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Señor Director
DIRECCIÓN DE NUEVAS CREACIONES
Superintendencia de Industria y Comercio
E. S. D.

Trámite : 011
Evento : 378
Actuación : 523

Referencia : Expediente No. **13.108.961**
Asunto : Solicitud de patente: "**HIDRATO DE TRATRATO DE 1-{(2S)-2-AMINO-4-[2,4-BIS(TRIFLUOROMETIL)-5,8-DIHIDROPIRIDO[3,4-D]PIRIMIDIN-7(6H)-IL]-4-OXOBUTIL}-5,5-DIFLUORO-PIPERIDIN-2-ONA**"
Solicitante : LG LIFE SCIENCES, LTD.
Fecha de solicitud : 30 de Abril del 2013

1. Yo, Luz Clemencia DE PÁEZ, en mi condición de apoderada de la sociedad solicitante de la patente de la referencia, me refiero al oficio No. **10462** notificado por fijación en lista el 26 de Agosto de 2014.

2. Mediante oficio No. **10462** se puso en conocimiento del solicitante el informe que contiene las observaciones hechas por su Despacho sobre la presente solicitud de patente. Las observaciones realizadas en el oficio se refieren a la presencia de reivindicaciones referentes a un uso o segundo uso, a la claridad del pliego reivindicatorio y al nivel inventivo de las reivindicaciones 1-5 en vista de los documentos **D1**: WO2006/104356 y **D2**: H.G. Brittain. Segunda Eddición, Informa Healthcare, NY, 2009.

3. **Respuesta a las objeciones**

De este modo y con el objeto de atender las objeciones arriba mencionadas, se desea presentar las siguientes modificaciones, aclaraciones y argumentos:

3.1. Modificación de una solicitud en trámite

De acuerdo con el artículo 34 de la Decisión 486 de la Comisión de la Comunidad Andina, donde se establece que la modificación de una solicitud es posible en cualquier momento del trámite mientras no implique una ampliación de la solicitud inicial, me permito presentar un nuevo pliego reivindicatorio conformado por 3 reivindicaciones.

Se han introducido las siguientes modificaciones al capítulo reivindicatorio:

- Se modificó la reivindicación 1, especificando cuáles son los valores característicos del pico (2θ) en el difractograma de XRD.
- Se eliminaron las reivindicaciones originales 2, 5 y 6. Lo anterior no puede ser considerado como un desistimiento de la materia allí revelada y mi representada se reserva el derecho de volver sobre la misma durante el trámite de la presente solicitud de patente.

De esta manera se aclara y precisa aún más el objeto de la presente invención, especialmente mediante el énfasis en sus características técnicas. Por lo anterior, las objeciones formuladas por el Examinador en cuanto a la presencia de reivindicaciones referentes al uso, la claridad y concisión del pliego reivindicatorio se ven superadas. En consecuencia, se solicita atentamente tener en cuenta este nuevo pliego reivindicatorio para el nuevo análisis de patentabilidad.

3.2. Argumentos con respecto a la falta de Nivel Inventivo

El artículo 18 de la Decisión 486 señala lo siguiente:

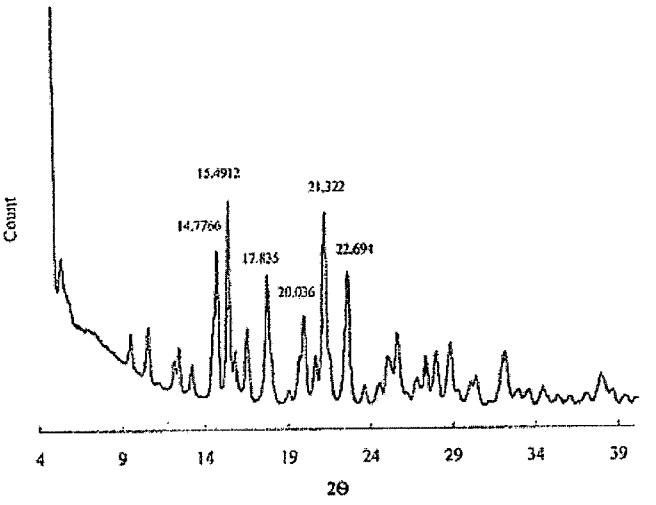
*"**Artículo 18.-** Se considerará que una invención tiene nivel inventivo, si para una persona del oficio normalmente versada en la materia técnica correspondiente, esa invención no hubiese resultado obvia ni se hubiese derivado de manera evidente del estado de la técnica".*

Una invención se considerará inventiva si la misma no hubiese resultado obvia a partir del arte previo para una persona del oficio normalmente versada en la materia. Esto a su vez implica que el Examinador a cargo de esta evaluación debe colocarse en el momento exacto en el que el inventor buscaba resolver el problema técnico contemplado en la solicitud y para el cual poseía la literatura y el conocimiento disponibles en dicho momento.

Siguiendo entonces los lineamientos de la Jurisprudencia aplicable al análisis del nivel inventivo de una solicitud de patente, se considera que una anterioridad o una combinación de dos anterioridades puede afectar dicho requerimiento de patentabilidad, si una persona medianamente versada en la materia encuentra enseñanzas o sugerencias claras que, a partir de un conocimiento medio en dicho campo, le permitan llegar de manera obvia a la invención reivindicada. Adicionalmente se considera que una mejora sustancial, un efecto inesperado o una ventaja con respecto al arte previo es un indicio de nivel inventivo, por cuanto aporta un salto tecnológico en la regla técnica.

A este respecto, respetuosamente solicitamos atentamente la reconsideración de las razones por las cuales se objeta el nivel inventivo, con base en la siguiente información:

En la reivindicación modificada 1, el 1,5 hidrato de sal de tartrato de 1-{(2S)-2-amino-4-[2,4-bis(trifluorometil)-5,8-dihidro-pirido[3,4-d]pirimidin-7(6H)-il]-4-oxobutil}-5,5-difluoropiperidin-2-ona es especificado por seis picos de XRPD de 14.6, 15.4, 18, 20, 21 y 23º con base a la Figura 1 del capítulo descriptivo de la presente invención. Como se puede observar en la Figura 1, los picos de XRD mencionados previamente son los más representativos.



Ahora, tal y como lo indica la Guía para Examen de Solicitudes de Patente de Invención y modelo de Utilidad, "la Difracción de Rayos X es la técnica más útil para el estudio del polimorfismo en lo que atañe a la estructura cristalina, dado que los patrones de difracción de los diversos polimorfos presentan siempre notables diferencias, por lo que deben incluir los picos de intensidad más representativa para el caso del cristal reivindicado", en este caso particular, los 6 picos presentados en la reivindicación 1 son suficientes para caracterizar el compuesto cristalino reivindicado.

Así mismo, como Anexo se presenta el artículo "*Chemical analysis by X-ray diffraction*" que también ratifica que los picos mencionados son suficientes para la caracterización. Además, la posibilidad de que el 1,5 hidrato de sal de tartrato de 1-{(2S)-2-amino-4-[2,4-bis(trifluorometil)-5,8-dihidro-pirido[3,4-d]pirimidin-7(6H)-il]-4-oxobutil}-5,5-difluoropiperidin-2-ona muestre picos de XRPD no sólo a los mencionados pero también diferentes, es extremadamente baja.

La presente invención está dirigida a el 1,5 hidrato de sal de tartrato de 1-{(2S)-2-amino-4-[2,4-bis(trifluorometil)-5,8-dihidro-pirido[3,4-d]pirimidin-7(6H)-il]-4-oxobutil}-5,5-difluoropiperidin-2-ona que tiene un contenido de agua de 3.5-5.5% y unos picos de XRPD de 14.6, 15.4, 18, 20, 21 y 23º.

El compuesto del ejemplo 83 de D1 se encuentra en forma de base libre y es un compuesto amina. La base libre es fácilmente degrada y por lo tanto su contenido decrece. Cuando esta base libre es preparada, el producto crudo es concentrado al remover el solvente. Sin embargo, cuando el compuesto es preparado en a gran escala, toma un largo tiempo, concentrar el producto crudo. Como resultado, es muy complicado obtener el compuesto del Ejemplo 83 de D1 con una alta pureza debido al incremento del producto de degradación. Además, la base libre del Ejemplo 83 de D1 es difícil de cristalizar y tiene baja estabilidad térmica.

En este sentido, los datos comparativos con respecto a la estabilidad térmica de la base libre y de la sal de tartrato se muestran a continuación.

Condición	Tiempo (Semanas)	Base libre (%)	Sal de tartrato (%)
40°C/75%RH	0	96.24	98.58
	2	96.22	98.12
	4	94.27	97.75
	6	-	97.74

Como se presentó previamente, la base libre del Ejemplo 83 de D1 tiene propiedades físicas que muestran su dificultad para ser desarrollada como un medicamento. D1 no presenta ninguna sugerencia o motivación para que una persona versada en la materia seleccione especifica una sal de tartrato, y específicamente el 1.5 hidrato de sal de tartrato.

Por su parte, D1 revela polimorfismo en solidos farmacéuticos. Como se mencionó en el capítulo descriptivo de la presente solicitud, en este campo técnico no existe una tendencia general par preferir el hidrato sobre el anhidro o viceversa, para el mejoramiento de la propiedades farmacéuticas incluyendo la estabilidad del medicamento, la propiedad higroscópica, etc. Específicamente, no podría ser anticipado entre cualquier forma concebible de un determinado medicamente, es decir, compuesto libre, sal, anhidro o hidrato, cuál podría exhibir estabilidad con la propiedad higroscópica que no cambia en función de la humedad a su alrededores, y entre

hidratos, el número de hidratación más estable, tampoco puede ser predicho. Además, así el número de hidratación sea el mismo, sigue siendo impredecible qué forma de cristal será más estable.

Por lo que es claro, que ni si quiera una persona ampliamente versada en la materia podría predecir qué forma de un medicamento en específico presentaría estabilidad. Adjuntos también se encuentran los documentos:

- R1: Polymorphism in molecular cystals.
- R2: Peddy Cishweshwar et al., L. Am. Chem. Soc. 2005.
- R3: Andrew Bond et al, Angew. Chem. Int. Ed. 2007.

R1 menciona que la posibilidad de polimorfismo puede existir para cualquier compuesto en particular, pero las condiciones necesarias para preparar polimorfos desconocidos, de ninguna manera son obvias, dado que no existen métodos sistemáticos comprensibles para determinar dichas condiciones. Además, en la actualidad se es totalmente ignorante con respecto a las propiedades que podrían esperar de un nuevo polimorfo que sea obtenido.

Por su parte D2 y D3, muestran estudios del polimorfismo de la aspirina, que fue sintetizada por primera vez en 1853, y que continúa en proceso. Por lo tanto, es claro con base a los argumentos presentados previamente que el 1.5 hidrato de sal de tartrato del compuesto I reivindicado en la presente invención en su forma cristalina, no es obvio con base al arte previo.

Así entonces, es claro que la materia de invención revelada en la presente solicitud de patente se debe tener como inventiva frente a las enseñanzas de los documentos D1 y D2 citados, toda vez que dichos documentos no enseñan ni sugieren como un todo las características técnicas esenciales de la presente invención y por lo tanto, la materia objeto de protección no podría derivarse de manera obvia u evidente a partir de las enseñanzas de este documento.

Además, el capítulo descriptivo de la presente invención muestra con claridad los efectos ventajosos de la misma. El ejemplo 8 muestra que la forma cristalina I (1.5 hidrato) presenta mayor estabilidad térmica que la forma cristalina II. Mientras que el Ejemplo 9, muestra que la forma cristalina I presenta una mayor densidad aparente que la forma cristalina II, por lo tanto la forma cristalina I, que presenta un menor índice de Carr puede ser fácilmente manipulado en el procesamiento de procesos. Dichos efectos mejorados con respecto al 1.5 hidrato de sal de tartrato del compuesto 1 son inesperados con base a los documentos D1 y D2. Por consiguiente, la presente solicitud posee la altura inventiva necesaria para que se le conceda el privilegio solicitado.

3.3 Conclusión

Por todo lo anterior, el documento D1, el documento D2, o su combinación, no resultan anterioridades válidas capaces de afectar el nivel inventivo de la invención de la presente solicitud.

Por lo tanto, consideramos que el Examinador está pasando por alto que una sola diferencia con respecto al estado de la técnica, permite concluir que el objeto reivindicado es nuevo. Además, está excluyendo el hecho de que el inventor en el momento de solucionar el problema técnico de la solicitud tuvo que emplear habilidad inventiva, pues la presente invención no resulta de la mera extrapolación de las enseñanzas del arte previo, como se afirma. Se está desconociendo el mérito investigativo empleado y que está aportando una ventaja al arte previo.

4. Puesto que se ha dado respuesta a todas las objeciones formuladas por el Examinador, se solicita atentamente proceder al otorgamiento de la solicitud de patente. En este sentido, respetuosamente recordamos al Examinador que la patente no podrá ser negada con base en objeciones diferentes a las expuestas en la acción oficial No. 10462, toda vez que al no haber sido trasladadas a mi representada, dicha decisión violaría tanto el tenor literal del artículo 45 de la Decisión 486 como el derecho constitucional al debido proceso. En este evento, y con base en el inciso 2 del artículo 45, respetuosamente solicitamos al Examinador expedir una nueva acción oficial que permita a mi representada

contra argumentar las mismas o modificar la solicitud con el fin de cumplir los requisitos de patentabilidad.

5. Anexos

- Nuevo pliego reivindicatorio conformado por 3 reivindicaciones.
- HANAWALT, J., RINN, H., FREVEL, L. "*Chemical analysis by X-Ray Diffraction: Classification and use of x-ray diffraction pattern*". The Dow Chemical Company.
- Nota de Aceptación de la Oficina de Patentes Europea.
- BERNSTEIN, J. "*Polymorphism in Molecular Crystals*". Department of Chemistry, Ben-Gurion University of the Negev.
- BOND, A., BOESE, R., DESIRAJU, G. "*On the polymorphism of aspirin: Crystalline aspirin as intergrowths of two "Polymorphic domains"*". Angew. Chem. Int. Ed. 2007.
- VISHWESHWAR, P., et al. "*The predictably elusive form II of aspirin*". Department of Chemistry, University of South Florida. 2005.

Señor Director,

LUZ CLEMENCIA DE PAEZ
C.C. 35.456.344 de Usaquén
T.P.A. No. 23.555

MCM
COLO-13548-0841-012-1
CPT\CPT\ID-274852\WPC13548
No. M-2014-274852\CPT

REIVINDICACIONES MODIFICADAS

1. Un 1,5 hidrato de sal de tartrato de 1-{(2S)-2-amino-4-[2,4-bis(trifluorometil)-5,8-dihidro-pirido[3,4-*d*]pirimidin-7(6H)-il]-4-oxobutil}-5,5-difluoropiperidin-2-ona, caracterizado porque tiene un contenido de agua en el rango que oscila entre 3,5 y 5,5 %,

en donde los valores característicos del pico (2θ) en el difractograma de XRD son de 14.6, 15.4, 18, 20, 21 y 23°.

2. Un proceso para preparar el 1,5 hidrato de acuerdo con la reivindicación 1, caracterizado porque la sal de tartrato de 1-{(2S)-2-amino-4-[2,4-bis(trifluorometil)-5,8-dihidropirido[3,4-*d*]-pirimidin-7(6H)-il]-4-oxobutil}-5,5-difluoropiperidin-2-ona se recristaliza a partir de solvente de agua, acetonitrilo/agua, etanol/agua, etanol/hexano o acetato de etilo/hexano.

3. El proceso de acuerdo con la reivindicación 2, caracterizado porque el solvente de recristalización es agua.

CPT\CPT\ID-274851\WPC13548

INDUSTRIAL and ENGINEERING CHEMISTRY

ANALYTICAL EDITION ◇ Harrison E. Howe, Editor

Chemical Analysis by X-Ray Diffraction

Classification and Use of X-Ray Diffraction Patterns

J. D. HANAWALT, H. W. RINN, AND L. K. FREVEL
The Dow Chemical Company, Midland, Mich.

INDUSTRIAL AND ENGINEERING CHEMISTRY considers itself fortunate in being able to present herewith a complete, new, workable system of analysis, for it is not often that this is possible in a single issue of any journal. Several qualified reviewers assure us that the authors present here a method that is not only workable but so clearly described that their scheme of chemical analysis will be readily understood by all those familiar with x-ray diffraction. The reader does not need to be skilled in crystal analysis; he needs only to be familiar with the bare principles of diffraction.

There is reason to believe that this publication, which is made possible in this form by the generous financial assistance of the Dow Chemical Company, will serve to bring this method of analysis into general use in industrial and consulting analytical laboratories.

THIS paper supplies tabulated data on the diffraction patterns of 1000 chemical substances and gives a scheme of classification which makes possible a routine and valuable use in the chemical laboratory of the Hull method of x-ray analysis.

In 1919 Hull (*9*) described a new method of chemical analysis by means of x-ray diffraction. He gave the experimental procedure and pointed out the various interesting and important features of the method, emphasizing the experimental simplicity of obtaining the diffraction pattern of a substance and the fact that it requires only a minute amount of material. He gave illustrations of the important fact that the diffraction method tells the state of chemical combination of the elements present in the unknown, and stated the basis for the method: "That every crystalline substance gives a pattern; that the same substance always gives the same pattern; and that in a mixture of substances, each produces its pattern independently of the other, so that the photograph obtained with a mixture is the superimposed sum of photographs that would be obtained by exposing each of the components separately for the same length of time. This law applies quantitatively to the intensities of the lines [provided absorption is negligible for each of the components], as well as to their positions, so that the method is capable of development as a quantitative analysis."

These unique features would appear to entitle the method to a place of real usefulness in chemical analysis. However, as yet no extensive use has been made of x-ray diffraction in this way. Probably one of the most important circumstances, which at present handicap the general use of the method, is that an adequate file of standard patterns is not available for reference. The method being empirical, standards are necessary. A certain limited amount of work could be done by determining crystal structure, but this is not a practical procedure. For any one person, the assembling of a large library of patterns would be a great task, since it would run into many thousands; also, it is not assured without test that it would be feasible to classify and make use of such a file were it available.

At The Dow Chemical Company it has been found that another useful fact concerning diffraction patterns may be added to those already given by Hull—namely, that the thousands of patterns representing the thousands of different chemical substances can be classified in such a way that they may be easily used for the identification of an unknown, even when the unknown is a mixture of substances.

The basis for this interesting conclusion and the scheme of classification were described in an earlier publication (*8*). Since that time, there have been many requests to make the data available for general use. The Dow Chemical Company has been very willing to do this, but has postponed publication until this time in order to determine a satisfactory form in which to put the data. When the original negatives are on file, the simplest procedure, after locating the standard by means of the classification system, is to compare negatives directly as to position and intensity of the lines. However, for publication, it is not feasible to make a true reproduction of the negatives. Microphotometer traces would give the data accurately, but would involve a more time-consuming technic than is desirable for routine and economical analysis.

The data of the pattern should be recorded as simply as possible and yet sufficiently accurately for analysis. During the past year such a means has been fully demonstrated and it is now possible to present the diffraction data in a form which may be used by a person in another laboratory. If it appears sufficiently interesting, data on more substances could be made available from this laboratory and perhaps from

Ind. Eng. Chem., Anal. Ed. 10, 457-512 (1938)

many others. The use of the x-ray method of analysis would be greatly extended if crystal structure workers, after they have taken care to get a pure material, would publish the powder data of the material in the same or in an equivalent form.

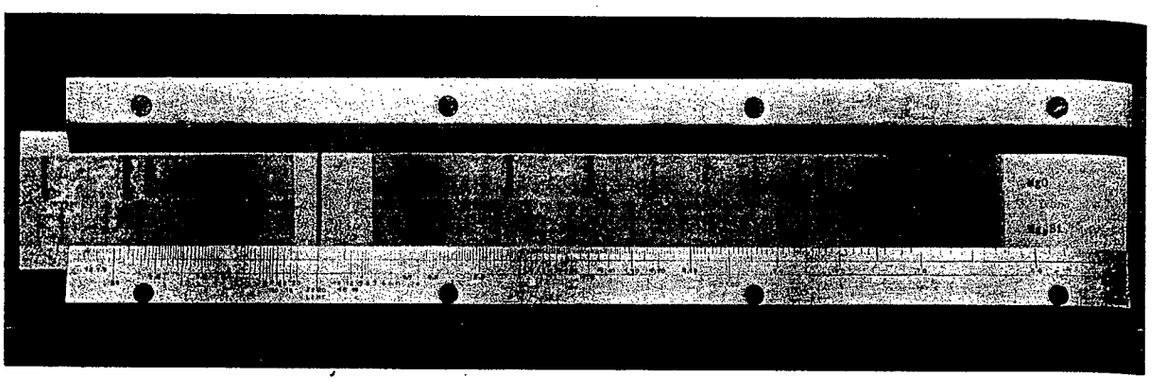


FIGURE 1. ANGSTROM SCALE WITH SYMMETRIC FILM

For those who are already equipped with x-ray diffraction apparatus, the only step necessary to use the data here presented is to compile the index book as described. For those who are not familiar with the details of what is involved in x-ray diffraction analysis, a survey view is given of the apparatus required, the technic of obtaining the patterns, and the method of interpreting the patterns, as well as some illustrations of the field of application of the general method. The present article is based on experience gained in carrying out several thousand actual analyses during the past five years.

The Classification System

The diffraction pattern, as commonly obtained, consists of a sequence of lines in certain definite positions (on an Å. scale giving the spacing of the crystal planes represented) and of certain relative intensities (Figure 1). The method of measuring the negatives is discussed below, but for the purpose of describing the classification system it can be assumed for the moment that the data have been obtained in the form given in the tables of patterns. The lines lie between 20 Å. and 0.5 Å., and for indexing purposes are grouped into 77 suitably chosen divisions. The sizes of these divisions are based upon experience and are determined by the consideration that they should be larger than the accuracy of measurement of the position of the lines, and should be no more numerous than is necessary to handle conveniently all the patterns without conflict. Actually the size of a division is 5 to 10 times the error of measurement.

From the data of the patterns, the positions of the three strongest lines are read off in the order of decreasing intensity. If two lines have the same intensity value, the rule is to list the one with the greater Å. spacing first. One thus has as a characteristic of each pattern, three numbers in a certain sequence. The patterns are then listed, at the proper place, in an indexed book which is divided and subdivided into the chosen regions. The first number determines the group, the second number the subgroup, and the third number the location within the subgroup. The index book thus consists of 77 sections or groups, each of which in turn contains 77 subgroups. For illustration, three sections of the index book are shown (Figures 2, 3, 4). The index book as it is actually being used provides 15 spaces in each subgroup, but in the illustration these spaces have been omitted. These sections are typical of the average section of the index book and show that among the 1000 patterns listed, it is hardly necessary to use more than the two strongest lines in order to index the patterns.

In the whole index book, there are only 27 subgroups which contain more than 3 patterns and only one which contains more than 5 patterns. The fact that two patterns fall in the same subgroup does not mean that they are identical with respect to their first two lines, since their positions within the divisions may be different and their relative intensities probably will be different. Considering now the coincidences of third lines within a subgroup, there are 11 subgroups in which 2 patterns have the same positions of the third line (within twice the ± error of measurement) and 4 subgroups in which 3 patterns have the same third line. In seven of these cases, a measurement of the fourth line serves to distinguish the patterns. (A column is included in the book for recording the fourth line.) However, in practice, after a pattern has been located in the index book (which gives its name and number in the file), the pattern data are referred to in the file and compared directly in all their details. When this is done, for the conflicts still remaining there are only three cases left in which the patterns are not immediately distinguishable from each other. In these cases, if there were nothing easier to do, a more accurate determination of planar spacings by a different x-ray technic would be sufficient. Probably, however, some other information would be available to assist in separating these very occasional conflicts.

Taking into account the number of subgroups and the distribution of the lines as they occur in the type of pattern studied, it is estimated that the index book in its present form, making use of three lines as described, would handle many thousands of patterns. If, for instance, there were 20,000 patterns in the file, there would be a total of only several hundred cases in which one would have to compare his unknown with two patterns from the file, and not more than about twenty cases in which one would have to compare with more than three patterns.

As practiced at The Dow Chemical Company, a second and independent method of listing the patterns is included in the index book. Each of the 77 major groups of the book is followed by a section called the Supplementary Group Index in which (1) all the patterns whose strongest line falls in the major group have their three strongest lines listed in the order 1, 2, 3; (2) all the patterns whose second strongest line falls in the major group have their three strongest lines listed in the order 2, 1, 3; and (3) all the patterns whose third strongest line falls in the major group have their three strongest lines listed in the order 3, 1, 2. An illustration of the use of the Supplementary Group Index will be found among the examples given below.

Procedure with Unknowns

Suppose that the pattern of an unknown has been obtained and the positions and relative intensities of the lines

FIGURE 2

Group 2.55–2.50

No.	Compound	3rd line	4th line	No.	Compound	3rd line	4th line	No.	Compound	3rd line	4th line	No.	Compound	3rd line	4th line
	20.00–15.00				4.50–4.40				2.75–2.70				1.75–1.70		
	15.00–12.00				4.40–4.30				2.70–2.65				1.70–1.65		
	12.00–10.00				4.30–4.20				2.65–2.60				1.65–1.60		
	10.00– 9.00				4.20–4.10				2.60–2.55				1.60–1.55		
	9.00– 8.50				4.10–4.00				2.55–2.50				1.55–1.50		
	8.50– 8.00				4.00–3.90				2.50–2.45			743	SiC (Cubic)	1.31	
	8.00– 7.50				3.90–3.80				2.45–2.40				1.50–1.45		
	7.50– 7.00				3.80–3.70				2.40–2.35			426	Fe_3O_4	1.62	
	7.00– 6.50				3.70–3.60				2.35–2.30			979	$ZnFe_2O_4$	2.97	
	6.50– 6.00				3.60–3.50			372	CuO	1.86		527	$MgFe_2O_4$	2.95	
	6.00– 5.75				3.50–3.40				2.30–2.25				1.45–1.40		
	5.75– 5.50				3.40–3.30				2.25–2.20				1.40–1.35		
	5.50– 5.25				3.30–3.20				2.20–2.15				1.35–1.30		
	5.25– 5.00				3.20–3.10				2.15–2.10				1.30–1.25		
108	$Ba(NO_2)_2 \cdot H_2O$	3.48		897	SrO_2	2.00			2.10–2.05				1.25–1.20		
	5.00– 4.90				3.10–3.00				2.05–2.00				1.20–1.15		
	4.90– 4.80				3.00–2.95				2.00–1.95				1.15–1.10		
	4.80– 4.70				2.95–2.90				1.95–1.90				1.10–1.05		
855	$Na_2SnO_3 \cdot 3H_2O$	1.85											1.05–1.00		
	4.70– 4.60				2.90–2.85				1.90–1.85				1.00– .90		
	4.60– 4.50				2.85–2.80				1.85–1.80				.90– .80		
					2.80–2.75				1.80–1.75				.80–		

SUPPLEMENTARY GROUP INDEX 2.55–2.50

No.	Compound	1st line	2nd line	3rd line	No.	Compound	2nd line	1st line	3rd line	No.	Compound	3rd line	1st line	2nd line
108	$Ba(NO_2)_2 \cdot H_2O$	2.52	5.1	3.48	127	$BeSO_4 \cdot 4H_2O$	2.52	3.90	3.20	362	$Cu_2Fe(CN)_6 \cdot 7H_2O$	2.50	5.0	3.55
855	$Na_2SnO_3 \cdot 3H_2O$	2.51	4.75	1.85	113	$Ba_3(PO_4)_2$	2.51	3.58	4.45	848	$Na_2PbO_3 \cdot 3H_2O$	2.53	4.80	4.62
897	SrO_2	2.52	3.14	2.00	679	KI	2.50	3.53	4.08	95	$BaCl_2 \cdot 2H_2O$	2.54	4.48	2.91
372	CuO	2.51	2.31	1.86	683	KNO_3	2.50	3.31	2.20	165	$CdWO_4$	2.53	3.80	3.05
743	SiC	2.51	1.54	1.31	74	SbI_3	2.54	3.30	2.14	589	$Hg(CN)_2$	2.51	3.72	4.85
979	$ZnFe_2O_4$	2.53	1.48	2.97	999	$ZrSiO_4$	2.51	3.29	1.71	164	$(CdSO_4)_3 \cdot 8H_2O$	2.51	3.55	4.90
426	Fe_3O_4	2.53	1.48	1.61	918	Th	2.53	2.92	1.79	87	Ba	2.51	3.54	2.04
527	$MgFe_2O_4$	2.51	1.48	2.95	749	Ag_3AsO_4	2.50	2.74	1.63	349	$2CuCO_3 \cdot Cu(OH)_2$	2.51	3.51	5.1
					423	Fe_3O_3	2.51	2.69	1.84	115	$Ba(H_2PO_2)_2 \cdot H_2O$	2.54	3.34	7.8
										84	As_2O_3	2.53	3.18	6.3
										726	$K_2WO_4 \cdot 2H_2O$	2.51	3.09	3.92
										724	KCNS	2.51	2.97	2.79

FIGURE 3

Group 2.70–2.65

No.	Compound	3rd line	4th line	No.	Compound	3rd line	4th line	No.	Compound	3rd line	4th line	No.	Compound	3rd line	4th line
	20.00–15.00				4.40–4.30				2.70–2.65				1.85–1.80		
	15.00–12.00				4.30–4.20				2.65–2.60				1.80–1.75		
	12.00–10.00				4.20–4.10				2.60–2.55				1.75–1.70		
	10.00– 9.00				4.10–4.00				2.55–2.50				1.70–1.65		
								423	Fe_2O_3	1.84					
	9.00– 8.50				4.00–3.90								1.65–1.60		
									2.50–2.45						
	8.50– 8.00				3.90–3.80			765	Ag_3PO_4	1.66			1.60–1.55		
	8.00– 7.50				3.80–3.70				2.45–2.40						
													1.55–1.50		
	7.50– 7.00				3.70–3.60				2.40–2.35						
													1.50–1.45		
	7.00– 6.50				3.60–3.50				2.35–2.30						
													1.45–1.40		
	6.50– 6.00				3.50–3.40				2.30–2.25						
													1.40–1.35		
	6.00– 5.75				3.40–3.30				2.25–2.20						
													1.35–1.30		
	5.75– 5.50				3.30–3.20				2.20–2.15						
								968	$ZnCrO_4$	9.50			1.30–1.25		
	5.50– 5.25				3.20–3.10										
									2.15–2.10				1.25–1.20		
	5.25– 5.00				3.10–3.00										
									2.10–2.05				1.20–1.15		
	5.00– 4.90				3.00–2.95			407	$FeCl_2$	5.90					
171	$5CaO.3Al_2O_3$	2.44											1.15–1.10		
					2.95–2.90				2.05–2.00						
	4.90– 4.80												1.10–1.05		
					2.90–2.85				2.00–1.95						
	4.80– 4.70			502	Mg_2Ca	3.14							1.05–1.00		
									1.95–1.90						
	4.70– 4.60				2.85–2.80								1.00– .90		
									1.90–1.85						
	4.60– 4.50				2.80–2.75			672	KF	3.08			.90– .80		
								846	$Na_2HPO_3.5H_2O$	1.54	4.23				
	4.50– 4.40				2.75–2.70			170	$3CaO.Al_2O_3$	1.54	4.05		.80–		
				752	Ag_2CO_3	2.27									

SUPPLEMENTARY GROUP INDEX 2.70–2.65

No.	Compound	1st line	2nd line	3rd line	No.	Compound	2nd line	1st line	3rd line	No.	Compound	3rd line	1st line	2nd line
171	$5CaO.3Al_2O_3$	2.68	4.90	2.44	354	$CuCl_2.2NH_4Cl.2H_2O$	2.68	5.5	2.75	138	$BiO_2C_{19}H_7$	2.67	20.0	9.9
502	Mg_2Ca	2.65	2.87	3.14	314	$Cr_2(C_2O_4)_3.H_2O$	2.68	4.75	9.2	120	$Ba(CNS)_2.2H_2O$	2.66	7.7	3.4
752	Ag_2CO_3	2.65	2.73	2.27	544	$MgSO_4.7H_2O$	2.66	4.22	5.9	532	$Mg_3(PO_4)_2.8H_2O$	2.69	6.7	2.94
423	Fe_2O_3	2.69	2.51	1.84	533	$MgNH_4PO_4.6H_2O$	2.69	4.28	2.93	566	$MnC_2O_4.2\frac{1}{2}H_2O$	2.67	4.80	3.00
765	Ag_3PO_4	2.68	2.45	1.66	448	$Pb_3(SbO_4)_2$	2.65	3.48	5.8	682	KNO_2	2.66	3.77	3.03
968	$ZnCrO_4$	2.67	2.14	9.5	133	BiOCl	2.67	3.45	7.4	650	K	2.65	3.75	2.16
407	$FeCl_2$	2.68	2.08	5.9	111	BaO_2	2.68	3.37	2.11	829	$NaHC_2O_4.H_2O$	2.67	2.97	2.45
846	$Na_2HPO_3.5H_2O$	2.67	1.89	1.54	907	$TeCl_2$	2.69	3.24	4.29	792	$Na_2CO_3.1H_2O$	2.67	2.76	2.37
170	$3CaO.Al_2O_3$	2.68	1.90	1.55	879	$Na_2C_8H_2O_8N_4.H_2O$	2.66	3.17	4.72	481	LiOH	2.67	2.75	4.35
672	KF	2.66	1.88	3.08	936	$SnSO_4$	2.67	3.08	2.10	442	FeS	2.65	2.06	2.98
					48	$(NH_4)_2C_2O_4.H_2O$	2.67	3.06	3.81	524	Mg_3N_2	2.66	1.76	2.12
					866	$Na_2SO_3.7H_2O$	2.66	2.87	4.26					
					315	Cr_2O_3	2.67	1.67	2.47					

FIGURE 4

Group 2.95–2.90

No.	Compound	3rd line	4th line
	20.00–15.00		
	15.00–12.00		
	12.00–10.00		
	10.00– 9.00		
	9.00– 8.50		
	8.50– 8.00		
	8.00– 7.50		
	7.50– 7.00		
	7.00– 6.50		
640	P_2S_5	4.90	
	6.50– 6.00		
600	$HgSO_4 \cdot 2HgO$	5.5	
	6.00– 5.75		
	5.75– 5.50		
	5.50– 5.25		
877	$Na_2S_2O_3 \cdot 5H_2O$	2.84	
	5.25– 5.00		
	5.00– 4.90		
	4.90– 4.80		
	4.80– 4.70		
	4.70– 4.60		
	4.60– 4.50		
	4.50– 4.40		
786	$(C_6H_4CO_2)_2$-BONa	3.45	

No.	Compound	3rd line	4th line
	4.40–4.30		
	4.30–4.20		
818	$NaIO_3$	3.19	
	4.20–4.10		
	4.10–4.00		
465	$Pb_3(PO_4)_2$	3.61	
	4.00–3.90		
	3.90–3.80		
	3.80–3.70		
152	$CdCO_3$	1.83	
	3.70–3.60		
93	$Ba(ClO_4)_2 \cdot 3H_2O$	2.14	
	3.60–3.50		
	3.50–3.40		
	3.40–3.30		
715	$C_{16}H_8O_2N_2(SO_3K)_2$	3.00	
	3.30–3.20		
797	$NaClO_3$	1.76	
	3.20–3.10		
	3.10–3.00		
	3.00–2.95		
	2.95–2.90		
	2.90–2.85		
	2.85–2.80		

No.	Compound	3rd line	4th line
	2.80–2.75		
925	Sn	2.01	
178	CaC_2 II	1.95	
	2.75–2.70		
801	Na_2CrO_4	4.09	
	2.70–2.65		
	2.65–2.60		
	2.60–2.55		
795	$NaHCO_3$	3.48	
	2.55–2.50		
918	Th	1.79	
	2.50–2.45		
685	$K_2C_2O_4$	2.32	
	2.45–2.40		
	2.40–2.35		
	2.35–2.30		
	2.30–2.25		
	2.25–2.20		
	2.20–2.15		
782	$Na_2B_4O_7 \cdot 5H_2O$	4.40	
	2.15–2.10		
	2.10–2.05		
	2.05–2.00		
	2.00–1.95		
	1.95–1.90		

No.	Compound	3rd line	4th line
	1.90–1.85		
	1.85–1.80		
779	NaN_3	2.42	
	1.80–1.75		
396	In_2O_3	1.52	
	1.75–1.70		
	1.70–1.65		
303	CsCl	4.11	
	1.65–1.60		
	1.60–1.55		
	1.55–1.50		
	1.50–1.45		
	1.45–1.40		
	1.40–1.35		
	1.35–1.30		
	1.30–1.25		
	1.25–1.20		
	1.20–1.15		
	1.15–1.10		
	1.10–1.05		
	1.05–1.00		
	1.00– .90		
	.90– .80		
	.80–		

SUPPLEMENTARY GROUP INDEX 2.95–2.90

No.	Compound	1st line	2nd line	3rd line
640	P_2S_5	2.90	6.7	4.90
600	$HgSO_4 \cdot 2HgO$	2.92	6.2	5.5
877	$Na_2S_2O_3 \cdot 5H_2O$	2.93	5.4	2.84
786	$(C_6H_4CO_2)_2BONa$	2.94	4.40	3.45
818	$NaIO_3$	2.93	4.25	3.19
465	$Pb_3(PO_4)_2$	2.91	4.03	3.61
152	$CdCO_3$	2.94	3.77	1.83
93	$Ba(ClO_4)_2 \cdot 3H_2O$	2.90	3.65	2.14
715	$C_{16}H_8O_2N_2(SO_3K)_2$	2.90	3.35	3.00
797	$NaClO_3$	2.94	3.28	1.76
925	Sn	2.91	2.79	2.01
178	CaC_2 II	2.93	2.79	1.95
801	Na_2CrO_4	2.91	2.73	4.09
795	$NaHCO_3$	2.94	2.58	3.49
918	Th	2.92	2.53	1.79
685	$K_2C_2O_4$	2.92	2.46	2.32
782	$Na_2B_4O_7 \cdot 5H_2O$	2.94	2.19	4.40
779	NaN_3	2.91	1.82	2.42
396	In_2O_3	2.91	1.78	1.52
303	CsCl	2.90	1.68	4.11

No.	Compound	2nd line	1st line	3rd line
532	$Mg_3(PO_4)_2 \cdot 8H_2O$	2.94	6.7	2.69
561	$MnCl_2 \cdot 1H_2O$	2.93	5.7	2.55
95	$BaCl_2 \cdot 2H_2O$	2.91	4.48	2.54
523	$Mg(NO_3)_2 \cdot 6H_2O$	2.93	4.42	3.29
543	$MgSO_4 \cdot 6H_2O$	2.92	4.40	4.04
693	KH_2PO_4	2.90	3.72	1.95
991	α-ZnS	2.91	3.29	1.76
462	PbO	2.93	3.06	2.72
179	CaC_2 III	2.92	2.86	2.05
597	Hg_2PO_4	2.94	2.60	3.09

No.	Compound	3rd line	1st line	2nd line
697	$C_6H_4(CO)_2NK$	2.90	14.5	6.4
129	$Bi(C_6H_5O_2)_3$	2.90	13.5	3.35
748	$AgC_2H_3O_2$	2.91	10.0	3.04
98	$Ba(CN)_2$	2.94	9.4	3.37
927	$SnCl_4 \cdot 5H_2O$	2.94	6.2	5.3
326	$CoCl_2 \cdot 6H_2O$	2.94	5.6	4.85
377	$CuOH \cdot CuPO_4$	2.91	4.81	2.63
533	$MgNH_4PO_4 \cdot 6H_2O$	2.93	4.28	2.69
586	$HgCl_2 \cdot 3HgO$	2.92	3.95	2.70
449	$PbHAsO_4$	2.93	3.39	3.17
707	$K_2S_2O_7$	2.90	3.23	3.07
755	Ag_2CrO_4	2.92	3.14	3.02
701	K_2SeO_3	2.94	3.08	4.35
49	$(NH_4)HC_2O_4 \cdot H_2O$	2.90	3.00	6.2
474	Li_2CO_3	2.91	2.80	4.16
853	$Na_2SiO_3 \cdot 9H_2O$	2.92	2.79	3.83

have been measured and tabulated. One opens the index book at the major group determined by the strongest line, turns to the subgroup determined by the second strongest line, and sees whether any of the lines of the unknown check lines in this subgroup. (This can be done at a glance since, of the subgroups which are occupied, the largest contains only seven patterns and most of them contain only one.) If the unknown is a single substance, the third strongest line will check and the pattern will have been located. However, if the unknown is a mixture of phases and if the second strongest line of the pattern happens to be the strongest line of the second component, the pattern will not have been found and one proceeds by using the third strongest line of the unknown pattern to determine the subgroup, and so on. When a match is found, the lines of the unknown coinciding with the standard are noted, as are also any intensity variations which would indicate superpositions of lines. The remaining unidentified lines of the unknown are then treated in the standard manner.

TABLE I. X-RAY DIFFRACTION DATA

d[a]	I[b]	I/I_1[c]
4.95	8	0.13
4.08	25	0.40
3.89	20	0.32
3.58	17.5	0.28
2.91	62.5	1.00
2.73	40	0.64
2.47	15	0.24
2.16	7	0.11
2.11	5	0.08
2.03	15	0.24
1.94	10	0.16
1.79	15	0.24
1.72	1	0.02
1.68	2	0.03
1.64	6	0.10
1.61	12.5	0.20

[a] d = interplanar spacing measured in Angstrom units.
[b] I = intensity of the diffraction line (arbitrary units).
[c] I_1 = intensity of the strongest line.

If the constituent corresponding to the strongest line of the unknown pattern is not contained in the file, or if the strongest line should happen to be so by virtue of the superposition of two lines, neither of which is the strongest line of any component present in a mixture, one will not find a match in the major group determined by the strongest line of the unknown pattern, so he must proceed by using the second strongest line to determine the major group, and so on. One cannot fail to find any or all components of a mixture which exists in the reference file. If the pattern is not found in the file, then even in this case one has obtained considerable negative information about the unknown.

Use of System in Identifying Unknowns

Probably the easiest way to become acquainted with the details of the system is to follow through the determinations of a few unknowns. For this purpose, three sections of the index book (Figures 2, 3, 4) have been chosen to be reprinted. (The complete index book is not reprinted here because it requires 462 pages, but it can, of course, be easily tabulated from the pattern data given.)

In working with a real unknown, one cannot, in general, tell by simply looking at the pattern whether it represents a single substance or a mixture, nor is it necessary to know this. However, for simplicity the illustrations are picked from different types of cases.

A. A SINGLE COMPONENT. Assume that the measurements of the pattern have been recorded as in Table I.

The three strongest lines in order of decreasing intensity are 2.91, 2.73, 4.08. Turn to the index book to group 2.95–2.90 (Figure 4) and look in subgroup 2.75–2.70. One finds that sodium chromate, pattern No. 801, has a third line at 4.09, which is also the third most intense line of the unknown. Then turn to pattern No. 801 and observe that within experimental error all positions and relative intensities check and there are no lines of either pattern not accounted for. The conclusion is that the unknown contains sodium chromate.

B. MIXTURE OF TWO SUBSTANCES (no superposed index lines). The data of such an unknown are reproduced in Table II.

TABLE II. X-RAY DIFFRACTION DATA

d	I	d	
4.65	6	1.82	4
3.79	12.5	1.75	30
3.28	30	1.71	2
2.93	50	1.63	1
2.67	20	1.58	10
2.52	50	1.54	1.5
2.32	50	1.50	15
2.18	15	1.465	1.5
2.07	2	1.430	6
1.97	6	1.406	10
1.86	10	1.372	10

Turn to group 2.95–2.90 (Figure 4) and to subgroup 2.55–2.50 and find that there is no compound with a third line corresponding to any of the lines of the unknown. Turn next to subgroup 2.35–2.30 and again find no match. Turn next to subgroup 3.30–3.20 and observe that sodium chlorate, pattern No. 797, has a third line at 1.76. Since there is a line at 1.75 in the unknown pattern, compare the data of sodium chlorate, pattern No. 797, with that of the unknown and list the relative intensities of the identified lines. This gives Table III in satisfactory agreement with sodium chlorate, pattern No. 797.

TABLE III. X-RAY DIFFRACTION DATA

d	I	I/I_1
4.65	6	0.12
3.79	12.5	0.25
3.28	30	0.60
2.93	50	1.00
2.67	20	0.40
2.18	15	0.30
2.07	2	0.04
1.97	6	0.12
1.82	4	0.08
1.75	30	0.60
1.63	1	0.02
1.58	(10)	(0.20)
1.54	1.5	0.03
1.50	(15)	(0.30)
1.465	1.5	0.03
1.430	6	0.12

The identification of one compound of the mixture is thus established. The strongest of the remaining lines is at 2.52; hence turn to group 2.55–2.50 (Figure 2), subgroup 2.35–2.30, and note the compound cupric oxide, pattern No. 372, with a third line at 1.86. Referring to the data of cupric oxide, pattern No. 372, note that all the remaining lines of the unknown are accounted for in position. List the relative intensities, Table IV.

TABLE IV. X-RAY DIFFRACTION DATA

d	I	I/I_1
2.52	50	1.00
2.32	50	1.00
1.86	10	0.20
1.71	2	0.04
1.58	(10)	(0.20)
1.50	(15)	(0.30)
1.406	10	0.20
1.372	10	0.20

These are seen to be in satisfactory agreement with the cupric oxide data. Since all the diffraction lines of the unknown have been satisfactorily accounted for, the qualitative compound analysis of the mixture is complete.

C. MIXTURE OF TWO COMPONENTS (superposed lines). The data for the unknown are recorded in Table V.

TABLE V. X-RAY DIFFRACTION DATA

d	I	d	I
4.90	2	1.309	4
3.68	4	1.274	2
2.96	7	1.256	3
2.69	25	1.220	1
2.52	50	1.189	2
2.43	1	1.160	2
2.21	7	1.140	2
2.08	8	1.120	1
1.84	15	1.103	1
1.69	17.5	1.089	2
1.61	15	1.054	2
1.480	25	1.040	1
1.450	10		

Turn to group 2.55–2.50 (Figure 2), subgroup 2.70–2.65, and find no compound listed with a third line corresponding to any of the lines of the unknown. Turn to subgroup 1.50–1.45 and find iron ferrite (ferrosoferric oxide), pattern No. 426, with a third line at 1.62. Compare the data of pattern No. 426 with the data of the unknown. On listing the relative intensities of the identified lines (Table VI), it is seen that the intensity of line 2.52 is decidedly too high, which suggests the possibility of a superposition of lines.

TABLE VI. X-RAY DIFFRACTION DATA

d	I	I/I_1
4.90	2	0.04
2.96	7	0.14
2.52	50	1.00
2.43	1	0.02
2.08	8	0.16
1.69	17.5	0.35
1.61	15	0.30
1.480	25	0.50
1.274	2	0.04
1.120	1	0.02
1.089	2	0.04
1.054	2	0.04

Therefore include line 2.52 along with the remaining unidentified lines. Inspection shows that the intensity of the superposed line on 2.52 of iron ferrite is about as strong as line 2.68. However, group 2.55–2.50, subgroup 2.70–2.65, gives no check, while group 2.70–2.65, subgroup 2.55–2.50, lists ferric oxide, pattern No. 423, with a third line at 1.84.

Comparing the data of ferric oxide, pattern No. 423, with the data of the unknown, it is found that the positions of the ferric oxide lines check with all of those of the remaining unidentified lines of the unknown as well as with three of the lines which had already been checked with the iron ferrite pattern. Thus there are superpositions of lines at three positions in the unknown pattern.

In order to show conclusively that the unknown is a mixture of ferric oxide and iron ferrite, it is necessary to account satisfactorily for the relative intensities of the lines of the unknown pattern. Since line 2.69 is not a superposed line, its intensity is due entirely to ferric oxide, and to get the value of the absolute intensities of all other ferric oxide lines of the unknown, it is only necessary to multiply the intensity of line 2.69 by the known relative intensities of ferric oxide as given in pattern No. 423. This is done in Table VII.

TABLE VII. X-RAY DIFFRACTION DATA

d		I
3.68	0.18 × 25 =	4.5
2.69	1.00 × 25 =	25
2.52	0.75 × 25 =	19
2.21	0.18 × 25 =	4.5
1.84	0.63 × 25 =	16
1.69	0.63 × 25 =	16
1.61	0.13 × 25 =	3
1.480	0.50 × 25 =	12.5
1.450	0.50 × 25 =	12.5
1.309	0.18 × 25 =	4.5
1.256	0.13 × 25 =	3
1.189	0.08 × 25 =	2
1.160	0.05 × 25 =	1
1.140	0.13 × 25 =	3

Then subtract these computed absolute intensities from those of the total unknown pattern (Table VIII). The resulting data must agree with those of iron ferrite, if the identification of the unknown is to be considered complete. This is found to be the case.

The low intensity in the case of line 1.48 can be explained by the fact that this line in the unknown pattern is a partially superposed line, and the intensity as read is not the sum of the intensities of the lines. The case could never exist where this phenomenon would cause the intensity of a line to be calculated too high.

It is worth while to point out an alternative method of identifying a mixture of the above type by making use of the Supplementary Group Index. If one inadvertently fails to recognize the anomalously high intensity of the spacing 2.52 for the identified iron ferrite pattern and proceeds to identify the second phase in the usual manner, he might easily neglect to reconsider the spacing 2.52 (inasmuch as the spacing has already been identified as the most intense line of iron ferrite) and consequently fail to locate the second phase. In that event, upon looking in group 2.70–2.65 in the standard manner, one fails to identify the remaining lines. He then refers to supplementary group 2.70–2.65 and finds listed along with 2.68 and 1.84 the line 2.51 which also occurs in the unknown pattern. The ferric oxide pattern would then be checked. The Supplementary Group Index in general is useful when for any reason the strongest line of a pattern is overlooked and one is attempting to identify a pattern from its second or third strongest lines.

While the illustrations have been limited to mixtures of only two unknowns, no new situation will be encountered in mixtures of three or more components. It has been found from experience in this laboratory that it is practical to use this method of analysis for mixtures with as many as four or five components. However, the ease of analysis becomes less as the number of components increases.

Apparatus and Technic

The x-ray literature describes many types of apparatus for diffraction work (*1*, *2*, *4*, *6*, *7*, *10*). The type to be used in any particular case depends on the kind of data desired and the accuracy necessary. A completely equipped x-ray laboratory which could handle all the x-ray technics for diverse purposes would require a large variety of apparatus. However, for the particular purpose of chemical analysis under discussion in this article, a satisfactory equipment and experimental procedure which is sufficiently accurate and at the same time economical will be described.

The diffraction unit most used in this laboratory is the G. E. multiple diffraction unit, Type VWC, Form E, as described by Davey (*3*) (Figure 5). (The production of this particular type of x-ray unit has been suspended at the present time, though other powder diffraction units are commercially available.) This unit consists of a transformer, x-ray tube with a molybdenum target, and cameras. Twelve slits 0.05 × 1.25 cm. (0.02 × 0.5 inch), located around the circumference of the cylinder containing the x-ray tube, define the x-ray beams. There is a switchboard holding the operating switches, meters, filament current stabilizer, a water pressure switch, and an overload circuit breaker. In this laboratory there have been added a recording milliammeter, which gives a record of the tube current during the exposure; a time switch, by which an exposure can be stopped at a predetermined time; and a temperature switch, which shuts off the voltage if the temperature of the cooling water reaches about 38° C. (100° F.).

The G. E. quadrant cassettes of 20.32-cm. (8.00-inch) radius (Figure 6) are used. A slight modification of these cameras makes it possible to record the diffraction lines on both sides of the beam. This produces a symmetrical pattern, which enables an accurate location of the setting of the primary beam on the zero of the measuring scale (Figure 1). In order to obtain a more uniform pattern, the specimen tube is rotated during the exposure. The power for rotating the specimen is supplied by an electric clock motor and is transmitted by a silk fish-line belt. A zirconium dioxide filter about 0.04 cm. (0.016 inch) thick is placed in front of the film to absorb the MoKβ radiation. (These filters are supplied by the Patterson Screen Company, Towanda, Pa.) Double-emulsion x-ray film 4.76 × 40 cm. (1.875 × 16 inches), costing about 7.5 cents each is used. A fluorazure intensifying screen (also supplied by the Patterson Screen Company) is placed immediately behind the film.

The specimens are loaded in powder form in Pyrex capillary tubes 0.04-cm. (0.016-inch) inside diameter (measured with a No. 78 drill) and 0.06-cm. (0.025-inch) outside diameter (measured with a No. 22 U. S. standard wire gage). These tubes can be

TABLE VIII. X-RAY DIFFRACTION DATA

d	I	I/I_1
4.90	2	0.07
2.96	7	0.23
2.52	31	1.00
2.43	1	0.03
2.08	8	0.26
1.69	1.5	0.05
1.61	12	0.39
1.480	12.5	0.40
1.274	2	0.07
1.220	1	0.03

readily made in large quantities. A plug of absorbent cotton about 0.1 cm. (0.04 inch) long is placed in the center of the tube. The samples are then loaded on either side of the central plug for a distance of 1 cm. (about 1 mg.) in a manner similar to that used in loading melting point tubes. Piano wire serves well as an aid in packing because it does not buckle and break the tube. After the sample is packed into the tube, another cotton plug is inserted and the ends of the tube are sealed in a flame. Brittle substances can be prepared for loading by grinding in an agate mortar. Samples of metals can be obtained by filing with a clean file. It has been found helpful to have available various dental tools for the purpose of obtaining samples of small inclusions in nonhomogeneous materials. A desiccator box equipped with glass top and rubber sleeves is more convenient for loading hygroscopic substances than loading under a protective liquid. Samples which contain elements of high atomic number should be diluted with an amorphous material such as flour or charcoal to decrease the absorption of the radiation. In general, about 200-mesh is a satisfactory powder size to use. The preparation and loading of a sample can usually be accomplished in 5 minutes or less.

The loaded tube is inserted in the pulley of the camera and secured by Picein wax. The camera is then placed on the diffraction unit and exposed for 6 hours at 30,000 volts and 20 milliamperes. The unit holds twelve cameras, so that 24 specimens may be exposed simultaneously. (When an analysis is desired in the least possible elapsed time, use of copper radiation and a different type of camera would require an exposure time of only about 15 minutes. This technic would not permit the simultaneous exposure of 24 specimens, however.) The exposed films are then developed as a batch in standard x-ray developer for 5 minutes at 18° C. (65° F.), fixed in x-ray hypo for about 12 minutes, washed in running water for 20 to 30 minutes, and dried in a film dryer. The drying takes about half an hour. The developed film, or pattern, is now ready to be measured.

TABLE IX. TIME STUDY OF OPERATIONS

	Time, *Man-minutes*
Preparation of specimens and filling of tubes (24 specimens)	120
Loading cameras, mounting specimen (24 specimens)	45
Removing cameras after exposure and filing specimen (24 specimens)	30
Darkroom operation (24 specimens)	20
Labeling and filing negatives (24 specimens)	30
Total	245
Preparation of pattern, average time per specimen	10
Measurement of pattern, average time per specimen	10–15
Identification of pattern, average time per specimen	5–15
Total man-minute time for analysis and permanent record, per specimen	25–40

The pattern is placed symmetrically in the measuring scale (Figure 1) and the positions of the different lines are read off in the order of decreasing Å. spacings. The scale divisions beginning at 20 Å. are 20, 15, 12, 10, 9; every 0.5 Å. from 9 to 6; every 0.25 Å. from 6 to 5; every 0.1 Å. from 5 to 3; every 0.05 Å. from 3 to 2; and every 0.01 Å. from 2 to 0.55.

The next step is to record the intensities of the lines with the aid of an intensity scale. The pattern is placed on top of the intensity scale, and the combination is viewed by eye in transmitted light. A match is then sought between the diffraction line and the standard lines of the intensity scale. The complete data of the diffraction pattern are thus recorded, giving the interplanar spacing and numerical intensity of each line.

The preparation of an intensity scale must be carried out very carefully. However, it need be done only once if the scale is protected from wear by sealing in a Cellophane envelope. (The diffraction patterns themselves can well be filed in Cellophane envelopes.)

While the pattern consists of diffraction lines formed by x-ray beams of very different intensities but of the same exposure time, the intensity scale can, by virtue of the reciprocity relation which holds for x-rays, be constructed by using an x-ray beam of constant intensity and varying the exposure times. The value of the intensity for each step of the intensity scale is therefore proportional to the time of exposure used for that step.

In order to have a beam of MoKα radiation of intensity comparable with the powder reflections, a calcite crystal monochromator was used in conjunction with an absorber further to reduce the intensity of the beam. The exposure times were determined to one-third second by a shutter system. The film was mounted on a drum which was turned by a 400-to-1 reduction gear, for the purpose of easily spacing the intensity steps. The secondary voltage was kept constant at about 25 kilovolts to within 0.5 per cent. The tube current was maintained constant by a stabilizer. The shortest exposure to produce a barely visible mark on the film was 10 seconds. This blackness was arbitrarily chosen to represent unit intensity. The longest exposure was 3250 seconds, corresponding to an intensity of 325. The steps of the intensity scale are such that easily observable differences in blackness exist between adjacent intensity marks, and are as follows: 1, 2, 4, 6, 8, 10, 15, 20, 30, 50, 75, 125, 175, 250, 325. The width of the intensity marks is made approximately the same as that of the diffraction lines.

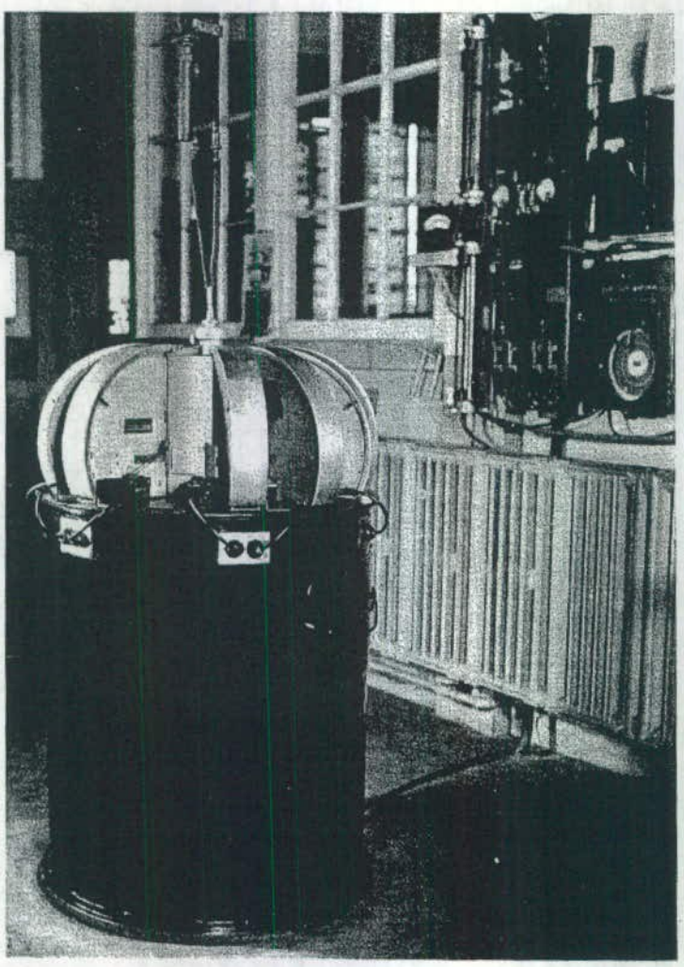


FIGURE 5. DIFFRACTION APPARATUS AND CONTROL BOARD

A fair idea of the approximate expense and time involved in carrying out analysis by the x-ray method can be obtained from data based on actual operation in this laboratory.

If only one specimen were run through instead of 24 at a batch, the time for preparation of the pattern would be about 25 minutes instead of 10.

TABLE X. COST OF SUPPLIES

	Cents
X-ray tube ($225 per tube, average life 12,000 hours' operation) per specimen	0.5
Darkroom supplies	0.7
X-ray film	3.7
Specimen tube	2.0
Power	0.3
Total cost of supplies per specimen	7.2

The expense of the analysis is almost entirely due to the labor involved (Table X).

Accuracy of the Data

SPACING MEASUREMENTS. In the experimental technic as given, the error of measurement of spacings increases in a smooth curve from ±0.001 Å., at 1.0 Å., through ±0.01 Å. at 3.5 Å. to ±0.06 Å. at 8.0 Å. Higher accuracy than this, of course, could be attained by modern precision x-ray methods, but only at the expense of the ease and speed of making the measurements. The use of MoKα radiation and a large camera radius of 20.32 cm. (8.00 inches), as described, makes possible the rapid measurement of the position of the lines on a scale, whereas use of a small precision camera and a comparator is not only tedious but also makes the measurement of weak lines very difficult. In order to secure the accuracy obtained, all cassettes are calibrated with sodium chloride. Since all films are treated under standardized conditions, the effect of film shrinkage is absorbed in the sodium chloride calibration. In 310 cases (the starred compounds) an independent check on the accuracy of the measured spacings was afforded by calculation of the spacings from published data listed by Wyckoff (*10*) and Ewald and Hermann (*5*). The agreement was within the experimental error. Each of the 1000 patterns was measured independently by two different observers.

INTENSITY MEASUREMENTS. The most objective method of measuring the intensities would be to use the microphotometer or densitometer. However, one year's experience with a direct comparison intensity scale has shown that it is sufficiently accurate for use with the classification system. It has the advantages of being rapid and easy to use. Weak lines can be measured in this way when they would be difficult to record with a microphotometer. The steps of the intensity scale are such that successive differences in blackness can easily be recognized. In use, one decides only whether the intensity of the diffraction line lies closer to one of two adjacent pairs of intensity marks, or lies nearer the mean. To check the accuracy of the intensity data, each of the 1000 patterns was read by two independent observers. The agreement was found to be within the steps of the intensity scale. It has been thoroughly tested that the relative intensities of the lines of a pattern remain essentially unchanged, even though the absolute strength of the pattern be different—for instance, because of different exposure times or amount of diffracting material in the tube. One can obtain on a single film the equivalent of two different exposures by covering half the x-ray film lengthwise with a suitable thickness of aluminum foil.

In order to attach a physical meaning to the seemingly arbitrary intensity values, microphotometer tracings were made of the intensity scale itself and of a number of sodium chloride films, for which the time of exposure and the concentration of sodium chloride were varied. This work showed that the use of the intensity scale eliminates the background and gives intensity values proportional to the peak intensities of the diffraction lines. The relative intensities as listed in the tables of data refer to intensities of the diffraction lines from rotated powdered specimens.

Besides the relative intensities, the values of the intensity of the three strongest lines of each compound are included in the tabulated data in order to have a measure of the absolute strength of the diffraction pattern. This information frequently permits a rough estimate of the sensitivity of detection of a compound in a mixture. In using the intensity data, one should bear in mind that the agreement between the tabulated relative intensities and those determined by the analyst for his film is only a semiquantitative one. While the recorded data for the 1000 compounds were obtained with MoKα radiation, it is possible to use the same data for CuKα radiation, provided due precautions are taken to reduce the effect of absorption.

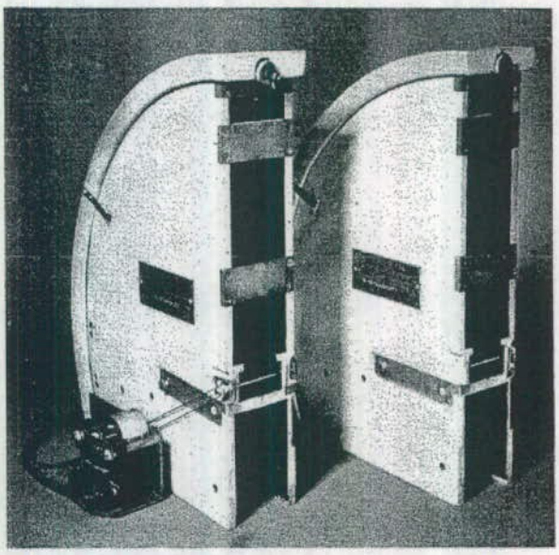


FIGURE 6. FILM CASSETTES WITH SPECIMEN TUBE AND ROTATING DEVICE

Sources and Reliability of Standards

The majority of the 1000 standards listed in this article have not been subjected to a complete chemical analysis. At The Dow Chemical Company, the patterns of a considerably larger number of substances have been entered in the index book and file. Whenever any one of these patterns is used as a standard, its reliability is invoked and, if questioned, is closely examined. However, to permit testing the usability of the classification system and x-ray method of chemical analysis, 1000 substances were selected whose compositions are thought to be reasonably certain.

The starred patterns are those for which it was possible to check all the lines of the pattern with published crystal structure data. This comprehensive check included the calculation of the spacings, the indexing of the lines, and the application of space group criteria. Since, in general, when a crystal structure investigation is made, the chemical formula of the substance must be definitely known, there is little reason to question the reliability of the starred patterns. There are 310 such patterns. Unfortunately, crystal structure data

are lacking for most of the balance of the 1000 patterns. Compounds rated chemically pure were obtained from Eimer & Amend, Merck & Co., Inc., Mallinckrodt Chemical Works, E. H. Sargent and Company, General Chemical Co., Vanadium Corporation of America, G. Frederick Smith Chemical Co., Central Scientific Company, Eastman Kodak Company, and The Dow Chemical Company. When it was not possible to obtain the desired compounds in a C. P. grade, the available grade was used. The less stable hydrates of a sizable group of compounds were prepared in this laboratory, and the degree of hydration was checked gravimetrically. In addition, about 50 compounds not commercially available were synthesized.

It is probable that a small number of cases exist among the unstarred patterns for which the data do not represent the exact formula as given. An idea of the type and extent of the errors to be expected can be obtained from a consideration of the results in those cases where a check with the crystal structure data was possible. Of the 342 cases so investigated, in 14 cases the degree of hydration was incorrectly given by the label on the reagent bottle, the diffraction pattern obtained being that of a different hydrate or of a mixture of hydrates. Seven cases resolved themselves as a mechanical mixture of the labeled substance and an impurity, and four cases as polymorphic mixtures of the same chemical substance. In seven instances, the diffraction pattern experimentally obtained differed completely from the data as published in the crystal structure literature.

Field of Application of X-Ray Diffraction in Chemical Analysis

It is well known that there are definite limitations to the field of application of the x-ray method of analysis, but the important question is as to the range of usefulness left when these things are taken into account. The method is limited in the first place to solids, and secondly to those solids which are crystalline, meaning by crystalline simply those substances which give a pattern. The only way to determine whether or not a material will give a pattern is to subject the material to x-ray diffraction. It has been found experimentally that about 5 per cent of the solid inorganic chemical substances are essentially amorphous and give no pattern by which they could be identified.

A considerable number of other substances give such weak patterns that, while they could be identified if they were the only constituents present, they might escape detection if they were mixed with something else. Depending to some extent on what the substances are mixed with, some would show if they represented less than 1.0 per cent of the material being examined, but many would not show at less than 10.0 per cent and some would not show plainly even when as much as 50.0 per cent was present. The magnitude of this figure can be estimated after the pattern has been obtained, but cannot be told beforehand. Still another weakness of the method is that appreciable percentages of elements may be present in solid solution without changing the pattern enough to be detected, at least without special technic.

Thus, while certainty of analysis is one of the valuable features of the x-ray method, this certainty applies only to what the pattern does show and not to what it does not show. If, for instance, one obtains the pattern of manganese chloride dihydrate it is certain that manganese chloride dihydrate is present. However, it is not certain that there is not a small amount of a more or less amorphous material mixed with it, nor that there is not in solid solution in the manganese chloride a substance which does not greatly change the characteristics of the manganese chloride pattern.

For these reasons the x-ray method is not independent and cannot, in general, stand alone as a means of chemical analysis. The x-ray data must be combined with other data for complete information. The combination of spectroscopy and x-ray diffraction is very fortunate, since they supplement each other's deficiencies by giving entirely different types of information about the same substance. In the arc or spark, the material is broken up into its elements, so that they show regardless of the state in which they were present, while the x-ray, without so much as changing the temperature of the material, records the existing chemical and physical state. The spectrograph is also sensitive in the region of small percentages, where the x-ray is not.

Installation of x-ray diffraction in the laboratory does not, in general, displace other technics, but gives the power to get more information or to obtain information under peculiarly difficult conditions. A practical procedure is to make a survey analysis before other work is attempted. In those cases in which the information obtained is sufficient, it does eliminate other work.

In the field of identification, the merits of x-ray diffraction analysis are sometimes compared with those of microscopic examination. The technics involved and the scientific principles invoked are different. The microscope is much more sensitive than the x-ray to the presence of small percentages of substances, and to amounts of sample of less than 0.1 mg., which is about the practical limit for the x-ray method. It is equally true that the x-ray is much more suited to the general problem of determining the chemical state and composition of the main components of an unknown. The x-rays are less affected by superficial differences, since they analyze the body of the substance. Furthermore, the interpretation of the diffraction pattern is direct. The experimental technic involved can be rapidly acquired. A further advantage of the x-ray method is that no special requirements are imposed upon the form of the specimen. It seems fair to say that, in general, no other single method will yield compound analysis of solids so reliably and economically.

The field of application of x-ray in chemical analysis might be summarized in a general way by saying that, wherever it is necessary to maintain an analytical laboratory, an invaluable supplementary technic will be found in x-ray diffraction. The following are some of the unique features which have been found of practical importance in this laboratory:

1. The substances present show in their true state of chemical combination.

The analysis of reaction mixtures is a good illustration of the application of this feature. The analysis of the residue or slag of a high-temperature reaction in this way shows which components of the charge react, and what the equation of the reaction is. For example, it is desired to determine whether the compounds calcium carbide and calcium silicide will react. About a gram of the two in molecular proportions is mixed and ground, and the mixture is heated to 1500° C. in a small electric vacuum furnace. Before heating, the mixture is a dark powder whose x-ray pattern is the superposition of the calcium carbide and calcium silicide patterns. After heating, the powder looks the same as before, but the x-ray pattern shows only silicon carbide. One concludes with certainty that reaction has taken place according to the equation

$$CaC_2 + CaSi_2 \longrightarrow 2Ca + 2SiC$$

The entire experiment is done with a minimum of expense and time.

A problem which resisted the usual chemical methods of attack was that of the chemicals added to molding sand to inhibit the oxidation of magnesium alloys on casting. A single compound such as ammonium fluoride or ammonium borofluoride may be added to the sand, but reactions begin to take place immediately. The question therefore arises as to what chemicals are actually present in the sand and which ones are actually effective in inhibiting oxidation. The chemical analysis for the ammonium radical present gave no hint as to the

TABLE XI. INDEX TO POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

Pattern No.	Name	Formula
60	Ammonium sulfite monohydrate	$(NH_4)_2SO_3 \cdot H_2O$
61	tartrate	$(CHOH)_2(CO_2NH_4)_2$
62	thiocyanate	NH_4CNS
63	thiosulfate	$(NH_4)_2S_2O_3$
64	tungstate	$(NH_4)_2WO_4 \cdot nH_2O$
65	phosphotungstate	$3(NH_4)_2O \cdot P_2O_5 \cdot 6WO_3 \cdot 9H_2O$
66	metavanadate	NH_4VO_3
67	Antimony	Sb
68	arsenate	$SbAsO_4$
69	arsenite	
70	tribromide	$SbBr_3$
71	trichloride	$SbCl_3$
72	oxychloride	SbOCl
73	trifluoride	SbF_3
74	triiodide	SbI_3
75	trioxide	Sb_2O_3
76	pentoxide	Sb_2O_5
77	potassium sulfurated	$K_2S \cdot Sb_2S_3$
78	sulfate	$Sb_2(SO_4)_3$
79	trisulfide (stibnite)	Sb_2S_3
80	tartrate	$Sb_2(C_4H_4O_6)_3 \cdot 6H_2O$
81	Antimonyl potassium tartrate	$(SbO)KC_4H_4O_6 \cdot {}^1/_2H_2O$
82	Arsenic metal	As
83	iodide (ous)	AsI_3
84	trioxide (ous)	As_2O_3
85	pentoxide	As_2O_5
86	trisulfide (ous), (orpiment)	As_2S_3
87	Barium metal	Ba
88	acetate monohydrate	$Ba(C_2H_3O_2)_2 \cdot H_2O$
89	borate	
90	carbonate	$BaCO_3$
91	chlorate	$Ba(ClO_3)_2$
92	chlorate monohydrate	$Ba(ClO_3)_2 \cdot H_2O$
93	perchlorate trihydrate	$Ba(ClO_4)_2 \cdot 3H_2O$
94	chloride	$BaCl_2$
95	chloride dihydrate	$BaCl_2 \cdot 2H_2O$
96	chromate	$BaCrO_4$
97	citrate	$Ba_3(C_6H_5O_7)_2 \cdot 7H_2O$
98	cyanide	$Ba(CN)_2$
99	fluoride	BaF_2
100	titanium fluoride	$BaTiF_6$
101	fluosilicate	$BaSiF_6$
102	formate	$Ba(HCO_2)_2$
103	hydroxide octahydrate	$Ba(OH)_2 \cdot 8H_2O$
104	iodate	$Ba(IO_3)_2 \cdot H_2O$
105	manganate	$BaMnO_4$
106	permanganate	$Ba(MnO_4)_2$
107	nitrate	$Ba(NO_3)_2$
108	nitrite monohydrate	$Ba(NO_2)_2 \cdot H_2O$
109	oxalate	BaC_2O_4
110	oxide	BaO
111	peroxide	BaO_2
112	phenolsulfonate	$Ba(C_6H_4OH \cdot SO_3)_2$
113	phosphate	$Ba_3(PO_4)_2$
114	phosphite	
115	hypophosphite	$Ba(H_2PO_2)_2 \cdot H_2O$
116	sulfate	$BaSO_4$
117	sulfide	BaS
118	sulfite	$BaSO_3$
119	tartrate	$BaC_4H_4O_6 \cdot H_2O$
120	thiocyanate	$Ba(CNS)_2 \cdot 2H_2O$
121	thiosulfate monohydrate	$BaS_2O_3 \cdot H_2O$
122	borotungstate	
123	valerianate	$Ba(C_4H_9CO_2)_2$
124	Beryllium metal	Be
125	oxide	BeO
126	sulfate	$BeSO_4$
127	sulfate tetrahydrate	$BeSO_4 \cdot 4H_2O$
128	Bismuth metal	Bi
129	acetate	$Bi(C_2H_3O_2)_3$
130	benzoate	$Bi(C_6H_5COO)_3$
131	oxybromide	BiOBr
132	subcarbonate	$Bi_2O_3 \cdot CO_2 \cdot H_2O$
133	oxychloride	BiOCl
134	chromate	$(BiO)_2CrO_4$
135	ammonium citrate	
136	hydroxide	$Bi(OH)_3$
137	lactate	$Bi(C_6H_9O_6) \cdot 7H_2O$
138	β-naphthol	$BiO_3 \cdot C_{10}H_7$
139	subnitrate	$BiO \cdot NO_3 \cdot H_2O$
140	osmate	
141	oxalate	$Bi_2(C_2O_4)_3$
142	trioxide (yellow)	Bi_2O_3
143	tetraoxide	$Bi_2O_4 \cdot 2H_2O$
144	phosphate	$BiPO_4$
145	salicylate	$Bi_2(C_6H_4OHCOO)_3$
146	sulfate	$Bi_2(SO_4)_3$
147	Boric acid	H_3BO_3
148	Boron carbide	B_4C
149	Cadmium metal	Cd
150	acetate	$Cd(C_2H_3O_2)_2 \cdot 2H_2O$
151	bromate	$Cd(BrO_3)_2 \cdot H_2O$
152	carbonate	$CdCO_3$
153	chloride	$CdCl_2$
154	chloride hydrated	$CdCl_2 \cdot 2{}^1/_2H_2O$
155	Cadmium hydroxide	$Cd(OH)_2$
156	potassium iodide	$2KI \cdot CdI_2 \cdot 2H_2O$
157	nitrate tetrahydrate	$Cd(NO_3)_2 \cdot 4H_2O$
158	oxalate	CdC_2O_4
159	oxalate trihydrate	$CdC_2O_4 \cdot 3H_2O$
160	oxide	CdO
161	ferrite	$CdFe_2O_4$
162	phosphate	$Cd_3(PO_4)_2$
163	salicylate	$Cd(C_6H_4OHCOO)_2 \cdot H_2O$
164	sulfate	$3CdSO_4 \cdot 8H_2O$
165	tungstate	$CdWO_4$
166	Calcium metal	Ca
167	acetate	$Ca(C_2H_3O_2)_2$
168	acetate monohydrate	$Ca(C_2H_3O_2)_2 \cdot H_2O$
169	aluminum alloy (22% Ca)	
170	Tricalcium aluminate	$3CaO \cdot Al_2O_3$
171	Pentacalcium aluminate	$5CaO \cdot 3Al_2O_3$
172	Calcium arsenate	$Ca_3(AsO_4)_2$
173	arsenite	
174	benzoate	$Ca(C_6H_5CO_2)_2 \cdot 3H_2O$
175	borate	
176	bromide	$CaBr_2 \cdot 6H_2O$
177	carbide (tetragonal)	CaC_2 I
178	carbide II	CaC_2 II
179	carbide III	CaC_2 III
180	carbonate (calcite)	$CaCO_3$
181	chlorate	$Ca(ClO_3)_2 \cdot 2H_2O$
182	chloride	$CaCl_2$
183	chloride monohydrate	$CaCl_2 \cdot H_2O$
184	chloride dihydrate	$CaCl_2 \cdot 2H_2O$
185	chloride tetrahydrate	$CaCl_2 \cdot 4H_2O$
186	chloride hexahydrate	$CaCl_2 \cdot 6H_2O$
187	chlorofluoride	$CaCl_2 \cdot CaF_2$
188	hypochlorite	$Ca(ClO)_2 \cdot 4H_2O$
189	chromate	$CaCrO_4$
190	chromate dihydrate	$CaCrO_4 \cdot 2H_2O$
191	dichromate	$CaCr_2O_7$
192	citrate	$Ca_3(C_6H_5O_7)_2 \cdot 4H_2O$
193	cyanamide	$CaCN_2$
194	cyanide	$Ca(CN)_2$
195	ferrocyanide	$Ca_2Fe(CN)_6 \cdot 12H_2O$
196	potassium ferrocyanide	$CaK_2Fe(CN)_6$
197	fluoride	CaF_2
198	fluosilicate	$CaSiF_6$
199	fluosilicate dihydrate	$CaSiF_6 \cdot 2H_2O$
200	formate	$Ca(HCO_2)_2$
201	glycolate	$Ca(CH_2OHCOO)_2$
202	glycolate trihydrate	$Ca(CH_2OHCOO)_2 \cdot 3H_2O$
203	glycolate hydrate	$Ca(CH_2OHCOO)_2 \cdot 3{}^1/_2H_2O$
204	hippurate	
205	hydride	CaH_2
206	hydroxide	$Ca(OH)_2$
207	iodate	$Ca(IO_3)_2$
208	iodide	$CaI_2 \cdot 4H_2O$
209	permanganate	$Ca(MnO_4)_2 \cdot 4H_2O$
210	nitrate	$Ca(NO_3)_2$
211	nitrate tetrahydrate	$Ca(NO_3)_2 \cdot 4H_2O$
212	nitrite	$Ca(NO_2)_2 \cdot H_2O$
213	oxalate	CaC_2O_4
214	oxide	CaO
215	peroxide	CaO_2
216	phenolsulfonate	$(C_6H_4OHSO_3)_2Ca \cdot H_2O$
217	hydrogen phosphate	$CaHPO_4$
218	hydrogen phosphate dihydrate	$CaHPO_4 \cdot 2H_2O$
219	dihydrogen phosphate	$Ca(H_2PO_4)_2$
220	dihydrogen phosphate monohydrate	$Ca(H_2PO_4)_2 \cdot H_2O$
221	orthophosphate	$Ca_3(PO_4)_2$
222	orthophosphate monohydrate	$Ca_3(PO_4)_2 \cdot H_2O$
223	chlorohydrophosphate	
224	glycerophosphate	$CaO_2 \cdot PO \cdot OC_3H_5(OH)_2$
225	lactophosphate	
226	pyrophosphate	$Ca_2P_2O_7$
227	phosphide	Ca_3P_2
228	hypophosphite	$Ca(H_2PO_2)_2$
229	sodium hypophosphite	$Ca(NaHPO_2)_2$
230	salicylate	$Ca(C_6H_4OHCOO)_2 \cdot 3H_2O$
231	silicate	$CaSiO_3$
232	Dicalcium silicate (low)	$\alpha\text{-}Ca_2SiO_4$
233	Dicalcium silicate (high)	$\beta\text{-}Ca_2SiO_4$
234	Tricalcium silicate	Ca_3SiO_5
235	Calcium silicide	$CaSi_2$
236	sulfate	$CaSO_4$
237	sulfate hemihydrate	$CaSO_4 \cdot {}^1/_2H_2O$
238	sulfate dihydrate (gypsum)	$CaSO_4 \cdot 2H_2O$
239	sulfide	CaS
240	sulfite	$CaSO_3$
241	tartrate	$CaC_4H_4O_6 \cdot 4H_2O$
242	thiocyanate	$Ca(CNS)_2 \cdot 3H_2O$
243	tungstate	$CaWO_4$
244	urate	$CaC_5H_2O_3N_4$
245	Carbon (graphite)	C
246	Acetaldehyde ammonia	$CH_3CH(NH_2)OH$
247	Acetamide	CH_3CONH_2
248	Acetanilide	$CH_3CONHC_6H_5$
249	Acetophenetidin (phenacetin)	$C_6H_4(OC_2H_5)(NH \cdot CH_3CO)$; 1:4
250	Antipyrine (1-phenyl-2,3-dimethyl pyrazolone)	$C_{11}H_{12}ON_2$
251	Aspirin (acetylsalicylic acid)	$C_6H_4CO_2HCO_2CH_3$
252	Benzoic acid	C_6H_5COOH
253	Benzophenone	$(C_6H_5)_2CO$
254	o-Chlorobenzoic acid	$C_6H_4ClCOOH$
255	β-Chloronaphthalene	$C_{10}H_7Cl$
256	p-Chloro-o-nitroaniline	$C_6H_3ClNO_2 \cdot NH_3$
257	Cinnamic acid	$C_6H_5CH:CHCOOH$
258	Citric acid	$H_3C_6H_5O_7 \cdot H_2O$

Pattern No.	Name
259	Coumarin
260	2,6-Dibror
261	p-Dichlorc
262	2,5-Dichlo
263	Diphenyle
264	Diphenyl
265	Diphenyl
266	Ethyl ami
267	Glycine
268	Glycollic a
269	Hexameth
270	Imino diac
271	Iodoacetyl
272	o-Iodophe
273	Isatin
274	Lactose
275	Maleic aci
276	Naphthale
277	α-Naphth
278	2-Naphth
279	Nitrile tri
280	p-Nitroani
281	m-Nitrobe
282	Oxalic aci
283	Pentachlo
284	o-Phenylp
285	p-Phenylp
286	Salicylic a
287	Sucrose (s
288	Sulfonal (t
289	Tartaric a
290	Tetrabron
291	p-Toluene
292	Trichlorob
293	Trional (n diethy
294	Urea
295	Cerium m
296	chloride
297	nitrate
298	oxalate
299	oxide (i
300	sulfate (
301	sulfate (
302	Cesium al
303	chloride
304	rubidiur
305	iodide
306	dichloro
307	nitrate
308	sulfate
309	Chromium
310	borate
311	bromide
312	fluoride
313	nitrate
314	oxalate
315	oxide (i
316	trioxide
317	ammoni (partl
318	ammoni
319	potassiu
320	Cobalt me
321	acetate
322	arsenate
323	bromide
324	carbona
325	chloride
326	chloride
327	chloride
328	chloride
329	chromat
330	hydroxi
331	mangan
332	nitrate
333	oxalate
334	oxide (o
335	oxide (o
336	phospha
337	stannate
338	sulfate
339	ammoni
340	Columbiu
341	Copper m
342	acetoar
343	alumina
344	benzoat
345	berylliu
346	borate (
347	bromide
348	bromide
349	carbona
350	carbona
351	chloride
352	chloride
353	chloride

TABLE XI. INDEX TO POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

Pattern No.	Name	Formula
259	Coumarin	$C_9H_6O_2$
260	2,6-Dibromo-4-nitrophenol	$NO_2C_6H_2Br_2OH$
261	*p*-Dichlorobenzene	$C_6H_4Cl_2$
262	2,5-Dichlorobenzophenone	$(C_6H_3Cl_2)_2CO$
263	Diphenylene oxide	$(C_6H_4)_2O$
264	Diphenyl sulfoxide	$(C_6H_5)_2SO$
265	Diphenyl urea	$(C_6H_5NH)_2CO$
266	Ethyl amine hydrochloride	$C_2H_5NH_2Cl$
267	Glycine	CH_2NH_2COOH
268	Glycollic acid	$CH_2OHCOOH$
269	Hexamethylenetetramine	$(CH_2)_6N_4$
270	Imino diacetic acid	$NH(CH_2COOH)_2$
271	Iodoacetylene	C_2I_2
272	*o*-Iodophenol	C_6H_4IOH
273	Isatin	$C_6H_4CO\cdot COH{:}N$
274	Lactose	$C_{12}H_{22}O_{11}\cdot H_2O$
275	Maleic acid	$C_2H_2(COOH)_2$
276	Naphthalene	$C_{10}H_8$
277	α-Naphthol	$C_{10}H_7OH$
278	2-Naphthol-6-sulfonic acid	$C_{10}H_6OHSO_2H$
279	Nitrile triacetic acid	$N(CH_2COOH)_3$
280	*p*-Nitroaniline	$NO_2C_6H_4\cdot NH_2$
281	*m*-Nitrobenzaldehyde	$NO_2C_6H_4CHO$
282	Oxalic acid dihydrate	$(COOH)_2\cdot 2H_2O$
283	Pentachlorobenzene	C_6HCl_5
284	*o*-Phenylphenol	$o\text{-}C_6H_5C_6H_4OH$
285	*p*-Phenylphenol	$p\text{-}C_6H_5C_6H_4OH$
286	Salicylic acid	$C_6H_4OHCOOH$
287	Sucrose (sugar)	$C_{12}H_{22}O_{11}$
288	Sulfonal (acetone diethyl sulfone)	$(CH_3)_2C(SO_2C_2H_5)_2$
289	Tartaric acid (*dl*)	$C_4H_6O_6\cdot H_2O$
290	Tetrabromobenzene	$C_6H_2Br_4$-(1,2,4,5)
291	*p*-Toluene sulfonylamide	$CH_3C_6H_4SO_2NH_2$
292	Trichlorobenzyl cyanide	$C_6H_2Cl_3\cdot CH_2CN$
293	Trional (methyl ethyl ketone diethyl sulfone)	$C_2H_5CH_3C{:}(SO_2C_2H_5)_2$
294	Urea	$NH_2\cdot CO\cdot NH_2$
295	Cerium metal (commercial)	Ce
296	chloride	$CeCl_3$
297	nitrate	$Ce(NO_3)_3\cdot 6H_2O$
298	oxalate	$Ce_2(C_2O_4)_3\cdot 9H_2O$
299	oxide (ic)	CeO_2
300	sulfate (ic)	$Ce(SO_4)_2\cdot 4H_2O$
301	sulfate (ous)	$Ce_2(SO_4)_3$
302	Cesium aluminum sulfate (alum)	$CsAl(SO_4)_2\cdot 12H_2O$
303	chloride	$CsCl$
304	rubidium chloride	$CsCl\cdot RbCl$
305	iodide	CsI
306	dichloroiodide	$CsICl_2$
307	nitrate	$CsNO_3$
308	sulfate	Cs_2SO_4
309	Chromium metal	Cr
310	borate	
311	bromide	$CrBr_3\cdot 6H_2O$
312	fluoride tetrahydrate	$CrF_3\cdot 4H_2O$
313	nitrate	$Cr(NO_3)_3\cdot 9H_2O$
314	oxalate	$Cr_2(C_2O_4)_3\cdot H_2O$
315	oxide (ic)	Cr_2O_3
316	trioxide (ic)	CrO_3
317	ammonium sulfate (partly dehydrated)	$Cr(NH_4)(SO_4)_2\cdot <12H_2O$
318	ammonium sulfate (alum)	$Cr(NH_4)(SO_4)_2\cdot 12H_2O$
319	potassium sulfate (alum)	$CrK(SO_4)_2\cdot 12H_2O$
320	Cobalt metal	Co
321	acetate (ous)	$Co(C_2H_3O_2)_2\cdot 4H_2O$
322	arsenate (ous)	$Co_2(AsO_4)_2\cdot 8H_2O$
323	bromide (ous)	$CoBr_2$
324	carbonate (ous)	$CoCO_3$
325	chloride (ous)	
326	chloride hexahydrate (ous)	$CoCl_2\cdot 6H_2O$
327	chloride (luteo)	$Co(NH_3)_4Cl_2$
328	chloride (purpureo)	$Co(NH_3)_5Cl_2$
329	chromate (ous)	$CoCrO_4$
330	hydroxide (ous)	$Co(OH)_2$
331	manganese spinel	$(Mn,Co)(Mn,Co)_2O_4$;2Co:Mn
332	nitrate hexahydrate	$Co(NO_3)_2\cdot 6H_2O$
333	oxalate (ous)	CoC_2O_4
334	oxide (ous)	CoO
335	oxide (ous), (ic)	$CoCo_2O_4$
336	phosphate (ous)	$Co_3(PO_4)_2\cdot 8H_2O$
337	stannate (ous)	
338	sulfate (ous)	$CoSO_4$
339	ammonium sulfate (ous)	$CoSO_4(NH_4)_2SO_4\cdot 6H_2O$
340	Columbium metal	Cb
341	Copper metal	Cu
342	acetoarsenite (ic), (Paris green)	$(CuOAs_2O_3)_2Cu(C_2H_3O_2)_2$
343	aluminate	$CuAl_2O_4$
344	benzoate (ic)	$Cu(C_6H_5COO)_2\cdot 2H_2O$
345	beryllium alloy (12% Be)	
346	borate (ic)	
347	bromide (ous)	$CuBr$
348	bromide (ic)	$CuBr_2$
349	carbonate (ic), (azurite)	$2CuCO_3\cdot Cu(OH)_2$
350	carbonate (ic), (malachite)	$CuCO_3\cdot Cu(OH)_2$
351	chloride (ous)	$CuCl$
352	chloride (ic)	$CuCl_2$
353	chloride (ic) dihydrate	$CuCl_2\cdot 2H_2O$
354	Copper ammonium chloride (ic)	$CuCl_2\cdot 2NH_4Cl\cdot 2H_2O$
355	potassium chloride (ic)	$CuCl_2\cdot 2KCl\cdot 2H_2O$
356	chromate (ic)	$CuCrO_4\cdot 2CuO\cdot 2H_2O$
357	ammonium chromate (ic)	
358	dichromate (ic)	$CuCr_2O_7\cdot 2H_2O$
359	citrate (ic)	$2Cu_3C_6H_5O_7\cdot 5H_2O$
360	cyanide (ous)	$CuCN$
361	potassium cyanide (ous)	$CuK_2(CN)_4$
362	ferrocyanide (ic)	$Cu_2Fe(CN)_6\cdot 7H_2O$
363	potassium ferrocyanide (ic)	$K_2CuFe(CN)_6$
364	fluoride dihydrate (ic)	$CuF_2\cdot 2H_2O$
365	ammonium fluoride	$(NH_4)_2CuF_4\cdot 2H_2O$
366	formate (ic)	$Cu(CHO_2)_2$
367	iodide (ous)	CuI
368	magnesium alloy	$CuMg_2$
369	magnesium alloy	Cu_2Mg
370	nitrate (ic)	$Cu(NO_3)_2\cdot 3H_2O$
371	oxide (ous)	Cu_2O
372	oxide (ic), (tennorite)	CuO
373	cobalt spinel	$CuCo_2O_4$
374	phenol sulfonate	$(C_6H_4OHSO_3)_2Cu\cdot 6H_2O$
375	phosphate (fused), (ic)	
376	phosphate (ic)	$Cu_3(PO_4)_2\cdot 3H_2O$
377	phosphate (ic), (libethenite)	$CuOH\cdot CuPO_4$
378	salicylate (ic)	$Cu(C_6H_4OHCOO)_2\cdot 4H_2O$
379	sulfate (ic)	$CuSO_4$
380	sulfate (ic) monohydrate	$CuSO_4\cdot H_2O$
381	sulfate (ic) pentahydrate	$CuSO_4\cdot 5H_2O$
382	ammonium sulfate (ic)	$CuSO_4(NH_4)_2SO_4\cdot 6H_2O$
383	potassium sulfate (ic)	$CuSO_4\cdot K_2SO_4\cdot 6H_2O$
384	Chalcopyrite	$CuFeS_2$
385	Copper sulfite (ous)	$Cu_2SO_3\cdot H_2O$
386	tartrate (ic)	$CuC_4H_4O_6\cdot 3H_2O$
387	thiocyanate (ous)	$CuCNS$
388	Erbium chloride	$ErCl_3\cdot 6H_2O$
389	oxide	Er_2O_3
390	Germanium dioxide	GeO_2
391	Gold metal	Au
392	cyanide (ous)	$AuCN$
393	potassium cyanide (ous)	$AuK(CN)_2$
394	Indium metal	In
395	trichloride	$InCl_3$
396	oxide	In_2O_3
397	Iodine	I_2
398	pentoxide	I_2O_5
399	Iridium metal	Ir
400	trichloride	$IrCl_3$
401	Iron	Fe
402	aluminum alloy I	$FeAl$
403	aluminum alloy II	$FeAl_2$
404	aluminum alloy III	Fe_2Al_5
405	arsenate (ous)	$Fe_3(AsO_4)_2\cdot 6H_2O$
406	cacodylate (ic)	$Fe[(CH_3)_2AsO_2]_3$
407	chloride (ic)	$FeCl_3$
408	chloride (ic) hexahydrate	$FeCl_3\cdot 6H_2O$
409	chloride (ous) dihydrate	$FeCl_2\cdot 2H_2O$
410	chloride (ous) tetrahydrate	$FeCl_2\cdot 4H_2O$
411	ammonium chloride	
412	ferrocyanide (ic), (Prussian blue)	$Fe_4[Fe(CN)_6]_3$
413	fluoride (ic)	$FeF_3\cdot 4\frac{1}{2}H_2O$
414	formate (ic)	$Fe(HCO_2)_3\cdot H_2O$
415	lactate (ous)	$Fe(C_3H_5O_3)_2\cdot 3H_2O$
416	nitrate (ic)	$Fe(NO_3)_3\cdot 9H_2O$
417	nitride I	Fe_3N
418	nitride II	Fe_4N
419	oxalate (ous)	$FeC_2O_4\cdot 2H_2O$
420	ammonium oxalate (ic)	$(NH_4)_3Fe(C_2O_4)_3$
421	potassium oxalate (ic)	$K_3Fe(C_2O_4)_3\cdot 3H_2O$
422	sodium oxalate (ic)	$2Na_3Fe(C_2O_4)_3\cdot 9H_2O$
423	oxide (ic)	Fe_2O_3
424	Goethite	$FeHO_2$
425	Iron oxide (ous)	FeO
426	ferrite (magnetite)	Fe_3O_4
427	chrome-aluminate	$FeO(Cr_2O_3\cdot Al_2O_3)$
428	phenolsulfonate (ous)	$(C_6H_4OHSO_3)_2\cdot Fe$
429	phosphide	Fe_2P
430	hypophosphite (ic)	$Fe(H_2PO_2)_3$
431	salicylate (ic)	
432	silicide	$FeSi$
433	disilicide	$FeSi_2$
434	sulfate (ic)	$Fe_2(SO_4)_3\cdot H_2O$
435	sulfate (ous)	$FeSO_4$
436	sulfate monohydrate (ous)	$FeSO_4\cdot H_2O$
437	sulfate trihydrate (ous)	$FeSO_4\cdot 3H_2O$
438	sulfate heptahydrate (ous)	$FeSO_4\cdot 7H_2O$
439	ammonium sulfate (partly dehydrated), (ic)	$FeNH_4(SO_4)_2\cdot <12H_2O$
440	ammonium sulfate (ic), (alum)	$FeNH_4(SO_4)_2\cdot 12H_2O$
441	ammonium sulfate (ous)	$FeSO_4\cdot(NH_4)_2SO_4\cdot 6H_2O$
442	sulfide (ous)	FeS
443	disulfide (pyrite)	FeS_2
444	tartrate (ous)	$FeC_4H_4O_6$
445	Lead metal	Pb
446	acetate	$Pb(C_2H_3O_2)_2\cdot 3H_2O$
447	acetate (basic)	$Pb(C_2H_3O_2)_2Pb(OH)_2\cdot H_2O$

TABLE XI. INDEX TO POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

Pattern No.	Name	Formula
448	Lead antimoniate	$Pb_2(SbO_4)_2$
449	hydrogen orthoarsenate	$PbHAsO_4$
450	bromide	$PbBr_2$
451	carbonate	$PbCO_3$
452	carbonate (basic)	$2PbCO_3 \cdot Pb(OH)_2$
453	chloride	$PbCl_2$
454	chromate	$PbCrO_4$
455	ferrocyanide	$Pb_2Fe(CN)_6 \cdot 3H_2O$
456	fluoride (cubic)	PbF_2
457	fluosilicate	$PbSiF_6 \cdot 2H_2O$
458	formate	$Pb(HCO_2)_2$
459	iodide	PbI_2
460	nitrate	$Pb(NO_3)_2$
461	oxalate	PbC_2O_4
462	oxide (litharge)	PbO
463	dioxide	PbO_2
464	oxide (minium)	Pb_3O_4
465	phosphate	$Pb_3(PO_4)_2$
466	sulfate	$PbSO_4$
467	sulfide	PbS
468	thiosulfate	PbS_2O_3
469	Lithium metal	Li
470	benzoate	$Li(C_6H_5COO)$
471	borate	$Li_2B_4O_7 \cdot 5H_2O$
472	bromide	$LiBr$
473	bromide dihydrate	$LiBr \cdot 2H_2O$
474	carbonate	Li_2CO_3
475	chloride	$LiCl$
476	chloride monohydrate	$LiCl \cdot H_2O$
477	chromate	Li_2CrO_4
478	chromate dihydrate	$Li_2CrO_4 \cdot 2H_2O$
479	dichromate	$Li_2Cr_2O_7 \cdot 2H_2O$
480	fluoride	LiF
481	hydroxide	$LiOH$
482	iodide	LiI
483	iodide trihydrate	$LiI \cdot 3H_2O$
484	lactate	$LiC_3H_5O_3$
485	nitrate	$LiNO_3$
486	oxalate	$Li_2C_2O_4$
487	salicylate	$LiC_6H_4OH \cdot COO$
488	sulfate	Li_2SO_4
489	sulfate monohydrate	$Li_2SO_4 \cdot H_2O$
490	tartrate	$Li_2C_4H_4O_6 \cdot H_2O$
491	acid tartrate	$LiHC_4H_4O_6$
492	Magnesium metal	Mg
493	acetate	$Mg(C_2H_3O_2)_2$
494	acetate tetrahydrate	$Mg(C_2H_3O_2)_2 \cdot 4H_2O$
495	aluminum alloy I	Mg_2Al_3
496	aluminum alloy II	Mg_2Al_3
497	aluminate	$MgAl_2O_4$
498	arsenate	$2MgHAsO_4 \cdot 13H_2O$
499	benzoate	$Mg(C_6H_5COO)_2 \cdot 3H_2O$
500	borate	
501	bromide hexahydrate	$MgBr_2 \cdot 6H_2O$
502	calcium alloy	Mg_2Ca
503	carbide	Mg_2C_3
504	carbonate trihydrate (nesquehonite)	$MgCO_3 \cdot 3H_2O$
505	carbonate (hydromagnesite)	$5MgO \cdot 4CO_2 \cdot 5H_2O$
506	Dolomite	$MgCO_3 \cdot CaCO_3$
507	Magnesium perchlorate	$Mg(ClO_4)_2$
508	perchlorate trihydrate	$Mg(ClO_4)_2 \cdot 3H_2O$
509	perchlorate hexahydrate	$Mg(ClO_4)_2 \cdot 6H_2O$
510	chloride	$MgCl_2$
511	chloride hexahydrate	$MgCl_2 \cdot 6H_2O$
512	ammonium chloride	$MgCl_2 \cdot NH_4Cl \cdot 6H_2O$
513	chromate	$MgCrO_4 \cdot 7H_2O$
514	citrate	$Mg_3(C_6H_5O_7)_2 \cdot 14H_2O$
515	fluoride	MgF_2
516	fluosilicate	$MgSiF_6 \cdot 6H_2O$
517	formate	$Mg(CHO_2)_2 \cdot 2H_2O$
518	hydroxide	$Mg(OH)_2$
519	iodide	$MgI_2 \cdot 8H_2O$
520	lactate	$Mg(C_3H_5O_3)_2 \cdot 3H_2O$
521	lead alloy	Mg_2Pb
522	mercury alloy	Mg_2Hg
523	nitrate	$Mg(NO_3)_2 \cdot 6H_2O$
524	nitride	Mg_3N_2
525	oxalate	$MgC_2O_4 \cdot 2H_2O$
526	oxide	MgO
527	ferrite	$MgFe_2O_4$
528	phenolsulfonate	$(C_6H_4OHSO_3)_2Mg$
529	phosphate monohydrogen	$MgHPO_4 \cdot 3H_2O$
530	phosphate dihydrogen	$Mg(H_2PO_4)_2$
531	phosphate tetrahydrate	$Mg_3(PO_4)_2 \cdot 4H_2O$
532	phosphate octahydrate	$Mg_3(PO_4)_2 \cdot 8H_2O$
533	ammonium phosphate	$MgNH_4PO_4 \cdot 6H_2O$
534	pyrophosphate	$Mg_2P_2O_7$
535	hypophosphite	$Mg(H_2PO_2)_2 \cdot 6H_2O$
536	lactophosphate	
537	silicate	$MgSiO_3$
538	Dimagnesium silicate	Mg_2SiO_4
539	Asbestos	$3MgO \cdot 2SiO_2 \cdot 2H_2O$
540	Magnesium silicide	Mg_2Si
541	sulfate	$MgSO_4$
542	sulfate monohydrate	$MgSO_4 \cdot H_2O$
543	sulfate hexahydrate	$MgSO_4 \cdot 6H_2O$
544	sulfate heptahydrate (Epsom salt)	$MgSO_4 \cdot 7H_2O$
545	ethyl sulfate	
546	sulfide	MgS
547	sulfite hexahydrate	$MgSO_3 \cdot 6H_2O$
548	tartrate	$MgC_4H_4O_6 \cdot 5H_2O$
549	thiosulfate	$MgS_2O_3 \cdot 6H_2O$
550	tin alloy	Mg_2Sn
551	Magnesium urate	$MgC_5H_2N_4O_3$
552	vanadate	
553	Manganese (α)	α-Mn
554	(β)	β-Mn
555	acetate	$Mn(C_2H_3O_2)_2 \cdot 4H_2O$
556	aluminate	$MnAl_2O_4$
557	benzoate	$Mn(C_6H_5COO)_2 \cdot 3H_2O$
558	borate	
559	carbonate	$MnCO_3$
560	chloride	$MnCl_2$
561	chloride monohydrate	$MnCl_2 \cdot H_2O$
562	chloride dihydrate	$MnCl_2 \cdot 2H_2O$
563	chloride tetrahydrate	$MnCl_2 \cdot 4H_2O$
564	fluoride	MnF_2
565	oxalate	MnC_2O_4
566	oxalate hydrate	$MnC_2O_4 \cdot 2^1/_2H_2O$
567	oxide	MnO
568	dioxide	MnO_2
569	manganic oxide (ous)	Mn_3O_4
570	cobalt spinel	$(Mn,Co)\ (Mn,Co)_2O_4;2Mn:Co$
571	phosphate	$Mn_3(PO_4)_2 \cdot 7H_2O$
572	hypophosphite	$Mn(H_2PO_2)_2 \cdot H_2O$
573	ammonium sulfate	$MnSO_4(NH_4)_2SO_4 \cdot 6H_2O$
574	sulfate tetrahydrate	$MnSO_4 \cdot 4H_2O$
575	sulfide	MnS
576	tartrate	$MnC_4H_4O_6$
577	Mercury acetate (ic)	$Hg(C_2H_3O_2)_2$
578	acetate (ous)	$(HgC_2H_3O_2)_2$
579	benzoate (ic)	$Hg(C_6H_5COO)_2$
580	bromide (ic)	$HgBr_2$
581	bromide (ous)	Hg_2Br_2
582	perchlorate (ic)	$Hg(ClO_4)_2$
583	chloride (ic)	$HgCl_2$
584	chloride (ous)	Hg_2Cl_2
585	ammonium chloride	
586	oxychloride (ic)	$HgCl_2 \cdot 3HgO$
587	chromate (ic)	$HgCrO_4$
588	chromate (ous)	Hg_2CrO_4
589	cyanide (ic)	$Hg(CN)_2$
590	iodide (ic)	HgI_2
591	iodide (ous)	Hg_2I_2
592	potassium iodide (ic)	$K_2HgI_4 \cdot 3H_2O$
593	nitrate (ous)	$HgNO_3 \cdot H_2O$
594	oxalate (ic)	HgC_2O_4
595	oxide (ic), (orthorhombic)	HgO
596	phosphate (ic)	$Hg_3(PO_4)_2$
597	phosphate (ous)	Hg_2PO_4
598	succinate (ic)	$Hg(CH_2COO)_2$
599	sulfate (ic)	$HgSO_4$
600	sulfate (basic)	$HgSO_4 \cdot 2HgO$
601	sulfate (ous)	Hg_2SO_4
602	sulfide (black)	HgS
603	sulfide (red), (cinnabar)	HgS
604	sulfide thiocyanate (ous)	$HgCNS$
605	Molybdenum metal	Mo
606	acid (ic)	H_2MoO_4
607	carbide	Mo_2C
608	oxalate	
609	oxide (ic)	MoO_2
610	sesquioxide	Mo_2O_3
611	silicide	$MoSi_2$
612	Neodymium chloride	$NdCl_3$
613	chloride hexahydrate	$NdCl_3 \cdot 6H_2O$
614	ammonium nitrate	
615	Nickel metal	Ni
616	acetate	$Ni(C_2H_3O_2)_2$
617	aluminate	$NiAl_2O_4$
618	chloride	$NiCl_2$
619	chloride dihydrate	$NiCl_2 \cdot 2H_2O$
620	chloride tetrahydrate	$NiCl_2 \cdot 4H_2O$
621	chloride hexahydrate	$NiCl_2 \cdot 6H_2O$
622	cyanide	$Ni(CN)_2 \cdot 4H_2O$
623	fluoride	
624	formate	$Ni(CHO_2)_2 \cdot 2H_2O$
625	hydroxide	$Ni(OH)_2$
626	nitrate	$Ni(NO_3)_2 \cdot 6H_2O$
627	oxalate	$NiC_2O_4 \cdot 2H_2O$
628	oxide	NiO
629	manganese spinel	$NiMn_2O_4$
630	sulfate hexahydrate	$NiSO_4 \cdot 6H_2O$
631	sulfate heptahydrate	$NiSO_4 \cdot 7H_2O$
632	ammonium sulfate	$NiSO_4 \cdot (NH_4)_2SO_4 \cdot 6H_2O$
633	tartrate (ous)	
634	Osmium metal	Os
635	Palladium metal	Pd
636	chloride	$PdCl_2$
637	nitrate	$Pd(NO_3)_2$
638	Phosphorus pentachloride	PCl_5
639	pentoxide	P_2O_5
640	pentasulfide	P_2S_5
641	Phosphomolybdic acid	$20MoO_3 \cdot 2H_3PO_4 \cdot 48H_2O$

Pattern No.	Name
642	Platinum m
643	ammoniu
644	potassiur
645	potassiur
646	sodium c
647	barium c
648	magnesiu
649	potassiur
650	Potassium
651	acetate
652	arsenate
653	arsenite
654	azide
655	benzoate
656	tetrabors
657	bromate
658	bromide
659	carbonat
660	bicarbon
661	chlorate
662	perchlora
663	chloride
664	chromate
665	dichroma
666	citrate
667	cyanate
668	cyanide
669	ferricyan
670	ferrocyar
671	ferrocyar
672	fluoride
673	fluoride c
674	fluosilica
675	hydroxid
676	iodate
677	iodate, a
678	periodat
679	iodide
680	permang
681	molybda
682	nitrate
683	nitrite
684	osmate
685	oxalate
686	oxalate r
687	oxalate,
688	phenolsu
689	phenylat
690	orthophc
691	hydroger
692	hydroger
693	dihydrog
694	ammoni
695	pyropho
696	hypopho
697	phthalin
698	hydroger
699	salicylat
700	selenate
701	selenite
702	selenocy
703	Feldspar (
704	Potassium
705	hydroge
706	persulfat
707	pyrosulf
708	ethyl sul
709	methyl s
710	sulfite
711	hydroge
712	pyrosulf
713	benzene
714	guaiacol
715	indigo s
716	toluene
717	tartrate
718	ammoni
719	hydroge
720	tellurite
721	thiocarb
722	thiosulf
723	thiosulf
724	thiocyar
725	titanate
726	tungstat
727	uranate
728	urate
729	vanadat
730	xanthog
731	Rhenium
732	Rhodium
733	Rubidium
734	chloride
735	iodide
736	nitrate
737	sulfate
738	aluminu
739	Ruthenium

TABLE XI. INDEX TO POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

Pattern No.	Name	Formula
642	Platinum metal	Pt
643	ammonium chloride (ic)	$(NH_4)_2PtCl_6$
644	potassium chloride (ic)	K_2PtCl_6
645	potassium chloride (ous)	K_2PtCl_4
646	sodium chloride	
647	barium cyanide tetrahydrate	$BaPt(CN)_4 \cdot 4H_2O$
648	magnesium cyanide	
649	potassium cyanide	$K_2Pt(CN)_4 \cdot 3H_2O$
650	Potassium metal	K
651	acetate	$KC_2H_3O_2$
652	arsenate	
653	arsenite	
654	aside	KN_3
655	benzoate	$K(C_6H_5COO) \cdot 3H_2O$
656	tetraborate	$K_2B_4O_7 \cdot 5H_2O$
657	bromate	$KBrO_3$
658	bromide	KBr
659	carbonate	K_2CO_3
660	bicarbonate	$KHCO_3$
661	chlorate	$KClO_3$
662	perchlorate	$KClO_4$
663	chloride	KCl
664	chromate	K_2CrO_4
665	dichromate	$K_2Cr_2O_7$
666	citrate	$K_3C_6H_5O_7 \cdot H_2O$
667	cyanate	KCNO
668	cyanide	KCN
669	ferricyanide	$K_3Fe(CN)_6$
670	ferrocyanide	$K_4Fe(CN)_6$
671	ferrocyanide trihydrate	$K_4Fe(CN)_6 \cdot 3H_2O$
672	fluoride	KF
673	fluoride dihydrate	$KF \cdot 2H_2O$
674	fluosilicate	K_2SiF_6
675	hydroxide	KOH
676	iodate	KIO_3
677	iodate, acid	$KIO_3 \cdot HIO_3$
678	periodate	KIO_4
679	iodide	KI
680	permanganate	$KMnO_4$
681	molybdate	K_2MoO_4
682	nitrate	KNO_3
683	nitrite	KNO_2
684	osmate	$K_2OsO_4 \cdot 2H_2O$
685	oxalate	$K_2C_2O_4$
686	oxalate monohydrate	$K_2C_2O_4 \cdot H_2O$
687	oxalate, acid	$KHC_2O_4 \cdot {}^1/_2H_2O$
688	phenolsulfonate	$K(C_6H_4OHSO_3)$
689	phenylate	C_6H_5OK
690	orthophosphate	K_3PO_4
691	hydrogen phosphate	K_2HPO_4
692	hydrogen phosphate trihydrate	$K_2HPO_4 \cdot 3H_2O$
693	dihydrogen phosphate	KH_2PO_4
694	ammonium phosphate	
695	pyrophosphate	$K_4P_2O_7 \cdot 3H_2O$
696	hypophosphite	KH_2PO_2
697	phthalimide	$C_6H_4(CO)_2NK$
698	hydrogen phthalate	$C_6H_4COOH \cdot COOK$
699	salicylate	$C_6H_4OHCOOK$
700	selenate	K_2SeO_4
701	selenite	K_2SeO_3
702	selenocyanide	KSeCN
703	Feldspar (microcline)	$KAlSi_3O_8$
704	Potassium sulfate	K_2SO_4
705	hydrogen sulfate	$KHSO_4$
706	persulfate	$K_2S_2O_8$
707	pyrosulfate	$K_2S_2O_7$
708	ethyl sulfate	$KC_2H_5SO_4$
709	methyl sulfate	$2KCH_3SO_4 \cdot H_2O$
710	sulfite	$K_2SO_3 \cdot 2H_2O$
711	hydrogen sulfite	$KHSO_3$
712	pyrosulfite	$K_2S_2O_5$
713	benzene sulfonate	$C_6H_5SO_3K$
714	guaiacol sulfonate	
715	indigo sulfonate	
716	toluene sulfonate	$p\text{-}CH_3C_6H_4SO_3K$
717	tartrate	$K_2C_4H_4O_6$
718	ammonium tartrate	$K(NH_4)C_4H_4O_6$
719	hydrogen tartrate	$KH(C_4H_4O_6)$
720	tellurite	K_2TeO_3
721	thiocarbonate	K_2CS_3
722	thiosulfate	$K_2S_2O_3$
723	thiosulfate hydrate	$3K_2S_2O_3 \cdot H_2O$
724	thiocyanate	KCNS
725	titanate	K_2TiO_3
726	tungstate	$K_2WO_4 \cdot 2H_2O$
727	uranate	K_2UO_4
728	urate	$KHC_5H_2N_4O_3$
729	vanadate, meta	KVO_3
730	xanthogenate	$KS_2COC_2H_5$
731	Rhenium metal	Re
732	Rhodium metal	Rh
733	Rubidium bromide	RbBr
734	chloride	RbCl
735	iodide	RbI
736	nitrate	$RbNO_3$
737	sulfate	Rb_2SO_4
738	aluminum sulfate (alum)	$RbAl(SO_4)_2 \cdot 12H_2O$
739	Ruthenium metal	Ru

Pattern No.	Name	Formula
740	Selenium (hexagonal)	Se
741	Selenium acid (ous)	H_2SeO_3
742	Silicon	Si
743	Silicon carbide (cubic)	SiC
744	Carborundum commercial (cubic and hexagonal forms)	SiC
745	Silicon dioxide (α-cristobalite)	SiO_2
746	dioxide (α-quartz)	SiO_2
747	Silver metal	Ag
748	acetate	$AgC_2H_3O_2$
749	arsenate	Ag_3AsO_4
750	bromate	$AgBrO_3$
751	bromide	AgBr
752	carbonate	Ag_2CO_3
753	perchlorate	$AgClO_4 \cdot H_2O$
754	chloride	AgCl
755	chromate	Ag_2CrO_4
756	citrate	$Ag_3C_6H_5O_7$
757	cyanide	AgCN
758	potassium cyanide	
759	iodide (cubic)	AgI
760	iodide (cubic and hexagonal)	AgI
761	molybdate	Ag_2MoO_4
762	nitrate	$AgNO_3$
763	nitrite	$AgNO_2$
764	oxide	Ag_2O
765	phosphate	Ag_3PO_4
766	sulfate	Ag_2SO_4
767	sulfide (orthorhombic)	Ag_2S
768	tartrate	$Ag_2C_4H_4O_6$
769	vanadate	$Ag_4V_2O_7$
770	Sodium metal	Na
771	acetate	$NaC_2H_3O_2$
772	acetate trihydrate	$NaC_2H_3O_2 \cdot 3H_2O$
773	uranyl zinc acetate	$Na(UO_2)Zn(C_2H_3O$
774	amide	$NaNH_2$
775	arsenate	$Na_2HAsO_4 \cdot 7H_2O$
776	arsenate (methyl)	$CH_3AsO(ONa)_2 \cdot 6H$
777	arsenite	Na_3HAsO_3
778	asparaginate	
779	azide	NaN_3
780	barbital	
781	bismuthate	$NaBiO_3$
782	tetraborate	$Na_2B_4O_7 \cdot 5H_2O$
783	tetraborate decahydrate (borax)	$Na_2B_4O_7 \cdot 10H_2O$
784	metaborate	$Na_2(B_2O_4)$
785	perborate	$NaBO_3 \cdot 2H_2O$
786	borobenzoate	
787	bromate	$NaBrO_3$
788	bromide	NaBr
789	butyrate	$CH_3CH_2CH_2COONa$
790	cacodylate	$(CH_3)_2AsO \cdot ONa \cdot 3H_2O$
791	carbonate	Na_2CO_3
792	carbonate monohydrate	$Na_2CO_3 \cdot H_2O$
793	carbonate hydrate	$Na_2CO_3 \cdot 2{}^1/_2H_2O$
794	carbonate decahydrate	$Na_2CO_3 \cdot 10H_2O$
795	hydrogen carbonate	$NaHCO_3$
796	potassium carbonate	$NaKCO_3$
797	chlorate	$NaClO_3$
798	perchlorate	$NaClO_4$
799	perchlorate monohydrate	$NaClO_4 \cdot H_2O$
800	chloride	NaCl
801	chromate	Na_2CrO_4
802	chromate tetrahydrate	$Na_2CrO_4 \cdot 4H_2O$
803	dichromate dihydrate	$Na_2Cr_2O_7 \cdot 2H_2O$
804	cinnamate	$C_6H_5CH{:}CHCOONa$
805	citrate dihydrate	$Na_3C_6H_5O_7 \cdot 2H_2O$
806	citrate hydrate	$2Na_3C_6H_5O_7 \cdot 11H_2O$
807	cyanide	NaCN
808	ethylate	C_2H_5ONa
809	ferrocyanide	$Na_4Fe(CN)_6$
810	ferrocyanide decahydrate	$Na_4Fe(CN)_6 \cdot 10H_2O$
811	nitroferrocyanide	$Na_2Fe(CN)_5NO \cdot 2H_2O$
812	fluoride	NaF
813	aluminum fluoride (cryolite)	Na_3AlF_6
814	fluosilicate	Na_2SiF_6
815	formate	$NaHCO_2$
816	hippurate	
817	hydroxide	NaOH
818	iodate	$NaIO_3$
819	periodate	$Na_2H_3IO_6$
820	iodide	NaI
821	permanganate	$NaMnO_4 \cdot 3H_2O$
822	molybdate	$Na_2MoO_4 \cdot 2H_2O$
823	phosphomolybdate	
824	naphthionate	
825	nitrate	$NaNO_3$
826	nitrate (cobaltic)	
827	nitrite	$NaNO_2$
828	oxalate	$Na_2C_2O_4$
829	hydrogen oxalate	$NaHC_2O_4 \cdot H_2O$
830	peroxide	Na_2O_2
831	p-phenolsulfonate	$p\text{-}C_6H_4OHSO_3Na \cdot 2H_2O$
832	nitrophenylate	
833	dinitrophenylate	
834	orthophosphate	Na_3PO_4
835	hydrogen phosphate	Na_2HPO_4
836	hydrogen phosphate dihydrate	$Na_2HPO_4 \cdot 2H_2O$
837	hydrogen phosphate dodecahydrate	$Na_2HPO_4 \cdot 12H_2O$
838	dihydrogen phosphate	NaH_2PO_4
839	dihydrogen phosphate monohydrate	$NaH_2PO_4 \cdot H_2O$

TABLE XI. INDEX TO POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Concluded*)

Pattern No.	Name	Formula
840	Sodium hypophosphate	$Na_4P_2O_6 \cdot 10H_2O$
841	metaphosphate	$NaPO_3$
842	pyrophosphate	$Na_4P_2O_7$
843	pyrophosphate decahydrate	$Na_4P_2O_7 \cdot 10H_2O$
844	ammonium hydrogen phosphate tetrahydrate	$NaNH_4HPO_4 \cdot 4H_2O$
845	calcium glycerophosphate (duotonal)	
846	phosphite	$Na_2HPO_3 \cdot 5H_2O$
847	hypophosphite	$NaH_2PO_2 \cdot H_2O$
848	plumbate	$Na_2PbO_3 \cdot 3H_2O$
849	salicylate	$Na(C_6H_4OHCOO)$
850	selenate	Na_2SeO_4
851	selenite	Na_2SeO_3
852	metasilicate	Na_2SiO_3
853	metasilicate nonahydrate	$Na_2SiO_3 \cdot 9H_2O$
854	aluminum silicate (albite)	$NaAlSi_3O_8$
855	stannate	$Na_2SnO_3 \cdot 3H_2O$
856	stearate	$Na(C_{17}H_{35}COO)$
857	succinate	$(CH_2COONa)_2 \cdot 6H_2O$
858	sulfate (orthorhombic)	Na_2SO_4
859	sulfate (heated)	Na_2SO_4
860	sulfate (decahydrate)	$Na_2SO_4 \cdot 10H_2O$
861	hydrogen sulfate	$NaHSO_4$
862	hydrogen sulfate monohydrate	$NaHSO_4 \cdot H_2O$
863	persulfate	$Na_2S_2O_8$
864	sulfide nonahydrate	$Na_2S \cdot 9H_2O$
865	sulfite	Na_2SO_3
866	sulfite heptahydrate	$Na_2SO_3 \cdot 7H_2O$
867	hyposulfite	$Na_2S_2O_4 \cdot 2H_2O$
868	pyrosulfite	$Na_2S_2O_5$
869	anthraquinone-β-sulfonate	$C_{14}H_7O_2SO_3Na$
870	naphthalene monosulfonate	$C_{10}H_7SO_3Na$
871	naphthalene α-disulfonate	$C_{10}H_6(SO_3Na)_2$
872	tartrate	$Na_2C_4H_4O_6 \cdot 2H_2O$
873	hydrogen tartrate	$NaHC_4H_4O_6 \cdot H_2O$
874	tellurite	Na_2TeO_3
875	thiocyanate	$NaCNS$
876	thiosulfate	$Na_2S_2O_3$
877	thiosulfate pentahydrate	$Na_2S_2O_3 \cdot 5H_2O$
878	tungstate	$Na_2WO_4 \cdot 2H_2O$
879	urate	$Na_2C_5H_2O_3N_4 \cdot H_2O$
880	metavanadate	$NaVO_3 \cdot H_2O$
881	orthovanadate	$Na_3VO_4 \cdot 16H_2O$
882	Strontium	Sr
883	acetate	$Sr(C_2H_3O_2)_2 \cdot {}^1/_2H_2O$
884	bromide hexahydrate	$SrBr_2 \cdot 6H_2O$
885	carbonate	$SrCO_3$
886	chlorate	$Sr(ClO_3)_2 \cdot 8H_2O$
887	chloride hexahydrate	$SrCl_2 \cdot 6H_2O$
888	chromate	$SrCrO_4$
889	formate	$Sr(HCO_2)_2$
890	formate dihydrate	$Sr(HCO_2)_2 \cdot 2H_2O$
891	fluoride	SrF_2
892	hydroxide octahydrate	$Sr(OH)_2 \cdot 8H_2O$
893	iodide hexahydrate	$SrI_2 \cdot 6H_2O$
894	lactate	$Sr(C_3H_5O_3)_2 \cdot 3H_2O$
895	nitrate	$Sr(NO_3)_2$
896	oxalate	$SrC_2O_4 \cdot H_2O$
897	peroxide	SrO_2
898	phosphate	$SrHPO_4$
899	salicylate	$Sr(C_7H_5O_3)_2 \cdot 2H_2O$
900	sulfate	$SrSO_4$
901	tartrate	$SrC_4H_4O_6 \cdot 4H_2O$
902	Sulfur	S
903	Tantalum metal	Ta
904	potassium fluoride	$KTaF_6$
905	pentoxide	Ta_2O_5
906	Tellurium	Te
907	dichloride (ic)	$TeCl_2$
908	dioxide (ic)	TeO_2
909	nitrate (ic) basic	$4TeO_2 \cdot N_2O_5 \cdot 1{}^1/_2H_2O$
910	nitrate (ic)	
911	acid (ic)	H_2TeO_4
912	acid dihydrate (ic)	$Te(OH)_6$
913	Thallium metal (hexagonal)	α-Tl
914	chloride (ous)	TlCl
915	nitrate (ic)	$Tl(NO_3)_3 \cdot 3H_2O$
916	oxide (ic)	Tl_2O_3
917	sulfate (ous)	Tl_2SO_4
918	Thorium metal	Th
919	acetate	
920	chloride	$ThCl_4$
921	Thorium nitrate	$Th(NO_3)_4 \cdot 12H_2O$
922	oxalate	$Th(C_2O_4)_2$
923	dioxide	ThO_2
924	sulfate	$Th(SO_4)_2$
925	Tin metal	Sn
926	antimony alloy	SnSb
927	chloride (ic)	$SnCl_4 \cdot 5H_2O$
928	ammonium chloride (ic)	$(NH_4)_2SnCl_6$
929	chloride dihydrate (ous)	$SnCl_2 \cdot 2H_2O$
930	iodide (ic)	SnI_4
931	oxalate (ous)	SnC_2O_4
932	oxide (ous)	SnO
933	oxide (ic)	SnO_2
934	phosphate (ous)	$Sn_3(PO_4)_2$
935	sulfate (ic)	$Sn(SO_4)_2 \cdot 2H_2O$
936	sulfate (ous)	$SnSO_4$
937	sulfide (ic)	SnS_2
938	sulfide (ous)	SnS
939	tartrate (ous)	$SnC_4H_4O_6$
940	Titanium metal	Ti
941	carbide	TiC
942	fluoride	TiF_4
943	potassium fluoride	$K_2TiF_6 \cdot H_2O$
944	dioxide (anatase)	TiO_2
945	dioxide (rutile)	TiO_2
946	Tungsten metal	W
947	acid (ic), (meta)	$H_2W_4O_{13}$
948	trioxide (ic)	WO_3
949	Uranyl acetate	$UO_2(C_2H_3O_2)_2 \cdot 2H_2O$
950	Uranyl nitrate hexahydrate	$UO_2(NO_3)_2 \cdot 6H_2O$
951	Vanadium	V
952	carbide (14% C)	VC
953	chloride	
954	trioxide	V_2O_3
955	pentoxide	V_2O_5
956	Vanadyl sulfate	$(VO)_2(SO_4)_3 \cdot 16H_2O$
957	Yttrium nitrate	$Y(NO_3)_3 \cdot 6H_2O$
958	oxide	Y_2O_3
959	Zinc metal	Zn
960	acetate	$Zn(C_2H_3O_2)_2$
961	acetate dihydrate	$Zn(C_2H_3O_2)_2 \cdot 2H_2O$
962	aluminate	$ZnAl_2O_4$
963	arsenate	$Zn_3(AsO_4)_2 \cdot 8H_2O$
964	arsenite	
965	benzoate	$Zn(C_6H_5COO)_2$
966	perchlorate	$Zn(ClO_4)_2 \cdot 6H_2O$
967	chloride (fused)	
968	chromate	$ZnCrO_4$
969	cyanide	$Zn(CN)_2$
970	potassium cyanide	
971	ferrocyanide	$Zn_2Fe(CN)_6 \cdot 3H_2O$
972	fluoride	ZnF_2
973	fluoride tetrahydrate	$ZnF_2 \cdot 4H_2O$
974	iodide	ZnI_2
975	lactate	$Zn(C_3H_5O_3)_2 \cdot 3H_2O$
976	oxalate	$ZnC_2O_4 \cdot 2H_2O$
977	oxide	ZnO
978	cobalt oxide	$ZnCo_2O_4$
979	iron oxide	$ZnFe_2O_4$
980	permanganate	$Zn(MnO_4)_2 \cdot 6H_2O$
981	phenolsulfonate	$Zn(C_6H_4OHSO_3)_2 \cdot 8H_2O$
982	phosphate	
983	phosphate tetrahydrate	$Zn_3(PO_4)_2 \cdot 4H_2O$
984	phosphite	$ZnHPO_3 \cdot 2{}^1/_2H_2O$
985	hypophosphite	$Zn(H_2PO_2)_2 \cdot H_2O$
986	salicylate	$Zn(C_6H_4OHCOO)_2 \cdot 3H_2O$
987	sulfate monohydrate	$ZnSO_4 \cdot H_2O$
988	sulfate heptahydrate	$ZnSO_4 \cdot 7H_2O$
989	ammonium sulfate	$ZnSO_4(NH_4)_2SO_4 \cdot 6H_2O$
990	potassium sulfate	$ZnSO_4 \cdot K_2SO_4 \cdot 6H_2O$
991	sulfide (hexagonal)	α-ZnS
992	sulfide (cubic)	β-ZnS
993	sulfide	$ZnSO_3 \cdot 2{}^1/_2H_2O$
994	valerate	$(CH_3CH_2CH_2CH_2COO)_2Zn \cdot 2H_2O$
995	Zirconium metal	Zr
996	Zirconyl chloride	$ZrOCl_2 \cdot 8H_2O$
997	Zirconium nitrate	$Zr(NO_3)_4 \cdot 5H_2O$
998	dioxide (monoclinic)	ZrO_2
999	silicate	$ZrSiO_4$
1000	Zirconyl sulfate	

d

1. Al
2.33 (100
2.02 (40
1.430 (30
1.219
1.168
1.011
0.928
0.905
0.826
0.778

2. $AlBr_3$
7.8
6.8
6.2
4.80
3.84 (7)
3.59 (6)
3.38 (6)
2.96
2.63
2.51
2.28
2.29
2.22
2.13
2.01
1.85
1.78
1.69
1.55
1.480
1.440

3. Al_4C
2.87 (25)
2.80 (25)
2.49
2.24
2.12
2.08
1.88
1.78
1.66 (25)
1.52
1.440
1.388
1.340
1.302

4. Al_2Cl
5.8 (40)
5.1
2.93
2.80 (40)
2.46 (62.5)
1.92
1.77
1.71
1.64
1.472
1.402
1.279
1.226
1.173
1.110
1.085
1.024
0.993
0.967

5. $AlCl_3.6$
6.0
5.2
3.89
3.69
3.41
3.29 (75)
2.95
2.75
2.57
2.30 (40)
2.18
2.05 (40)
1.99
1.94
1.82
1.76
1.68
1.65
1.51
1.475
1.412
1.380
1.353
1.316
1.290
1.225

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES

(Starred patterns were checked with published crystal structure data. B = broad line)

1. Al*

d		I/I₁
2.33	(100)	1.00
2.02	(40)	0.40
1.430	(30)	0.30
1.219		0.30
1.166		0.07
1.011		0.02
0.928		0.04
0.905		0.04
0.826		0.01
0.778		0.01

2. $AlBr_3.6H_2O$

7.8		0.29
6.8		0.29
6.2		0.14
4.80		0.14
4.34	(7)	1.00
4.09	(6)	0.86
3.88	(6)	0.86
3.66		0.29
3.53		0.14
3.51		0.14
3.38		0.57
3.29		0.14
3.22		0.43
3.13		0.71
3.01		0.43
2.85		0.43
2.78		0.14
2.69		0.14
2.55		0.29
1.480		0.14
1.440		0.29

3. Al_4C_3*

2.87	(25)	1.00
2.80	(25)	1.00
2.49		0.60
2.24		0.80
2.12		0.04
2.08		0.32
1.88		0.20
1.78		0.16
1.66	(25)	1.00
1.52		0.20
1.440		0.12
1.388		0.04
1.340		0.12
1.302		0.40

4. Al_2Cl_6*

5.8	(40)	0.64
5.1		0.14
4.93		0.40
4.80	(40)	0.64
4.46	(62.5)	1.00
3.92		0.14
3.77		0.20
3.71		0.64
3.54		0.11
3.472		0.32
3.402		0.24
3.279		0.06
3.226		0.10
3.173		0.03
3.110		0.20
3.085		0.16
3.024		0.05
2.993		0.08
2.967		0.10

5. $AlCl_3.6H_2O$

6.0		0.17
5.2		0.20
4.89		0.13
4.69		0.27
4.41		0.11
4.29	(75)	1.00
2.95		0.12
2.75		0.11
2.57		0.40
2.30	(40)	0.53
2.18		0.27
2.05	(40)	0.53
1.99		0.08
1.94		0.27
1.82		0.08
1.76		0.27
1.68		0.13
1.65		0.11
1.51		0.11
1.475		0.17
1.412		0.11
1.390		0.13
1.353		0.05
1.316		0.09
1.290		0.05
1.225		0.13

6. $AlNaCl_4$

d		I/I₁
5.3		0.23
4.93		0.23
4.62		0.06
3.62		0.40
3.10	(17.5)	1.00
2.95	(15)	0.86
2.80		0.57
2.55		0.71
2.47		0.29
2.30		0.23
2.22		0.23
2.10		0.29
1.99		0.11
1.87		0.23
1.76		0.34
1.64	(17.5)	1.00
1.57		0.11
1.52		0.17
1.480		0.06

7. $AlF_3.3^1/_2H_2O$

d		I/I₁
5.5	(50)	1.00
3.86	(25)	0.50
3.63		0.06
3.28	(25)	0.50
3.03		0.30
2.73		0.16
2.65		0.14
2.51		0.16
2.44		0.40
2.18		0.02
2.09		0.02
2.03		0.16
1.93		0.06
1.84		0.04
1.77		0.40
1.72		0.50
1.66		0.04
1.61		0.04
1.56		0.02
1.51		0.02
1.390		0.10
1.330		0.02
1.304		0.04

8. $Al_2(SiF_6)_3$

d		I/I₁
3.52	(15)	1.00
2.98		0.07
2.77		0.07
2.11	(1.5)	0.10
1.76	(2)	0.13
1.58		0.10

9. AlI_3

d		I/I₁
3.70		0.05
3.50	(40)	1.00
3.08	(20)	0.50
2.98		0.05
2.14	(20)	0.50
1.84		0.38
1.80		0.10
1.75		0.13
1.53		0.10
1.490		0.03
1.390		0.13
1.365		0.05
1.240		0.05
1.175		0.05

10. $Al(NO_3)_3.9H_2O$

7.0		0.20
6.8		0.30
6.3		0.50
5.7		0.10
5.3		0.05
4.90		0.30
4.50		0.40
4.05	(20)	1.00
3.78		0.40
3.60		0.50
3.43		0.10
3.25		0.50
3.10		0.10
3.01	(15)	0.75
2.90		0.20
2.77		0.10
2.59		0.63
2.52		0.40
2.36	(15)	0.75
2.30		0.10
2.25		0.10
2.18		0.25
2.12		0.05
2.07		0.10
2.03		0.20
1.95		0.20
1.88		0.25

11. α-Al_2O_3*

d		I/I₁
3.47		0.50
2.55	(15)	0.75
2.37		0.30
2.08	(20)	1.00
1.74		0.50
1.59	(20)	1.00
1.54		0.05
1.50		0.05
1.402		0.40
1.370		0.50
1.233		0.20
1.186		0.10
1.144		0.05
1.122		0.05
1.095		0.05
1.080		0.05
1.040		0.08
1.015		0.05
0.995		0.05

12. $AlHO_2$*

d		I/I₁
4.70		0.09
3.99	(75)	1.00
3.20		0.08
2.55		0.33
2.37		0.05
2.31	(75)	1.00
2.12		0.67
2.06		0.67
1.81		0.07
1.71		0.20
1.63	(62.5)	0.83
1.60		0.05
1.52		0.08
1.477		0.33
1.420		0.27
1.400		0.08
1.370		0.20
1.330		0.10
1.290		0.08
1.260		0.05
1.240		0.07
1.215		0.03
1.200		0.05
1.170		0.09
1.140		0.03
1.090		0.08
1.063		0.07
1.037		0.04
1.000		0.03

13. $Al_2O_3.2H_2O$

d		I/I₁
4.88	(125)	1.00
4.39	(62.5)	0.50
3.33		0.12
3.18		0.07
2.45	(40)	0.32
2.38		0.32
2.29		0.03
2.25		0.08
2.17		0.12
2.05		0.24
1.99		0.12
1.92		0.10
1.81		0.20
1.75		0.20
1.69		0.20
1.64		0.03
1.59		0.06
1.460		0.12
1.410		0.12
1.361		0.05
1.321		0.05
1.273		0.01
1.251		0.03
1.215		0.04

14. $Na_2O.11Al_2O_3$*

d		I/I₁
11.8	(40)	0.53
5.7		0.13
4.45		0.09
4.08		0.05
3.78		0.01
2.79		0.17
2.67		0.40
2.51		0.27
2.40		0.27
2.23		0.27
2.13		0.27
2.08		0.03
2.02		0.40
1.93		0.27
1.84		0.13
1.74		0.12
1.69		0.01
1.65		0.04
1.59	(40)	0.53
1.56		0.20
1.480		0.20
1.400	(75)	1.00
1.340		0.33
1.238		0.17
1.210		0.11
1.190		0.01
1.170		0.03
1.152		0.03
1.135		0.03
1.113		0.03
1.098		0.03
1.051		0.11
1.042		0.13
1.017		0.12
0.993		0.13
0.968		0.12

15. Al_2SiO_5*

d		I/I₁
5.3		0.25
3.40	(40)	1.00
2.88		0.20
2.68		0.30
2.54		0.45
2.41		0.13
2.28		0.15
2.20	(30)	0.75
2.11		0.30
1.97		0.03
1.88		0.13
1.84		0.15
1.69		0.25
1.59		0.20
1.52	(30)	0.75
1.440		0.20
1.395		0.08
1.328		0.25
1.275		0.20
1.265		0.20

16. $H_2KAl_3(SiO_4)_3$*

d		I/I₁
9.9	(9)	0.60
5.0		0.27
4.47	(8)	0.53
3.88		0.20
3.72		0.13
3.49		0.13
3.33		0.33
3.19		0.20
2.99		0.47
2.86		0.27
2.79		0.20
2.56	(15)	1.00
2.47		0.27
2.38		0.20
2.28		0.07
2.21		0.20
2.13		0.53
1.99		0.40
1.72		0.07
1.64		0.20
1.498		0.33

17. $Al_2Si_2O_5(OH)_4$

d		I/I₁
7.2	(10)	0.80
4.45	(10)	0.80
4.30		0.64
4.20		0.48
4.04		0.32
3.59	(12.5)	1.00
2.56		0.48
2.50		0.48
2.34		0.80
1.99		0.32
1.90		0.08
1.85		0.08
1.80		0.08
1.67		0.40
1.54		0.16
1.490		0.56
1.310		0.08
1.289		0.16
1.240		0.16

18. Bentonite

d		I/I₁
12.2	(40)	1.00
4.48	(20)	0.50
3.14	(8)	0.20
2.56		0.15
1.68		0.05
1.498		0.15
1.288		0.03
1.250		0.03

19. $Al_2(SO_4)_3$

d		I/I₁
5.8	(15)	0.30
4.23		0.14
3.50	(50)	1.00
2.92		0.25
2.65	(15)	0.30
2.35		0.02
2.22		0.08
2.03		0.08
1.95		0.04
1.87		0.02
1.82		0.02
1.75		0.08
1.66		0.08
1.63		0.04
1.57		0.02
1.53		0.10
1.490		0.04
1.430		0.04
1.395		0.02
1.350		0.04

20. $Al_2(SO_4)_3.18H_2O$

d		I/I₁
13.7		0.20
7.2		0.20
4.95		0.02
4.42	(50)	1.00
3.95	(30)	0.60
3.67		0.30
3.37		0.20
3.00		0.30
2.84		0.08
2.75		0.06
2.62		0.16
2.48	(20)	0.40
2.34		0.12
2.18		0.08
2.02		0.12
1.97		0.08
1.91		0.10
1.86		0.10
1.82		0.16
1.76		0.06
1.71		0.04
1.67		0.04

21. $AlNH_4(SO_4)_2.12H_2O$*

d		I/I₁
7.0		0.30
5.4	(30)	0.60
4.97		0.30
4.30	(40)	0.80
4.07		0.60
3.67		0.40
3.26	(50)	1.00
3.05		0.30
2.95		0.08
2.79		0.12
2.60		0.12
2.34		0.08
2.25		0.08
2.12		0.08
2.02		0.08
1.93		0.35
1.86		0.04
1.81		0.16
1.70		0.12
1.62		0.12
1.58		0.02
1.54		0.02
1.48		0.12

22. $AlK(SO_4)_2.12H_2O$*

d		I/I₁
7.0		0.04
5.4		0.20
4.96		0.08
4.29	(50)	1.00
4.03	(20)	0.40
3.65		0.04
3.24	(20)	0.40
3.03		0.16
2.93		0.12
2.85		0.10
2.78		0.20
2.71		0.06
2.64		0.06
2.58		0.06
2.47		0.06
2.33		0.08
2.25		0.04
2.21		0.06
2.11		0.06
2.02		0.08
1.97		0.06
1.91		0.16
1.85		0.02
1.68		0.04
1.61		0.08

23. $AlNa(SO_4)_2.12H_2O$

d		I/I₁
4.23	(50)	1.00
3.98	(20)	0.40
3.65	(25)	0.50
3.15		0.08
3.05		0.06
2.90		0.06
2.72		0.12
2.60		0.02
2.47		0.08
2.32		0.06
2.19		0.04
2.04		0.02
1.90		0 04
1.82		0.02
1.75		0.02
1.69		0.02
1.62		0.04
1.50		0.02

24. Al_2S_3

d		I/I₁
5.3		0.13
4.70		0.23
3.47		0.13
3.22	(30)	1.00
2.95		0.27
2.82	(25)	0.83
2.66		0.13
2.54		0.20
2.47		0.13
2.37		0.13
2.18		0.13
2.13		0.07
2.07		0.33
1.99		0.20
1.86	(20)	0.66
1.74		0.20
1.69		0.33
1.60		0.33
1.56		0.33
1.50		0.27
1.401		0.10
1.370		0.20

25. CH_3COONH_4

d		I/I₁
6.5		0.16
4.69	(8)	0.32
4.30		0.08
4.05	(25)	1.00
3.89		0.32
3.62	(9)	0.36
3.39		0.04
3.25		0.04
3.09		0.24
2.95		0.08
2.80		0.32
2.77		0.32
2.61		0.04
2.52		0.20
2.24		0.28
2.18		0.04
2.03		0.08
1.97		0.06
1.89		0.08

26. $(NH_4)_3AsO_4.3H_2O$

d		I/I₁
5.4	(40)	0.64
3.86	(30)	0.48
3.15	(62.5)	1.00
2.72		0.20
2.43		0.03
2.05		0.48
1.93		0.02
1.81		0.13
1.72		0.14
1.64		0.13
1.57		0.06
1.50		0.14
1.405		0.13
1.359		0.08
1.320		0.03
1.280		0.05
1.250		0.10
1.212		0.03
1.187		0.02
1.135		0.05

27. $C_6H_5COONH_4$

d		I/I₁
4.70	(30)	1.00
4.45		0.20
4.09		0.03
3.83		0.20
3.71		0.07
3.50	(7)	0.23
3.09	(8)	0.27
2.97		0.07
2.88		0.07
2.79		0.03
2.54		0.03
2.44		0.07
2.27		0.03
2.18		0.03
2.04		0.03
1.92		0.03

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

28. Ammonium Borate

d		I/I1
12.1		0.50
8.5	(6)	1.00
5.8	(6)	1.00
3.39	(4)	0.66
3.04		0.66
2.65		0.33
2.52		0.17
2.32		0.17
2.21		0.17
1.99		0.17

29. NH_4Br*

d		I/I1
4.07		0.17
2.85	(30)	1.00
2.33		0.10
2.02		0.10
1.81	(7)	0.23
1.65	(12.5)	0.42
1.429		0.10
1.350		0.13
1.280		0.10
1.220		0.03
1.169		0.03
1.081		0.67
0.955		0.03

30. $NH_4CO_2NH_2$

d		I/I1
5.2		0.08
4.50	(30)	0.40
4.30		0.27
4.10		0.27
3.89		0.03
3.70		0.11
3.30	(30)	0.40
3.00		0.07
2.93	(75)	1.00
2.82		0.23
2.76		0.23
2.62		0.13
2.45		0.05
2.33		0.08
2.25		0.07
2.17		0.07
2.04		0.08
1.98		0.05
1.89		0.04
1.84		0.07
1.78		0.08
1.76		0.05

31. $(NH_4)_2CO_3.H_2O$

d		I/I1
6.9		0.04
5.7		0.05
5.3		0.10
5.0		0.04
4.52		0.10
4.05		0.10
3.71	(40)	0.40
3.40	(30)	0.30
3.00	(100)	1.00
2.89		0.30
2.61		0.04
2.45		0.15
2.28		0.20
2.15		0.15
2.09		0.13
1.93		0.03
1.86		0.15
1.80		0.04
1.75		0.06
1.68		0.08
1.62		0.04
1.54		0.04
1.475		0.04
1.436		0.04
1.360		0.02
1.290		0.04

32. $(NH_4)HCO_3$

d		I/I1
5.3	(12.5)	0.42
4.02	(8)	0.27
3.61		0.27
3.39		0.07
3.19		0.07
3.06		0.10
2.99	(30)	1.00
2.79		0.03
2.69		0.07
2.61		0.07
2.42		0.10
2.28		0.03
2.15		0.20
2.09		0.03
1.69		0.03

33. NH_4ClO_4*

d		I/I1
5.8		0.16
4.61	(50)	1.00
3.93		0.30
3.70		0.30
3.60	(30)	0.60
3.25	(30)	0.60
2.97		0.60
2.90		0.40
2.60		0.40
2.21		0.35
1.85		0.20
1.68		0.25
1.60		0.02
1.54		0.02
1.45		0.08
1.392		0.06
1.362		0.02
1.311		0.04
1.211		0.02

34. NH_4Cl*

d		I/I1
3.85	(15)	0.15
2.72	(100)	1.00
2.22		0.05
1.92		0.12
1.72		0.08
1.57	(25)	0.25
1.370		0.05
1.288		0.03
1.221		0.07
1.165		0.01
1.115		0.01
1.033		0.04
0.912		0.01
0.864		0.01

35. $(NH_4)_2CrO_4$

d		I/I1
6.9		0.10
5.6	(12.5)	0.62
4.80	(20)	1.00
3.91		0.35
3.74		0.10
3.65		0.10
3.45		0.40
3.18	(15)	0.75
2.94		0.40
2.84		0.20
2.77		0.10
2.32		0.62
2.23		0.05
2.10		0.05
2.01		0.15
1.92		0.05
1.87		0.05
1.82		0.10
1.77		0.05
1.70		0.10

36. $(NH_4)_2Cr_2O_7$*

d		I/I1
6.6	(17.5)	0.58
5.1	(30)	1.00
3.77		0.16
3.37	(25)	0.83B
3.04		0.40
2.77		0.27
2.48		0.30
2.33		0.18
2.05		0.25
2.00		0.10
1.92		0.10
1.87		0.10
1.82		0.25
1.50		0.10
1.465		0.10
1.425		0.10
1.350		0.07
1.290		0.07

37. $(NH_4)_2HC_6H_5O_7$

d		I/I1
5.8		0.40
5.5	(15)	0.60
5.1		0.16
4.09		0.08
3.98	(25)	1.00
3.69		0.24
3.15	(12.5)	0.50
3.07		0.12
2.92		0.24
2.68		0.24
2.60		0.04
2.47		0.08
2.36		0.16
2.25		0.28
2.17		0.12
2.02		0.12
1.97		0.04
1.84		0.04
1.77		0.04
1.72		0.04
1.68		0.04
1.57		0.04
1.53		0.04

38. NH_4F*

d		I/I1
3.85	(50)	1.00
3.59	(30)	0.60
3.39	(30)	0.60
2.62		0.20
2.22		0.60
2.02		0.40
1.88		0.16
1.490		0.04
1.450		0.02
1.420		0.02
1.340		0.04
1.270		0.02
1.240		0.04

39. NH_4BF_4

d		I/I1
5.7		0.15
4.50	(40)	1.00
3.84		0.20
3.65		0.63
3.55	(30)	0.75
3.35		0.03
3.18	(30)	0.75
2.89		0.50
2.84		0.38
2.53		0.75
2.40		0.15
2.33		0.25
2.28		0.25
2.22		0.15
2.16		0.75
2.09		0.15
1.81		0.13
1.72		0.05
1.65		0.38
1.450		0.15

40. $(NH_4)_2SiF_6$*

d		I/I1
4.85	(100)	1.00
4.19		0.15
2.96		0.20
2.52		0.08
2.42	(50)	0.50
2.09	(50)	0.50
1.92		0.02
1.88		0.02
1.61		0.30
1.481		0.15
1.415		0.10
1.325		0.08
1.210		0.02
1.174		0.08
1.120		0.02
1.092		0.02
0.968		0.01

41. $HCOONH_4$

d		I/I1
4.55		0.33
4.19	(15)	0.50
3.82		0.25
3.25		0.03
2.96	(30)	1.00
2.82		0.33
2.46	(12.5)	0.42
2.27		0.33
1.93		0.03
1.85		0.03
1.78		0.03
1.65		0.03
1.53		0.03
1.460		0.03
1.425		0.03

42. NH_4I*

d		I/I1
4.18	(62.5)	1.00
3.62	(62.5)	1.00
2.56	(50)	0.80
2.18		0.48
2.08		0.20
1.81		0.10
1.66		0.16
1.62		0.30
1.476		0.13
1.391		0.13
1.278		0.03
1.223		0.04
1.208		0.04
1.144		0.03
1.012		0.02

43. $(NH_4)_6Mo_7O_{24}.4H_2O$

d		I/I1
7.2		0.20
6.4	(30)	1.00
5.4		0.07
5.1		0.20
4.80		0.20
4.10		0.05
3.63		0.27
3.35	(15)	0.50
3.20	(10)	0.33
3.10		0.05
3.01		0.10
2.66		0.07
2.56		0.03
2.48		0.20
2.40		0.07
2.25		0.20
2.18		0.33
2.08		0.07
1.95		0.10
1.90		0.17
1.82		0.27
1.69		0.10
1.61		0.14

44. $(NH_4)_3PO_4.12MoO_3.3H_2O$

d		I/I1
8.3	(25)	0.50
5.8		0.25
4.82		0.10
4.18		0.25
3.70		0.14
3.39	(50)	1.00
2.92		0.50
2.75		0.16
2.49		0.50
2.29		0.30
2.06		0.25
1.94		0.12
1.89		0.25
1.84		0.12
1.80		0.20
1.76		0.20
1.69		0.12
1.65		0.40
1.59		0.12
1.480	(30)	0.60
1.440		0.30
1.360		0.12
1.290		0.08
1.260		0.04
1.230		0.02
1.205		0.12
1.180		0.08
1.156		0.12
1.135		0.08
1.055		0.06
1.005		0.04

45. NH_4NO_3*

d		I/I1
4.93		0.40
3.95		0.50
3.09	(20)	1.00
2.86		0.05
2.72	(15)	0.75
2.47		0.13
2.38		0.10
2.25	(15)	0.75
2.10		0.05
1.97		0.05
1.83		0.05
1.78		0.06
1.73		0.05
1.63		0.09
1.57		0.10
1.51		0.10
1.495		0.10
1.463		0.15
1.430		0.05

46. NH_4NO_2

d		I/I1
4.94		0.17
4.67		0.03
4.10		0.27
3.69		0.20
2.95	(20)	0.67
2.84	(30)	1.00
2.65		0.03
2.45		0.20
2.33		0.13
2.20		0.03
2.04	(15)	0.50
1.99		0.03
1.86		0.07
1.66		0.10
1.64		0.10
1.59		0.03
1.55		0.07
1.470		0.03
1.420		0.07

47. $C_6H_4N.NO.ONH_4$

d		I/I1
4.75	(25)	1.00
4.20	(6)	0.24
3.98		0.16
3.60		0.16
3.37		0.16
3.01	(10)	0.40
2.83		0.04
2.68		0.08
2.45		0.08
2.36		0.04
2.21		0.08
2.06		0.08
1.99		0.04
1.94		0.04
1.86		0.08

48. $(NH_4)_2C_2O_4.H_2O$*

d		I/I1
6.3		0.60
5.1		0.10
3.81	(8)	0.80
3.57		0.10
3.43		0.10
3.26		0.60
3.06	(10)	1.00
2.86		0.80
2.76		0.10
2.67	(10)	1.00
2.58		0.60
2.43		0.60
2.36		0.60
2.14		0.30
2.01		0.20
1.86		0.20
1.82		0.20

49. $(NH_4)HC_2O_4.H_2O$

d		I/I1
6.2	(15)	0.75
5.6		0.10
4.32		0.10
4.13		0.10
3.45		0.35
3.30		0.05
3.17		0.15
3.00	(20)	1.00
2.90	(8)	0.40
2.70		0.05
2.56		0.35
2.38		0.30
2.31		0.05
2.25		0.25
2.19		0.20
2.13		0.05
2.08		0.05
1.95		0.05
1.84		0.05
1.78		0.05
1.70		0.05
1.65		0.05

50. $C_6H_4(OH)SO_2NH$

d		I/I1
5.8	(20)	0.80
5.3		0.24
5.0		0.24
4.48	(25)	1.00
4.15	(10)	0.40
3.61		0.28
3.32		0.32
3.14		0.04
3.00		0.16
2.86		0.12
2.65		0.04
2.50		0.04
2.35		0.04
2.25		0.04
2.02		0.04
1.95		0.04
1.89		0.04
1.83		0.04
1.75		0.04

51. $(NH_4)_2HPO_4$

d		I/I1
5.5		0.71
5.0	(17.5)	1.00
4.04		0.34
3.75		0.57
3.42		0.23
3.20	(17.5)	1.00
3.04	(15)	0.86
2.80		0.57
2.54		0.57
2.45		0.29
2.30		0.23
2.07		0.23
2.00		0.46
1.91		0.17
1.87		0.23
1.77		0.11
1.69		0.34
1.56		0.11
1.490		0.11

52. $(NH_4)H_2PO_4$*

d		I/I1
5.3	(62.5)	0.83
3.76	(40)	0.53
3.07	(75)	1.00
2.65		0.09
2.37		0.09
2.00		0.05
1.77		0.27
1.68		0.03
1.60		0.03
1.54		0.05
1.473		0.03
1.373		0.03
1.328		0.04
1.291		0.01
1.254		0.03
1.220		0.03
1.188		0.01
1.161		0.01
1.108		0.01

53. $(NH_4)H_2PO_3$*

d		I/I1
5.7		0.30
3.97		0.33
3.75		0.33
3.27	(20)	0.67
3.14	(17.5)	0.53
2.73	(30)	1.00
2.58		0.23
2.46		0.07
2.27		0.03
2.08		0.03
1.98		0.10
1.91		0.10
1.87		0.10
1.71		0.10
1.68		0.07
1.62		0.17
1.56		0.03
1.470		0.07
1.435		0.10
1.335		0.03
1.290		0.07
1.267		0.07

54. $C_6H_2(NO_2)_3.ONH_4.H_2O$

d		I/I1
10.1		0.64
6.8		0.08
5.5		0.12
5.3		0.12
4.98		0.64
3.95	(9)	0.72
3.56		0.64
3.40	(9)	0.72
3.16	(12.5)	1.00
3.02		0.32
2.91		0.08
2.77		0.32
2.67		0.08
2.57		0.08
2.43		0.16
2.25		0.12
2.18		0.08
2.13		0.08
2.05		0.08

55. $C_6H_4(OH)COONH_4$

d		I/I1
10.5	(4)	0.57
5.9		0.14
5.3		0.43
5.1		0.29
4.60		0.43
3.87	(5)	0.72
3.39	(7)	1.00
3.11		0.29
2.92		0.14
2.82		0.29
2.54		0.14
2.38		0.14
2.33		0.14
2.23		0.14
2.12		0.14
2.00		0.14
1.94		0.14
1.84		0.14

56. $(CH_2COONH_4)_2$

d		I/I1
6.0		0.08
4.74	(25)	1.00
3.89	(10)	0.40
3.72		0.06
3.55		0.08
3.38		0.28
3.06	(17.5)	0.70
2.76		0.40
2.57		0.28
2.38		0.20
2.31		0.08
2.20		0.08
2.13		0.04
2.05		0.08
1.95		0.08
1.86		0.04
1.83		0.04
1.74		0.04
1.66		0.04

57. (NH_4)

d		I/I1
5.2		
4.36		(100
3.91		
3.12		(40
3.03		(40
2.67		
2.51		
2.32		
2.18		
2.05		
1.97		
1.93		
1.77		
1.73		
1.70		
1.63		
1.56		
1.52		
1.490		

58. (NH_4)

d		I/I1
5.6		(10)
5.0		
4.02		
3.52		(15)
3.35		(20)
3.13		
3.03		
2.93		
2.85		
2.61		
2.51		
2.47		
2.41		
2.31		
2.21		
2.02		
1.93		
1.86		
1.77		
1.71		
1.65		
1.59		
1.53		

59. NH_4

d		I/I1
4.75		(15)
3.90		
3.69		(15)
3.15		
3.06		
2.84		
2.61		(15)
2.43		
2.35		
2.24		
2.18		
2.11		
2.01		
1.95		
1.87		
1.80		
1.66		
1.62		
1.58		
1.493		

60. (NH_4)

d		I/I1
5.3		
4.35		(4
4.10		
3.90		
3.12		(12.
3.02		(12.
2.66		
2.51		
2.31		
2.17		
1.97		
1.94		
1.77		
1.63		
1.56		
1.52		
1.493		

61. $(CHOH)_2($

d		I/I1
5.0		
4.65		
4.38		(5)
4.13		
3.23		(8)
3.07		
2.88		
2.70		(6)
2.52		
2.32		
2.12		
2.07		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

d	I/I1
$(NH_4)H_2PO_4$*	
(62.5)	0.83
(40)	0.53
(75)	1.00
	0.09
	0.05
	0.27
	0.03
	0.03
	0.05
	0.03
	0.04
	0.03
	0.04
	0.01
	0.03
	0.03
	0.01
	0.01
	0.01
$(NH_4)H_2PO_4$*	
	0.30
	0.33
	0.33
(20)	0.67
(17.5)	0.58
(30)	1.00
	0.23
	0.07
	0.03
	0.03
	0.10
	0.10
	0.10
	0.10
	0.07
	0.17
	0.03
	0.07
	0.10
	0.03
	0.07
	0.07
$NO_3.ONH_4.H_2O$	
	0.64
	0.08
	0.12
	0.12
	0.64
(9)	0.72
	0.64
(9)	0.72
(12.5)	1.00
	0.32
	0.08
	0.32
	0.08
	0.08
	0.16
	0.12
	0.08
	0.08
	0.08
55. $_4$(OH)COONH$_4$	
(4)	0.57
	0.14
	0.43
	0.29
	0.43
(5)	0.72
(7)	1.00
	0.29
	0.14
	0.29
	0.14
	0.14
	0.14
	0.14
	0.14
	0.14
	0.14
$(CH_2COONH_4)_2$	
	0.08
	1.00
(25)	0.40
(10)	0.06
	0.08
	0.28
(17.5)	0.70
	0.40
	0.28
	0.20
	0.08
	0.08
	0.04
	0.08
	0.08
	0.04
	0.04
	0.04
	0.04

d	I/I1
57. $(NH_4)_2SO_4$*	
	0.20
5.2 (100)	1.00
4.36	0.20
3.91 (40)	0.40
3.12 (40)	0.40
3.03	0.07
2.67	0.07
2.51	0.20
2.32	0.20
2.18	0.20
2.05	0.01
1.97	0.04
1.93	0.02
1.77	0.02
1.73	0.02
1.70	0.02
1.63	0.05
1.56	0.02
1.52	0.02
1.490	0.05
58. $(NH_4)_2S_2O_8$*	
(10)	0.50
	0.50
	0.45
	0.75
(15)	1.00
(20)	1.00
	0.50
	0.05
	0.30
	0.15
	0.05
	0.05
	0.35
	0.10
	0.25
	0.15
	0.05
	0.05
	0.05
59. NH_4HSO_4	
4.75 (15)	1.00
3.90	0.83
3.69 (15)	1.00
3.15	0.40
3.06	0.40
2.84	0.40
2.61 (15)	1.00
2.43	0.27
2.35	0.07
2.24	0.13
2.18	0.13
2.11	0.20
2.01	0.07
1.95	0.27
1.87	0.07
1.80	0.20
1.66	0.13
1.62	0.13
1.58	0.07
1.493	0.27
60. $(NH_4)_2SO_3.H_2O$	
5.3	0.15
4.35 (40)	1.00
4.10	0.05
3.90	0.10
3.12 (12.5)	0.31
3.02 (12.5)	0.31
2.66	0.08
2.51	0.08
2.31	0.13
2.17	0.13
1.97	0.03
1.94	0.03
1.77	0.03
1.63	0.03
1.56	0.03
1.52	0.03
1.493	0.03
61. $(CHOH)_2(CO_2NH_4)_2$	
5.0	0.25
4.65	0.25
4.38 (5)	0.63
4.13	0.50
3.23 (8)	1.00
3.07	0.50
2.88	0.50
2.70 (6)	0.75
2.52	0.13
2.32	0.13
2.12	0.25
2.07	0.25
62. NH_4CNS	
	0.10
	0.10
	0.10
	0.60
(10)	1.00
	0.20
	0.60
(8)	0.80
(7)	0.70
	0.70
	0.50
	0.40
	0.10
	0.10
	0.10
	0.10
	0.10
	0.10
	0.10
	0.08
	0.08
	0.08
	0.08
	0.08
63 $(NH_4)_2S_2O_3$	
5.0	0.32
4.75	0.56
4.58 (10)	0.80
3.91	0.16
3.46	0.08
3.34	0.08
3.20	0.08
3.02 (12.5)	1.00
2.77	0.08
2.62 (9)	0.72
2.36	0.16
2.27	0.08
2.18	0.08
1.95	0.08
1.81	0.24
1.72	0.16
1.69	0.08
1.56	0.08
1.440	0.08
64. $(NH_4)_2WO_4.nH_2O$	
10.7 (3)	1.00
8.5	0.66
6.4	0.33
5.1	0.66
3.23	0.66
2.99 (3)	1.00
2.89	0.66
2.78	0.33
2.50 (3)	1.00
2.38	0.33
2.01	0.33
1.86	0.33
1.71	0.33
1.54	0.33
1.470	0.33
65. $3(NH_4)_2O.P_2O_5.6WO_3.9H_2O$	
8.5	0.27
7.2	0.07
5.9	0.13
4.12	0.40
3.37 (15)	1.00
3.10	0.07
2.92 (7)	0.47
2.75	0.07
2.61	0.07
2.48 (7)	0.47
2.28	0.40
2.18	0.07
2.13	0.13
2.06	0.27
1.95	0.13
1.89	0.20
1.80	0.13
1.77	0.07
1.65	0.47
1.59	0.13
1.480	0.47
1.440	0.27
66. NH_4VO_3	
5.9	0.33
4.92 (20)	0.66
4.14 (25)	0.84
3.78	0.23
3.17 (30)	1.00
2.91	0.42
2.72	0.13
2.62	0.27
2.45	0.23
2.12	0.10
1.86	0.03
1.79	0.03
1.72	0.03
1.63	0.10
1.55	0.06
1.52	0.03
1.460	0.03
1.420	0.03
1.390	0.03
67. Sb*	
3.71	0.15
3.10 (40)	1.00
2.24 (25)	0.63
2.14 (25)	0.63
1.86	0.15
1.76	0.44
1.55	0.20
1.470	0.13
1.410	0.20
1.360	0.25
1.310	0.08
1.258	0.15
1.243	0.10
1.215	0.03
1.190	0.03
1.120	0.03
1.075	0.10
1.047	0.03
1.031	0.08
68. $SbAsO_4$	
6.4	0.12
4.54	0.02
4.21	0.02
3.68	0.20
3.49	0.35
3.22 (50)	1.00
3.13	0.25
2.79	0.35
2.55	0.08
2.47	0.08
2.40	0.06
2.27	0.04
2.13	0.02
2.05	0.02
1.97 (30)	0.60
1.92	0.02
1.81	0.02
1.73	0.02
1.68 (30)	0.60
1.61	0.12
1.57	0.18
1.475	0.02
1.40	0.06
1.367	0.06
1.280	0.18
1.250	0.12
1.183	0.02
1.140	0.08
1.075	0.12
1.042	0.02
0.973	0.02
0.943	0.06
69. Antimony Arsenite	
6.4	0.25
5.3	0.03
3.18 (100)	1.00
2.75	0.25
2.52	0.13
2.24	0.02
2.11	0.04
1.95 (30)	0.30
1.86 (30)	0.01
1.66 (30)	0.30
1.58	0.06
1.54	0.10
1.430	0.07
1.370	0.02
1.340	0.08
1.295	0.02
1.260	0.06
1.240	0.06
1.205	0.04
1.153	0.03
1.122	0.01
1.064	0.06
0.962	0.03
70 $SbBr_3$	
5.2 (10)	1.00
3.82	0.60
3.57	0.10
3.18 (10)	1.00
2.98 (10)	1.00
2.86	0.60
2.79	0.60
2.62	0.20
2.50	0.15
2.26	0.60
2.14	0.40
1.98	0.80
1.80	0.70
1.74	0.50
1.68	0.40
1.63	0.10
1.59	0.10
1.470	0.10
71. $SbCl_3$	
8.0	0.30
5.0 (20)	1.00
4.69	0.30
4.10	0.30
3.44	0.50
3.08	0.50
2.80	0.40
2.63	0.30
2.50	0.40
2.20 (20)	1.00
2.04	0.40
1.88	0.50
1.71 (15)	0.75
1.66	0.25
1.60	0.25
1.57	0.25
1.54	0.25
1.50	0.35
1.410	0.05
1.380	0.05
1.350	0.05
1.310	0.05
1.240	0.30
72 SbOCl	
13.2	0.05
9.0	0.05
6.2	0.30
4.80	0.05
4.03	0.20
3.70	0.20
3.27 (20)	1.00
3.10 (12.5)	0.63
2.81	0.05
2.64	0.05
2.55 (8)	0.40
2.37	0.10
2.25	0.05
2.12	0.10
2.04	0.25
1.98	0.10
1.86	0.05
1.79	0.05
1.65	0.05
1.54	0.05
1.480	0.10
73. SbF_3	
13.5	0.20
6.0	0.03
4.91 (17.5)	0.44
4.32	0.13
3.60 (40)	1.00
3.40 (20)	0.50
3.12	0.25
3.00	0.20
2.80	0.25
2.64	0.03
2.47	0.08
2.24	0.10
2.11	0.23
2.02	0.03
1.98	0.03
1.91	0.20
1.85	0.10
1.79	0.25
1.71	0.08
74. SbI_3	
6.2	0.03
5.5	0.13
3.97	0.01
3.70	0.03
3.45	0.04
3.30 (75)	1.00
2.54 (30)	0.40
2.42	0.01
2.14 (30)	0.40
1.97	0.20
1.80	0.17
1.73	0.01
1.64	0.10
1.57	0.01
1.450	0.07
1.380	0.10
1.350	0.08
1.300	0.10
1.200	0.05
75. Sb_2O_3*	
6.4	0.10
3.22 (100)	1.00
2.78	0.30
2.56	0.08
1.96 (50)	0.50
1.68 (50)	0.50
1.61	0.10
1.56	0.10
1.450	0.02
1.394	0.06
1.355	0.04
1.283	0.15
1.247	0.10
1.217	0.01
1.184	0.01
1.138	0.04
1.073	0.08
76. Sb_2O_4	
6.0 (25)	1.00
3.10 (20)	0.80
2.97 (20)	0.80
2.58	0.16
2.36	0.04
1.98	0.16
1.82	0.50
1.73	0.16
1.55	0.36
1.480	0.08
1.440	0.08
1.340	0.12
1.180	0.08
1.150	0.04
1.075	0.04
1.048	0.04
0.990	0.04
77. $K_2S.Sb_2S_3$	
3.00 (4)	0.40
2.89 (10)	1.00
2.40	0.10
2.22	0.10
2.08 (2)	0.20
1.88	0.10
1.56	0.10
1.440	0.10
78. $Sb_2(SO_4)_3$	
5.4	0.20
5.2	0.15
4.25 (40)	1.00
3.45	0.03
3.30 (12.5)	0.31
3.15 (20)	0.50
2.90	0.15
2.80	0.03
2.69	0.20
2.61	0.10
2.46	0.03
2.41	0.05
2.34	0.10
2.27	0.05
2.13	0.18
2.04	0.31
1.97	0.08
1.89	0.18
1.82	0.15
1.78	0.03
1.70	0.05
1.65	0.05
1.57	0.05
1.51	0.03
1.475	0.08
1.420	0.05
1.370	0.05
1.32	0.05
1.26	0.05
79. Sb_2S_3*	
8.2	0.06
5.6	0.23
5.0	0.46
3.97	0.23
3.57 (17.5)	1.00
3.02 (15)	0.86
2.75	0.86
2.66	0.34
2.60	0.06
2.50	0.34
2.42	0.23
2.23	0.29
2.09	0.40
1.92 (17.5)	1.00
1.72	0.23
1.68	0.57
1.63	0.06
1.53	0.17
1.475	0.06
1.400	0.06
1.350	0.06
1.305	0.11
80. $Sb_2(C_4H_4O_6)_3.6H_2O$	
7.7 (5)	0.33
6.2	0.20
5.7	0.13
4.31 (15)	1.00
3.70 (6)	0.40
3.03	0.27
2.70	0.13
2.52	0.27
2.43	0.13
2.32	0.13
2.06	0.07
1.93	0.20
1.86	0.13
1.77	0.07
1.67	0.13
1.60	0.07
1.54	0.07
1.48	0.07
81. (SbO)$KC_4H_4O_6$.-$\frac{1}{2}H_2O$	
6.8 (25)	0.83
5.8 (17.5)	0.58
4.73	0.50
3.90	0.42
3.64 (30)	1.00
3.38	0.33
3.14	0.20
2.96	0.23
2.87	0.23
2.75	0.23
2.59	0.13
2.50	0.27
2.42	0.07
2.30	0.17
2.19	0.23
2.06	0.07
1.99	0.20
1.96	0.20
1.91	0.10
1.86	0.13
1.81	0.10
1.77	0.10
1.65	0.07
1.61	0.07
1.57	0.07
1.51	0.10
1.470	0.07
1.340	0.07
1.315	0.03
1.260	0.03
1.213	0.07
82. As	
3.51	0.04
2.76 (75)	1.00
2.04 (10)	0.13
1.88 (15)	0.20
1.77	0.05
1.66	0.04
1.56	0.08
1.382	0.04
1.368	0.01
1.281	0.04
1.196	0.05
1.100	0.02
1.085	0.01
1.062	0.01
83. AsI_3*	
5.9	0.07
5.4	0.07
3.59 (25)	0.33
3.21 (75)	1.00
2.53 (17.5)	0.23
2.08	0.23
1.97	0.17
1.79	0.13
1.74	0.11
1.60	0.08
1.430	0.04
1.352	0.01
1.330	0.04
1.267	0.03
1.185	0.01
1.135	0.01
1.080	0.01
1.035	0.01
84. As_2O_3*	
6.3 (7)	0.56
3.18 (12.5)	1.00
2.75	0.24
2.53 (4)	0.32
2.24	0.08
2.12	0.16
1.95	0.24
1.66	0.16
1.59	0.08
1.54	0.16
1.438	0.08
1.343	0.08
1.301	0.08
1.266	0.08
1.205	0.08
1.064	0.08
85. As_2O_5	
7.1	0.30
5.6	0.30
4.88 (10)	1.00
4.01	0.10
3.58 (6)	0.60
3.40 (6)	0.60
3.21	0.20
3.05	0.50
2.70	0.20
2.62	0.40
2.34	0.10
2.26	0.20
2.18	0.20
2.10	0.10
2.02	0.10
1.89	0.10
1.84	0.10
1.77	0.10
1.71	0.20

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

86. As_2S_3

d		I/I₁
4.82	(15)	1.00
4.42		0.07
4.00	(7)	0.47
3.70		0.47
3.19		0.20
3.05		0.13
2.85		0.47
2.70	(8)	0.53
2.55		0.07
2.45		0.47
2.31		0.13
2.12		0.13
2.07		0.13
2.02		0.07
1.91		0.13
1.85		0.13
1.74		0.13
1.68		0.27
1.64		0.07

87. Ba*

d		I/I₁
3.54	(40)	1.00
2.51	(20)	0.50
2.04	(40)	1.00
1.77		0.50
1.58		0.50
1.443		0.05
1.340		0.44
1.181		0.15
1.120		0.05
1.066		0.03
1.022		0.03
0.981		0.08
0.915		0.03

88. $Ba(C_2H_3O_2)_2.H_2O$

d		I/I₁
9.3	(40)	1.00
7.0		0.38
4.88		0.15
4.43		0.38
3.55		0.25
3.40	(30)	0.75
3.10	(17.5)	0.44
2.76		0.10
2.65		0.10
2.49		0.25
2.34		0.20
2.21		0.25
2.07		0.25
2.00		0.38
1.93		0.38
1.70		0.31
1.450		0.18
1.390		0.18
1.290		0.15
1.260		0.10
1.225		0.08
1.185		0.08
1.093		0.08

89. Barium Borate

d		I/I₁
9.0		0.08
6.3		0.10
5.2		0.15
4.53	(25)	0.63
3.70		0.15
3.41	(30)	0.75
3.20		0.25
3.00	(40)	1.00
2.72		0.50
2.62		0.15
2.50		0.15
2.32		0.15
2.26		0.63
2.12		0.50
2.06		0.38
1.97		0.15
1.93		0.38
1.84		0.08
1.71		0.13
1.67		0.10
1.63		0.05
1.495		0.10
1.375		0.08

90. $BaCO_3$*

d		I/I₁
4.56		0.07
3.72	(100)	1.00
3.25		0.08
3.05		0.02
2.63	(40)	0.40
2.27		0.03
2.14	(20)	0.20
2.03		0.20
1.94		0.20
1.85		0.01
1.65		0.06
1.56		0.02
1.52		0.05
1.375		0.10
1.340		0.04
1.300		0.01
1.239		0.04
1.173		0.01
1.120		0.02B
1.070		0.01B
1.022		0.01B
0.992		0.01

91. $Ba(ClO_4)_2$

d		I/I₁
7.0		0.13
5.7		0.25
5.2		0.08
4.37		0.15
4.20		0.13
3.78		0.05
3.58	(40)	1.00
3.34	(30)	0.75
3.23		0.50
2.89		0.38
2.80		0.50
2.60		0.03
2.38		0.18
2.33		0.18
2.19	(25)	0.63
2.10		0.10
2.03		0.05
1.99		0.31
1.89		0.20
1.82		0.13
1.75		0.18
1.67		0.08
1.64		0.05
1.54		0.23
1.52		0.03
1.50		0.03
1.443		0.08
1.411		0.13

92. $Ba(ClO_3)_2.H_2O$

d		I/I₁
6.0	(62.5)	1.00
4.70		0.02
3.70		0.24
3.35	(40)	0.64
3.14		0.40
3.00		0.24
2.90		0.48
2.78		0.02
2.50		0.32
2.32	(50)	0.80
2.21		0.32
2.12		0.20
2.01		0.13
1.94		0.10
1.85		0.13
1.80		0.24
1.73		0.14
1.66		0.13
1.61		0.02
1.57		0.02
1.52		0.10
1.470		0.10
1.440		0.10
1.390		0.10
1.320		0.10
1.290		0.06
1.270		0.06
1.190		0.10
1.170		0.06

93. $Ba(ClO_4)_2.3H_2O$

d		I/I₁
6.4		0.20
4.87		0.27
3.84		0.09
3.65	(50)	0.67
2.90	(75)	1.00
2.64		0.13
2.39		0.20
2.25		0.27
2.14	(30)	0.40
2.10		0.08
2.00		0.11
1.92		0.33
1.82		0.13
1.75		0.01
1.70		0.20
1.65		0.09
1.58		0.11
1.55		0.05
1.492		0.03
1.475		0.03
1.450		0.05
1.415		0.04
1.378		0.13
1.324		0.17
1.295		0.01
1.277		0.07
1.240		0.05
1.212		0.05
1.190		0.11
1.150		0.01
1.124		0.03

94. $BaCl_2$

d		I/I₁
4.05	(25)	0.83
3.88		0.13
3.72		0.07
3.07		0.50
2.89		0.50
2.80		0.50
2.63		0.33
2.48		0.23
2.33	(30)	1.00
2.18		0.07
2.02	(25)	0.83
1.85		0.07
1.79		0.10
1.65		0.58
1.52		0.83
1.450		0.07
1.415		0.17
1.340		0.33
1.275		0.33
1.210		0.13
1.168		0.17
1.117		0.17
1.040		0.13
1.010		0.17

95. $BaCl_2.2H_2O$

d		I/I₁
5.5		0.50
4.98		0.33
4.48	(30)	1.00
3.64		0.42
3.39		0.50
3.21		0.33
2.91	(30)	1.00
2.70		0.50
2.54	(20)	0.66
2.40		0.33
2.23		0.33
2.08		0.58
2.00		0.33
1.70		0.10
1.60		0.12
1.56		0.17
1.52		0.16
1.450		0.07
1.385		0.10
1.340		0.03
1.305		0.10

96. $BaCrO_4$

d		I/I₁
4.50		0.11
4.00		0.27
3.54	(30)	0.40
3.19	(62.5)	0.83
2.90		0.33
2.78		0.27
2.53		0.08
2.37		0.07
2.25		0.07
2.16	(75)	1.00
1.97		0.01
1.91		0.17
1.80		0.10
1.71		0.33
1.66		0.11
1.62		0.11
1.56		0.23
1.50		0.05
1.450		0.13
1.410		0.03
1.380		0.07
1.350		0.03
1.325		0.03
1.288		0.13
1.250		0.04
1.225		0.05
1.170		0.08
1.120		0.10
1.055		0.04

97. $Ba_3(C_6H_5O_7)_2.7H_2O$

d		I/I₁
15.1	(25)	1.00
9.0	(25)	1.00
6.9		0.08
4.60		0.40
3.99		0.32
3.63		0.24
3.32	(15)	0.60
3.21		0.32
3.08		0.24
2.92		0.32
2.65		0.16
2.51		0.32
2.37		0.36
2.31		0.24
2.21		0.16
2.10		0.04
2.03		0.04
1.93		0.16
1.83		0.12

98. $Ba(CN)_2$

d		I/I₁
9.4	(62.5)	1.00
6.9		0.24
4.80		0.13
4.40		0.24
3.68		0.13
3.50		0.24
3.37	(40)	0.64
3.08		0.32
2.94	(30)	0.48
2.73		0.10
2.63		0.16
2.46		0.24
2.40		0.10
2.33		0.16
2.20		0.24
2.06		0.16
1.99		0.32
1.92		0.28
1.87		0.03
1.78		0.03
1.73		0.03
1.69		0.20
1.59		0.03
1.56		0.06
1.52		0.05
1.485		0.02
1.446		0.10
1.382		0.10
1.341		0.03
1.288		0.08
1.254		0.05
1.215		0.05
1.180		0.03
1.149		0.06

99. BaF_2*

d		I/I₁
3.58	(125)	1.00
3.09		0.25
2.19	(125)	1.00
1.86	(100)	0.80
1.78		0.15
1.55		0.15
1.420		0.32
1.382		0.18
1.262		0.32
1.190		0.20
1.095		0.05
1.045		0.15
1.031		0.03
0.978		0.06
0.944		0.03
0.933		0.02
0.866		0.03
0.859		0.02
0.827		0.05

100. $BaTiF_6$

d		I/I₁
4.79		0.11
3.68	(62.5)	1.00
3.15	(40)	0.64
2.40		0.16
2.28		0.40
2.12		0.06
2.00	(40)	0.64
1.84		0.10
1.74		0.05
1.58		0.06
1.450		0.14
1.390		0.05
1.355		0.03
1.262		0.03
1.230		0.02
1.200		0.05
1.143		0.05
1.090		0.02
1.007		0.02

101. $BaSiF_6$

d		I/I₁
4.65		0.18
3.58	(100)	1.00
3.05		0.50
2.85		0.08
2.33		0.20
2.23	(62.5)	0.63
2.07		0.06
1.95	(100)	1.00
1.79		0.08
1.68		0.04
1.55		0.06
1.52		0.06
1.420		0.06
1.405		0.15
1.360		0.07
1.320		0.06
1.228		0.05
1.198		0.04
1.170		0.04
1.110		0.04
1.064		0.03
1.015		0.02

102. $Ba(HCO_2)_2$

d		I/I₁
5.8		0.30
5.4	(40)	0.80
4.42		0.40
3.80		0.35
3.34		0.60
3.11	(50)	1.00
2.92		0.30
2.75		0.60
2.66		0.20
2.54		0.40
2.44		0.30
2.30		0.25
2.21		0.60
2.10	(40)	0.80
2.02		0.40
1.92		0.30
1.85		0.40
1.79		0.20
1.67		0.30
1.62		0.16
1.57		0.16
1.461		0.16
1.411		0.04
1.375		0.40
1.332		0.30
1.305		0.02
1.274		0.16
1.260		0.16
1.220		0.16
1.187		0.08
1.151		0.10
1.130		0.04
1.100		0.14

103. $Ba(OH)_2.8H_2O$

d		I/I₁
6.6		0.50
6.0	(25)	1.00
5.5		0.32
4.62	(15)	0.60
4.33		0.50
4.13		0.08
3.92		0.24
3.71		0.12
3.53		0.32
3.38		0.16
3.22		0.50
3.07		0.32
3.00		0.32
2.78	(15)	0.60
2.73		0.32
2.66		0.60
2.56		0.16
2.37		0.16
2.30		0.40
2.17		0.20
2.12		0.20
2.07		0.50
2.02		0.16
1.97		0.16
1.93		0.12
1.81		0.20
1.74		0.08
1.67		0.20
1.63		0.04
1.59		0.12
1.55		0.08
1.468		0.24

104. $Ba(IO_3)_2.H_2O$

d		I/I₁
6.0		0.50
4.52		0.32
4.00		0.44
3.70		0.44
3.41	(30)	0.75
3.29		0.50
3.06	(40)	1.00
2.58		0.38
2.42		0.25
2.31		0.20
2.26	(40)	1.00
2.13		0.10
1.97		0.20
1.91		0.25
1.85		0.50
1.79		0.50
1.75		0.15
1.69		0.13
1.64		0.20
1.59		0.20
1.50		0.15
1.460		0.25
1.420		0.10
1.350		0.03
1.320		0.23
1.230		0.18
1.205		0.32
1.165		0.05
1.140		0.05
1.096		0.05
1.066		0.08
1.030		0.05

105. $BaMnO_4$

d		I/I₁
4.42		0.07
3.97		0.33
3.68		0.20
3.50	(30)	1.00
3.40		0.42
3.16	(25)	0.83
2.89		0.56
2.74		0.38
2.53		0.03
2.35		0.03
2.24		0.03
2.15	(25)	0.83
1.96		0.03
1.91		0.13
1.80		0.03
1.71		0.23
1.65		0.03
1.61		0.03
1.56		0.13

106. $Ba(MnO_4)_2$

d		I/I₁
5.7		0.38
3.68	(25)	0.63
3.39	(40)	1.00
3.31	(30)	0.71
2.95		0.15
2.84		0.63
2.38		0.15
2.24		0.63
2.20		0.38
2.05		0.10
1.92		0.31
1.85		0.18
1.80		0.15
1.74		0.10
1.65		0.10
1.57		0.31
1.475		0.15
1.440		0.15
1.375		0.08
1.332		0.08
1.294		0.08
1.258		0.10

107. $Ba(NO_3)_2$*

d		I/I₁
4.69	(75)	0.75
4.06		0.30
3.62		0.15
3.31		0.10
2.87		0.40
2.44	(100)	1.00
2.34	(50)	0.50
2.02		0.20
1.86		0.40
1.81		0.30
1.65		0.20
1.56		0.50
1.433		0.15
1.370		0.40
1.351		0.10
1.318		0.01
1.281		0.08
1.238		0.13
1.222		0.13
1.170		0.04
1.137		0.19
1.126		0.06
1.085		0.13
1.056		0.20

108. $Ba(NO_3)_2.H_2O$

d		I/I₁
6.1		0.44
5.1	(30)	0.75
4.29		0.63
3.60		0.25
3.48	(30)	0.75
3.01		0.75
2.77		0.38
2.68		0.38
2.52	(40)	1.00
2.30		0.63
2.24		0.50
2.16		0.38
2.06		0.25
1.94		0.32
1.89		0.20
1.70		0.25
1.64		0.10
1.60		0.05
1.53		0.05
1.475		0.44
1.420		0.15
1.385		0.13
1.335		0.13
1.305		0.05
1.278		0.05
1.252		0.10
1.215		0.03
1.180		0.05
1.150		0.05
1.120		0.10
1.096		0.08
1.066		0.05

109. BaC_2

d		I/I₁
8.5		0.07
7.7	(15)	0.33
4.81		0.20
4.40		1.00
3.80	(20)	0.42
3.41	(25)	0.83
3.20		0.56
3.10		0.38
2.83		0.03
2.65		0.03
2.53		0.03
2.41		0.83
2.39		0.03
2.20		0.13
2.10		0.03
1.95		0.23
1.87		0.03
1.82		0.03
1.64		0.13
1.54		
1.50		
1.430		
1.380		

110. BaO

d		I/I₁
3.20	(20)	
2.75	(17.5)	
1.95	(15)	
1.66		
1.59		
1.380		
1.265		
1.231		
1.128		
1.060		
0.975		
0.933		
0.920		

111. BaO

d		I/I₁
3.37	(53)	
2.68	(40)	
2.11	(40)	
1.95		
1.89		
1.65		
1.443		
1.380		
1.282		
1.250		
1.200		
1.137		
1.108		
1.063		
1.045		
0.980		
0.958		
0.930		
0.915		
0.879		
0.828		

112. $Ba(C_2H_4OH.$

d		I/I₁
18.0	(30)	
11.5	(30)	
9.5		
7.0		
5.4		
4.60		
4.25	(10)	
3.53		
3.33		
3.20		
2.80		
2.65		
2.14		
2.07		
1.98		
1.91		
1.69		

113. $Ba_3(P$

d		I/I₁
4.45	(17.5)	
3.85		
3.58	(75)	
3.20		
3.00		
2.85		
2.51	(30)	
2.19		
1.99		
1.88		
1.83		
1.76		
1.68		
1.58		
1.490		
1.420		
1.330		
1.150		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

105. $BaMnO_4$

d	I/I1
	0.07
	0.32
	0.20
(30)	1.00
	0.42
(25)	0.82
	0.50
	0.30
	0.03
	0.03
(25)	0.03
	0.82
	0.03
	0.13
	0.03
	0.23
	0.03
	0.03
	0.13

[illegible] $Ba(MnO_4)_2$

	0.38
(25)	0.63
(40)	1.00
(30)	0.71
	0.15
	0.63
	0.15
	0.63
	0.38
	0.19
	0.31
	0.18
	0.15
	0.10
	0.10
	0.31
	0.15
	0.15
	0.08
	0.08
	0.10

[illegible] $Ba(NO_3)_2$*

(75)	0.75
	0.30
	0.15
	0.10
	0.40
(100)	1.00
(50)	0.50
	0.20
	0.40
	0.30
	0.30
	0.30
	0.15
	0.40
	0.10
	0.01
	0.08
	0.13
	0.13
	0.04
	0.10
	0.06
	0.13
	0.20

$Ba(NO_3)_2.H_2O$

	0.44
(30)	0.75
	0.03
	0.25
(30)	0.75
	0.75
	0.38
	0.38
	1.00
	0.63
	0.50
	0.38
	0.25
	0.32
	0.20
	0.25
	0.10
	0.05
	0.05
	0.44
	0.15
	0.13
	0.13
	0.05
	0.05
	0.10
	0.05
	0.08
	0.05
	0.10
	0.08
	0.05

109. BaC_2O_4

d	I/I1
	0.40
(15)	0.60
	0.60
	0.16
(20)	0.80
	0.60
(25)	1.00
	0.40
	0.04
	0.24
	0.24
	0.32
	0.24
	0.24
	0.04
	0.28
	0.12
	0.08
	0.04
	0.16
	0.08
	0.04
	0.08

110. BaO*

d	I/I1
(20)	1.00
(17.5)	0.88
(15)	0.75
	0.50
	0.25
	0.10
	0.20
	0.25
	0.15
	0.20
	0.05

111. BaO_2*

d	I/I1
(50)	1.00
(40)	0.80
(40)	0.80
	0.50
	0.30
	0.80
	0.08
	0.40
	0.16
	0.16
	0.10
	0.16
	0.06
	0.16
	0.08
	0.04
	0.06
	0.02
	0.04
	0.02

112. $Ba(C_6H_4OH.SO_3)_2$

d	I/I1
(30)	1.00
(30)	1.00
	0.13
	0.10
	0.07
	0.13
(10)	0.33
	0.27
	0.20
	0.20
	0.13
	0.20
	0.13
	0.07
	0.07
	0.03
	0.03

113. $Ba_3(PO_4)_2$

d	I/I1
(17.5)	0.23
	0.09
(75)	1.00
	0.01
	0.13
	0.20
(30)	0.40
	0.08
	0.10
	0.03
	0.03
	0.05
	0.05
	0.08
	0.03
	0.04
	0.03
	0.04

114. Barium Phosphite

d	I/I1
4.49	0.12
3.29 (30)	0.60
3.49 (50)	1.00
3.37	0.40
3.02	0.04
2.80	0.40
2.36 (25)	0.59
2.14	0.40
2.10	0.35
2.05	0.30
1.93	0.16
1.78	0.08
1.71	0.08
1.60	0.06
1.50	0.10
1.445	0.04
1.420	0.06
1.370	0.04
1.320	0.04
1.280	0.04

115. $Ba(H_2PO_2)_2.H_2O$

d	I/I1
7.8 (100)	0.80
4.23	0.24
3.34 (125)	1.00
3.12	0.32
2.88	0.24
2.61	0.05
2.54 (75)	0.60
2.43	0.12
2.20	0.20
2.11	0.16
1.99	0.24
1.95	0.32
1.84	0.32
1.67	0.16
1.65	0.12
1.61	0.06
1.55	0.06
1.455	0.08
1.410	0.08
1.325	0.06
1.295	0.06
1.222	0.07
1.193	0.06
1.180	0.06
1.143	0.05
1.130	0.05

116. $BaSO_4$*

d	I/I1
4.35	0.20
3.89	0.25
3.57	0.10
3.44 (25)	0.63
3.31	0.35
3.10 (25)	0.63
2.83	0.40
2.72	0.45
2.47	0.15
2.31	0.10
2.20	0.15
2.10 (40)	1.00
2.04	0.10
1.92	0.05
1.85	0.15
1.74	0.08
1.67	0.15
1.63	0.08
1.58	0.10
1.52	0.25
1.465	0.07
1.420	0.20
1.255	0.18
1.190	0.08
1.093	0.13
1.028	0.05

117. BaS*

d	I/I1
3.67 (40)	0.53
3.18 (75)	1.00
2.25 (62.5)	0.83
1.91	0.40
1.83	0.27
1.59	0.15
1.460	0.11
1.421	0.45
1.299	0.25
1.225	0.10
1.125	0.05
1.076	0.05
1.061	0.08
1.005	0.04
0.960	0.04
0.891	0.01
0.883	0.01
0.851	0.05
0.829	0.01

118. $BaSO_3$

d	I/I1
4.20 (12.5)	0.63
3.44 (20)	1.00
3.20 (15)	0.75
2.75	0.63
2.33	0.35
2.08	0.45
1.99	0.10
1.77	0.10
1.69	0.10
1.59	0.05
1.490	0.05
1.380	0.05
1.320	0.05
1.260	0.05
1.182	0.05

119. $BaC_4H_4O_6.H_2O$

d	I/I1
6.1 (40)	1.00
4.95	0.38
4.52	0.38
4.20	0.20
3.69	0.50
3.45 (30)	0.75
3.05	0.20
2.85 (30)	0.75
2.67	0.38
2.49	0.63
2.33	0.50
2.23	0.10
2.09	0.10
2.04	0.25
1.97	0.50
1.91	0.15
1.86	0.10
1.82	0.20
1.72	0.08
1.68	0.08
1.61	0.20

120. $Ba(CNS)_2.2H_2O$

d	I/I1
7.7 (20)	1.00
6.5	0.75
6.0	0.50
4.22	0.88
3.91	0.50
3.69	0.30
3.40 (20)	1.00
3.16	0.50
3.02	0.20
2.92	0.20
2.80	0.20
2.66 (20)	1.00
2.54	0.75
2.41	0.15
2.22	0.20
2.15	0.50
2.02	0.10
1.97	0.40
1.92	0.10
1.86	0.10
1.78	0.20
1.74	0.10
1.71	0.15
1.65	0.15
1.59	0.20
1.53	0.10
1.460	0.10
1.370	0.05
1.330	0.10

121. $BaS_2O_3.H_2O$

d	I/I1
10.1 (40)	1.00
5.0 (12.5)	0.32
4.60	0.20
3.62 (20)	0.50
3.34	0.20
2.93	0.08
2.56	0.10
2.46	0.32
2.25	0.18
2.04	0.08
1.75	0.03
1.68	0.03
1.63	0.03
1.58	0.03
1.51	0.03
1.450	0.03
1.410	0.03
1.290	0.03
1.220	0.03

122. Barium Borotungstate

d	I/I1
11.0 (4)	1.00
9.2	0.25
4.50 (4)	1.00
3.40	0.50
3.18 (3)	0.75
3.05	0.50
2.70	0.25
1.52	0.25
1.470	0.25
1.430	0.25

123. $Ba(C_6H_5CO_2)_2$

d	I/I1
13.0 (62.5)	1.00
7.4 (10)	0.16
5.9	0.05
4.43	0.06
3.96	0.06
3.50	0.10
3.37 (8)	0.13
2.83	0.02
2.70	0.03
2.56	0.02
2.48	0.02
2.32	0.02
2.10	0.03
1.93	0.05
1.81	0.02

124. Be*

d	I/I1
1.97 (10)	0.20
1.79 (7)	0.14
1.73 (50)	1.00
1.328	0.12
1.137	0.12
1.022	0.12
0.983	0.02
0.963	0.08
0.955	0.06

125. BeO*

d	I/I1
2.34 (100)	0.80
2.19 (62.5)	0.50
2.06 (125)	1.00
1.59	0.24
1.350	0.32
1.239	0.32
1.170	0.04
1.150	0.20
1.130	0.04
1.032	0.03
0.915	0.08
0.884	0.02
0.870	0.02
0.822	0.08
0.780	0.03
0.758	0.08

126. $BeSO_4$

d	I/I1
3.77 (75)	1.00
3.45	0.05
3.19	0.08
2.34 (25)	0.33
1.93 (7)	0.09
1.88	0.05
1.59	0.01
1.51	0.08
1.365	0.03
1.315	0.03
1.250	0.01
1.225	0.03
1.135	0.01
1.095	0.01

127. $BeSO_4.4H_2O$

d	I/I1
5.7	0.13
3.90 (75)	1.00
3.40	0.13
3.20 (15)	0.20
3.06	0.01
2.84	0.03
2.52 (40)	0.53
2.42	0.01
2.30	0.01
2.23	0.01
2.17	0.17
2.00	0.04
1.94	0.03
1.88	0.13
1.84	0.07
1.78	0.05
1.70	0.03
1.60	0.05
1.490	0.04
1.458	0.08
1.414	0.04
1.330	0.04

128. Bi*

d	I/I1
3.28 (30)	1.00
2.35 (15)	0.50
2.27 (15)	0.50
2.01	0.07
1.96	0.13
1.86	0.30
1.63	0.20
1.54	0.03
1.490	0.20
1.440	0.20
1.327	0.27
1.180	0.13
1.135	0.03
1.089	0.10
1.073	0.07
1.045	0.07
1.020	0.03
	0.03

129. $Bi(C_2H_3O_2)_3$

d	I/I1
13.5 (40)	1.00
3.35 (12.5)	0.31
2.90 (8)	0.20
2.72	0.05
2.52	0.02
2.10	0.08
1.97	0.05
1.87	0.08
1.70	0.08
1.63	0.05
1.55	0.02
1.473	0.02
1.395	0.02
1.260	0.02

130. $Bi(C_6H_5COO)_3$

d	I/I1
10.0 (3)	1.00
4.95	0.33
3.99	0.33
3.70	0.33
3.45 (3)	1.00
3.10 (2)	0.66
2.75	0.66

131. BiOBr

d	I/I1
8.1	0.12
3.52 (5)	0.20
2.80 (25)	1.00
2.29	0.08
1.95	0.12
1.80	0.08
1.71	0.04
1.61 (7)	0.28
1.386	0.04
1.320	0.04
1.238	0.08
1.049	0.04

132. $Bi_2O_3.CO_2.H_2O$

d	I/I1
3.73 (8)	0.27
3.43	0.03
2.97 (30)	1.00
2.73 (10)	0.33
2.28	0.03
2.15	0.13
1.94	0.13
1.75	0.17
1.62	0.23
1.475	0.03
1.420	0.03
1.370	0.03
1.300	0.03
1.225	0.03
1.145	0.03
1.080	0.03
1.044	0.03

133. BiOCl

d	I/I1
7.4 (17.5)	0.70
3.71	0.08
3.45 (25)	1.00
2.75	0.40
2.67 (20)	0.80
2.45	0.08
2.20	0.24
1.94	0.24
1.87	0.04
1.83	0.24
1.69	0.24
1.66	0.16
1.57	0.36
1.52	0.16
1.375	0.16
1.263	0.16
1.225	0.20
1.200	0.04
1.165	0.08
1.121	0.08
1.095	0.08
1.065	0.08
1.036	0.12

134. $(BiO)_2CrO_4$

d	I/I1
10.5 (10)	0.50
4.90	0.05
3.55	0.05
3.20 (20)	1.00
2.93	0.05
2.80	0.05
2.70	0.05
2.58 (2)	0.10
2.40	0.05
2.32	0.05
2.05	0.05
1.88	0.05
1.65	0.05
1.58	0.10

135. Bismuth Ammonium Citrate

d	I/I1
14.0 (6)	1.00
11.2	0.67
8.9 (6)	1.00
7.9 (6)	1.00
5.6	0.50
5.0	0.33
3.47	0.67
2.80	0.12
2.43	0.33
2.33	0.17
2.23	0.17
2.16	0.17
2.07	0.17
1.72	0.17
1.68	0.17
1.59	0.17
1.55	0.17

136. $Bi(OH)_3$

d	I/I1
6.9	0.05
3.72	0.38
2.96 (40)	1.00
2.72 (20)	0.50
2.54	0.03
2.28	0.03
2.13	0.23
1.93	0.31
1.85	0.05
1.81	0.03
1.75	0.31
1.71	0.10
1.68	0.03
1.61 (17.5)	0.44
1.470	0.05
1.412	0.05
1.365	0.05
1.295	0.05
1.235	0.08
1.219	0.08
1.170	0.03
1.142	0.05
1.073	0.08

137. $Bi(C_6H_7O_8).7H_2O$

d	I/I1
8.7 (17.5)	1.00
5.0 (4)	0.23
4.08 (3)	0.17
3.42	0.17
2.62	0.11
2.49	0.07
2.35	0.07
2.26	0.11
2.03	0.06
1.95	0.06

138. $BiO_2.C_{12}H_7$

d	I/I1
20.0 (40)	1.00
9.9 (7)	0.18
3.40	0.05
3.22	0.03
3.15	0.03
2.98	0.03
2.67 (4)	0.10
2.06	0.03
1.93	0.05
1.88	0.10
1.61	0.05
1.57	0.03
1.52	0.03
1.330	0.03
1.240	0.03
1.190	0.05

139. $BiO.NO_3.H_2O$

d	I/I1
8.2	0.20
4.1	0.08
3.52	0.20
2.80 (50)	1.00
2.60	0.04
2.29	0.10
1.96 (15)	0.30
1.80	0.08
1.71	0.12
1.63	0.04
1.61 (20)	0.40
1.410	0.04
1.390	0.06
1.325	0.06
1.241	0.16
1.210	0.02
1.188	0.04
1.050	0.08

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

140. Bismuth Osmate

d		I/I1
10.6	(10)	0.80
9.4	(10)	0.80
6.2		0.32
5.5		0.32
4.80	(12.5)	1.00
3.94		0.08
3.20		0.08
3.01		0.48
2.78		0.32
2.62		0.08
2.41		0.64
1.97		0.40
1.83		0.24
1.79		0.24
1.66		0.48
1.61		0.16
1.52		0.40
1.467		0.16
1.394		0.16
1.342		0.16
1.250		0.16
1.202		0.24
1.180		0.24
1.108		0.32

141. $Bi_2(C_2O_4)_3$

9.9		0.20
6.4	(20)	1.00
5.6		0.10
5.1		0.30
4.79		0.10
4.17	(8)	0.40
3.81		0.30
3.61		0.10
3.45		0.30
3.22		0.15
3.09		0.05
3.00		0.10
2.88		0.20
2.82		0.20
2.76		0.15
2.62		0.30
2.52		0.10
2.40	(7)	0.35
2.17		0.30
2.08		0.35
2.00		0.15
1.91		0.20
1.85		0.15
1.80		0.20
1.73		0.10
1.70		0.05
1.63		0.05
1.60		0.15
1.52		0.10
1.486		0.08
1.435		0.15
1.390		0.10

142. Bi_2O_3

3.42		0.05
3.25	(20)	1.00
2.69	(17.5)	0.88
2.54		0.05
2.39		0.15
2.03		0.05
1.95	(5)	0.25
1.87		0.15
1.82		0.05
1.75		0.20
1.66		0.10
1.58		0.10
1.490		0.10
1.395		0.05
1.305		0.05
1.270		0.05
1.225		0.05
1.195		0.05
1.120		0.05

143. $Bi_2O_4.2H_2O$

3.73		0.17
3.20		0.17
2.95	(6)	1.00
2.74	(2)	0.33
2.14		0.17
1.93		0.17
1.75		0.17
1.62	(2)	0.33

144. $BiPO_4$

4.68		0.40
4.20	(3)	0.60
3.52		0.20
3.30		0.20
3.08	(5)	1.00
2.87	(5)	1.00
2.60		0.20
2.45		0.20
2.33		0.20
2.18		0.20
2.12		0.20
1.95		0.20
1.81		0.40
1.73		0.40
1.58		0.20
1.53		0.40

145. $Bi_2(C_6H_4OHCOO)_2$

d		I/I1
16.0	(30)	1.00
7.5		0.07
6.8		0.13
6.2	(10)	0.33
4.95		0.10
4.48		0.10
3.98	(7)	0.23
3.40		0.03
3.13		0.03
2.75		0.03
2.52		0.03
2.40		0.03
2.26		0.03
2.08		0.07
2.02		0.03
1.93		0.03
1.72		0.03
1.62		0.03

146. $Bi_2(SO_4)_3$

5.6	(6)	0.75
5.2	(6)	0.75
4.30	(8)	1.00
3.36		0.37
3.13		0.50
2.94		0.13
2.74		0.75
2.62		0.25
2.45		0.13
2.36		0.13
2.17		0.25
2.07		0.25
1.99		0.13
1.91		0.13
1.87		0.13
1.71		0.13
1.67		0.13
1.60		0.13
1.53		0.13
1.490		0.13
1.440		0.13
1.360		0.13
1.225		0.13

147. H_3BO_3

5.9	(17.5)	0.28
3.16	(62.5)	1.00
2.90		0.03
2.81		0.02
2.62		0.06
2.55		0.02
2.49		0.02
2.23	(8)	0.13
2.16		0.03
2.08		0.06
2.02		0.03
1.68		0.03
1.63		0.02
1.58		0.03

148. B_4C

4.00		0.05
3.79		0.15
3.39	(40)	1.00
2.57		0.23
2.38	(15)	0.38
2.03	(15)	0.38
1.81		0.03
1.69		0.03
1.54		0.03
1.50		0.03
1.450		0.05
1.400		0.05
1.320		0.05
1.260		0.03
1.230		0.05
1.158		0.05

149. Cd*

2.80	(40)	0.40
2.58	(30)	0.30
2.34	(100)	1.00
1.89		0.20
1.51		0.25
1.486		0.18
1.400		0.03
1.310		0.27
1.286		0.02
1.252		0.20
1.228		0.02
1.170		0.03
1.060		0.05
1.020		0.04
0.959		$0.10\alpha_1$
0.921		$0.02\alpha_1$
0.863		$0.04\alpha_1$
0.821		$0.02\alpha_1$

150. $Cd(C_2H_3O_2)_2.2H_2O$

d		I/I1
11.8		0.25
9.9	(20)	1.00
8.6	(15)	0.75
7.7		0.20
7.1		0.30
6.2		0.10
5.6		0.40
5.2		0.20
4.84		0.30
4.55		0.40
4.00		0.35
3.76		0.40
3.56		0.40
3.35		0.20
3.25	(10)	0.50
3.12		0.10
3.00		0.10
2.96		0.10
2.90		0.10
2.77		0.15
2.66		0.10
2.45		0.05
2.40		0.05
2.29		0.05
2.20		0.15
2.09		0.20
2.02		0.10
1.98		0.10
1.92		0.10
1.83		0.10
1.72		0.10

151. $Cd(BrO_3)_2.H_2O$

6.2		0.08
5.6		0.08
4.40	(12.5)	1.00
4.00		0.08
3.71		0.08
3.51		0.08
3.17	(6)	0.48
3.08	(4)	0.32
2.81		0.08
2.74		0.08
2.49		0.08
2.37		0.16
2.26		0.08
2.19		0.32
2.05		0.32
1.93		0.16
1.81		0.16
1.69		0.16
1.370		0.16

152. $CdCO_3$*

3.77	(25)	0.80
2.94	(30)	1.00
2.46		0.50
2.23		0.03
2.06		0.45
1.88		0.33
1.83	(25)	0.80
1.58		0.40
1.50		0.17
1.470		0.05
1.419		0.15
1.355		0.05
1.295		0.05
1.260		0.17
1.230		0.05
1.190		0.08
1.142		0.08
1.120		0.08
1.022		0.08
0.976		0.07
0.942		0.07
0.880		0.07

153. $CdCl_2$*

5.8	(50)	1.00
3.27	(30)	0.60
2.64	(40)	0.80
2.40		0.25
1.99		0.12
1.92		0.40
1.87		0.04
1.83		0.50
1.66		0.08
1.56		0.12
1.50		0.06
1.445		0.04
1.388		0.02
1.368		0.04
1.324		0.06
1.252		0.06
1.210		0.08
1.184		0.04
1.162		0.06
1.125		0.02
1.114		0.02
1.092		0.06

154. $CdCl_2.2^1/_2H_2O$

d		I/I1
7.3	(25)	0.63
5.9	(40)	1.00
4.65		0.31
3.63		0.44
3.37		0.50
2.99		0.25
2.84		0.13
2.62	(40)	1.00
2.42		0.38
2.35		0.31
2.08		0.23
1.97		0.50
1.88		0.44
1.81		0.15
1.76		0.10
1.68		0.15
1.64		0.15
1.60		0.10
1.50		0.15
1.450		0.08
1.390		0.05
1.330		0.08
1.250		0.08
1.193		0.10
1.153		0.05
1.103		0.10

155. $Cd(OH)_2$*

4.70	(100)	1.00
3.02	(62.5)	0.63
2.55	(100)	1.00
1.86		0.40
1.74		0.30
1.63		0.30
1.51		0.13
1.440		0.20
1.400		0.20
1.271		0.15
1.165		0.07
1.139		0.08
1.110		0.13
1.090		0.03
1.028		0.10
1.005		0.03
0.980		0.04
0.925		0.05

156. $2KI.CdI_2.2H_2O$

7.3		0.08
5.9		0.32
4.25	(12.5)	1.00
3.60	(8)	0.64
3.45		0.48
3.16		0.48
2.85		0.64
2.70		0.08
2.27		0.16
2.19	(12.5)	1.00
2.02		0.08
1.93		0.48
1.85		0.08
1.72		0.08
1.58		0.16

157. $Cd(NO_3)_2.4H_2O$

6.5		0.30
5.0	(50)	1.00
4.40	(30)	0.60
3.65	(25)	0.50
3.39		0.02
3.23		0.02
3.06		0.16
2.99		0.50
2.92		0.30
2.66		0.20
2.55		0.16
2.40		0.40
2.35		0.20
2.13		0.25
2.10		0.16
2.00		0.30
1.98		0.16
1.91		0.08
1.86		0.16
1.81		0.30
1.68		0.16
1.63		0.08
1.50		0.10
1.450		0.04
1.430		0.04
1.395		0.08
1.368		0.08

158. CdC_2O_4

d		I/I1
8.0		0.04
6.5		0.20
5.7	(100)	1.00
4.69		0.07
4.50		0.30
3.98		0.07
3.70	(40)	0.40
3.43		0.15
3.22		0.15
3.08		0.15
2.85	(40)	0.40
2.73		0.40
2.65		0.20
2.56		0.07
2.49		0.07
2.41		0.02
2.33		0.20
2.25		0.07
2.21		0.07
2.13		0.06
2.04		0.13
1.98		0.20
1.90		0.10
1.85		0.10
1.81		0.13
1.74		0.04
1.70		0.03
1.65		0.07
1.58		0.06
1.53		0.04
1.50		0.06
1.473		0.07
1.420		0.03
1.358		0.06
1.310		0.04
1.275		0.02
1.237		0.08
1.201		0.03
1.161		0.04
1.137		0.02
1.120		0.04

159. $CdC_2O_4.3H_2O$

6.5		0.05
5.7	(50)	0.40
4.90		0.16
4.51		0.06
3.75	(125)	1.00
3.42		0.05
3.20		0.12
3.07		0.02
2.85		0.08
2.72		0.14
2.66		0.24
2.54	(50)	0.40
2.45		0.05
2.37		0.06
2.31		0.24
2.22		0.06
2.13		0.02
2.02		0.16
1.93		0.32
1.87		0.24
1.79		0.12
1.76		0.16
1.67		0.12
1.59		0.04
1.55		0.08
1.50		0.14
1.450		0.06
1.417		0.01
1.385		0.08
1.359		0.03
1.338		0.05
1.315		0.10
1.272		0.08
1.247		0.05
1.228		0.03
1.212		0.02

160. CdO*

2.70	(100)	1.00
2.34	(100)	1.00
1.65	(100)	1.00
1.412		0.75
1.352		0.30
1.171		0.15
1.075		0.30
1.047		0.40
0.957		0.25
0.902		0.18
0.830		0.02
0.793		0.15
0.782		0.10

161. $CdFe_2O_4$*

d		I/I1
3.08	(17.5)	0.5
2.62	(30)	1.0
2.52		0.1
2.19		0.2
2.00		0.1
1.78		0.2
1.67	(12.5)	0.5
1.54		0.2
1.489		0.2
1.455		0.2
1.377		0.2
1.329		0.1
1.313		0.1
1.259		0.1
1.165		0.1
1.135		0.1

162. $Cd_3(PO_4)_2$

8.5	(4)	0.17
7.4		0.33
7.0		0.33
6.6		0.33
6.0		0.33
4.68	(4)	0.67
4.21	(6)	1.00
3.22		0.67
3.08		0.67
2.95		0.67
2.77		0.17
2.68		0.33
2.50		0.17
2.38		0.17
2.23		0.17
2.09		0.17
2.02		0.17
1.97		0.17
1.89		0.17
1.85		0.17
1.78		0.33
1.74		0.33
1.68		0.33
1.62		0.33

163. $Cd(C_6H_4OHCOO)_2.H_2O$

16.0	(75)	1.00
10.0		0.08
6.6	(15)	0.20
6.3		0.13
5.8		0.05
5.2		0.03
4.80		0.11
4.55		0.05
4.22		0.07
3.98		0.01
3.82	(20)	0.25
3.65		0.20
3.45		0.13
3.24		0.07
3.10		0.07
2.87		0.05
2.51		0.05
2.41		0.03
2.34		0.05
2.22		0.03
2.06		0.04
1.99		0.04
1.92		0.03

164. $3CdSO_4.8H_2O$

4.90	(40)	0.80
3.70		0.20
3.55	(50)	1.00
3.20		0.60
3.10		0.15
2.51	(40)	0.80
2.38		0.60
2.30		0.35
2.10		0.25
2.05		0.25
1.94		0.12
1.86		0.15
1.77		0.25
1.71		0.30
1.68		0.20
1.63		0.35
1.56		0.20
1.52		0.04
1.470		0.08
1.440		0.08
1.400		0.04
1.325		0.14
1.270		0.04
1.170		0.08

165. $CdWO_4$

5.9		0.25
5.0		0.38
3.80	(8)	1.00
3.05	(8)	1.00
2.93		0.50
2.53	(6)	0.75
1.91		0.38
1.81		0.38
1.76		0.13
1.53		0.25
1.465		0.13
1.410		0.13

166. Ca(

d		
3.21	(40)	
2.80	(12.5)	
1.97	(8)	
1.68		
1.61		
1.28		
1.246		
1.138		

167. $Ca(C_2H$

11.0	(50)	
8.5	(10)	
6.7		
5.9		
5.5		
3.80		
3.58		
3.34	(25)	
3.13		
2.96		
2.68		
2.34		
2.23		
2.15		
2.03		
1.97		
1.88		
1.84		
1.66		
1.52		

168. $Ca(C_6H_7O_2)_2$.

10.0	(75)	
6.7		
6.0	(10)	
5.2		
4.10		
3.78		
3.61		
3.28	(40)	
2.97		
2.89		
2.72		
2.41		
2.33		
2.23		
2.17		
2.08		
1.97		
1.87		
1.81		

169. Ca-Al . (22% Ca

3.09		
2.83	(30)	
2.70	(50)	
2.42		
2.33		
2.25		
2.18	(30)	
2.07		
1.99		
1.73		
1.59		
1.55		
1.51		
1.47		
1.425		
1.395		
1.340		
1.236		
1.175		

170. $3CaO_.$

4.08		
3.30		
2.68	(25)	
2.39		
2.19		
2.03		
1.90	(6)	
1.55	(6)	
1.342		
1.203		
1.015		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

166. Ca*

d	I/I₁
3.21	1.00
(40)	
2.80	0.30
(12.5)	
1.97	0.20
(8)	
1.68	0.20
1.61	0.10
1.28	0.05
1.246	0.03
1.138	0.05

167. $Ca(C_2H_3O_2)_2$

d	I/I₁
11.0	1.00
(50)	
8.5	0.20
(10)	
6.7	0.06
5.9	0.12
5.5	0.10
3.80	0.08
3.58	0.08
3.34	0.50
(25)	
3.13	0.16
2.96	0.08
2.68	0.18
2.34	0.10
2.23	0.16
2.15	0.16
2.03	0.08
1.97	0.16
1.88	0.08
1.84	0.20
1.66	0.04
1.52	0.04

168. $Ca(C_2H_3O_2)_2.H_2O$

d	I/I₁
10.0	1.00
(75)	
6.7	0.11
6.0	0.13
(10)	
5.2	0.05
4.10	0.08
3.78	0.08
3.61	0.01
3.28	0.53
(40)	
2.97	0.09
2.89	0.11
2.72	0.04
2.41	0.11
2.33	0.11
2.23	0.03
2.17	0.07
2.08	0.11
1.97	0.09
1.87	0.05
1.81	0.05

169. Ca–Al Alloy (22% Ca)

d	I/I₁
3.09	0.18
2.83	0.60
(30)	
2.70	1.00
(50)	
2.42	0.04
2.33	0.02
2.25	0.02
2.18	0.60
(30)	
2.07	0.20
1.99	0.35
1.73	0.30
1.59	0.08
1.55	0.25
1.51	0.02
1.47	0.20
1.425	0.02
1.395	0.06
1.340	0.25
1.236	0.04
1.175	0.08

170. $3CaO.Al_2O_3$*

d	I/I₁
4.08	0.20
3.30	0.04
2.68	1.00
(25)	
2.39	0.04
2.19	0.08
2.03	0.04
1.90	0.24
(6)	
1.55	0.24
(6)	
1.342	0.12
1.203	0.08
1.015	0.04

171. $5CaO.3Al_2O_3$*

d	I/I₁
4.95	0.67
(20)	
3.19	0.20
3.01	0.23
2.68	1.00
(30)	
2.44	0.50
(15)	
2.19	0.50
1.94	0.50
1.73	0.13
1.66	0.42
1.59	0.50
1.52	0.13
1.478	0.10
1.395	0.27
1.344	0.10
1.309	0.17
1.261	0.07
1.236	0.07
1.209	0.10
1.174	0.10
1.141	0.07
1.112	0.13
1.091	0.03

172. $Ca_3(AsO_4)_2$

d	I/I₁
8.7	0.16
6.0	0.04
5.5	0.04
4.90	0.04
4.01	0.40
3.51	0.50
(12.5)	
3.22	0.04
3.05	0.20
2.90	1.00
(25)	
2.82	0.80
(20)	
2.69	0.16
2.34	0.12
2.30	0.12
2.22	0.16
2.00	0.28
1.88	0.50
1.75	0.16
1.69	0.20
1.65	0.08
1.52	0.12
1.485	0.24

173. Calcium Arsenite

d	I/I₁
9.0	0.48
4.97	0.32
4.49	0.64
(8)	
3.54	0.16
3.05	1.00
(12.5)	
2.85	0.40
2.65	0.56
(7)	
2.56	0.16
2.09	0.16
2.01	0.16
1.94	0.16
1.81	0.56
1.69	0.24
1.52	0.16
1.425	0.08
1.315	0.08
1.230	0.08
1.115	0.08

174. $Ca(C_2H_3CO_2)_2.3H_2O$

d	I/I₁
6.4	0.07
5.8	0.13
5.3	0.47
(7)	
4.41	0.33
4.22	0.83
(12.5)	
3.98	0.07
3.48	1.00
(15)	
2.97	0.27
2.67	0.27
2.54	0.07
2.48	0.07
2.30	0.07
2.23	0.07
2.12	0.07
2.06	0.07
2.01	0.07
1.98	0.07
1.93	0.07
1.87	0.07

175. Calcium Borate

d	I/I₁
5.8	0.07
3.40	0.42
(12.5)	
3.04	1.00
(30)	
2.90	0.23
2.76	0.07
2.62	0.33
2.25	0.07
2.14	0.42
(12.5)	
2.01	0.03
1.95	0.42
1.86	0.33
1.70	0.10
1.65	0.07
1.51	0.13
1.310	0.07
1.200	0.03
1.070	0.03

176. $CaBr_2.6H_2O$*

d	I/I₁
4.03	1.00
(25)	
3.49	0.50
(12.5)	
2.85	0.50
2.65	0.50
2.34	0.50
2.21	0.60
(15)	
2.01	0.16
1.92	0.08
1.80	0.16
1.75	0.24
1.60	0.16
1.53	0.24
1.495	0.08
1.430	0.16
1.395	0.04
1.353	0.08
1.312	0.04
1.285	0.04
1.259	0.08
1.219	0.08
1.190	0.04

177. CaC_2 I*

d	I/I₁
3.32	0.25
3.18	0.50
(20)	
2.74	1.00
(40)	
2.08	0.44
(17.5)	
1.93	0.31
1.86	0.25
1.67	0.18
1.375	0.08
1.348	0.08
1.263	0.05
1.232	0.08
1.147	0.05
1.028	0.03

178. CaC_2 II*

d	I/I₁
3.49	0.20
3.32	0.16
3.17	0.16
2.93	1.00
(62.5)	
2.79	0.40
(25)	
2.28	0.14
2.09	0.24
2.06	0.16
2.00	0.13
1.95	0.28
(17.5)	
1.88	0.08
1.80	0.20
1.76	0.10
1.71	0.06
1.67	0.08
1.59	0.05
1.52	0.05
1.470	0.05
1.300	0.13

179. CaC_2 III

d	I/I₁
3.52	0.60
3.20	0.10
2.92	0.80
(8)	
2.86	1.00
(10)	
2.27	0.40
2.15	0.20
2.05	0.80
(8)	
1.93	0.60
1.78	0.60

180. $CaCO_3$*

d	I/I₁
3.86	0.08
3.04	1.00
(125)	
2.49	0.20
2.28	0.24
(30)	
2.09	0.20
1.92	0.32
(40)	
1.87	0.24
1.60	0.16
1.51	0.12
1.475	0.05
1.439	0.08
1.425	0.05
1.350	0.03
1.295	0.05
1.243	0.03
1.179	0.03
1.150	0.05
1.045	0.06
1.011	0.03

181. $Ca(ClO_3)_2.2H_2O$

d	I/I₁
6.0	0.30
5.6	0.12
5.4	0.12
4.68	0.14
4.30	0.50
(25)	
3.62	0.06
3.30	0.10
3.05	0.60
(30)	
2.94	0.12
2.80	1.00
(50)	
2.70	0.10
2.64	0.16
2.48	0.14
2.37	0.18
2.32	0.06
2.26	0.08
2.20	0.04
2.16	0.10
2.10	0.30
1.99	0.08
1.92	0.04
1.87	0.10
1.85	0.10
1.77	0.08
1.70	0.04
1.66	0.10
1.62	0.04
1.50	0.04
1.470	0.12
1.402	0.08
1.321	0.06

182. $CaCl_2$*

d	I/I₁
4.49	1.00
(25)	
3.46	0.16
3.05	0.80
(20)	
2.85	0.32
2.33	0.60
(15)	
2.24	0.16
2.09	0.16
1.90	0.36
1.79	0.08
1.68	0.12
1.56	0.04
1.51	0.08
1.490	0.04
1.330	0.12
1.243	0.12
1.210	0.12
1.165	0.04

183. $CaCl_2.H_2O$

d	I/I₁
5.9	0.40
(10)	
4.38	0.12
3.41	0.12
3.22	0.24
3.03	0.40
2.81	0.24
2.55	1.00
(25)	
2.40	0.24
2.26	0.60
(15)	
2.17	0.04
2.11	0.28
1.93	0.12
1.69	0.04
1.60	0.12
1.53	0.08
1.50	0.12
1.460	0.04
1.410	0.04
1.360	0.12

184. $CaCl_2.2H_2O$

d	I/I₁
6.1	0.40
4.34	0.50
3.05	0.70
(17.5)	
2.82	1.00
(25)	
2.68	0.16
2.51	0.20
2.35	0.20
2.26	0.16
2.16	0.24
2.12	0.60
(15)	
2.01	0.08
1.87	0.20
1.78	0.12
1.71	0.12
1.67	0.16
1.62	0.04
1.52	0.04
1.475	0.16
1.405	0.04

185. $CaCl_2.4H_2O$

d	I/I₁
6.0	0.27
5.2	0.20
4.70	0.42
(12.5)	
3.58	0.27
3.30	0.13
3.02	0.13
2.94	0.13
2.81	0.42
2.72	0.27
2.63	1.00
(30)	
2.39	0.42
2.22	0.67
(20)	
2.16	0.13
2.08	0.20
2.00	0.27
1.91	0.07
1.75	0.13
1.70	0.07
1.62	0.07
1.57	0.07
1.49	0.13

186. $CaCl_2.6H_2O$

d	I/I₁
6.9	0.15
3.93	0.75
(30)	
3.41	0.31
2.78	0.63
(25)	
2.58	0.50
2.27	0.50
2.16	1.00
(40)	
1.97	0.50
1.90	0.15
1.76	0.13
1.70	0.38
1.57	0.10
1.489	0.38
1.452	0.20
1.393	0.15
1.365	0.05
1.313	0.13
1.290	0.10
1.225	0.15
1.189	0.10
1.170	0.10
1.079	0.13
1.006	0.10

187. $CaCl_2.CaF_2$

d	I/I₁
6.8	0.04
3.39	0.08
3.18	0.02
2.75	0.50
(25)	
2.56	1.00
(50)	
2.14	0.40
1.94	0.50
(25)	
1.75	0.02
1.68	0.02
1.55	0.25
1.450	0.02
1.374	0.12
1.215	0.08
1.155	0.04
1.115	0.02
1.028	0.04
0.973	0.02
0.910	0.02
0.871	0.02

188. $Ca(ClO)_2.4H_2O$

d	I/I₁
4.95	0.25
3.18	0.63
(25)	
2.47	0.05
2.36	1.00
(40)	
1.93	0.50
(20)	
1.80	0.10
1.70	0.05
1.52	0.15
1.490	0.20
1.300	0.05
1.262	0.15
1.182	0.15
1.115	0.03
1.085	0.03
1.050	0.03
1.002	0.03

189. $CaCrO_4$*

d	I/I₁
4.80	0.06
3.63	1.00
(100)	
2.90	0.15
2.70	0.75
(75)	
2.57	0.15
2.39	0.20
2.27	0.08
1.86	0.75
(75)	
1.81	0.20
1.62	0.15
1.58	0.02
1.50	0.23
1.45	0.18
1.345	0.13
1.293	0.10
1.210	0.06
1.188	0.05
1.154	0.08
1.130	0.08
1.027	0.08
1.000	0.05
0.973	0.08

190. $CaCrO_4.2H_2O$

d	I/I₁
8.0	0.50
(15)	
4.30	1.00
(30)	
4.02	0.07
3.90	0.07
3.66	0.23
3.11	0.67
(20)	
2.94	0.42
2.70	0.30
2.62	0.13
2.55	0.03
2.45	0.17
2.20	0.10
2.10	0.07
2.02	0.03
1.98	0.07
1.91	0.20
1.87	0.07
1.82	0.13
1.69	0.10

191. $CaCr_2O_7$

d	I/I₁
7.0	0.60
(9)	
6.4	0.07
5.3	0.27
4.98	0.27
4.20	0.07
4.08	0.07
3.90	1.00
(15)	
3.73	0.53
3.50	0.83
(12.5)	
3.39	0.53
3.08	0.40
2.98	0.53
2.78	0.27
2.62	0.53
2.39	0.27
2.30	0.27
2.20	0.27
2.06	0.13
1.99	0.13
1.93	0.33
1.78	0.40
1.74	0.40

192. $Ca_3(C_6H_5O_7)_2.4H_2O$

d	I/I₁
15.3	1.00
(6)	
3.95	0.67
(4)	
3.09	0.67
(4)	
2.98	0.33
2.78	0.17
2.58	0.17
2.39	0.33
2.23	0.33
2.03	0.33
1.96	0.17
1.81	0.17
1.75	0.17
1.66	0.17

193. $CaCN_2$

d	I/I₁
4.90	0.40
(4)	
3.36	0.20
3.03	1.00
(10)	
2.62	0.80
(8)	
2.50	0.10
2.29	0.10
2.08	0.40
1.92	0.10
1.87	0.10
1.79	0.10
1.68	0.10
1.59	0.10

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TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

194. $Ca(CN)_2$

d		I/I1
5.4		0.20B
3.36		0.07
3.15		0.20
2.87	(30)	1.00
2.77		0.07
2.40	(12.5)	0.42
2.02	(12.5)	0.42
1.92		0.03
1.70		0.27
1.66		0.07
1.56		0.03
1.451		0.05
1.389		0.05
1.279		0.03
1.200		0.03
1.075		0.03

195. $Ca_2Fe(CN)_6.12H_2O$

8.0		0.13
5.5	(15)	0.50
5.1	(30)	1.00
4.70	(12.5)	0.42
4.29		0.23
3.68		0.33
3.25		0.13
3.09		0.20
3.01		0.13
2.77		0.20
2.66		0.42
2.54		0.30
2.37		0.20
2.29		0.07
2.23		0.33
2.15		0.10
2.10		0.10
1.99		0.13
1.86		0.10

196. $CaK_2Fe(CN)_6$

6.0		0.07
5.1	(9)	0.30
4.60		0.03
3.72		0.13
3.64	(30)	1.00
3.07		0.10
2.85		0.03
2.57	(12.5)	0.42
2.35		0.03
2.30		0.10
2.13		0.07
2.06		0.10
1.63		0.03

197. CaF_2*

3.16	(100)	0.67
1.93	(150)	1.00
1.65	(75)	0.50
1.370		0.23
1.256		0.23
1.117		0.30
1.050		0.10
0.968		0.05
0.925		0.07
0.866		0.05
0.835		0.02
0.789		0.01
0.767		0.02
0.731		0.05
0.713		0.03
0.644		0.01

198. $CaSiF_6$

6.1		0.03B
4.43		0.04B
3.83	(100)	1.00
3.02		0.03
2.74		0.08
2.30	(30)	0.30
1.91	(30)	0.30
1.73		0.30
1.70		0.10
1.55		0.09
1.470		0.04
1.370		0.07
1.337		0.02
1.305		0.03
1.276		0.02
1.261		0.06
1.220		0.04
1.151		0.02
1.073		0.04
1.011		0.04

199. $CaSiF_6.2H_2O$

d		I/I1
5.3	(25)	1.00
4.85		0.36
4.61		0.08
4.25	(15)	0.60
3.80		0.28
3.44	(20)	0.80
3.31		0.60
3.19		0.16
3.05		0.16
2.88		0.08
2.70		0.32
2.29		0.40B
2.11		0.32
2.05		0.08
1.99		0.32
1.89		0.50
1.81		0.40B
1.69		0.40B
1.63		0.08

200. $Ca(HCO_2)_2$

6.6		0.08
5.6	(50)	1.00
5.0		0.50
3.82		0.12
3.43	(50)	1.00
3.10		0.16
2.99	(40)	0.80
2.86		0.25
2.77		0.08
2.56		0.06
2.52		0.20
2.41		0.06
2.31		0.25
2.25		0.40
2.19		0.12
2.00		0.25
1.94		0.08
1.88		0.12
1.79		0.10
1.74		0.10

201. $Ca(CH_3OHCOO)_2$

6.0	(17.5)	0.88
4.89		0.40
4.10		0.50
3.88		0.50
3.60	(15)	0.75
3.19	(20)	1.00
3.00		0.10
2.79		0.05
2.60		0.30
2.47		0.05
2.42		0.10
2.32		0.50
2.24		0.20
2.18		0.30
2.12		0.50
2.00		0.10
1.93		0.10
1.85		0.10
1.78		0.40
1.75		0.30
1.68		0.10
1.65		0.20
1.62		0.10
1.58		0.10
1.302		0.10
1.268		0.10
1.238		0.10
1.175		0.05
1.120		0.10

202. $Ca(CH_3OHCOO)_2.3H_2O$

9.8	(25)	1.00
7.3		0.24
6.4	(8)	0.32
4.98		0.16
4.58		0.24
4.10		0.16
3.64		0.28
3.19	(17.5)	0.83
2.89		0.08
2.71		0.04
2.50		0.32
2.38		0.32
2.20		0.32
2.02		0.16
1.95		0.16
1.88		0.16
1.80		0.20
1.72		0.12
1.61		0.04

203. $Ca(CH_3OHCOO)_2.3^1/_2H_2O$

d		I/I1
10.0	(25)	1.00
4.65		0.20
4.34		0.16
3.98		0.08
3.58		0.16
3.39		0.16
3.05	(9)	0.36
2.81	(7)	0.28
2.64		0.08
2.46		0.08
2.34		0.16
2.14		0.08
2.03		0.16
1.99		0.16
1.92		0.08
1.85		0.08
1.74		0.04
1.70		0.04
1.63		0.08
1.490		0.04
1.265		0.04
1.160		0.04

204. Calcium Hippurate

8.5	(20)	1.00
6.7		0.50
5.2		0.50
4.80	(12.5)	0.62
4.25		0.50
3.85		0.50
3.61		0.30
3.40	(17.5)	0.87
3.19		0.20
2.96		0.20
2.80		0.40
2.64		0.10
2.54		0.10
2.27		0.15
2.15		0.10
2.05		0.10
1.96		0.10
1.92		0.05
1.84		0.05

205. CaH_2

4.99		0.08
3.18	(10)	0.40
2.97	(25)	1.00
2.81	(20)	0.80
2.63		0.08
2.40		0.08
2.17		0.40
1.92		0.28
1.82		0.08
1.79		0.20
1.71		0.24
1.68		0.24
1.61		0.20
1.54		0.36
1.480		0.08
1.380		0.04
1.350		0.04
1.245		0.36
1.180		0.08
1.145		0.08
1.120		0.04
1.073		0.04
1.015		0.04

206. $Ca(OH)_2$*

4.93	(30)	0.50
3.11		0.25
2.63	(62.5)	1.00
1.93	(30)	0.50
1.79		0.40
1.69		0.30
1.55		0.02
1.485		0.20
1.450		0.20
1.315		0.16
1.178		0.02
1.145		0.15
1.063		0.10
1.035		0.05
1.012		0.08
0.955		0.05
0.850		0.02

207. $Ca(IO_3)_2$

d		I/I1
6.7		0.07
6.0		0.27
5.1		0.33
4.27	(30)	1.00
3.75		0.30
3.51		0.27
3.35		0.23
3.24	(20)	0.67
3.04	(30)	1.00
2.83		0.07
2.69		0.33
2.59		0.07
2.53		0.50
2.43		0.27
2.37		0.30
2.30		0.07
2.23		0.13
2.12		0.27
2.04		0.23
2.00		0.03
1.95		0.20
1.85		0.20
1.78		0.42
1.75		0.42
1.71		0.13
1.67		0.23
1.63		0.13
1.60		0.13
1.56		0.13
1.485		0.07
1.450		0.13
1.407		0.17
1.362		0.13

208. $CaI_2.4H_2O$

4.98	(20)	0.67
4.52		0.58
3.92	(30)	1.00
3.60		0.03
3.35		0.50
3.20		0.50
2.96		0.50
2.49	(20)	0.67
2.42		0.33
2.25		0.13
2.18		0.33
2.05		0.03
2.02		0.13
1.96		0.13
1.87		0.33
1.71		0.20
1.67		0.07
1.64		0.07
1.60		0.17
1.56		0.17
1.480		0.13
1.437		0.07
1.410		0.07
1.360		0.13
1.313		0.07
1.290		0.07

209. $Ca(MnO_4)_2.4H_2O$

7.1		0.27
6.2		0.42
5.7		0.07
5.0		0.27
4.55	(30)	1.00
3.99		0.27
3.75	(20)	0.67
3.58		0.33
3.43		0.13
3.30		0.33
3.20	(25)	0.83
3.02		0.50
2.86		0.03
2.76		0.20
2.57		0.13
2.51		0.23
2.35		0.13
2.27		0.07
2.18		0.27
2.12		0.07
2.04		0.13
2.01		0.13
1.95		0.13
1.90		0.17
1.85		0.07
1.80		0.23
1.74		0.20

210. $Ca(NO_3)_2$*

d		I/I1
4.39	(30)	0.60
3.39		0.50
3.09		0.50
2.67		0.02
2.52		0.04
2.29	(40)	0.80
2.19	(50)	1.00
2.01		0.02
1.89		0.30
1.78		0.12
1.73		0.10
1.69		0.10
1.65		0.02
1.61		0.02
1.54		0.04
1.457		0.10
1.405		0.04
1.338		0.14
1.280		0.10
1.142		0.04

211. $Ca(NO_3)_2.4H_2O$

7.8	(9)	0.45
6.0		0.05
5.4		0.20
5.2	(20)	1.00
4.40		0.30
3.60		0.20
3.32		0.05
3.13		0.35
3.00		0.30
2.81	(8)	0.40
2.71		0.05
2.58		0.05
2.45		0.20
2.32		0.40
2.27		0.05
2.18		0.20
2.08		0.10
2.03		0.40
1.92		0.10
1.53		0.05
1.398		0.05
1.343		0.05
1.291		0.05

212. $Ca(NO_3)_2.H_2O$

7.1	(25)	0.40
6.1	(25)	0.40
5.0		0.28
4.13		0.16
3.82		0.13
3.02		0.32
2.85	(62.5)	1.00
2.58		0.32
2.34		0.40
2.20		0.24
2.10		0.28
2.00		0.40
1.95		0.06
1.89		0.03
1.84		0.06
1.78		0.06
1.73		0.13
1.485		0.10
1.450		0.10
1.415		0.20
1.340		0.06
1.300		0.03
1.265		0.16
1.242		0.05
1.152		0.16
1.110		0.06
1.078		0.06
1.060		0.03
1.000		0.03
0.942		0.05
0.868		0.03
0.850		0.02

213. CaC_2O_4

5.9	(30)	1.00
3.65	(25)	0.83
2.98	(17.5)	0.58
2.85		0.06
2.50		0.33
2.35		0.58
2.26		0.20
2.21		0.03
2.13		0.03
2.07		0.20
1.95		0.13
1.82		0.07
1.73		0.10
1.69		0.03
1.64		0.03
1.58		0.03
1.55		0.03
1.480		0.03
1.390		0.03
1.340		0.03
1.300		0.03
1.215		0.03
1.180		0.07
1.155		0.03
1.095		0.03

214. CaO*

d		I/I1
2.76	(40)	0.40
2.39	(100)	1.00
1.69	(62.5)	0.63
1.445		0.20
1.382		0.20
1.200		0.10
1.100		0.07
1.071		0.25
0.979		0.13
0.922		0.03
0.847		0.03
0.810		0.03
0.800		0.06
0.759		0.02
0.731		0.01
0.723		0.02
0.671		0.01
0.666		0.01

215. CaO_2

5.7		0.05
4.29		0.10
3.90		0.03
3.59		0.38
3.30	(30)	0.75
3.04		0.50
2.73	(40)	1.00
2.51		0.25
2.30		0.15
2.11		0.05
2.06	(25)	0.63
1.99		0.10
1.93		0.18
1.87		0.18
1.83		0.50
1.74		0.05
1.65		0.25
1.54		0.10
1.480		0.10
1.414		0.05
1.366		0.08
1.315		0.08
1.290		0.15

216. $(C_6H_4OHSO_3)_2.Ca.H_2O$

4.39	(3)	0.30
3.98	(10)	1.00
3.55	(4)	0.40
3.07		0.10
2.67		0.10

217. $CaHPO_4$

6.8		0.08
3.35	(40)	1.00
3.11		0.10
2.95	(30)	0.75
2.74	(25)	0.63
2.50		0.15
2.24		0.10
1.98		0.05
1.91		0.13
1.84		0.20
1.79		0.10
1.72		0.25
1.67		0.15
1.64		0.10
1.60		0.05
1.56		0.03
1.53		0.03
1.50		0.03
1.470		0.03
1.410		0.03
1.350		0.06
1.260		0.05
1.230		0.05
1.200		0.05
1.180		0.03

218. $CaHPO_4.2H_2O$*

7.6	(20)	0.67
4.24	(30)	1.00
3.04	(20)	0.67
2.93		0.50
2.62		0.67
2.42		0.23
2.26		0.07
2.16		0.27
2.08		0.13
2.00		0.17
1.87		0.20
1.81		0.27
1.71		0.10
1.66		0.07
1.60		0.07
1.55		0.10
1.52		0.10
1.452		0.10
1.370		0.07

219. $Ca(H_2$

d		I/I1
7.1		
6.5		
5.8		
4.35		
3.63		(17.5)
3.50		(10)
3.19		
3.04		
2.96		
2.80		
2.57		(15
2.32		
2.11		
1.93		
1.82		
1.76		
1.71		
1.59		
1.51		

220. $Ca(H_2PO_4)_2$

12.0		(15
5.6		
4.95		
3.88		(20
3.69		(15
3.36		
3.18		
2.96		
2.81		
2.65		
2.56		
2.44		
2.14		
2.07		
2.00		
1.93		
1.84		
1.78		
1.74		
1.70		
1.65		
1.60		
1.57		
1.53		
1.460		
1.405		
1.365		
1.333		
1.266		
1.230		

221. Ca_3

6.6		
5.2		
4.11		
3.47		
3.22		(25
2.89		(40
2.78		
2.62		(30
2.54		
2.42		
2.27		
2.20		
2.09		
2.02		
1.94		
1.90		
1.83		
1.79		
1.74		
1.69		
1.64		
1.61		
1.56		
1.470		
1.420		
1.390		
1.315		
1.260		
1.225		
1.190		
1.155		
1.128		
1.102		
1.063		
1.038		
1.018		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

d	*I/I*₁

219. $Ca(H_2PO_4)_2$*

d	*I/I*₁
7.1	0.23
6.5	0.23
5.8	0.11
4.35	0.23
3.63	(17.5) 1.00
3.50	(10) 0.57
3.19	0.46
3.04	0.57
2.95	0.17
2.80	0.11
2.57	(15) 0.86
2.32	0.11
2.11	0.46
1.93	0.17
1.82	0.23
1.76	0.11
1.71	0.23
1.59	0.17
1.51	0.11

220. $Ca(H_2PO_4)_2.H_2O$*

d	*I/I*₁
12.0	(15) 0.75
5.6	0.20
4.95	0.40
3.88	(20) 1.00
3.69	(15) 0.75
3.56	0.30
3.18	0.40
2.96	0.63
2.81	0.20
2.65	0.75
2.56	0.50
2.44	0.40
2.14	0.30
2.07	0.20
2.00	0.40
1.93	0.75
1.84	0.05
1.78	0.30
1.74	0.15
1.70	0.20
1.65	0.20
1.60	0.15
1.57	0.10
1.53	0.20
1.460	0.15
1.405	0.25
1.365	0.10
1.333	0.15
1.266	0.15
1.230	0.20

221. $Ca_3(PO_4)_2$

d	*I/I*₁
5.6	0.10
5.2	0.15
4.11	0.10
3.47	0.20
3.22	(25) 0.63
2.89	(40) 1.00
2.78	0.15
2.62	(30) 0.75
2.54	0.10
2.42	0.15
2.27	0.20
2.20	0.15
2.09	0.15
2.02	0.15
1.94	0.31
1.90	0.25
1.83	0.15
1.79	0.15
1.74	0.50
1.69	0.10
1.64	0.08
1.61	0.10
1.56	0.22
1.470	0.05
1.420	0.07
1.390	0.05
1.315	0.03
1.260	0.10
1.225	0.05
1.190	0.05
1.155	0.05
1.128	0.15
1.102	0.05
1.083	0.03
1.038	0.07
1.018	0.05

222. $Ca_3(PO_4)_2.H_2O$

d	*I/I*₁
3.44	(10) 0.40
3.11	0.08
2.79	(25) 1.00
2.62	0.08
2.27	0.16
2.13	0.04
2.06	0.04
1.94	(5) 0.20
1.84	0.20
1.71	0.16
1.450	0.08
1.310	0.08
1.240	0.04
1.109	0.08

223. Calcium Chlorohydrophosphate

d	*I/I*₁
4.32	(17.5) 0.43
3.25	(40) 1.00
2.99	0.31
2.84	0.25
2.66	(15) 0.37
2.58	0.05
2.42	0.05
2.29	0.20
2.22	0.15
2.12	0.05
2.01	0.05
1.92	0.02
1.86	0.05
1.74	0.07
1.66	0.02
1.51	0.02
1.465	0.05
1.192	0.02

224. $CaO_2.PO.OC_6H_4(OH)_2$

d	*I/I*₁
14.2	(100) 1.00
7.0	0.03
5.2	(7) 0.07
3.48	(7) 0.07
3.10	0.01
2.21	0.01
2.05	0.02
1.81	0.01
1.73	0.02

225. Calcium Lactophosphate

d	*I/I*₁
10.0	(8) 0.89
8.9	(9) 1.00
7.7	0.44
4.30	0.22
4.04	(6) 0.67
3.28	0.11
3.09	0.33
2.95	0.22
2.62	0.33
2.45	0.22
2.28	0.11
2.18	0.22
2.01	0.11
1.88	0.11

226. $Ca_2P_2O_7$

d	*I/I*₁
4.92	0.16
4.30	0.24
3.80	0.16
3.31	(12.5) 1.00
3.20	0.48
3.03	(8) 0.64
2.78	(12.5) 1.00
2.65	0.16
2.56	0.16
2.33	0.24
2.22	0.24
2.10	0.56
1.98	0.64
1.95	0.16
1.89	0.08
1.83	0.48
1.77	0.40
1.72	0.08
1.68	0.08
1.62	0.40
1.57	0.16
1.53	0.16
1.495	0.16
1.458	0.16
1.420	0.08
1.390	0.08
1.332	0.24
1.300	0.16
1.229	0.16
1.200	0.08

227. Ca_3P_2

d	*I/I*₁
4.92	0.05
4.00	0.15
3.45	0.20
3.10	0.20
2.82	(20) 1.00
2.73	(8) 0.40
2.62	(10) 0.50
2.27	0.16
2.16	0.05
2.05	0.05
1.95	0.45
1.89	0.05
1.83	0.30
1.80	0.30
1.72	0.10
1.54	0.05
1.50	0.05
1.480	0.05
1.460	0.20
1.315	0.05
1.285	0.05
1.110	0.05

228. $Ca(H_2PO_2)_2$

d	*I/I*₁
7.4	(25) 0.63
3.70	0.63
3.48	(40) 1.00
3.25	(30) 0.75
3.01	0.23
2.75	0.31
2.60	0.25
2.26	0.15
2.20	0.10
2.05	0.08
2.02	0.13
1.86	0.25
1.76	0.13
1.71	0.10
1.60	0.03
1.50	0.05
1.375	0.03
1.225	0.03
1.180	0.03

229. $Ca(NaHPO_2)_2$

d	*I/I*₁
7.0	(20) 0.67
5.7	0.10
4.90	0.20
4.00	(20) 0.67
3.48	0.07
3.24	0.17
3.09	(30) 1.00
2.95	0.03
2.86	0.03
2.71	0.03
2.60	0.23
2.44	0.07
2.36	0.10
2.30	0.17
2.12	0.07
1.99	0.03
1.91	0.20
1.87	0.03
1.81	0.03
1.78	0.03
1.69	0.03
1.62	0.03
1.57	0.03
1.51	0.03
1.450	0.03
1.328	0.03

230. $Ca(C_6H_4OHCOO)_2.3H_2O$

d	*I/I*₁
9.9	(40) 1.00
6.0	(20) 0.50
5.0	0.31
4.17	0.31
3.59	0.25
2.99	(17.5) 0.44
2.76	0.03
2.50	0.05
2.38	0.10
2.28	0.15
2.11	0.03
2.02	0.15
1.88	0.08
1.80	0.05
1.72	0.03
1.66	0.03
1.62	0.03

231. $CaSiO_3$

d	*I/I*₁
5.7	0.05
3.42	0.15
3.23	(40) 1.00
2.80	(30) 0.75
2.45	0.10
1.98	(25) 0.63
1.83	0.08
1.69	0.03
1.61	0.08
1.54	0.03
1.476	0.08
1.400	0.05
1.293	0.03
1.250	0.08
1.180	0.03
1.140	0.03
1.110	0.03
1.040	0.03

232. α-Ca_2SiO_4

d	*I/I*₁
5.6	0.08
4.32	0.24
4.05	0.06
3.80	0.24
3.38	0.09
3.01	(30) 0.48
2.89	0.09
2.74	(62.5) 1.00
2.60	0.06
2.51	0.09
2.44	0.06
2.32	0.06
2.24	0.05
2.18	0.06
2.02	0.06
1.90	(30) 0.48
1.80	0.32
1.75	0.20
1.68	0.20
1.63	0.28
1.53	0.08
1.495	0.06
1.470	0.09
1.440	0.05
1.405	0.05
1.300	0.03
1.268	0.03
1.254	0.09
1.230	0.05
1.180	0.02
1.160	0.09
1.134	0.09
1.092	0.06
1.075	0.02
1.013	0.03
0.957	0.03

233. β-Ca_2SiO_4

d	*I/I*₁
2.77	(25) 1.00
2.62	(10) 0.40
2.43	0.16
2.28	0.12
2.19	(12.5) 0.50
2.03	0.16
1.98	0.32
1.90	0.16
1.80	0.12
1.70	0.08
1.62	0.16
1.52	0.12
1.485	0.12
1.370	0.08
1.290	0.04
1.250	0.04
1.180	0.04
1.125	0.04

234. Ca_3SiO_5

d	*I/I*₁
3.02	0.44
2.75	(40) 1.00
2.61	(30) 0.75
2.30	0.08
2.18	(20) 0.50
1.98	0.05
1.92	0.10
1.81	0.03
1.76	0.38
1.63	0.31
1.54	0.10
1.480	0.31
1.441	0.20
1.380	0.18
1.195	0.08
1.160	0.03
1.130	0.03
1.094	0.05

235. $CaSi_2$

d	*I/I*₁
3.31	0.12
3.08	0.12
2.66	(25) 0.40
2.55	(17.5) 0.28
2.13	0.16
1.92	(62.5) 1.00
1.64	0.16
1.55	0.12
1.465	0.03
1.432	0.06
1.355	0.03
1.245	0.11
1.215	0.02
1.119	0.02
1.165	0.06
1.150	0.02
1.110	0.06
1.045	0.02
1.020	0.02
0.991	0.02
0.961	0.02
0.920	0.03
0.904	0.02
0.881	0.02

236. $CaSO_4$

d	*I/I*₁
3.89	0.03
3.49	(75) 1.00
3.11	0.03
2.85	(50) 0.67
2.46	0.07
2.32	(25) 0.33
2.26	0.01
2.20	0.33
2.08	0.11
1.99	0.11
1.93	0.04
1.86	0.27
1.74	0.20
1.64	0.27
1.59	0.03
1.56	0.05
1.52	0.07
1.487	0.08
1.420	0.08
1.395	0.07
1.360	0.01
1.318	0.09
1.296	0.03
1.275	0.09
1.215	0.05
1.197	0.01
1.163	0.07
1.103	0.09

237. $CaSO_4.1/2H_2O$

d	*I/I*₁
6.0	0.40
3.48	0.30
3.00	(30) 0.60
2.80	(50) 1.00
2.34	0.02
2.13	0.18
1.85	(30) 0.60
1.74	0.02
1.69	0.10
1.53	0.04
1.470	0.02
1.445	0.02
1.350	0.02
1.300	0.08
1.262	0.04
1.243	0.04
1.210	0.02
1.150	0.04
1.125	0.02
1.070	0.02
1.038	0.02
1.012	0.02
1.000	0.02
0.958	0.02
0.920	0.02

238. $CaSO_4.2H_2O$

d	*I/I*₁
7.7	0.50
4.29	(40) 1.00
3.81	0.15
3.06	(25) 0.63
2.87	(25) 0.63
2.68	0.50
2.48	0.20
2.22	0.20
2.07	0.50
1.88	0.25
1.79	0.20
1.66	0.10
1.62	0.15
1.58	0.10
1.435	0.13
1.360	0.10
1.325	0.10
1.270	0.03
1.240	0.15
1.200	0.10
1.138	0.08
1.083	0.05
1.037	0.03
0.997	0.05

239. CaS*

d	*I/I*₁
2.84	(125) 1.00
2.00	(125) 1.00
1.63	0.50
1.419	0.16
1.268	(75) 0.60
1.158	0.32
1.004	0.06
0.946	0.14
0.897	0.08
0.856	0.06
0.788	0.05
0.759	0.08
0.689	0.03
0.670	0.02

240. $CaSO_3$

d	*I/I*₁
5.5	(10) 0.40
4.85	0.08
4.32	0.08
3.80	0.32
3.16	(25) 1.00
2.82	0.24
2.62	(15) 0.60
2.45	0.16
2.22	0.16
2.12	0.16
2.06	0.16
1.95	0.36
1.85	0.40
1.81	0.32
1.67	0.28
1.62	0.24
1.52	0.24
1.480	0.12
1.440	0.08
1.410	0.04
1.350	0.08
1.320	0.04
1.280	0.04
1.245	0.08
1.222	0.08
1.112	0.08

241. $CaC_4H_6O_6.4H_2O$

d	*I/I*₁
7.2	(8) 0.40
6.7	(8) 0.40
5.3	0.20
4.85	0.20
4.18	0.10
3.30	0.15
3.05	0.40
2.80	0.10
2.68	0.05
2.55	(20) 1.00
2.34	0.05
2.24	0.15
2.07	0.20
1.95	0.10
1.87	0.15
1.78	0.10

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

242. $Ca(CNS)_2.3H_2O$

d	I/I1
6.1	0.08
4.86	0.08
4.41 (20)	0.27
4.20 (20)	0.27
3.93	0.17
3.34	0.05
3.05 (75)	1.00
2.69	0.04
2.60	0.03
2.46	0.11
2.38	0.07
2.28	0.05
2.20	0.03
2.13	0.09
2.06	0.08
1.95	0.09
1.91	0.09
1.79	0.01
1.73	0.01
1.70	0.01
1.66	0.05
1.60	0.09
1.55	0.03
1.52	0.01
1.462	0.03
1.412	0.03
1.379	0.04
1.345	0.01
1.295	0.01
1.263	0.03

243. $CaWO_4$*

d	I/I1	
4.76	(12.5)	0.31
3.09	(40)	1.00
2.83		0.08
2.61		0.13
2.28		0.10
1.98		0.05
1.92	(9)	0.23
1.85		0.08
1.67		0.10
1.62		0.05
1.58		0.20
1.54		0.10
1.243		0.10
1.200		0.03
1.165		0.03
1.080		0.05
1.010		0.03

244. $CaC_3H_3O_3N_4$

d	I/I1	
9.9		0.07
8.3		0.03
7.0		0.17
6.0		0.07
5.5		0.07
4.85	(7)	0.23
4.45		0.20
4.00		0.07
3.61		0.13
3.25	(30)	1.00
3.05		0.20
2.88		0.03
2.72	(7)	0.23
2.48		0.03
2.40		0.07
2.31		0.03
2.21		0.03
2.08		0.10
1.94		0.10
1.83		0.10
1.62		0.10

245. C*

d	I/I1	
3.38	(100)	1.00
2.12		0.05
2.02	(10)	0.10
1.69		0.10
1.227	(17.5)	0.18
1.150		0.09
1.120		0.01
1.049		0.01
0.991		0.03
0.828		0.01
0.796		0.01
0.707		0.01
0.695		0.01

246. $CH_3CH(NH_2)OH$

d	I/I1	
8.5	(15)	0.60
6.2	(25)	1.00
5.7		0.08
4.22		0.08
3.98		0.08
3.70	(17.5)	0.70
3.29		0.20
3.10		0.16
2.81		0.08
2.67		0.04
2.59		0.12
2.42		0.08
2.32		0.04
2.24		0.12
2.16		0.08
2.08		0.12
1.99		0.04

247. CH_3CONH_2

d	I/I1	
6.4		0.03
5.7	(25)	0.63
4.22		0.03
4.02		0.03
3.56	(40)	1.00
3.30		0.10
3.20		0.10
2.87	(7)	0.18
2.52		0.08
2.33		0.08
2.17		0.08
2.00		0.03
1.86		0.03
1.81		0.03
1.76		0.05
1.72		0.05
1.59		0.03

248. $CH_3CONHC_6H_5$

d	I/I1	
10.0	(8)	0.89
8.6		0.22
8.0		0.22
7.5		0.22
6.8		0.56
5.8	(8)	0.89
5.2		0.33
4.77		0.22
4.45		0.67
4.02	(9)	1.00
3.75		0.89
3.45		0.67
3.21		0.11
3.04		0.67
2.81		0.11
2.56		0.11
2.36		0.11
2.27		0.22
2.20		0.11
2.13		0.11

249. $C_6H_4(OC_2H_5)$-$(NH.CH_3CO)$; 1:4

d	I/I1	
7.9		0.10
6.0	(12.5)	0.31
4.85		0.15
4.01	(40)	1.00
3.65	(12.5)	0.31
3.41		0.31
2.92		0.10
2.79		0.05
2.68		0.05
2.46		0.03
2.43		0.03
2.27		0.05
1.99		0.03
1.93		0.03
1.90		0.03
1.70		0.03

250. $C_{11}H_{12}ON_2$

d	I/I1	
7.7		0.24
6.7	(17.5)	0.70
5.8		0.24
4.49	(25)	1.00
4.18	(12.5)	0.50
3.77		0.32
3.12		0.50
2.95		0.08
2.77		0.16
2.65		0.12
2.30		0.08
2.25		0.04
2.12		0.08
1.90		0.04
1.83		0.04
1.71		0.04

251. $C_6H_4CO_2HCO_2CH_3$

d	I/I1	
11.7		0.20
5.7	(25)	1.00
4.29		0.20
3.92	(8)	0.32
3.30	(10)	0.40
2.84		0.04
2.73		0.08
2.60		0.08
2.47		0.08
2.39		0.04
2.32		0.04
2.15		0.12
2.06		0.04
1.87		0.04
1.80		0.04

252. C_6H_5COOH

d	I/I1	
11.0		0.20
5.5		0.25
5.2	(40)	0.80
4.66		0.20
4.20		0.12
3.75	(40)	0.80
3.45	(50)	1.00
3.21		0.60
2.98		0.50
2.74		0.02
2.58		0.12
2.50		0.02
2.42		0.12
2.32		0.20
2.21		0.08
2.10		0.10
2.02		0.04
1.92		0.06
1.87		0.02
1.81		0.04
1.72		0.08
1.67		0.04
1.61		0.06
1.55		0.04

253. $(C_6H_5)_2CO$

d	I/I1	
6.3		0.16
5.6		0.72
4.80	(12.5)	1.00
4.38	(12.5)	1.00
4.03	(10)	0.80
3.78		0.24
3.59		0.32
3.17		0.80
3.05		0.48
2.92		0.08
2.80		0.16
2.76		0.16
2.72		0.16
2.60		0.08
2.48		0.08
2.39		0.08
2.17		0.08
1.97		0.08
1.92		0.08

254. $C_6H_4ClCOOH$

d	I/I1	
6.8		0.50
5.9		0.30
3.68	(7)	0.70
3.47	(6)	0.60
3.25	(10)	1.00
2.96		0.30
2.56		0.30
2.41		0.30
2.34		0.10
2.26		0.20
2.12		0.10
1.97		0.10
1.68		0.10

255. $C_{10}H_7Cl$

d	I/I1	
9.2		0.16
4.69	(25)	1.00
4.45		0.16
3.82	(17.5)	0.70
3.20	(17.5)	0.70
3.00		0.08
2.77		0.08
2.37		0.12
1.94		0.12
1.83		0.12

256. $C_6H_3ClNO_2.NH_3$

d	I/I1	
7.3		0.30
6.5		0.05
5.6	(12.5)	0.63
5.0		0.05
4.45		0.05
4.19		0.05
3.53	(20)	1.00
3.28	(15)	0.75
3.15		0.30
3.00		0.20
2.88		0.20
2.67		0.30
2.48		0.10
2.12		0.10
2.03		0.10
1.86		0.05
1.69		0.05
1.56		0.05

257. $C_6H_5CH{:}CHCOOH$

d	I/I1	
9.0		0.16
5.9		0.16
4.82	(25)	1.00
4.29		0.08
4.11		0.08
3.89		0.50
3.50	(17.5)	0.70
3.30		0.04
3.17		0.04
3.02	(20)	0.80
2.63		0.08
2.23		0.12
2.16		0.04

258. $H_2C_6H_6O_7.H_2O$

d	I/I1	
6.4		0.25
5.4		0.08
4.94	(40)	1.00
4.57		0.43
4.10		0.10
3.73		0.31
3.42	(40)	1.00
3.10		0.25
2.86	(30)	0.75
2.66		0.31
2.55		0.15
2.48		0.50
2.42		0.20
2.30		0.10
2.20		0.13
2.09		0.25
1.77		0.08

259. $C_6H_6O_2$

d	I/I1	
5.6	(20)	1.00
4.45		0.63
3.97	(15)	0.75
3.52		0.63
3.23	(20)	1.00
2.99		0.63
2.49		0.10
2.38		0.05
2.29		0.10
2.04		0.05
1.82		0.05

260. $NO_2C_6H_2Br_2OH$

d	I/I1	
4.12		0.27
3.59	(10)	0.66
3.35	(15)	1.00
2.74	(5)	0.33
2.67		0.33
2.35		0.13
2.08		0.07
1.97		0.13
1.71		0.07
1.65		0.13

261. $C_6H_4Cl_2$

d	I/I1	
6.8		0.04
6.0		0.04
5.3		0.28
4.41	(25)	1.00
3.73	(25)	1.00
3.29	(25)	1.00
3.10		0.32
2.94		0.28
2.84		0.24
2.55		0.04
2.47		0.04
2.38		0.04
2.29		0.08
2.18		0.04
2.00		0.16
1.89		0.12
1.84		0.08
1.78		0.12
1.72		0.04
1.65		0.04

262. $(C_6H_3Cl_2)_2CO$

d	I/I1	
6.7		0.20
5.6	(10)	0.66
4.60		0.27
4.46		0.40
4.19		0.53
3.74	(15)	1.00
3.53	(10)	0.66
3.17		0.27
3.04		0.40
2.92		0.13
2.85		0.27
2.50		0.13
2.34		0.07
2.27		0.20
2.21		0.07
2.11		0.07
2.01		0.13
1.94		0.13
1.77		0.13

263. $(C_6H_4)_2O$

d	I/I1	
10.0		0.25
4.59	(40)	1.00
3.78	(30)	0.75
3.55		0.05
3.16	(40)	1.00
2.92		0.05
2.48		0.05
2.33		0.13
2.25		0.05
2.19		0.03
1.92		0.08
1.86		0.05
1.81		0.10
1.350		0.03

264. $(C_6H_4)_2SO$

d	I/I1	
6.7		0.20
6.1		0.20
5.4	(20)	1.00
4.12	(20)	1.00
3.85	(7)	0.35
3.48		0.20
3.25		0.20
2.98		0.10
2.69		0.15
2.32		0.10
2.01		0.10
1.92		0.05
1.82		0.05

265. $(C_6H_5NH)_2CO$

d	I/I1	
8.0		0.31
5.9		0.08
5.2		0.13
4.53	(25)	0.63
4.24	(40)	1.00
3.94		0.15
3.65		0.08
3.38		0.20
3.31	(15)	0.38
2.97		0.05
2.69		0.08
2.60		0.05
2.39		0.03
2.25		0.05
2.06		0.03
1.96		0.03
1.87		0.03
1.77		0.03
1.70		0.03

266. $C_7H_5NH_2Cl$

d	I/I1	
9.7		0.04
8.3		0.12
4.08		0.04
3.89	(9)	0.36
3.39	(25)	1.00
3.25		0.16
3.00	(8)	0.32
2.81		0.04
2.72		0.08
2.65		0.24
2.40		0.16
2.37		0.24
2.17		0.04
2.12		0.12
2.02		0.08
1.87		0.04
1.79		0.12

267. CH_3NH_2COOH

d	I/I1	
6.0		0.02
4.69		0.40
4.40		0.16
3.73	(30)	0.48
3.13		0.16
3.00	(62.5)	1.00
2.54		0.32
2.46	(40)	0.64
2.34		0.02
2.22		0.02
2.15		0.06
2.12		0.03
2.04		0.13
2.01		0.05
1.93		0.10
1.86		0.05
1.80		0.10
1.63		0.13
1.57		0.03
1.52		0.03
1.475		0.05

268. $CH_3OHCOOH$

d	I/I1	
6.5		0.16
4.44		0.20
4.20		0.16
4.09	(15)	0.30
3.80		0.02
3.52	(50)	1.00
3.35		0.08
3.20		0.02
2.94		0.08
2.80		0.12
2.71		0.02
2.63		0.14
2.47	(20)	0.40
2.27		0.12
2.19		0.04
2.11		0.04
2.03		0.10
1.95		0.02
1.89		0.04
1.70		0.06

269. $(CH_2)_6N_4$

d	I/I1	
7.0	(4)	0.13
5.9		0.07
4.97	(30)	1.00
4.00		0.13
3.85		0.13
3.52	(5)	0.16
3.22		0.12
2.86		0.13
2.75		0.10
2.65		0.13
2.49		0.10
2.33		0.10
2.02		0.10
1.88		0.07
1.78		0.03
1.72		0.03
1.37		0.03

270. $NH(CH_2COOH)_2$

d	I/I1	
6.4		0.16
5.1		0.16
4.70		0.24
4.18	(20)	0.80
3.74		0.50
3.53		0.32
3.31	(25)	1.00
3.05	(20)	0.80
2.80		0.24
2.65		0.32
2.47		0.24
2.35		0.32
2.26		0.24
2.13		0.32
2.06		0.24
1.93		0.08
1.83		0.08
1.75		0.16
1.71		0.16
1.66		0.16

271. C_5I_5

d	I/I1	
6.2		0.04
5.5		0.06
4.14		0.20
3.91	(50)	1.00
3.67	(30)	0.60
3.50		0.16
3.30	(30)	0.60
3.05		0.40
2.84		0.12
2.76		0.60
2.67		0.05
2.52		0.60
2.40		0.12
2.20		0.12
2.13		0.20
2.04		0.20
1.98		0.30
1.88		0.30
1.82		0.08
1.76		0.40
1.72		0.04
1.69		0.12
1.57		0.04
1.485		0.04
1.420		0.08
1.385		0.06
1.355		0.04
1.326		0.06
1.275		0.06
1.240		0.06
1.200		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

d	I/I₁
272. C_6H_4IOH	
9.8	0.33
7.2	(20) 0.66
6.5	0.17
5.7	0.20
5.1	(25) 0.83
4.86	0.27
4.60	0.27
4.37	0.13
3.97	0.42
3.79	0.66
3.60	0.40
3.38	0.27
3.22	(30) 1.00
3.05	0.27
2.97	0.66
2.79	0.17
2.70	0.17
2.57	0.10
2.41	0.27
2.25	0.20
2.17	0.13
2.13	0.42
1.98	0.20
1.93	0.20
1.88	0.23
1.81	0.10
1.69	0.10

273. $C_6H_4CO.COH:N$

6.5	0.13
5.7	(15) 0.50
5.2	0.10
4.66	0.03
3.49	(20) 0.66
3.21	(30) 1.00
2.86	0.03
2.60	0.03
2.14	0.03
2.06	0.03
1.74	0.03
1.60	0.03
1.470	0.03

274. $C_{12}H_{22}O_{11}.H_2O$

7.1	0.20
5.4	(7) 0.35
4.51	(20) 1.00
4.20	(6) 0.30
3.91	0.10
3.73	0.25
3.50	0.15
3.22	0.10
2.87	0.10
2.70	0.10
2.59	0.15
2.37	0.15
2.12	0.10
1.90	0.05

275. $C_2H_2(COOH)_2$

5.3	0.10
5.0	(15) 0.38
3.97	(15) 0.38
3.18	(40) 1.00
2.98	0.03
2.77	0.20
2.66	0.15
2.47	0.03
2.35	0.25
2.27	0.08
2.22	0.15
2.00	0.03
1.95	0.05
1.91	0.05
1.77	0.03
1.73	0.03
1.68	0.03
1.58	0.03
1.480	0.03

276. $C_{10}H_8$

11.5	0.07
9.9	0.13
8.7	0.13
7.9	0.20
7.2	0.20
4.52	(15) 1.00
4.10	(8) 0.53
3.49	0.27
3.37	(10) 0.67
3.00	0.40
2.75	0.07
2.42	0.20
1.91	0.07
1.84	0.07

277. $C_{10}H_7OH$

5.9	(20) 0.80
4.40	0.20
3.66	(25) 1.00
3.21	(7) 0.28
2.95	0.16
2.70	0.16
2.19	0.04
2.11	0.04
2.02	0.04
1.94	0.12
1.75	0.04

278. $C_{10}H_6OHSO_3H$

14.0	0.07
5.3	0.07
4.55	(15) 1.00
3.67	(6) 0.40
3.44	0.27
3.09	(8) 0.53
2.77	0.13
2.65	0.13
2.44	0.08
2.25	0.07
2.18	0.07
2.00	0.07
1.88	0.20
1.455	0.07

279. $N(CH_2COOH)_3$

6.0	0.08
4.48	(25) 1.00
3.69	0.12
3.47	0.08
3.15	(17.5) 0.70
2.99	(10) 0.40
2.65	0.16
2.58	0.08
2.44	0.32
2.32	0.04
2.22	0.12
2.11	0.24
1.99	0.28
1.97	0.08
1.83	0.08
1.77	0.08
1.58	0.08
1.50	0.04
1.445	0.04
1.410	0.04

280. $NO_2C_6H_4.NH_2$

7.1	0.07
5.4	0.23
4.95	0.23
4.58	(17.5) 0.58
3.80	0.50
3.48	(30) 1.00
3.13	(17.5) 0.58
3.01	0.27
2.90	0.13
2.74	0.07
2.62	0.07
2.58	0.07
2.40	0.03
2.03	0.03
1.96	0.03
1.86	0.03
1.75	0.03
1.70	0.03

281. $NO_2C_6H_4CHO$

6.2	(12.5) 0.63
4.74	(12.5) 0.63
4.22	0.63
3.69	0.10
3.53	0.30
3.35	0.25
3.18	(20) 1.00
3.05	0.05
2.88	0.10
2.70	0.10
2.53	0.05
2.38	0.05
2.23	0.05
2.15	0.05
2.04	0.10
1.58	0.05

282. $(COOH)_2.2H_2O$

6.0	0.20
4.75	0.20
3.95	0.07
3.45	0.09
3.08	(75) 1.00
2.87	0.13
2.60	0.08
2.41	(25) 0.33
2.27	(25) 0.33
2.17	0.01
1.98	0.05
1.93	0.03
1.83	0.05
1.77	0.01
1.72	0.03
1.58	0.01
1.54	0.07
1.486	0.01
1.433	0.01

283. C_6HCl_5

8.4	0.27
7.1	0.33
6.6	(10) 0.67
5.2	0.07
4.00	0.40
3.60	0.67
3.34	(15) 1.00
3.10	(12.5) 0.83
2.87	0.40
2.79	0.40
2.60	0.53
2.53	0.27
2.13	0.27
2.01	0.13
1.91	0.07
1.84	0.27
1.75	0.07
1.65	0.13
1.58	0.07
1.490	0.13

284. o-$C_6H_5C_6H_4OH$

6.0	0.06
5.2	(12.5) 0.71
4.40	(17.5) 1.00
3.58	(10) 0.57
3.40	0.34
3.17	0.29
2.87	0.29
2.42	0.23
2.12	0.05
1.84	0.06
1.76	0.05

285. p-$C_6H_5C_6H_4OH$

4.55	(25) 1.00
4.25	(20) 0.80
3.88	(25) 1.00
3.15	0.80
3.00	0.04
2.39	0.12
2.23	0.04
2.17	0.04
1.89	0.04
1.82	0.04
1.66	0.04
1.58	0.04

286. $C_6H_4OHCOOH$

8.2	(30) 0.48
5.2	(30) 0.48
4.52	0.11
3.52	(62.5) 1.00
3.11	0.32
2.92	0.24
2.67	0.11
2.51	0.03
2.45	0.03
2.36	0.13
2.26	0.16
2.10	0.02
2.05	0.06
1.95	0.08
1.86	0.03
1.78	0.02
1.67	0.06
1.53	0.03

287. $C_{12}H_{22}O_{11}$

7.6	(8) 0.53
6.9	0.53
6.0	0.07
5.7	0.33
5.4	0.13
4.71	(12.5) 0.83
4.50	0.47
4.30	0.40
4.00	0.53
3.79	0.27
3.59	(15) 1.00
3.37	0.07
3.22	0.13
3.10	0.13
2.88	0.47
2.80	0.13
2.67	0.07
2.58	0.13
2.49	0.13
2.41	0.33
2.34	0.33
2.24	0.13
2.18	0.27
2.06	0.07
1.95	0.13
1.90	0.13
1.80	0.07
1.74	0.20
1.69	0.07
1.64	

288. $(CH_2)_2C(SO_2C_2H_4)_2$

6.7	(25) 1.00
6.0	(10) 0.40
5.3	0.32
4.9	(10) 0.40
4.54	0.32
4.29	0.32
4.06	0.24
3.60	0.24
2.92	0.28
2.69	0.16
2.51	0.08
2.42	0.08
2.34	0.04
2.14	0.08
2.02	0.12
1.98	0.04
1.89	0.04
1.77	0.04

289. $C_4H_4O_4.H_2O$

7.7	0.10
4.76	0.20
4.34	(30) 1.00
4.00	0.13
3.57	0.27
3.04	(17.5) 0.58
2.81	0.42
2.70	0.03
2.52	(17.5) 0.58
2.44	0.27
2.32	0.13
2.14	0.10
2.02	0.03
1.93	0.13
1.77	0.03
1.68	0.06

290. $C_6H_3Br_4$-(1,2,4,5)

4.65	(10) 0.66
4.58	0.66
4.50	0.53
3.65	0.66
3.34	0.27
3.18	0.53
2.90	(15) 1.00
2.81	0.66
2.58	(12.5) 0.83
2.43	0.66
2.25	0.13
2.08	0.13
1.97	0.13
1.74	0.13
1.67	0.13
1.57	0.13
1.51	0.20
1.460	0.27

291. $CH_3C_6H_4SO_2NH_2$

8.2	(3) 0.60
6.2	0.60
5.7	0.40
4.92	(4) 0.80
4.20	0.40
3.78	0.40
3.50	0.20
3.32	(5) 1.00

292. $C_6H_2Cl_3.CH_2CN$

7.5	(20) 0.80
5.5	0.08
4.30	0.08
3.88	0.24
3.60	(25) 1.00
3.35	0.32
3.15	(12.5) 0.50
3.00	0.04
2.81	0.08
2.68	0.08
2.51	0.04
2.32	0.04
2.17	0.08
2.08	0.08
1.95	0.04
1.88	0.04
1.79	0.04

293. $C_6H_5CH_2C:(SO_2C_2H_5)_2$

6.6	(50) 1.00
5.4	(10) 0.20
4.98	0.10
4.65	0.16
4.38	0.04
4.15	(10) 0.20
3.78	0.12
3.60	0.12
3.27	0.08
2.94	0.12
2.80	0.04
2.68	0.06
2.57	0.10
2.35	0.06
2.31	0.02
2.17	0.02
2.08	0.06

294. $NH_2.CO.NH_2$

4.00	(75) 1.00
3.61	(30) 0.40
3.04	(40) 0.53
2.82	0.11
2.52	0.20
2.41	0.20
2.34	0.03
2.23	0.08
2.17	0.20
2.08	0.01
2.01	0.08
1.84	0.13
1.75	0.01
1.67	0.13
1.51	0.08
1.368	0.03
1.329	0.07
1.259	0.01
1.230	0.01
1.177	0.04

295. Ce

3.20	(12.5) 1.00
2.96	0.16
2.81	(9) 0.72
2.47	0.16
2.25	0.16
1.96	0.24
1.85	(5) 0.40
1.68	0.16
1.57	0.08

296. $CeCl_3$

8.6	0.12
7.9	0.08
6.8	(50) 1.00
5.7	0.06
5.3	(15) 0.30
5.0	0.12
4.50	0.16
4.30	(15) 0.30
3.99	0.25
3.82	0.30
3.31	0.20
3.17	0.12
3.07	0.02
2.83	0.12
2.63	0.16
2.53	0.04
2.48	0.16
2.38	0.10
2.30	0.08
2.21	0.30
2.08	0.02
2.01	0.08
1.93	0.08
1.89	0.08
1.82	0.04
1.73	0.08

297. $Ce(NO_3)_3.6H_2O$

11.5	0.24
10.0	0.16
8.7	0.16
8.1	0.64
6.8	0.80
6.3	(12.5) 1.00
5.8	0.64
5.4	0.80
5.2	0.48
4.70	(12.5) 1.00
4.39	(12.5) 1.00
3.97	0.80
3.80	0.48
3.64	0.32
3.35	0.64
3.25	0.64
3.00	0.32
2.91	0.64
2.84	0.64
2.62	0.80
2.53	0.48
2.45	0.40
2.41	0.32
2.30	0.40
2.25	0.40
2.19	0.32
2.11	0.64
2.03	0.24
2.00	0.16
1.95	0.48
1.86	0.32

298. $Ce_2(C_2O_4)_3.9H_2O$

5.4	(12.5) 1.00
4.89	(7) 0.56
4.32	0.24
3.20	(6) 0.48
2.90	0.32
2.67	0.24
2.10	0.48
1.95	0.48
1.66	0.08
1.59	0.16
1.490	0.08
1.460	0.08

299. CeO_2*

3.11	(50) 1.00
2.69	0.25
1.90	(40) 0.80
1.62	(30) 0.60
1.55	0.10
1.347	0.10
1.237	0.25
1.207	0.16
1.101	0.20
1.037	0.18
0.954	0.04
0.912	0.14
0.899	0.02
0.853	0.04
0.816	0.02B
0.756	0.04
0.722	0.04
0.703	0.02

300. $Ce(SO_4)_2.4H_2O$

6.8	0.13
5.8	0.05
5.4	0.03
4.65	(30) 1.00
4.41	0.13
3.96	0.07
3.69	0.07
3.45	(5) 0.17
3.33	0.03
3.22	(10) 0.33
2.98	0.07
2.91	0.03
2.82	0.10
2.70	0.13
2.60	0.07
2.48	0.03
2.39	0.03
2.33	0.03
2.23	0.03
2.10	0.10
2.05	0.07
2.00	0.10
1.88	0.03
1.83	0.07
1.76	0.05
1.67	0.05
1.62	0.05
1.54	0.03

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

301. $Ce_2(SO_4)_3$

d	I/I1
9.5	0.06
8.0	0.02
6.7	0.04
6.1	0.50
5.5 (50)	1.00
4.85	0.04
4.33	0.16
3.50	0.50
3.03 (40)	0.80
2.85 (50)	1.00
2.71	0.04
2.60	0.02
2.47	0.14
2.37	0.14
2.27	0.14
2.15	0.35
2.08	0.04
2.01	0.08
1.93	0.06
1.87	0.60
1.82	0.02
1.76	0.12
1.71	0.20
1.68	0.12
1.63	0.04
1.56	0.14
1.495	0.04
1.463	0.04
1.430	0.04
1.370	0.04
1.320	0.20
1.275	0.08
1.260	0.08
1.220	0.06
1.185	0.02
1.165	0.04
1.138	0.02
1.108	0.02
1.084	0.04
1.052	0.04

302. $CsAl(SO_4)_2.12H_2O$*

d	I/I1
7.1	0.18
6.1	0.23
5.5 (15)	0.38
5.0	0.03
4.35 (40)	1.00
4.10	0.15
3.56	0.15
3.29	0.18
3.08	0.18
2.83 (30)	0.75
2.75	0.25
2.51	0.20
2.37	0.20
2.17	0.05
2.06	0.08
1.95	0.25
1.88	0.10
1.71	0.08
1.65	0.20
1.60	0.05
1.495	0.10
1.455	0.08

303. CsCl*

d	I/I1
4.11 (15)	0.38
2.90 (40)	1.00
2.37	0.08
2.05	0.18
1.84	0.15
1.68 (17.5)	0.44
1.454	0.08
1.375	0.05
1.301	0.10
1.240	0.03
1.188	0.03
1.140	0.03
1.100	0.10

304. CsCl.RbCl

d	I/I1
4.45	0.40
4.15	0.30
3.81	0.30
3.30 (10)	1.00
3.16 (10)	1.00
2.91	0.70
2.59	0.30
2.33 (10)	1.00
2.23	0.30
2.05	0.10
1.99	0.70
1.90	0.30
1.82	0.40
1.67	0.20
1.64	0.10
1.475	0.40
1.405	0.10
1.345	0.20
1.300	0.10
1.185	0.10
1.098	0.10
1.043	0.10
0.995	0.10
0.970	0.10

305. CsI*

d	I/I1
3.22 (40)	1.00
2.27 (6)	0.15
1.86 (15)	0.38
1.61	0.10
1.435	0.13
1.218	0.10
1.074	0.04

306. $CsICl_2$*

d	I/I1
4.07 (40)	0.53
3.16 (75)	1.00
2.66	0.40
2.50	0.20
2.03	0.27
1.96	0.20
1.82	0.20
1.71 (40)	0.53
1.58	0.13
1.472	0.13
1.387	0.20
1.331	0.07
1.250	0.08
1.225	0.08
1.191	0.11
1.161	0.07
1.115	0.04
1.051	0.07
1.030	0.05

307. $CsNO_3$*

d	I/I1
4.45	0.27
3.15 (75)	1.00
2.57	0.27
2.23	0.23
1.99 (30)	0.40
1.82 (25)	0.33
1.57	0.13
1.485	0.20
1.409	0.17
1.344	0.10
1.283	0.01
1.235	0.05
1.190	0.12
1.112	0.01
1.080	0.04
1.050	0.04
1.021	0.03
0.995	0.01
0.971	0.03

308. Cs_2SO_4*

d	I/I1
4.55	0.10
3.68	0.35
3.28 (20)	1.00
3.14 (20)	1.00
2.90	0.05
2.72	0.10
2.65	0.20
2.58	0.20
2.41	0.10
2.27 (9)	0.45
2.20	0.05
2.11	0.05
2.04	0.10
1.93	0.05
1.84	0.15
1.80	0.05
1.75	0.05
1.71	0.05
1.57	0.10

309. Cr*

d	I/I1
2.03 (30)	1.00
1.437 (5)	0.17
1.174 (9)	0.30
1.018	0.03
0.910	0.03
0.770	0.03

310. Chromium Borate

d	I/I1
8.4 (6)	0.66B
3.28 (9)	1.00B
2.35	0.11
1.96 (8)	0.89
1.90	0.22
1.89	0.44
1.495	0.22
1.360	0.22
1.190	0.22

311. $CrBr_3.6H_2O$

d	I/I1
6.2 (2)	1.00
5.5 (2)	1.00
5.3	0.75
4.90	0.50
4.49	0.50
4.15	0.50
3.92	0.75
3.52 (2)	1.00
3.42	1.00
3.30	1.00
3.12	0.75
2.96	0.75
2.82	0.50
2.66	1.00
2.57	0.50
2.51	0.50
2.44	0.75
2.36	0.50
2.21	0.50
2.15	0.50
2.08	0.50
1.97	1.00
1.94	1.00
1.91	0.50
1.88	0.50
1.80	0.50
1.75	0.75
1.69	0.50

312. $CrF_3.4H_2O$

d	I/I1
4.70 (75)	1.00
4.09 (50)	0.67
3.09	0.03
2.57 (50)	0.67
2.04	0.09
1.87	0.40
1.82	0.01
1.77	0.11
1.73	0.11
1.67	0.01
1.63	0.17
1.56	0.01
1.53	0.03
1.490	0.03
1.460	0.08
1.423	0.01
1.395	0.03
1.360	0.07
1.300	0.03

313. $Cr(NO_3)_3.9H_2O$

d	I/I1
6.7 (15)	0.75
6.3 (15)	0.75
5.7	0.05
4.90	0.35
4.51	0.50
4.04 (20)	1.00
3.80	0.50
3.63	0.50
3.43	0.10
3.27	0.45
3.13	0.05
3.01	0.45
2.92	0.15
2.78	0.10
2.61	0.75
2.54	0.30
2.39	0.75
2.32	0.05
2.25	0.15
2.20	0.20
2.13	0.10
2.09	0.35
2.04	0.30
1.95	0.10
1.90	0 40
1.82	0.10
1.78	0.20
1.73	0.05
1.69	0.25
1.62	0.10
1.58	0.10
1.53	0.05
1.490	0.05
1.460	0.10
1.410	0.10
1.367	0.10
1.319	0.10

314. $Cr_2(C_2O_4)_3.H_2O$

d	I/I1
9.2 (1)	0.14
4.75 (7)	1.00
3.60	0.14
2.68 (2)	0.29
2.05	0.14

315. Cr_2O_3*

d	I/I1
3.62	0.45
2.67 (40)	0.70
2.47 (40)	0.70
2.17	0.30
2.03	0.04
1.81	0.45
1.67 (50)	1.00
1.58	0.06
1.465	0.30
1.432	0.45
1.294	0.16
1.236	0.06
1.209	0.06
1.172	0.05
1.148	0.06
1.123	0.06
1.087	0.12
1.041	0.10
1.025	0.02
0.946	0.06α1

316. CrO_3*

d	I/I1
4.20 (100)	0.75
3.40 (125)	1.00
2.86 (30)	0.25
2.36	0.20
2.25	0.20
2.00	0.07
1.96	0.10
1.84	0.05
1.74	0.15
1.71	0.03
1.68	0.01
1.60	0.03
1.56	0.01
1.54	0.01
1.50	0.05
1.470	0.01
1.431	0.03
1.405	0.05
1.376	0.02
1.353	0.06
1.273	0.02
1.230	0.02

317. $Cr(NH_4)(SO_4)_2.<12H_2O$

d	I/I1
7.1	0.40
5.5	0.27
4.75	0.13
4.34 (15)	1.00
3.84 (10)	0.66
3.71 (12.5)	0.83
3.29	0.47
3.08	0.27
2.79	0.07
2.61	0.13
2.50	0.07
2.38	0.07
2.25	0.07
2.03	0.13
1.94	0.07
1.71	0.07
1.495	0.07
1.430	0.07

318. $Cr(NH_4)(SO_4)_2.12H_2O$*

d	I/I1
7.1 (40)	0.64
5.5	0.32
5.0	0.14
4.35 (62.5)	1.00
4.11	0.40
3.71	0.64
3.55	0.02
3.29 (50)	0.80
3.08	0.40
2.98	0.05
2.90	0.03
2.82	0.03
2.75	0.13
2.67	0.03
2.62	0.03
2.52	0.10
2.42	0.03
2.37	0.13
2.28	0.03
2.25	0.03
2.18	0.02
2.14	0.02
2.06	0.16
1.99	0.03
1.94	0.32
1.89	0.02
1.81	0.03
1.72	0.16
1.64	0.14
1.60	0.10
1.487	0.08
1.449	0.06
1.368	0.06

19. $CrK(SO_4)_2.12H_2O$*

d	I/I1
7.0	0.12
5.5	0.16
4.98	0.08
4.31 (50)	1.00
4.08	0.30
3.68 (30)	0.60
3.26 (17.5)	0.35
3.04	0.30
2.87	0.02
2.81	0.12
2.72	0.12
2.59	0.06
2.48	0.12
2.34	0.06
2.25	0.06
2.15	0.04
2.03	0.12
1.97	0.06
1.93	0.16
1.85	0.04
1.74	0.04
1.69	0.08
1.63	0.10

320. Co*

d	I/I1
2.04 (40)	1.00
1.77 (17.5)	0.44
1.253 (9)	0.22
1.066	0.22
1.021	0.05
0.886	0.03
0.813	0.03
0.792	0.03
0.723	0.03
0.682	0.03

321. $Co(C_2H_3O_2)_2.4H_2O$

d	I/I1
6.8	0.08
4.88	0.16
4.35	0.06
4.13 (25)	0.50
3.90 (50)	1.00
3.65	0.12
3.42	0.04
3.05	0.04
2.84 (30)	0.60
2.68	0.02
2.60	0.04
2.42	0.04
2.29	0.04
2.06	0.08
2.00	0.02
1.95	0.08
1.87	0.04
1.82	0.14
1.77	0.06
1.70	0.02
1.55	0.02
1.48	0.03
1.418	0.02
1.360	0.02

322. $Co_3(AsO_4)_2.8H_2O$

d	I/I1
8.0	0.11
6.7 (17.5)	1.00
4.48	0.05
3.24 (10)	0.57
3.01 (12.5)	0.71
2.73	0.51
2.55	0.11
2.47	0.34
2.34	0.46
2.21	0.17
2.10	0.23
1.97	0.11
1.92	0.11
1.83	0.05
1.68	0.34
1.61	0.17
1.55	0.05
1.50	0.11
1.463	0.11
1.425	0.05
1.390	0.05
1.350	0.11
1.260	0.05

323. $CoBr_2$*

d	I/I1
6.1 (6)	0.75
3.08	0.25
2.82 (4)	0.50
2.04	0.13
1.86 (8)	1.00
1.59	0.25
1.55	0.25
1.185	0.50

324. $CoCO_3$*

d	I/I1
3.64 (7)	0.40
2.76 (17.5)	1.00
2.34	0.11
2.12	0.11
1.96	0.11
1.71 (12.5)	0.71
1.50	0.11
1.415	0.11
1.355	0.06

325. Cobaltous Chloride

d	I/I1
5.8 (50)	1.00
4.31	0.06
3.04	0.04
2.84	0.02
2.71	0.06
2.48	0.06
2.38	0.04
2.30	0.04
2.23	0.02
2.14	0.02
2.07	0.03
1.98	0.02
1.92	0.02
1.86	0.02
1.77 (30)	0.60
1.70 (10)	0.20
1.64	0.02
1.59	0.02
1.53	0.02
1.443	0.04
1.307	0.02
1.181	0.02
1.157	0.03
1.120	0.08
1.025	0.06
0.970	0.03

326. $CoCl_2.6H_2O$

d	I/I1
5.6 (40)	1.00
4.85 (40)	1.00
3.52	0.31
3.11	0.10
2.94 (25)	0.63
2.73	0.50
2.56	0.20
2.40	0.63
2.20	0.50
2.07	0.05
2.02	0.03
1.98	0.31
1.94	0.03
1.89	0.20
1.86	0.10
1.81	0.03
1.76	0.13
1.70	0.18
1.60	0.23
1.55	0.18
1.50	0.03
1.460	0.05
1.375	0.05
1.270	0.03
1.235	0.03
1.205	0.03

327. $Co(NH_3)_4Cl_2$

d	I/I1
5.8 (40)	0.80
5.3	0.10
4.98	0.12
3.60 (50)	1.00
3.47	0.16
3.15	0.04
3.02	0.04
2.93	0.04
2.63	0.20
2.48 (15)	0.30
2.36	0.02
2.30	0.04
2.20	0.02
2.12	0.06
2.05	0.12
2.02	0.10
1.92	0.06
1.82	0.02
1.78	0.03
1.75	0.02
1.70	0.04
1.66	0.04
1.58	0.06

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

328. $Co(NH_3)_3Cl_3$

d		I/I1
6.7		0.05
6.1		0.05
5.7	(40)	1.00
5.2		0.10
4.75		0.05
4.08		0.20
3.92		0.25
3.50	(15)	0.38
3.29		0.20
3.08		0.13
2.99		0.13
2.80		0.18
2.68		0.08
2.58	(15)	0.38
2.38		0.10
2.16		0.03
2.04		0.20
1.97		0.20
1.86		0.18
1.79		0.05
1.74		0.08
1.71		0.08
1.66		0.08
1.62		0.18
1.50		0.08
1.433		0.08

329. $CoCrO_4$

d		I/I1
3.30	(2)	0.50
3.10	(2)	0.50
2.89		0.50
2.62	(4)	1.00
2.36		0.50
2.04		0.25
1.73		0.50
1.65		0.25
1.55		0.50

330. $Co(OH)_2$

d		I/I1
4.40	(75)	1.00
2.44		0.23
2.31	(62.5)	0.83
1.80	(30)	0.40
1.50		0.08
1.425		0.40
1.367		0.27
1.215		0.05
1.196		0.01
1.162		0.04
1.120		0.04

331. (Mn, Co)(Mn, Co)$_2$O$_4$; 2Co:Mn*

d		I/I1
4.76		0.10
2.91		0.30
2.48	(100)	1.00
2.37		0.07
2.05		0.20
1.68		0.10
1.58	(40)	0.40
1.452	(50)	0.50
1.302		0.03
1.256		0.08
1.242		0.02
1.190		0.02
1.101		0.03
1.073		0.13
1.031		0.03
0.951		0.04

332. $Co(NO_3)_2.6H_2O$

d		I/I1
6.7		0.05
5.8		0.20
5.5		0.20
4.60	(40)	1.00
3.88		0.20
3.70		0.15
3.50		0.13
3.29	(30)	0.75
3.16		0.18
3.05		0.03
2.93		0.15
2.82		0.03
2.70		0.20
2.60		0.10
2.19	(30)	0.75
2.11		0.08
2.05		0.03
2.01		0.13
1.92		0.13
1.87		0.13
1.72		0.18
1.66		0.08
1.58		0.10
1.53		0.10
1.479		0.08
1.448		0.03

333. CoC_2O_4

d		I/I1
4.73	(40)	1.00
3.90		0.15
3.60	(12.5)	0.31
2.95	(25)	0.50
2.65		0.31
2.55		0.15
2.23		0.20
2.16		0.03
2.08		0.15
2.02		0.15
1.89		0.18
1.78		0.20
1.70		0.03
1.64		0.10
1.58		0.05
1.54		0.05
1.480		0.05
1.430		0.05
1.365		0.03
1.335		0.03
1.170		0.03
1.115		0.03

334. CoO*

d		I/I1
2.45	(50)	0.67
2.12	(75)	1.00
1.50	(75)	1.00
1.281		0.40
1.227		0.40
1.060		0.10
0.975		0.10
0.951		0.30
0.869		0.20
0.819		0.07

335. $CoCo_2O_4$*

d		I/I1
4.68		0.08
2.86		0.20
2.43	(100)	1.00
2.34		0.06
2.02		0.13
1.65		0.04
1.56	(25)	0.25
1.432	(30)	0.30
1.235		0.02
1.084		0.01
1.055		0.04
1.012		0.01
0.931		0.02
0.850		0.01
0.828		0.02

336. $Co_3(PO_4)_2.8H_2O$

d		I/I1
8.0		0.20
6.7	(50)	1.00
4.87		0.40
4.51		0.14
4.04		0.12
3.81		0.30
3.60		0.04
3.19		0.40
2.95	(30)	0.60
2.69	(30)	0.60
2.60		0.08
2.50		0.20
2.40		0.20
2.30		0.20
2.20		0.20
2.17		0.20
2.05		0.16
2.00		0.04
1.92		0.20
1.88		0.14
1.80		0.08
1.76		0.16
1.66		0.30
1.57		0.14
1.53		0.02
1.51		0.04
1.472		0.10
1.409		0.06
1.370		0.04
1.330		0.14
1.255		0.04
1.230		0.04
1.205		0.02
1.170		0.04

337. Cobalt Stannate (ous)

d		I/I1
3.40	(8)	0.80
2.67	(6)	0.60
2.45	(10)	1.00
2.02		0.30
1.77		0.60
1.56		0.30
1.430		0.60
1.230		0.20
1.080		0.10
1.055		0.10
0.850		0.10

338. $CoSO_4$

d		I/I1
4.82	(40)	0.64
3.80		0.08
3.40	(62.5)	1.00
3.30		0.16
3.08	(30)	0.48
2.57		0.16
2.51		0.48
2.40		0.02
2.35		0.20
2.20		0.24
2.10		0.16
2.05		0.10
1.97		0.20
1.90		0.11
1.81		0.13
1.74		0.03
1.70		0.10
1.67		0.24
1.62		0.10
1.59		0.13
1.56		0.06
1.53		0.05
1.498		0.11
1.448		0.08
1.412		0.08
1.360		0.03
1.329		0.06
1.282		0.08
1.262		0.10
1.194		0.05
1.168		0.05

339. $CoSO_4(NH_4)_2SO_4.6H_2O$

d		I/I1
6.3		0.13
6.0		0.13
5.4		0.38
4.20	(40)	1.00
3.79	(25)	0.63
3.60		0.13
3.41		0.25
3.14		0.03
3.04	(15)	0.38
2.80		0.31
2.55		0.03
2.45		0.20
2.23		0.15
2.15		0.18
2.08		0.10
1.99		0.05
1.91		0.15
1.86		0.03
1.80		0.10
1.75		0.03
1.72		0.05
1.68		0.03
1.62		0.03
1.55		0.05
1.480		0.05
1.430		0.03
1.380		0.03
1.255		0.03
1.220		0.03
1.188		0.03
1.158		0.03

340. Cb*

d		I/I1
2.33	(125)	1.00
1.65	(25)	0.20
1.34	(40)	0.32
1.16		0.06
1.041		0.10
0.950		0.01
0.879		0.06
0.775		0.02
0.736		0.01

341. Cu*

d		I/I1
2.08	(75)	1.00
1.81	(40)	0.53
1.277	(25)	0.33
1.089		0.33
1.043		0.09
0.905		0.03

342. $(CuOAs_2O_2)_2.Cu(C_2H_3O_2)_2$

d		I/I1
10.0	(25)	1.00
4.55		0.12
3.99		0.12
3.48		0.08
3.30		0.04
3.06	(5)	0.20
2.68	(6)	0.24
2.40		0.04
1.69		0.08
1.62		0.04
1.55		0.08
1.450		0.04

343. $CuAl_2O_4$*

d		I/I1
2.85	(5)	0.33
2.43	(15)	1.00
2.01		0.27
1.85		0.07
1.64		0.07
1.55		0.20
1.423	(10)	0.67
1.230		0.07

344. $Cu(C_6H_5COO)_2.2H_2O$

d		I/I1
6.9	(7)	0.56
5.9		0.24
4.51	(12.5)	1.00
4.01		0.40
3.50	(7)	0.56
3.07		0.08
2.84		0.24
2.62		0.08
2.45		0.08
2.32		0.08
2.15		0.16
1.92		0.08
1.86		0.08

345. Copper-Beryllium Alloy (12% Be)

d		I/I1
2.73	(6)	0.24
2.06	(4)	0.16
1.93	(25)	1.00
1.56		0.16
1.350		0.08
1.205		0.08
1.105		0.16
0.958		0.04

346. Copper Borate (ic)

d		I/I1
6.4		0.44
5.3	(7)	0.78
3.88	(9)	1.00
3.17		0.33
2.91		0.22
2.66		0.33
2.51	(9)	1.00
2.37		0.11
2.17		0.11
1.95		0.11
1.73		0.33
1.58		0.11
1.55		0.11
1.53		0.11
1.425		0.11B

347. CuBr*

d		I/I1
3.29	(30)	1.00
2.01	(20)	0.67
1.71	(15)	0.50
1.420		0.07
1.305		0.13
1.160		0.13
1.094		0.07
1.008		0.03
0.962		0.03

348. $CuBr_2$

d		I/I1
6.2		0.35
3.62		0.30
3.08	(20)	1.00
2.49	(20)	1.00
2.02		0.05
1.96	(10)	0.50
1.92		0.45
1.79		0.30
1.74		0.25
1.67		0.05
1.62		0.05
1.57		0.20
1.52		0.40
1.415		0.05
1.322		0.15
1.297		0.10
1.246		0.15
1.152		0.15
1.126		0.05
1.101		0.10
1.072		0.05

349. $2CuCO_3.Cu(OH)_2$

d		I/I1
5.1	(12.5)	0.71
3.68		0.23
3.51	(17.5)	1.00
3.02		0.23
2.51	(9)	0.51
2.27		0.40
2.09		0.06
1.94		0.17
1.82		0.11
1.79		0.06
1.59		0.17
1.52		0.17
1.470		0.06
1.430		0.06
1.380		0.06
1.345		0.06
1.295		0.06

350. $CuCO_3.Cu(OH)_2$

d		I/I1
6.0		0.35
5.1	(8)	0.40
3.68	(10)	0.50
2.86	(20)	1.00
2.49		0.25
2.31		0.05
2.16		0.05
2.04		0.05
1.94		0.05
1.78		0.05
1.67		0.10
1.59		0.05
1.51		0.05
1.475		0.05
1.420		0.05

351. CuCl*

d		I/I1
3.12	(50)	1.00
2.70		0.08
1.91	(30)	0.60
1.63	(15)	0.30
1.353		0.06
1.240		0.08
1.104		0.06
1.043		0.04

352. $CuCl_2$

d		I/I1
5.7	(30)	1.00
5.4		0.03
4.01		0.07
3.42		0.42
2.90	(20)	0.66
2.62		0.10
2.36	(20)	0.66
2.20		0.03
2.00		0.03
1.86		0.33
1.80		0.20
1.70		0.20
1.64		0.17
1.58		0.07
1.490		0.07
1.435		0.20
1.260		0.07
1.220		0.07
1.182		0.03
1.082		0.03
1.046		0.03

353. $CuCl_2.2H_2O$*

d		I/I1
5.4	(50)	1.00
4.03	(20)	0.40
3.73		0.08
3.33		0.08
3.08		0.25
2.72		0.03
2.63	(15)	0.30
2.52		0.08
2.36		0.06
2.20		0.16
2.10		0.06
2.01		0.20
1.88		0.02
1.85		0.16
1.81		0.02
1.77		0.08
1.73		0.02
1.68		0.08
1.64		0.02
1.61		0.20
1.58		0.02
1.55		0.02
1.51		0.02
1.460		0.06
1.402		0.02
1.370		0.14

354. $CuCl_2.2NH_4Cl.2H_2O$

d		I/I1
5.5	(30)	1.00
4.00		0.23
3.39		0.07
3.20		0.20
3.12		0.20
2.75	(15)	0.50
2.68	(20)	0.66
2.58		0.07
2.51		0.03
2.40		0.03
2.23		0.13
2.09		0.07
2.04		0.07
1.98		0.07
1.90		0.13
1.79		0.07
1.72		0.07
1.67		0.07
1.60		0.13
1.490		0.03
1.375		0.03
1.190		0.03

355. $CuCl_2.2KCl.2H_2O$

d		I/I1
5.4	(30)	0.75
3.95		0.15
3.73		0.08
3.31		0.10
3.17		0.44
3.07		0.25
2.71	(30)	0.75
2.64	(40)	1.00
2.56		0.03
2.48		0.05
2.37		0.03
2.19		0.05
2.06		0.08
2.02		0.20
1.98		0.15
1.86		0.25
1.80		0.05
1.76		0.05
1.70		0.03
1.64		0.03
1.58		0.25
1.54		0.05
1.490		0.03
1.460		0.03
1.430		0.03
1.360		0.08

356. $CuCrO_4.2CuO.2H_2O$

d		I/I1
6.1		0.05
5.4		0.20
4.90	(20)	1.00
3.62		0.45
3.43		0.20
2.70		0.45
2.57	(20)	1.00
2.14	(12.5)	0.62
2.05		0.05
1.94		0.10
1.83		0.20
1.63		0.15
1.56		0.10
1.480		0.20
1.440		0.15
1.380		0.05
1.319		0.10
1.281		0.10
1.108		0.05
1.062		0.05

357. Copper Ammonium Chromate (ic)

d		I/I1
5.1	(20)	0.50
4.20	(10)	0.25
3.57	(40)	1.00
3.35		0.15
2.93		0.08
2.82		0.08
2.62		0.03
2.38		0.08
2.30		0.10
2.25		0.10
2.16		0.05
2.08		0.05
1.87		0.03
1.81		0.08
1.76		0.03
1.65		0.03
1.59		0.03
1.54		0.03
1.423		0.05
1.240		0.03

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

358. $CuCr_2O_7.2H_2O$

d		I/I1
6.7		0.33
5.5		0.17
4.78		0.33
4.50		0.33
4.21		0.33
3.95		0.67
3.67		0.83
3.55	(6)	1.00
3.40	(6)	1.00
3.15	(6)	1.00
2.99		0.67
2.71		0.33
2.61		0.83
2.48		1.00
2.24		0.17
2.16		0.17
2.06		0.17
2.01		0.17
1.86		0.17
1.83		0.17
1.74		0.17
1.52		0.17
1.49		0.17

359. $2Cu_3C_6H_3O_7.5H_2O$

d		I/I1
7.4	(12.5)	0.25
5.6	(50)	1.00
4.55	(12.5)	0.25
3.85		0.25
3.56		0.12
3.13		0.08
2.92		0.08
2.66		0.08
2.49		0.04
2.41		0.02
2.19		0.08
1.99		0.08
1.93		0.08
1.88		0.06
1.82		0.04
1.70		0.04
1.66		0.04
1.56		0.02
1.325		0.02

360. CuCN

d		I/I1
3.78	(20)	1.00
3.18	(17.5)	0.88
3.02		0.15
2.89		0.05
2.62		0.15
2.35	(8)	0.40
2.25		0.05
2.15		0.05

361. $CuK_3(CN)_4$

d		I/I1
7.4	(15)	0.24
4.22		0.20
3.45		0.09
3.13	(62.5)	1.00
2.75		0.16
2.51		0.09
2.22	(20)	0.32
2.00		0.06
1.81		0.13
1.69		0.02
1.57		0.05
1.405		0.06
1.375		0.02
1.310		0.02
1.283		0.05
1.115		0.02
1.050		0.02

362. $Cu_2Fe(CN)_6.7H_2O$

d		I/I1
10.1		0.03
7.1		0.03
5.8		0.05
5.0	(40)	1.00
3.55	(30)	0.75
3.02		0.03
2.50	(20)	0.50
2.23		0.25
2.04		0.20
1.76		0.15
1.67		0.08
1.58		0.10
1.50		0.03
1.450		0.03
1.385		0.05
1.335		0.05
1.212		0.03
1.180		0.03

363. $K_2CuFe(CN)_6$

d		I/I1
5.1		0.38
3.63	(40)	1.00
3.06		0.20
2.86		0.08
2.57	(30)	0.75
2.36		0.15
2.29		0.31
2.13		0.25
2.06	(25)	0.63
1.82		0.15
1.63		0.25
1.58		0.03
1.52		0.03
1.460		0.05
1.390		0.05
1.360		0.05
1.340		0.03
1.275		0.03
1.215		0.05
1.150		0.05

364. $CuF_2.2H_2O$

d		I/I1
4.73	(50)	1.00
4.31		0.08
3.50		0.12
2.66		0.10
2.57	(30)	0.60
2.44		0.20
2.34		0.06
2.14		0.12
1.98	(20)	0.40
1.89		0.20
1.69		0.04
1.63		0.06
1.59		0.16
1.54		0.08
1.490		0.06
1.443		0.06
1.330		0.02
1.310		0.04
1.238		0.02
1.217		0.04
1.165		0.02
1.140		0.02
1.113		0.02

365. $(NH_4)_2CuF_4.2H_2O$

d		I/I1
6.6		0.04
5.5		0.04
4.70	(25)	1.00
3.02		0.04
2.57	(9)	0.36
2.43		0.08
2.14		0.08
1.97	(4)	0.16
1.88		0.08
1.60		0.04
1.55		0.04

366. $Cu(CHO_2)_2$

d		I/I1
4.90	(17.5)	1.00
4.60	(12.5)	0.71
4.29		0.46
3.60		0.11
3.39		0.11
2.84		0.17
2.61	(12.5)	0.71
2.44		0.11
2.20		0.11
2.12		0.06
2.02		0.06
1.95		0.11
1.81		0.11
1.75		0.11
1.64		0.06
1.53		0.06

367. CuI*

d		I/I1
3.49	(50)	1.00
3.01		0.06
2.14	(40)	0.80
1.82	(30)	0.60
1.51		0.12
1.386		0.20
1.350		0.04
1.233		0.25
1.162		0.12
1.070		0.02
1.020		0.08
0.956		0.06
0.921		0.02
0.847		0.02
0.809		0.02
0.787		0.02

368. $CuMg_2$*

d		I/I1
4.60	(20)	0.50
4.43		0.50
3.67		0.25
2.53		0.15
2.41		0.38
2.28	(40)	1.00
2.13		0.08
2.03	(40)	1.00
1.86		0.10
1.72		0.05
1.66		0.05
1.61		0.08
1.56		0.05
1.475		0.05
1.439		0.15
1.408		0.10
1.313		0.20
1.268		0.10
1.137		0.15

369. Cu_2Mg*

d		I/I1
4.07	(12.5)	0.50
2.12	(25)	1.00
2.03	(17.5)	0.70
1.76		0.28
1.61		0.20
1.354		0.50
1.245		0.50
1.190		0.20
1.074		0.12
1.061		0.32
1.016		0.04
0.986		0.04
0.916		0.24

370. $Cu(NO_2)_2.3H_2O$

d		I/I1
5.8	(17.5)	1.00
5.4		0.06
4.70		0.34
4.04	(12.5)	0.72
3.65		0.46
3.38		0.34
3.00		0.46
2.63	(12.5)	0.72
2.46		0.23
2.25		0.06
2.09		0.17
1.81		0.06
1.69		0.06
1.57		0.06

371. Cu_2O*

d		I/I1
3.00		0.03
2.45	(40)	1.00
2.12	(12.5)	0.31
1.51	(17.5)	0.44
1.283		0.31
1.228		0.05
1.065		0.03
0.977		0.05
0.953		0.03
0.869		0.03
0.819		0.03

372. CuO*

d		I/I1
2.51	(62.5)	1.00
2.31	(62.5)	1.00
1.85	(12.5)	0.20
1.70		0.08
1.57		0.08
1.50		0.15
1.408		0.20
1.370		0.20
1.298		0.05
1.258		0.10
1.159		0.05B
1.086		0.03
1.007		0.03
0.978		0.03
0.885		0.03

373. $CuCo_2O_4$*

d		I/I1
4.65		0.15
2.85		0.25
2.43	(40)	1.00
2.31		0.20
2.11		0.05
1.64		0.10
1.55	(12.5)	0.31
1.421	(15)	0.38
1.361		0.03
1.227		0.08
1.160		0.03
1.076		0.03
1.047		0.08

374. $(C_6H_4OHSO_3)_2Cu.6H_2O$

d		I/I1
11.7	(17.5)	0.44
5.8		0.15
5.5		0.20
5.2		0.10
4.63	(40)	1.00
3.95	(9)	0.23
3.52		0.15
3.27		0.03
3.00		0.15
2.91		0.08
2.81		0.03
2.70		0.10
2.58		0.10
2.44		0.05
2.28		0.08
2.21		0.03
1.95		0.08
1.90		0.08
1.82		0.03
1.75		0.03
1.72		0.03
1.65		0.03
1.61		0.03
1.56		0.03
1.51		0.03

375. Cupric Phosphate (Fused)

d		I/I1
4.15		0.32
3.76		0.32
3.10		0.32
2.96	(25)	1.00
2.80	(17.5)	0.70
2.69		0.08
2.58	(15)	0.60
2.42		0.40
2.18		0.16
2.06		0.32
1.98		0.24
1.82		0.20
1.74		0.04
1.69		0.08
1.65		0.16
1.62		0.04
1.59		0.08
1.460		0.32
1.435		0.32
1.400		0.16
1.305		0.08
1.250		0.04
1.180		0.04
1.150		0.04
1.120		0.04

376. $Cu_3(PO_4)_2.3H_2O$

d		I/I1
9.9	(20)	1.00
6.9	(5)	0.25
4.80		0.08
4.32		0.15
3.90		0.05
3.34		0.10
3.02	(17.5)	0.87
2.65		0.20
2.54		0.05
2.49		0.05
2.41		0.05
2.34		0.05
2.15		0.08
1.93		0.08
1.71		0.15
1.66		0.05
1.61		0.05
1.50		0.10
1.430		0.05
1.365		0.08
1.300		0.05

377. $CuOH.CuPO_4$*

d		I/I1
5.8		0.40
4.81	(25)	1.00
3.71		0.28
2.91	(12.5)	0.50
2.63	(25)	1.00
2.55		0.12
2.41		0.16
2.30		0.16
2.07		0.06
1.91		0.12
1.71		0.20
1.66		0.08
1.61		0.12
1.58		0.16
1.54		0.12
1.474		0.06
1.455		0.06
1.430		0.04
1.395		0.04
1.370		0.04
1.340		0.04
1.313		0.04

378. $Cu(C_6H_4OHCOO)_2.4H_2O$

d		I/I1
14.9	(10)	0.57
13.0		0.17
9.9		0.46
9.0		0.46
7.6	(15)	0.86
6.5		0.11
5.8		0.11
4.80	(17.5)	1.00
4.48		0.29
3.51		0.40
3.25		0.23
3.12		0.23
2.96		0.23
2.79		0.11
2.70		0.11
2.58		0.11
2.43		0.11
2.34		0.11
2.27		0.11
2.13		0.11
2.07		0.11
1.97		0.11

379. $CuSO_4$

d		I/I1
4.20	(40)	0.53
3.92		0.03
3.55	(40)	0.53
2.62	(75)	1.00
2.41		0.40
2.31		0.09
2.08		0.05
2.01		0.03
1.96		0.12
1.77		0.33
1.67		0.09
1.58		0.13
1.55		0.08
1.461		0.01
1.430		0.27
1.400		0.03
1.375		0.11
1.305		0.03
1.290		0.01
1.243		0.01
1.210		0.03
1.182		0.01
1.150		0.03
1.096		0.04
1.074		0.04

380. $CuSO_4.H_2O$

d		I/I1
5.1		0.15
4.81	(25)	0.63
4.43		0.38
4.00		0.13
3.64		0.31
3.40	(40)	1.00
3.15		0.50
3 00		0.15
2.81		0.25
2.58		0.08
2.47	(25)	0.63
2.35		0.13
2.27		0.38
2.07		0.10
2.01		0.20
1.92		0.10
1.81		0.18
1.67		0.25
1.62		0.20
1.59		0.38
1.56		0.10
1.480		0.05
1.450		0.15
1.405		0.03
1.385		0.03
1.352		0.03
1.251		0.18
1.207		0.05
1.178		0.08

381. $CuSO_4.5H_2O$

d		I/I1
5.7		0.33
5.6		0.42
5.2		0.03
4.70	(30)	1.00
4.00	(17.5)	0.58
3.70	(15)	0.50
3.50		0.03
3.29		0.33
3.03		0.20
2.83		0.27
2.74		0.27
2.66		0.13
2.56		0.10
2.42		0.33
2.33		0.07
2.19		0.07
2.14		0.07
2.08		0.03
2.02		0.10
1.98		0.03
1.91		0.10
1.83		0.10
1.77		0.03
1.74		0.03
1.62		0.13
1.57		0.03
1.52		0.03
1.487		0.03

382. $CuSO_4(NH_4)_2SO_4.6H_2O$

d		I/I1
6.1		0.27
5.4	(9)	0.30
4.19	(30)	1.00
3.74	(17.5)	0.58
3.38		0.13
3.04		0.30
2.82		0.17
2.70		0.03
2.53		0.10
2.42		0.23
2.21		0.03
2.16		0.03
2.08		0.03
1.96		0.03
1.90		0.07
1.82		0.03
1.72		0.03
1.460		0.03
1.425		0.03

383. $CuSO_4.K_2SO_4.6H_2O$

d		I/I1
6.0		0.20
5.3		0.16
4.21	(17.5)	0.70
3.68	(25)	1.00
3.30		0.12
2.99		0.40
2.83		0.36
2.65		0.08
2.50		0.08
2.37	(12.5)	0.50
2.19		0.40
2.12		0.08
2.06		0.24
1.99		0.12
1.92		0.08
1.87		0.08
1.79		0.08
1.69		0.04
1.62		0.04
1.57		0.04
1.480		0.08
1.405		0.04
1.290		0.04
1.250		0.04

384. CuFeS2*

d		I/I1
3.03	(30)	1.00
2.62		0.07
1.86	(25)	0.83
1.59	(6)	0.20
1.323		0.03
1.206		0.07
1.077		0.03

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

385. $Cu_2SO_3.H_2O$

d	I/I1
4.65	(12.5) 0.50
4.15	(12.5) 0.50
3.03	0.50
2.77	0.12
2.49	(25) 1.00
2.35	0.04
2.25	0.16
2.19	0.08
2.03	0.04
1.89	0.16
1.78	0.12
1.66	0.04
1.62	0.04
1.58	0.16
1.55	0.08
1.52	0.16
1.483	0.12
1.205	0.08

386. $CuC_4H_4O_6.3H_2O$

d	I/I1
7.6	(15) 0.60
5.9	(25) 1.00
4.60	0.50
4.33	0.50
4.10	0.50
3.80	0.40
3.54	(25) 1.00
3.30	0.04
3.06	0.16
2.90	0.32
2.54	0.32
2.43	0.40
2.35	0.04
2.22	0.04
2.15	0.16
2.03	0.08
1.91	0.40
1.85	0.12
1.81	0.16
1.65	0.24
1.61	0.08
1.50	0.16
1.450	0.12
1.370	0.12
1.300	0.08
1.218	0.08

387. CuCNS

d	I/I1
5.5	(40) 1.00
3.25	(40) 1.00
3.10	0.03
2.72	0.05
2.59	0.25
1.92	(20) 0.50
1.82	0.20
1.75	0.03
1.66	0.05
1.57	0.08
1.470	0.05
1.360	0.05
1.260	0.03
1.110	0.03

388. $ErCl_3.6H_2O$

d	I/I1
6.8	0.20
6.6	0.20
5.9	0.40
5.4	0.40
5.0	0.20
4.86	0.20
4.50	0.20
4.38	0.20
3.94	(4) 0.80
3.55	(5) 1.00
3.39	(5) 1.00
3.08	0.20
2.84	0.40
2.52	0.20
2.39	0.40
2.32	0.20
2.27	0.20
2.11	0.20
2.03	0.20
1.91	0.20
1.76	0.20
1.66	0.20
1.51	0.20
1.446	0.20
1.408	0.20
1.370	0.20

389. Er_2O_3*

d	I/I1
4.31	0.07
3.06	(30) 1.00
2.64	0.27
2.49	0.03
2.25	0.03
2.07	0.13
1.87	(15) 0.50
1.81	0.07
1.71	0.07
1.59	(12.5) 0.42
1.52	0.07
1.323	0.03
1.220	0.07
1.185	0.03
1.145	0.03
1.087	0.07

390. GeO_2*

d	I/I1
4.31	0.20
3.41	(50) 1.00
2.48	0.14
2.35	(12.5) 0.25
2.28	0.16
2.15	0.20
2.00	0.02
1.87	(12.5) 0.25
1.71	0.12
1.62	0.02
1.56	0.25
1.495	0.08
1.445	0.04
1.410	0.25
1.386	0.08
1.339	0.10
1.301	0.02
1.277	0.10
1.248	0.02
1.228	0.06

391. Au*

d	I/I1
2.35	(75) 1.00
2.03	(40) 0.53
1.439	0.33
1.227	(30) 0.40
1.173	0.09
1.019	0.03
0.935	0.09
0.910	0.07
0.832	0.04
0.784	0.04

392. AuCN*

d	I/I1
5.1	(30) 0.60
2.94	(50) 1.00
2.54	(50) 1.00
1.92	0.40
1.69	0.16
1.61	0.12
1.467	0.20
1.410	0.16
1.271	0.04
1.200	0.04
1.165	0.04
1.110	0.04
1.086	0.04
1.018	0.04
0.961	0.04

393. $AuK(CN)_2$

d	I/I1
9.0	(10) 1.00
6.1	0.10
5.7	0.10
4.52	(2) 0.20
4.00	0.10
3.67	0.10
3.36	0.10
3.10	(10) 1.00
2.84	0.20
2.40	0.10
2.27	0.10
2.03	0.10
1.81	0.10
1.68	0.10
1.56	0.10

394. In*

d	I/I1
(62.5)	1.00
	0.25
(25)	0.40
(20)	0.30
	0.15
	0.20
	0.30
	0.15
	0.02
	0.10
	0.02
	0.02
	0.02
	0.06
	0.02
	0.02

395. $InCl_3$

d	I/I1
(62.5)	1.00
	0.13
	0.20
	0.24
	0.24
	0.06
	0.32
	0.10
(25)	0.40
	0.32
	0.10
(30)	0.48
	0.10
	0.24
	0.13
	0.03
	0.16
	0.13
	0.10
	0.24
	0.08
	0.11
	0.03
	0.03
	0.06
	0.06
	0.06

396. In_2O_3*

d	I/I1
4.12	0.14
2.91	(175) 1.00
2.70	0.03
2.52	0.43
2.38	0.10
2.26	0.02
2.15	0.10
2.06	0.02
1.98	0.17
1.84	0.04
1.78	(125) 0.71
1.73	0.03
1.68	0.02
1.63	0.10
1.60	0.03
1.55	0.06
1.52	(100) 0.57
1.490	0.07
1.458	0.07
1.429	0.03
1.401	0.02
1.375	0.05
1.350	0.03
1.281	0.04
1.262	0.05
1.241	0.05
1.225	0.02
1.205	0.03
1.190	0.01
1.175	0.03
1.159	0.14
1.130	0.09

397. I_2*

d	I/I1
3.69	(25) 1.00
3.09	(25) 1.00
2.52	0.08
2.44	0.18
2.33	0.15
2.11	0.15
2.02	0.20
1.97	(7) 0.30
1.81	0.10
1.76	0.10
1.71	0.20
1.51	0.10
1.460	0.08
1.400	0.05

398. I_2O_5

d	I/I1
4.03	0.15
3.79	(20) 0.50
3.40	(30) 0.75
3.28	(40) 1.00
3.18	0.15
2.92	0.05
2.83	0.03
2.74	0.05
2.53	0.13
2.44	0.13
2.35	0.05
2.28	0.05
2.18	0.13
2.08	0.10B
2.02	0.05
1.96	0.05
1.90	0.05
1.83	0.10
1.79	0.08
1.74	0.05
1.71	0.13
1.66	0.05
1.62	0.03
1.59	0.10
1.56	0.13

399. Ir*

d	I/I1
2.20	(25) 1.00
1.91	(12.5) 0.50
1.352	0.28
1.153	(9) 0.36
1.104	0.08
0.878	0.08
0.857	0.08
0.782	0.04
0.737	0.04
0.647	0.04

400. $IrCl_3$

d	I/I1
5.7	(25) 1.00
5.1	0.24
2.95	0.80
2.81	0.24
2.44	(25) 1.00
2.24	0.28
1.95	0.16
1.88	0.32
1.73	(25) 1.00
1.65	0.50
1.490	0.24
1.470	0.20
1.437	0.08
1.410	0.32
1.370	0.16
1.272	0.20
1.222	0.08
1.190	0.04
1.150	0.04
1.128	0.16
1.092	0.28
1.074	0.04
1.027	0.04
1.000	0.16

401. Fe*

d	I/I1
2.01	(40) 1.00
1.428	(6) 0.15
1.166	(15) 0.38
1.010	0.10
0.904	0.08
0.825	0.03
0.764	0.10
0.676	0.03

402. FeAl

d	I/I1
2.89	(15) 0.12
2.04	(125) 1.00
1.67	0.04
1.445	0.08
1.295	0.03
1.180	(25) 0.20
1.025	0.02
0.915	0.02
0.834	0.01
0.776	0.02

403. $FeAl_3$*

d	I/I1
4.07	0.17
3.68	0.11
3.54	0.11
3.34	0.07
3.25	0.07
2.26	0.08
2.15	0.08
2.08	(62.5) 0.83
2.02	(75) 1.00
1.93	0.09
1.80	0.03
1.445	(15) 0.20
1.395	0.05
1.355	0.01
1.287	0.05
1.263	0.03
1.250	0.05
1.225	0.07
1.180	0.04
1.169	0.05
1.127	0.03
1.089	0.04
1.061	0.04

404. Fe_2Al_3

d	I/I1
4.90	0.11
3.86	0.24
3.20	(25) 0.40
2.39	0.10
2.11	(62.5) 1.00
2.05	(62.5) 1.00
1.94	0.10
1.90	0.08
1.84	0.03
1.76	0.08
1.70	0.02
1.63	0.02
1.59	0.03
1.55	0.02
1.52	0.10
1.475	0.16
1.418	0.02
1.390	0.10
1.350	0.02
1.300	0.02
1.272	0.10
1.240	0.08
1.212	0.16
1.180	0.02
1.145	0.02
1.102	0.08
1.090	0.02
1.068	0.10
1.031	0.03
1.018	0.02

405. $Fe_2(AsO_4)_2.6H_2O$

d	I/I1
9.0	0.20
6.7	(5) 1.00
3.99	(2) 0.40
3.70	(2) 0.40
3.36	0.20
3.18	0.40
2.95	0.40
2.82	0.40
2.72	0.20
2.63	0.20
2.55	0.20
2.32	0.20
2.08	0.20
1.67	0.20
1.61	0.20
1.51	0.20
1.470	0.20

406. $Fe[(CH_2)_2AsO_2]_3$

d	I/I1
10.0	(15) 1.00
7.7	(8) 0.53
5.3	0.53
5.1	(10) 0.67
4.37	0.07
3.73	0.13
3.34	0.27
3.23	0.07
3.06	0.27
2.98	0.07
2.84	0.07
2.66	0.33
2.52	0.07
2.35	0.20
2.27	0.07
2.18	0.13
2.05	0.07
1.97	0.07
1.90	0.07
1.86	0.07
1.81	0.07
1.61	0.07
1.56	0.07
1.450	

407. $FeCl_2$

d	I/I1
5.9	(20) 0.32
5.7	0.32
5.1	0.05
4.79	0.06
4.50	0.03
3.49	0.03
3.09	0.03
3.03	0.03
2.90	0.03
2.68	(62.5) 1.00
2.52	0.02
2.40	0.02
2.23	0.02
2.08	(25) 0.40
2.02	0.02
1.96	0.03
1.75	0.32
1.67	0.06
1.63	0.16
1.460	0.06
1.340	0.05
1.300	0.02
1.190	0.03
1.116	0.05
1.080	0.02
1.063	0.03
1.009	0.02
0.985	0.03

408. $FeCl_2.6H_2O$

d	I/I1
6.0	(40) 1.00
4.40	0.38
4.00	0.20
3.50	0.38
3.14	(30) 0.75
3.00	0.03
2.76	(20) 0.50
2.57	0.31
2.42	0.38
2.19	0.25
2.04	0.03
1.99	0.03
1.94	0.38
1.90	0.20
1.84	0.03
1.79	0.05
1.75	0.10
1.69	0.08
1.63	0.03
1.60	0.03
1.56	0.03
1.53	0.03
1.50	0.03
1.450	0.03
1.417	0.03
1.390	0.03
1.359	0.03
1.338	0.03
1.301	0.03
1.273	0.03
1.238	0.03

409. $FeCl_3.2H_2O$

d	I/I1
5.5	0.13
4.28	(25) 0.83
3.63	0.07
3.17	0.07
2.88	0.50
2.75	(30) 1.00
2.65	0.23
2.39	(20) 0.67
2.32	0.33
2.13	0.33
2.08	0.67
1.84	0.07
1.81	0.20
1.75	0.20
1.72	0.17
1.69	0.20
1.66	0.17
1.59	0.27
1.52	0.10
1.490	0.07
1.430	0.07
1.377	0.23
1.338	0.13

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

410. $FeCl_2.4H_2O$

d		I/I1
5.9		0.10
5.4	(40)	1.00
4.40		0.50
3.98	(40)	1.00
3.45		0.31
3.11		0.05
3.00	(40)	1.00
2.87		0.03
2.77		0.25
2.63		0.18
2.48		0.18
2.36		0.03
2.26		0.08
2.19		0.13
2.12		0.31
2.04		0.10
1.98		0.05
1.92		0.03
1.87		0.05
1.83		0.13
1.79		0.08
1.74		0.20
1.68		0.05
1.64		0.08
1.52		0.25
1.470		0.10
1.408		0.05
1.381		0.08
1.280		0.05
1.242		0.03

411. Iron Ammonium Chloride

d		I/I1
5.7	(17.5)	1.00
4.95	(12.5)	0.71
3.01		0.06
2.82	(17.5)	1.00
2.48		0.57
2.22		0.17
2.16		0.06
2.11		0.06
2.02		0.06
1.90		0.11
1.85		0.23
1.74		0.23
1.62		0.11
1.480		0.11
1.425		0.06
1.370		0.06

412. $Fe_4[Fe(CN)_6]_3$

d		I/I1
5.1	(62.5)	1.00
3.60	(20)	0.32
2.55	(30)	0.48
2.28		0.32
2.07		0.03
1.80		0.14
1.70		0.13
1.61		0.14
1.53		0.03
1.470		0.02
1.410		0.10
1.360		0.08
1.271		0.02
1.235		0.03
1.201		0.02
1.170		0.02
1.138		0.02
1.110		0.02
1.087		0.02
1.060		0.02
1.040		0.02
1.021		0.02
1.000		0.02
0.981		0.02
0.947		0.02
0.930		0.02

413. $FeF_3.4^1/_2H_2O$

d		I/I1
5.5	(50)	1.00
3.91	(25)	0.50
3.48	(20)	0.40
3.18		0.20
2.77		0.20
2.59		0.04
2.47		0.25
2.08		0.12
1.95		0.08
1.88		0.30
1.84		0.02
1.75		0.25
1.70		0.20
1.66		0.02
1.59		0.02
1.55		0.02
1.53		0.04
1.445		0.12
1.354		0.12
1.265		0.02
1.235		0.02
1.213		0.02
1.160		0.02

414. $Fe(HCO_2)_2.H_2O$

d		I/I1
13.0		0.13
11.0		0.13
9.4		0.13
8.4	(5)	0.63
7.6	(3)	0.38
6.6		0.13
6.2	(8)	1.00
5.7		0.25
5.2		0.13
4.90		0.13
4.40		0.13
4.06		0.13
3.88		0.13
3.78		0.13
3.60		0.25
3.37		0.25
3.17		0.25
3.00		0.25
2.88		0.13
2.75		0.13
2.60		0.13
2.54		0.13
2.41		0.13
2.31		0.13
2.25		0.13
2.17		0.13
2.08		0.13
1.77		0.13
1.68		0.13
1.54		0.13

415. $Fe(C_6H_5O_2)_2.3H_2O$

d		I/I1
9.5	(40)	1.00
7.0		0.05
6.3		0.05
5.5		0.10
5.2	(15)	0.38
4.70		0.05
4.50	(6)	0.15
4.30		0.03
4.10		0.03
3.70		0.05
3.52		0.05
3.32		0.03
3.02		0.05
2.89		0.03
2.75		0.05
2.69		0.05
2.60		0.03
2.48		0.03
2.41		0.03
2.36		0.03
2.28		0.03
2.22		0.03
2.08		0.03
2.02		0.03
1.97		0.03
1.89		0.03
1.85		0.03
1.79		0.03
1.74		0.03

416. $Fe(NO_3)_3.9H_2O$

d		I/I1
6.6	(25)	1.00
5.6		0.16
4.91		0.24
4.52		0.80
4.10	(25)	1.00
3.81		0.40
3.64		0.50
3.45		0.16
3.29		0.80
3.05		0.60
2.92		0.24
2.80		0.08
2.62	(25)	1.00
2.55		0.32
2.40		0.50
2.27		0.08
2.21		0.28
2.10		0.20
2.05		0.20
1.96		0.04
1.90		0.32
1.84		0.08
1.79		0.20
1.74		0.08
1.70		0.28
1.63		0.08
1.59		0.08
1.53		0.08
1.468		0.08
1.416		0.08
1.372		0.08
1.325		0.12
1.276		0.04
1.201		0.12

417. Fe_3N

d		I/I1
2.38		0.20
2.19	(10)	0.25
2.09	(40)	1.00
1.61	(10)	0.25
1.370		0.25
1.240		0.25
1.160		0.20
1.140		0.10
1.095		0.03
1.040		0.05
0.918		0.05
0.875		0.08
0.855		0.08
0.822		0.03
0.762		0.03

418. Fe_4N*

d		I/I1
2.18	(10)	1.00
1.88	(4)	0.40
1.332		0.20
1.136	(3)	0.30

419. $FeC_2O_4.2H_2O$

d		I/I1
4.75	(17.5)	1.00
3.83		0.23
3.58		0.23
2.98	(6)	0.34
2.61	(6)	0.34
2.23		0.06
2.09		0.06
2.02		0.06
1.93		0.06
1.87		0.06
1.81		0.11

420. $(NH_4)_2Fe(C_2O_4)_2$

d		I/I1
7.0	(50)	1.00
5.0		0.12
4.50		0.20
4.20		0.02
3.62	(12.5)	0.25
3.52		0.16
3.35		0.04
3.19	(12.5)	0.25
2.90		0.08
2.73		0.04
2.63		0.04
2.56		0.04
2.47		0.04
2.37		0.04
2.22		0.16
2.12		0.02
2.04		0.02
1.98		0.02
1.92		0.02
1.84		0.02
1.75		0.02
1.67		0.02

421. $K_2Fe(C_2O_4)_2.3H_2O$

d		I/I1
10.2		0.53
6.9	(15)	1.00
6.6		0.07
4.96		0.53
4.68		0.07
4.43		0.27
4.09		0.27
3.61	(10)	0.67
3.48		0.07
3.34		0.27
3.16		0.47
3.03		0.40
2.85		0.13
2.67		0.60
2.58		0.33
2.51		0.07
2.46		0.07
2.36		0.07
2.31		0.13
2.18	(10)	0.67
2.12		0.13
2.03		0.07
1.96		0.07
1.90		0.07
1.85		0.07
1.81		0.07
1.75		0.13
1.71		0.07
1.67		0.13
1.52		0.07
1.318		0.07

422. $2Na_2Fe(C_2O_4)_2.9H_2O$

d		I/I1
10.0		0.08
7.7		0.40
6.9		0.24
6.2		0.04
5.1	(15)	0.60
4.83	(25)	1.00
4.50		0.08
4.33		0.24
4.12		0.50
3.93		0.50
3.75		0.16
3.65		0.16
3.45		0.16
3.09		0.16
2.95		0.08
2.84		0.12
2.72		0.12
2.62	(20)	0.80
2.42		0.24
2.36		0.24
2.17		0.32
2.05		0.24
1.96		0.20
1.90		0.24
1.82		0.40
1.71		0.40
1.65		0.16
1.59		0.04
1.56		0.04
1.52		0.16
1.483		0.04
1.460		0.16

423. Fe_2O_3*

d		I/I1
3.68		0.18
2.69	(40)	1.00
2.51	(30)	0.75
2.20		0.18
1.84	(25)	0.63
1.69		0.63
1.60		0.13
1.485		0.50
1.452		0.50
1.351		0.03
1.308		0.18
1.259		0.13
1.230		0.03
1.190		0.08
1.163		0.05
1.140		0.13
1.104		0.10
1.056		0.08
0.962		0.10
0.954		0.05
0.900		0.03
0.881		0.05
0.843		0.05

424. $FeHO_2$*

d		I/I1
4.98		0.04
4.21	(25)	1.00
3.39		0.12
2.70	(9)	0.36
2.58		0.24
2.45	(20)	0.80
2.25		0.12
2.19		0.20
1.92		0.08
1.80		0.08
1.72		0.36
1.68		0.04
1.65		0.04
1.60		0.08
1.56		0.28
1.50		0.24
1.455		0.12
1.420		0.04
1.355		0.08
1.315		0.12

425. FeO*

d		I/I1
2.47	(20)	0.50
2.14	(40)	1.00
1.51	(25)	0.63
1.293		0.15
1.238		0.08
1.072		0.03
0.984		0.03
0.959		0.05
0.876		0.03

426. Fe_3O_4*

d		I/I1
4.85		0.06
2.97		0.28
2.53	(62.5)	1.00
2.42		0.11
2.10		0.32
1.71		0.16
1.61	(40)	0.64
1.483	(50)	0.80
1.326		0.06
1.279		0.20
1.210		0.05
1.121		0.10
1.092		0.32
1.049		0.10
0.970		0.16
0.966		0.08
0.940		0.06
0.880		0.10
0.859		0.20
0.853		0.08
0.825		0.02
0.814		0.10
0.809		0.05

427. $FeO(Cr_2O_3.Al_2O_3)$*

d		I/I1
4.76		0.30
2.91		0.25
2.48	(50)	1.00
2.05		0.25
1.67		0.04
1.58	(17.5)	0.35
1.455	(20)	0.40
1.255		0.04
1.212		0.04
1.186		0.02
1.072		0.08
0.942		0.02

428. $(C_6H_4OHSO_3)_2.Fe$

d		I/I1
9.5		0.03
7.5		0.03
6.5		0.03
5.9		0.03
5.6	(15)	0.38
5.3		0.25
4.59	(40)	1.00
4.20	(15)	0.38
3.94		0.03
3.60		0.38
3.33		0.13
3.20		0.08
3.09		0.08
2.93		0.05
2.82		0.03
2.75		0.15
2.56		0.04
2.39		0.04
2.27		0.05
2.22		0.05
2.12		0.04
2.03		0.03
1.97		0.03
1.88		0.04
1.83		0.03
1.79		0.03
1.74		0.05
1.64		0.03
1.60		0.03
1.54		0.03

429. Fe_2P

d		I/I1
2.90		0.17
2.72		0.51
2.23	(17.5)	1.00
2.03	(10)	0.57
1.92	(10)	0.57
1.72		0.11
1.68		0.11
1.407		0.06
1.354		0.06
1.303		0.06
1.282		0.11
1.269		0.06
1.208		0.17
1.102		0.11
1.070		0.06
1.043		0.11

430. $Fe(H_2PO_2)_2$

d		I/I1
5.7	(50)	1.00
4.46	(5)	0.10
3.82		0.04
3.44	(10)	0.20
3.20		0.02
3.11		0.02
2.76		0.12
2.65		0.04
2.50		0.02
2.42		0.04
2.28		0.04
1.95		0.02
1.91		0.02
1.84		0.02
1.71		0.02
1.68		0.02
1.480		0.02
1.405		0.02
1.330		0.02

431. Ferric Salicylate

d		I/I1
9.8	(20)	1.00
8.3		0.10
7.0		0.10
5.7		0.10
5.1	(12.5)	0.63
4.71		0.35
4.49		0.05
4.00		0.10
3.90		0.10
3.51	(15)	0.75
3.40		0.15
3.19		0.50
2.90		0.40
2.75		0.05
2.66		0.10
2.37		0.15
2.25		0.10
2.16		0.15
2.05		0.10
2.00		0.10
1.94		0.15
1.76		0.05
1.72		0.10
1.59		0.05
1.53		0.05
1.490		0.05

432. FeSi*

d		I/I1
3.16		0.15
2.59		0.10
2.00	(100)	1.00
1.82	(40)	0.40
1.414		0.01
1.345		0.10
1.238		0.04
1.193	(20)	0.20
1.116		0.04
1.052		0.01
1.023		0.02
0.974		0.05
0.875		0.01
0.830		0.02

433. $FeSi_2$*

d		I/I1
5.1	(30)	0.30
2.37	(62.5)	0.63
1.89		0.30
1.84	(100)	1.00
1.78		0.15
1.70		0.08
1.434		0.01
1.343		0.13
1.298		0.01
1.269		0.08
1.165		0.07
1.084		0.20
1.058		0.05
0.950		0.02
0.923		0.02
0.846		0.01
0.775		0.01

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

434. $Fe_2(SO_4)_3.H_2O$

d		I/I1
10.2		0.20
9.2		0.10
7.1		0.10
6.8	(8)	0.80
4.75	(8)	0.80
4.41		0.50
4.16		0.30
4.00		0.20
3.53	(10)	1.00
3.35		0.50
3.20		0.60
3.11		0.20
3.02		0.10
2.88		0.10
2.77		0.10
2.67		0.20
2.33		0.10
2.28		0.10
2.20		0.10
2.15		0.10
2.03		0.10
1.94		0.10
1.88		0.20
1.82		0.10
1.77		0.20
1.68		0.10
1.63		0.10
1.60		0.10
1.55		0.10
1.50		0.10
1.460		0.10
1.422		0.10
1.390		0.10
1.353		0.10

435. $FeSO_4$

d		I/I1
4.78	(15)	0.24
3.58		0.13
3.25	(62.5)	1.00
2.56		0.13
2.40		0.02
2.28		0.13
2.23		0.10
2.05		0.11
1.99	(12.5)	0.20
1.83		0.16
1.78		0.02
1.70		0.03
1.63		0.20
1.59		0.20
1.55		0.10
1.440		0.06
1.420		0.02
1.361		0.05
1.281		0.13
1.251		0.02
1.200		0.08
1.140		0.03
1.110		0.02
1.014		0.02
1.000		0.03

436. $FeSO_4.H_2O$

d		I/I1
4.85	(20)	0.50
3.42	(40)	1.00
3.25		0.25
3.13	(15)	0.38
2.57		0.25
2.50		0.25
2.24		0.15
2.07		0.18
2.00		0.15
1.93		0.08
1.82		0.08
1.71		0.10
1.68		0.13
1.60		0.31
1.50		0.05
1.450		0.08
1.330		0.03
1.290		0.10
1.264		0.05
1.210		0.05
1.111		0.03

437. $FeSO_4.3H_2O$

d		I/I1
6.9		0.38
5.5	(40)	1.00
4.49	(40)	1.00
3.99	(30)	0.75
3.60		0.03
3.40		0.50
3.24		0.50
2.97		0.75
2.75		0.20
2.58		0.38
2.43		0.38
2.36		0.38
2.27		0.38
2.18		0.03
2.11		0.08
2.04		0.03
1.97		0.38
1.89		0.20
1.80		0.18
1.76		0.08
1.72		0.10
1.67		0.10
1.63		0.08
1.59		0.03
1.57		0.03
1.55		0.03
1.51		0.10
1.488		0.03
1.452		0.18
1.398		0.10
1.370		0.10
1.288		0.15
1.230		0.03
1.201		0.05
1.140		0.03

438. $FeSO_4.7H_2O$

d		I/I1
8.0		0.02
6.8		0.05
6.0		0.02
5.5		0.13
4.90	(62.5)	1.00
4.55		0.08
4.02		0.08
3.78	(40)	0.64
3.23	(12.5)	0.20
3.09		0.06
2.92		0.03
2.75		0.11
2.63		0.16
2.50		0.03
2.42		0.02
2.31		0.10
2.17		0.02
2.11		0.02
2.07		0.05
2.01		0.08
1.96		0.08
1.92		0.02
1.87		0.08
1.81		0.02
1.75		0.05
1.70		0.06
1.63		0.05
1.56		0.03
1.53		0.03
1.50		0.03
1.468		0.02

439. $FeNH_4(SO_4)_2.<12H_2O$

d		I/I1
9.2	(10)	0.07
8.2	(7)	0.47
7.0	(15)	1.00
5.9		0.07
5.5		0.07
4.72		0.13
4.51		0.27
4.14		0.33
3.72		0.07
3.57		0.13
3.40		0.40
3.29		0.40
3.20		0.13
3.10		0.13
2.95		0.10
2.70		0.10
2.58		0.07
2.42		0.20
2.34		0.07
2.29		0.13
2.21		0.07
2.15		0.07
2.13		0.07
2.10		0.07
2.07		0.07
2.02		0.10
1.90		0.07
1.86		0.07
1.80		0.07
1.70		0.07
1.65		0.07
1.61		0.07
1.57		0.10
1.52		0.10
1.450		0.10
1.396		0.07

440. $FeNH_4(SO_4)_2.12H_2O$*

d		I/I1
7.1	(40)	0.80
5.5		0.50
5.0		0.25
4.37	(50)	1.00
4.12		0.60
3.73	(40)	0.80
3.30		0.80
3.09		0.40
2.75		0.14
2.62		0.06
2.52		0.14
2.37		0.16
2.26		0.06
2.15		0.04
2.06		0.20
2.00		0.04
1.95		0.35
1.82		0.04
1.72		0.20
1.65		0.18
1.61		0.12
1.497		0.12
1.455		0.08
1.425		0.10
1.376		0.08
1.337		0.02
1.310		0.04

441. $FeSO_4.(NH_4)_2SO_4.6H_2O$

d		I/I1
6.2		0.20
6.0		0.20
5.4		0.50
5.12		0.20
4.46		0.20
4.20	(30)	1.00
3.97		0.03
3.80	(20)	0.67
3.61		0.07
3.43		0.27
3.15		0.13
3.03	(17.5)	0.58
2.87		0.03
2.80		0.27
2.71		0.03
2.64		0.03
2.56		0.07
2.52		0.03
2.45		0.23
2.32		0.03
2.23		0.20
2.16		0.16
2.08		0.13
2.04		0.03
1.98		0.03
1.91		0.07
1.86		0.03
1.81		0.07
1.76		0.03
1.73		0.03
1.69		0.03
1.63		0.03
1.55		0.03
1.51		0.07
1.480		0.07
1.441		0.03
1.384		0.03
1.335		0.03
1.254		0.03
1.222		0.03
1.197		0.03
1.182		0.03
1.159		0.03
1.134		0.03
1.112		0.03

442. FeS*

d		I/I1
2.97	(25)	0.33
2.88		0.04
2.65	(25)	0.33
2.06	(75)	1.00
2.71		0.33
1.61		0.07
1.48		0.04
1.442		0.09
1.321		0.13
1.299		0.05
1.179		0.01
1.105		0.13
1.050		0.07
0.995		0.01

443. FeS_2*

d		I/I1
3.12		0.27
2.70	(50)	0.75
2.42	(30)	0.45
2.21		0.35
1.91		0.45
1.63	(62.5)	1.00
1.56		0.15
1.50		0.17
1.450		0.25
1.240		0.10
1.210		0.15
1.180		0.10
1.153		0.05
1.105		0.12
1.041		0.25
1.005		0.03
0.987		0.02
0.957		0.10
0.903		0.03
0.878		0.02
0.855		0.02

444. $FeC_4H_4O_5$

d		I/I1
7.3		0.15
5.8	(15)	0.75
4.64		0.40
4.44	(20)	1.00
3.63		0.75
3.51	(17.5)	0.88
3.29		0.15
3.09		0.10
2.64		0.25
2.56		0.40
2.43		0.75
2.27		0.10
2.21		0.10
2.06		0.50
1.96		0.10
1.92		0.25
1.86		0.10
1.81		0.05
1.75		0.10
1.70		0.15
1.67		0.10
1.64		0.15
1.58		0.10
1.54		0.05
1.494		0.20

445. Pb*

d		I/I1
2.85	(6)	1.00
2.47	(3)	0.50
1.74	(3)	0.50
1.490		0.50
1.428		0.17
1.134		0.17
1.105		0.17

446. $Pb(C_2H_3O_2)_2.3H_2O$

d		I/I1
11.7	(20)	1.00
7.7	(8)	0.40
4.90		0.30
4.36		0.40
4.24		0.40
3.50	(20)	1.00
3.36		0.40
2.90		0.25
2.81		0.20
2.69		0.10
2.62		0.10
2.53		0.10
2.43		0.05
2.28		0.40
2.17		0.30
2.10		0.25
1.98		0.15
1.92		0.05
1.88		0.05
1.78		0.05
1.73		0.10
1.67		0.10
1.63		0.05
1.59		0.08
1.52		0.05
1.470		0.10
1.432		0.05
1.403		0.05
1.360		0.05
1.298		0.10
1.247		0.05
1.220		0.05
1.180		0.05
1.160		0.08
1.068		0.05
1.042		0.05

447. $Pb(C_2H_3O_2)_2.Pb(OH)_2.H_2O$

d		I/I1
13.0	(40)	1.00
3.38	(7)	0.18
3.05	(15)	0.38
2.88		0.15
2.73		0.08
2.60		0.08
2.48		0.05
2.24		0.03
2.07		0.05
1.95		0.04
1.88		0.03
1.81		0.03
1.77		0.03
1.69		0.08
1.65		0.05
1.53		0.05
1.485		0.04
1.443		0.05

448. $Pb_3(SbO_4)_2$

d		I/I1
5.8	(3)	0.30
4.55		0.10
4.35		0.10
3.88		0.10
3.48	(10)	1.00
3.20		0.10
3.00		0.20
2.82		0.10
2.65	(4)	0.40
2.08		0.20
1.87		0.30
1.82		0.10
1.64		0.20
1.55		0.10
1.52		0.10
1.40		0.10
1.316		0.10
1.233		0.10
1.185		0.10
1.121		0.10

449. $PbHAsO_4$

d		I/I1
6.7		0.20
4.88		0.10
4.43		0.15
3.39	(20)	1.00
3.17	(17.5)	0.87
2.93	(6)	0.30
2.56		0.10
2.42		0.10
2.20		0.20
1.95		0.20
1.78		0.20
1.68		0.15
1.55		0.10
1.475		0.10
1.390		0.05
1.338		0.05
1.300		0.05
1.275		0.05
1.250		0.05
1.220		0.10

450. $PbBr_2$

d		I/I1
6.0		0.33
4.18	(5)	0.83
3.92		0.50
3.72		0.33
3.40	(6)	1.00
2.94		0.67
2.62		0.67
2.39	(5)	0.83
2.29		0.17
2.21		0.17
2.12		0.33
2.05		0.33
1.94		0.33
1.84		0.33
1.76		0.33
1.69		0.33
1.62		0.33
1.58		0.33
1.56		0.17
1.51		0.17

451. $PbCO_3$*

d		I/I1
4.40		0.06
4.24		0.04
3.56	(25)	1.00
3.47		0.12
3.05		0.16
2.57		0.08
2.47	(8)	0.32
2.19		0.04
2.07	(7)	0.28
1.99		0.06
1.96		0.06
1.91		0.20
1.83		0.24
1.79		0.04
1.74		0.04
1.62		0.06
1.58		0.06
1.55		0.04
1.50		0.04
1.469		0.04

452. $2PbCO_3.Pb(OH)_2$

d		I/I1
4.45		0.33
4.24		0.33
3.61	(5)	0.83
3.28	(6)	1.00
2.62	(6)	1.00
2.23		0.25
2.11		0.25
2.03		0.17
1.86		0.25
1.69		0.17

453. $PbCl_2$*

d		I/I1
4.04		0.20
3.87	(17.5)	0.88
3.57	(20)	1.00
2.90		0.20
2.77	(15)	0.75
2.50		0.50
2.26		0.30
2.21		0.15
2.15		0.50
2.08		0.50
1.94		0.45
1.63		0.20
1.58		0.20
1.50		0.05
1.460		0.10
1.425		0.05
1.393		0.10
1.350		0.05
1.269		0.05
1.213		0.05

454. $PbCrO_4$

d		I/I1
4.97		0.23
4.38	(8)	0.46
3.75		0.11
3.48		0.40
3.28	(17.5)	1.00
3.01	(15)	0.86
2.71		0.11
2.61		0.11
2.53		0.11
2.32		0.11
2.25		0.34
2.15		0.06
2.08		0.17
1.97		0.40
1.91		0.06
1.85		0.34
1.80		0.06
1.74		0.06
1.69		0.11
1.65		0.06
1.61		0.06
1.54		0.06
1.422		0.09
1.358		0.06
1.303		0.06

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

455. $Pb_2Fe(CN)_6.3H_2O$

d		I/I1
7.3		0.40
6.3	(10)	0.67
5.7		0.40
4.10	(15)	1.00
3.67	(15)	1.00
3.32		0.27
3.11		0.13
2.99		0.27
2.82		0.07
2.66		0.53
2.42		0.40
2.14		0.67
2.05		0.40
1.91		0.07
1.84		0.13
1.76		0.53
1.67		0.13
1.63		0.27
1.56		0.13
1.490		0.13
1.420		0.13
1.360		0.07
1.310		0.07
1.243		0.07
1.208		0.07
1.181		0.07
1.158		0.07

456. PbF_2*

d		I/I1
3.44	(15)	1.00
2.96		0.13
2.10	(8)	0.53
1.78	(8)	0.53
1.71		0.07
1.483		0.07
1.362		0.20
1.324		0.13
1.212		0.13
1.142		0.07
1.003		0.07

457. $PbSiF_6.2H_2O$

d		I/I1
8.8		0.25
7.9	(6)	0.75
6.3	(6)	0.75
5.7		0.25
5.1	(8)	1.00
4.25		0.75
3.86		0.50
3.55		0.75
3.43		0.75
3.24		0.13
2.92		0.50
2.75		0.75
2.49		0.50
2.36		0.13
2.32		0.75
2.18		0.50
2.03		0.13
1.98		0.13
1.85		0.25
1.79		0.13
1.76		0.13
1.69		0.13
1.64		0.13

458. $Pb(HCO_2)_2$*

d		I/I1
5.7	(8)	0.80
5.2	(10)	1.00
4.36		0.40
3.70		0.40
3.25		0.60
3.02	(8)	0.80
2.82		0.20
2.71		0.40
2.59		0.20
2.45		0.20
2.36		0.20
2.22		0.10
2.18		0.10
2.07		0.10
2.02		0.40
1.87		0.30
1.80		0.10
1.74		0.20B
1.71		0.20B
1.63		0.20
1.59		0.30
1.54		0.20

459. PbI_2*

d		I/I1
7.0		0.13
3.95		0.02
3.43	(75)	1.00
2.62	(30)	0.40
2.27	(20)	0.27
2.16		0.07
2.00		0.11
1.90		0.13
1.71		0.08
1.63		0.05
1.50		0.03
1.454		0.08
1.381		0.08
1.370		0.08
1.314		0.04
1.287		0.01
1.258		0.03
1.137		0.03
1.080		0.02
1.045		0.02
1.020		0.01

460. $Pb(NO_3)_2$*

d		I/I1
4.54	(30)	1.00
3.92	(10)	0.33
2.77		0.33
2.36	(20)	0.67
2.26		0.33
1.96		0.13
1.80		0.27
1.75		0.30
1.60		0.17
1.50		0.23
1.387		0.10
1.325		0.20
1.307		0.07
1.240		0.07
1.196		0.07
1.183		0.03
1.098		0.07
1.048		0.07
1.022		0.07

461. PbC_2O_4

d		I/I1
4.77	(7)	1.00
4.50		0.14
4.25	(7)	1.00
3.76	(6)	0.86
3.39		0.86
3.28		0.86
3.00		0.43
2.75		0.29
2.62		0.14
2.53		0.43
2.40		0.14
2.32		0.14
2.16		0.29
2.09		0.14
2.02		0.21
1.91		0.14
1.87		0.14
1.82		0.14
1.78		0.21
1.69		0.14
1.63		0.14
1.59		0.14
1.54		0.14
1.50		0.14
1.371		0.14
1.331		0.14
1.291		0.14
1.248		0.14

462. PbO*

d		I/I1
3.06	(40)	1.00
2.93	(10)	0.25
2.72	(10)	0.25
2.36		0.20
1.99		0.20
1.84		0.20
1.79		0.15
1.71		0.25
1.63		0.23
1.52		0.18
1.467		0.20
1.287		0.08
1.245		0.05
1.200		0.05
1.170		0.05
1.135		0.03
1.115		0.03
1.100		0.03
1.050		0.03
1.020		0.05
0.923		0.03

463. PbO_2*

d		I/I1
3.49	(25)	1.00
2.78	(25)	1.00
2.46		0.28
1.84	(25)	1.00
1.74		0.20
1.68		0.08
1.56		0.20
1.51		0.24
1.480		0.24
1.390		0.12
1.268		0.16
1.210		0.08
1.145		0.08
1.125		0.08
1.000		0.12
0.948		0.04

464. Pb_3O_4

d		I/I1
3.35	(7)	1.00
2.88	(3)	0.43
2.76	(3)	0.43
2.62		0.28
1.95		0.14
1.89		0.28
1.82		0.28
1.74		0.43
1.62		0.14
1.58		0.14
1.51		0.14
1.405		0.14

465. $Pb_3(PO_4)_2$

d		I/I1
4.03	(3)	0.24
3.61	(2)	0.16
3.31		0.16
3.18		0.16
2.91	(12.5)	1.00
2.82		0.08
2.15		0.08
2.02		0.16
1.96		0.08
1.91		0.16
1.86		0.08
1.82		0.16
1.57		0.08
1.51		0.16
1.480		0.08
1.315		0.08
1.285		0.08
1.264		0.08
1.094		0.08
1.017		0.08

466. $PbSO_4$*

d		I/I1
4.26	(20)	0.80
3.80		0.28
3.61		0.08
3.47		0.08
3.33		0.60
3.21		0.40
3.00	(25)	1.00
2.75		0.32
2.68		0.32
2.40		0.12
2.27		0.12
2.16		0.16
2.06	(25)	1.00
2.02		0.40
1.97		0.20
1.90		0.04
1.87		0.04
1.78		0.12
1.73		0.06
1.70		0.12
1.65		0.04
1.61		0.20
1.57		0.04
1.490		0.16

467. PbS*

d		I/I1
3.43	(20)	0.80
2.97	(25)	1.00
2.09	(15)	0.60
1.79		0.32
1.71		0.16
1.484		0.08
1.361		0.08
1.327		0.16
1.212		0.08
1.144		0.08
1.050		0.04
1.004		0.04

468. PbS_2O_3

d		I/I1
4.80		0.33
4.25	(6)	1.00
4.02	(6)	1.00
3.61	(4)	0.67
3.41		0.33
2.91		0.50
2.68		0.50
2.48		0.33
2.37		0.67
2.27		0.33
2.18		0.50
2.12		0.17
2.04		0.17
1.98		0.17
1.92		0.17
1.87		0.17
1.74		0.17
1.70		0.17
1.65		0.17
1.59		0.17
1.382		0.17
1.346		0.17

469. Li*

d		I/I1
2.48	(30)	1.00
1.75	(5)	0.17
1.430	(6)	0.20
1.240		0.03

470. $Li(C_6H_5COO)$

d		I/I1
4.46	(10)	1.00
4.37	(9)	0.90
4.12	(9)	0.90
3.92		0.90
3.65		0.80
3.34		0.20
3.13		0.10
2.98		0.10
2.84		0.10
2.64		0.10
2.38		0.10
2.23		0.10
2.12		0.10
1.93		0.10

471. $Li_2B_4O_7.5H_2O$

d		I/I1
6.9	(10)	1.00
6.3		0.20
4.26		0.20
3.88		0.40
3.60		0.20
3.46		0.20
3.16	(10)	1.00
2.88		0.10
2.64		0.40
2.45		0.10
2.40		0.10
2.26	(8)	0.80
2.14		0.30
2.03		0.10
1.87		0.20
1.80		0.10
1.76		0.10
1.70		0.10
1.63		0.10
1.58		0.10
1.55		0.10
1.490		0.10
1.420		0.10

472. LiBr*

d		I/I1
3.17	(8)	1.00
2.74	(6)	0.75
1.94	(6)	0.75
1.65		0.75
1.58		0.25
1.372		0.13
1.259		0.38
1.227		0.25
1.121		0.13
1.056		0.13

473. $LiBr.2H_2O$

d		I/I1
5.3	(15)	1.00
4.2		0.13
3.97	(4)	0.27
3.68		0.13
3.47	(3)	0.20
2.70		0.20
2.55		0.13
2.39		0.13
2.23		0.20
2.16		0.13
2.02		0.07
1.83		0.07
1.73		0.07
1.60		0.07
1.54		0.07
1.490		0.07

474. Li_2CO_3

d		I/I1
4.16	(25)	0.63
3.80		0.05
3.02		0.05
2.91	(20)	0.50
2.80	(40)	1.00
2.62		0.25
2.47		0.10
2.42		0.38
2.26		0.18
2.07		0.03
1.86		0.13
1.81		0.03
1.61		0.03
1.59		0.05
1.57		0.05
1.54		0.05
1.51		0.05
1.460		0.05
1.422		0.03
1.389		0.03
1.350		0.03
1.311		0.03
1.280		0.03

475. LiCl*

d		I/I1
2.96	(125)	1.00
2.56	(125)	1.00
1.81	(75)	0.60
1.55		0.32
1.482		0.12
1.283		0.05
1.178		0.12
1.148		0.14
1.048		0.06
0.989		0.05
0.909		0.02
0.869		0.03
0.857		0.02

476. $LiCl.H_2O$*

d		I/I1
3.82		0.10
2.70	(150)	1.00
2.58		0.03
2.43		0.03
2.21		0.05
2.04		0.01
1.94		0.03
1.91	(20)	0.13
1.86		0.01
1.71		0.03
1.57	(30)	0.20
1.358		0.05
1.275		0.01
1.210		0.04
1.155		0.01
1.105		0.01
1.025		0.02

477. Li_2CrO_4

d		I/I1
7.0		0.16
5.3		0.05
4.39	(20)	0.32
4.10	(62.5)	1.00
3.70		0.05
3.50	(20)	0.32
3.27		0.20
3.15		0.13
2.85		0.32
2.64		0.24
2.54		0.08
2.47		0.10
2.32		0.08
2.22		0.03
2.14		0.05
2.08		0.02
2.01		0.03
1.94		0.08
1.86		0.11
1.80		0.02
1.73		0.03
1.69		0.06
1.64		0.02
1.60		0.03
1.56		0.03
1.52		0.02
1.457		0.02
1.420		0.13
1.367		0.05
1.343		0.03
1.215		0.02
1.113		0.02

478. $Li_2CrO_4.2H_2O$

d		I/I1
6.6		0.40
5.3		0.27
4.78		0.83
4.50		0.67
4.25		0.83
4.08		0.83
3.70		0.67
3.57		0.67
3.38		0.40
3.18		0.53
3.07	(15)	1.00
3.00	(15)	1.00
2.76	(15)	1.00
2.65		0.27
2.55		0.27
2.49		0.53
2.37		0.53
2.18		0.40
2.10		0.27
2.03		0.40
1.92		0.13
1.87		0.07
1.81		0.27
1.75		0.13
1.70		0.07
1.66		0.40
1.63		0.40
1.59		0.13
1.53		0.07
1.50		0.27
1.452		0.40
1.400		0.13
1.370		0.07
1.340		0.13

479. $Li_2Cr_2O_7.2H_2O$

d		I/I1
6.4		0.04
5.4	(15)	0.60
5.1	(15)	0.60
4.31		0.50
3.92		0.04
3.72		0.60
3.42		0.32
3.19	(25)	1.00
3.08		0.20
2.86		0.20
2.69		0.28
2.58		0.12
2.42		0.08
2.36		0.08
2.19		0.16
2.12		0.12
2.01		0.08
1.76		0.08
1.70		0.08
1.65		0.12
1.485		0.04
1.350		0.04

480. LiF*

d		I/I1
2.32	(20)	0.67
2.00	(30)	1.00
1.419	(7)	0.23
1.211		0.03
1.160		0.03

481. LiOH*

d		I/I1
4.35	(10)	0.33
2.98		0.20
2.75	(30)	1.00
2.67	(7)	0.23
2.51		0.13
2.42		0.17
2.08		0.03
1.97		0.03
1.85		0.05
1.77		0.07
1.74		0.03
1.65		0.07
1.490		0.07
1.280		0.03
1.257		0.03

482. LiI*

d		I/I1
3.47	(100)	1.00
3.00	(75)	0.75
2.12	(40)	0.40
1.81		0.40
1.73		0.10
1.50		0.06
1.378		0.15
1.343		0.15
1.226		0.08
1.157		0.08
1.062		0.01
1.016		0.06
0.998		0.02
0.950		0.02
0.917		0.01
0.907		0.01
0.842		0.01
0.804		0.01
0.783		0.01

483. LiI.3

d		
6.4		
4.19	(75)	
3.72	(50)	
3.22		
2.78	(75)	
2.44		
2.22		
2.15		
2.08		
2.00		
1.86		
1.82		
1.75		
1.70		
1.58		
1.54		
1.50		
1.460		
1.431		
1.409		
1.360		
1.280		
1.256		
1.195		

484. LiC

d		
11.1	(20)	
5.5		
5.3		
4.90		
4.50		
4.30	(6)	
4.04		
3.73		
3.30	(6)	
3.13		
2.90		
2.65		
2.48		
2.24		
2.12		

485. Li

d		
3.58	(50)	
2.78	(40)	
2.53		
2.13	(75)	
1.95		
1.72		
1.53		
1.420		
1.371		
1.355		
1.265		
1.194		
1.140		
1.117		
1.082		
1.025		
1.008		
0.982		
0.932		
0.927		
0.895		
0.890		

486. Li

d		
4.49	(40	
3.29		
3.08		
2.83		
2.75	(25	
2.64	(75	
2.57		
2.25		
2.15		
2.05		
1.97		
1.82		
1.74		
1.69		
1.61		
1.53		
1.498		
1.466		
1.420		
1.380		
1.290		
1.244		
1.205		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

483. LiI.3H₂O*

d		I/I₁
5.4		0.11
4.19	(75)	1.00
3.72	(50)	0.67
3.22		0.23
2.78	(75)	1.00
2.44		0.17
2.22		0.40
2.15		0.09
2.08		0.11
2.00		0.03
1.86		0.11
1.82		0.11
1.75		0.09
1.70		0.33
1.58		0.11
1.54		0.13
1.50		0.03
1.460		0.05
1.431		0.08
1.409		0.05
1.360		0.01
1.280		0.07
1.256		0.07
1.195		0.04

484. $LiC_2H_3O_2$

d		I/I₁
11.1	(20)	1.00
5.5		0.05
5.3		0.10
4.90		0.05
4.50		0.05
4.30	(6)	0.30
4.04		0.20
3.73		0.15
3.30	(6)	0.30
3.13		0.05
2.90		0.05
2.65		0.10
2.48		0.15
2.24		0.10
2.12		0.10

485. $LiNO_3$*

d		I/I₁
3.58	(50)	0.67
2.78	(40)	0.53
2.53		0.20
2.13	(75)	1.00
1.95		0.01
1.72		0.11
1.53		0.27
1.420		0.01
1.371		0.20
1.355		0.13
1.255		0.04
1.194		0.04
1.140		0.01
1.117		0.03
1.082		0.04
1.025		0.01
1.008		0.03
0.982		0.03
0.932		0.01
0.927		0.01
0.895		0.01
0.890		0.01

486. $Li_2C_2O_4$

d		I/I₁
4.49	(40)	0.53
3.29		0.12
3.08		0.23
2.83		0.09
2.75	(25)	0.33
2.64	(75)	1.00
2.57		0.17
2.25		0.12
2.15		0.20
2.05		0.13
1.97		0.01
1.82		0.03
1.74		0.09
1.69		0.27
1.61		0.09
1.53		0.01
1.498		0.03
1.466		0.09
1.420		0.04
1.380		0.04
1.290		0.03
1.244		0.07
1.205		0.01

487. $Li(C_2H_4OH.COO)$

d		I/I₁
11.3		0.07
8.4		0.07
6.5		0.13
5.4	(12.5)	0.83
5.2		0.13
4.86		0.13
4.52	(10)	0.67
4.28		0.53
3.55	(15)	1.00
3.30		0.20
3.15		0.13
2.92		0.07
2.82		0.13
2.70		0.13
2.42		0.07
2.31		0.07

488. Li_2SO_4*

d		I/I₁
4.01	(62.5)	1.00
3.49		0.11
3.16	(25)	0.40
2.78		0.06
2.68		0.03
2.62		0.05
2.47	(8)	0.13
2.40		0.06
2.31		0.06
2.20		0.03
2.09		0.05
2.01		0.02
1.95		0.13
1.88		0.05
1.81		0.03
1.77		0.02
1.67		0.02
1.60		0.03
1.56		0.02
1.53		0.03
1.487		0.06
1.424		0.02
1.400		0.03
1.340		0.03
1.279		0.03
1.215		0.02
1.185		0.03

489. $Li_2SO_4.H_2O$*

d		I/I₁
7.8		0.07
5.1	(20)	0.67
4.12	(30)	1.00
3.84		0.58
3.68		0.07
3.54	(20)	0.67
3.02		0.50
2.93		0.33
2.72		0.33
2.65		0.03
2.48		0.03
2.41		0.27
2.33		0.03
2.28		0.03
2.18		0.07
2.04		0.07
1.91		0.07
1.81		0.07
1.72		0.07
1.70		0.07
1.63		0.03
1.59		0.07
1.55		0.07
1.490		0.07
1.378		0.07

490. $Li_2C_4H_4O_6.H_2O$

d		I/I₁
5.6		0.13
4.57	(8)	1.00
4.06	(5)	0.63
3.80	(8)	1.00
3.55		0.25
3.42		0.25
3.30		0.13
2.97		0.13
2.84		0.13
2.75		0.13
2.59		0.25
2.43		0.13
2.38		0.13
2.24		0.13
2.15		0.13
2.08		0.13
2.00		0.13
1.93		0.13
1.83		0.13
1.77		0.13
1.66		0.13
1.59		0.13
1.480		0.13
1.425		0.13

491. $LiHC_4H_4O_8$

d		I/I₁
5.3		0.10
5.0		0.20
4.27	(10)	1.00
3.70	(6)	0.60
3.48		0.10
3.35		0.60
3.00		0.20
2.77		0.10
2.64		0.20
2.56		0.20
2.36	(8)	0.80
2.29		0.10
2.17		0.10
2.08		0.10
2.02		0.10
1.90		0.10
1.83		0.10
1.77		0.10
1.74		0.10
1.69		0.10

492. Mg*

d		I/I₁
2.77	(30)	0.30
2.60	(25)	0.25
2.45	(100)	1.00
1.90		0.20
1.60		0.20
1.471		0.20
1.378		0.18
1.341		0.13
1.303		0.08
1.225		0.08
1.180		0.08
1.084		0.04
1.030		0.07
1.010		0.03
0.974		0.04
0.925		0.01
0.898		0.03
0.870		0.01
0.763		0.01
0.740		0.01

493. $Mg(C_2H_3O_2)_2$

d		I/I₁
9.8		0.13
8.9	(30)	1.00
6.3		0.03
5.5		0.13
5.3		0.03
4.37		0.07
4.15		0.07
3.95		0.05
3.51	(10)	0.33
3.30		0.20
3.14		0.03
3.01		0.03
2.89	(6)	0.20
2.76		0.05
2.58		0.10
2.43		0.10
2.33		0.03
2.19		0.13
2.10		0.03
2.04		0.06
1.98		0.03
1.91		0.03
1.88		0.03
1.82		0.03
1.78		0.05
1.76		0.05
1.68		0.03
1.65		0.03
1.61		0.03
1.55		0.03
1.50		0.03

494. $Mg(C_2H_3O_2)_2.4H_2O$

d		I/I₁
6.9	(50)	1.00
4.78	(10)	0.20
4.47		0.02
4.07		0.06
3.77		0.02
3.22	(30)	0.60
3.05		0.12
2.93		0.20
2.70		0.02
2.54		0.12
2.40		0.10
2.28		0.06
2.23		0.02
2.14		0.14
2.08		0.02
2.03		0.06
1.95		0.02
1.89		0.10
1.86		0.10
1.80		0.04
1.72		0.04
1.67		0.02
1.63		0.02
1.59		0.02
1.53		0.02
1.430		0.02
1.410		0.02
1.360		0.02
1.269		0.02
1.170		0.02

495. Mg_2Al_3

d		I/I₁
2.47	(75)	1.00
2.38	(40)	0.53
2.32		0.17
2.21		0.20
2.12		0.13
2.05		0.05
1.99		0.04
1.94		0.03
1.57		0.07
1.490		0.17
1.423	(30)	0.40
1.325		0.05
1.240		0.07
1.215		0.08
1.138		0.03
1.105		0.03
1.080		0.03
0.972		0.03
0.928		0.01

496. Mg_2Al_3*

d		I/I₁
2.80		0.01B
2.64		0.07
2.48	(150)	1.00
2.24	(50)	0.33
2.15		0.12
2.06		0.20
1.92		0.01
1.81		0.01
1.75		0.01
1.71		0.01
1.60		0.02
1.52		0.05
1.490		0.10
1.434	(50)	0.33
1.412		0.04
1.386		0.05
1.342		0.06
1.245		0.10
1.195		0.01
1.165		0.03
1.140		0.03
1.115		0.04

497. $MgAl_2O_4$*

d		I/I₁
4.63		0.13
2.83		0.30
2.41	(100)	1.00
2.31		0.02
2.00	(62.5)	0.63
1.63		0.08
1.54		0.40
1.417	(75)	0.75
1.358		0.01
1.268		0.02
1.223		0.06
1.168		0.03
1.067		0.02
1.040		0.08
0.998		0.03
0.941		0.01
0.923		0.02
0.893		0.01
0.838		0.02
0.817		0.04
0.773		0.02

498. $2MgHAsO_4.13H_2O$

d		I/I₁
6.0		0.13
4.87		0.25
4.25	(40)	1.00
3.90		0.13
2.99	(20)	0.50
2.69		0.05
2.44	(25)	0.63
2.36		0.38
2.10		0.03
1.88		0.13
1.80		0.13
1.65		0.03
1.60		0.50
1.58		0.10
1.51		0.10
1.486		0.10
1.406		0.08
1.372		0.03
1.332		0.10
1.305		0.03
1.275		0.08
1.179		0.05
1.090		0.03
1.060		0.05

499. $Mg(C_6H_5COO)_2.3H_2O$

d		I/I₁
14.8	(15)	1.00
10.3		0.13
7.8		0.13
6.8		0.27
6.0	(12.5)	0.84
4.82		0.13
4.45	(12.5)	0.84
4.12		0.13
3.73		0.10
3.57		0.10
3.38		0.13
3.25		0.27
3.13		0.13
2.93		0.10
2.74		0.20
2.58		0.07
2.38		0.07
2.22		0.07
2.16		0.07
2.06		0.07
2.01		0.07
1.94		0.07
1.87		0.07

500. Magnesium Borate

d		I/I₁
7.7		0.12
6.1		0.16
5.3		0.08
4.39		0.24
3.57		0.12
3.18		0.12
3.07	(10)	0.80
2.82	(12.5)	1.00
2.18		0.24
2.07		0.32
1.99	(5)	0.40
1.91		0.08
1.86		0.12
1.77		0.08
1.71		0.08
1.63		0.12
1.50		0.08
1.445		0.08
1.412		0.08
1.375		0.08
1.262		0.16
1.151		0.08

501. $MgBr_2.6H_2O$

d		I/I₁
4.25	(12.5)	0.83
4.03		0.07
3.68		0.40
3.11	(8)	0.53
3.00		0.40
2.80		0.47
2.71	(15)	1.00
2.40		0.07
2.37		0.13
2.33		0.27
2.21		0.20
2.11		0.20
1.98		0.13
1.90		0.40
1.78		0.20
1.72		0.13
1.67		0.13
1.63		0.13
1.57		0.07
1.55		0.13

502. Mg_2Ca

d		I/I₁
3.14	(17.5)	0.44
2.87	(30)	0.75
2.65	(40)	1.00
2.54		0.15
2.40		0.08
2.29		0.05
1.90		0.05
1.80		0.05
1.75		0.31
1.70		0.25
1.62		0.20
1.56		0.15
1.435		0.08
1.372		0.08
1.335		0.05
1.230		0.03
1.210		0.03
1.170		0.03
1.150		0.03
1.125		0.03

503. Mg_2C_3*

d		I/I₁
3.24	(10)	0.80
3.05		0.24
2.77		0.24
2.45	(12.5)	1.00
2.21	(5)	0.40
1.99		0.16
1.87		0.32
1.80		0.16
1.75		0.16
1.58		0.24
1.51		0.32

504. $MgCO_3.3H_2O$*

d		I/I₁
6.5	(12.5)	1.00
5.8		0.08
4.96		0.08
3.86	(10)	0.80
3.58		0.16
3.23		0.16
3.02		0.24
2.77		0.16
2.61	(6)	0.48
2.51		0.40
2.35		0.08
2.17		0.16
2.01		0.08
1.92		0.32
1.83		0.08
1.79		0.24
1.71		0.16
1.64		0.08
1.55		0.12
1.50		0.08
1.450		0.08
1.430		0.08
1.390		0.08

505. $5MgO.4CO_2.5H_2O$*

d		I/I₁
5.8	(3)	1.00
2.89	(3)	1.00
2.70		0.33
2.48		0.33
2.17	(3)	1.00B
2.00		1.00
1.72		0.66
1.55		0.33
1.390		0.33

506. $MgCO_3.CaCO_3$*

d		I/I₁
3.71		0.02
2.89	(100)	1.00
2.68		0.02
2.55		0.02
2.40		0.13
2.19	(40)	0.40
2.06		0.02
2.02		0.20
1.85		0.02
1.80	(40)	0.40
1.57		0.02
1.55		0.10
1.50		0.01
1.408		0.06
1.418		0.01
1.389		0.08
1.337		0.02
1.300		0.01
1.270		0.01
1.237		0.02
1.202		0.01
1.172		0.01

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

d		*I*/*I*$_1$
507. $Mg(ClO_4)_2$		
6.9		0.10
4.90	(25)	0.63
3.39	(40)	1.00
3.20		0.23
2.69		0.05
2.60	(10)	0.25
2.17		0.08
2.04		0.13
1.90		0.05
1.80		0.08
1.71		0.03
1.68		0.03
1.61		0.13
508. $Mg(ClO_4)_2.3H_2O$		
6.9		0.02
5.5		0.12
4.80	(50)	1.00
3.99	(30)	0.60
3.35		0.60
3.22	(50)	1.00
3.06		0.02
2.95		0.04
2.85		0.06
2.75		0.08
2.59		0.20
2.43		0.04
2.34		0.10
2.25		0.02
2.18		0.02
2.03		0.12
1.99		0.10
1.90		0.14
1.84		0.16
1.76		0.02
1.72		0.04
1.67		0.02
1.62		0.10
509. $Mg(ClO_4)_2.6H_2O$		
6.8		0.02
4.91		0.05
4.18	(100)	0.80
3.91	(75)	0.60
3.41		0.03
2.85	(125)	1.00
2.64		0.24
2.55		0.24
2.45		0.06
2.30		0.24
2.07		0.10
1.95		0.16
1.83		0.20
1.76		0.20
1.70		0.08
1.60		0.02
1.56		0.08
1.53		0.02
1.480		0.10
1.420		0.06
1.385		0.02
1.300		0.08
1.280		0.03
1.242		0.04
1.183		0.03
1.162		0.03
510. $MgCl_2$*		
5.9	(25)	0.63
2.94		0.31
2.55	(25)	0.63
1.96		0.05
1.80	(40)	1.00
1.72		0.18
1.53		0.18
1.470		0.18
1.272		0.05
1.140		0.20
1.040		0.08
0.983		0.05
511. $MgCl_2.6H_2O$*		
5.8		0.15
4.10	(40)	1.00
3.57		0.15
2.98		0.20
2.88	(20)	0.50
2.72		0.44
2.65	(30)	0.75
2.55		0.03
2.46		0.03
2.31		0.15
2.23		0.25
2.15		0.08
2.05		0.18
1.84		0.31
1.78		0.08
1.72		0.10
1.63		0.03
1.59		0.03
1.480		0.10
1.420		0.03
1.390		0.10
1.365		0.03
512. $MgCl_2.NH_4Cl.6H_2O$		
6.7		0.18
4.75		0.03
4.30		0.03
3.85	(30)	0.75
3.33	(40)	1.00
2.97		0.50
2.73	(30)	0.75
2.48		0.03
2.35		0.50
2.23		0.18
2.10		0.13
2.00		0.63
1.94		0.15
1.90		0.15
1.77		0.05
1.73		0.05
1.67		0.13
1.58		0.15
1.53		0.10
1.490		0.23
1.370		0.15
1.349		0.05
1.285		0.10
1.224		0.05
1.180		0.03
1.120		0.05
513. $MgCrO_4.7H_2O$		
10.8		0.20
6.0	(12.5)	0.42
5.2		0.33
5.0	(30)	1.00
4.45		0.27
4.08		0.20
3.77	(15)	0.50
3.60		0.13
3.36		0.33
3.23		0.20
3.12		0.27
2.99		0.33
2.86		0.30
2.76		0.42
2.61		0.27
2.48		0.07
2.40		0.07
2.31		0.20
2.23		0.03
2.12		0.17
2.06		0.13
2.00		0.10
1.95		0.07
1.92		0.20
1.88		0.03
1.78		0.13
1.71		0.10
514. $Mg_3(C_6H_5O_7)_2.14H_2O$		
8.4		0.13
6.8		0.13
6.3		0.03
5.7	(30)	1.00
5.2		0.13
4.90		0.33
4.50		0.17
4.10		0.23
3.75		0.23
3.58		0.03
3.40	(20)	0.67
3.10		0.13
2.87	(25)	0.83
2.74		0.03
2.68		0.03
2.62		0.03
2.54		0.03
2.48		0.03
2.40		0.23
2.35		0.17
2.24		0.33
2.13		0.13
2.05		0.07
2.00		0.07
1.94		0.20
1.88		0.13
1.82		0.07
1.77		0.07
1.73		0.07
1.69		0.13
1.59		0.07
1.56		0.03
1.52		0.03
1.480		0.03
1.446		0.03
1.415		0.03
1.334		0.05
515. MgF_2*		
3.29	(100)	0.80
3.14		0.05
2.56		0.20
2.24	(125)	1.00
2.07		0.32
1.93		0.12
1.72	(125)	1.00
1.64		0.32
1.53		0.20
1.460		0.05
1.437		0.01
1.408		0.01
1.378		0.60
1.340		0.01
1.319		0.08
1.227		0.06
1.155		0.02
1.116		0.16
1.090		0.05
1.052		0.06
516. $MgSiF_6.6H_2O$		
6.4		0.08
5.3		0.03
4.79	(62.5)	1.00
4.54		0.02
4.22	(20)	0.32
2.98		0.06
2.64	(17.5)	0.28
2.33		0.05
2.24		0.05
2.10		0.02
1.92		0.13
1.87		0.02
1.81		0.02
1.77		0.03
1.67		0.06
1.64		0.02
1.60		0.02
1.50		0.02
1.425		0.02
1.401		0.02
1.384		0.02
1.330		0.02
1.255		0.02
1.228		0.02
517. $Mg(CHO_2)_2.2H_2O$		
4.93	(10)	1.00
4.62	(8)	0.80
4.35		0.30
3.68		0.30
3.37	(6)	0.60
3.06		0.20
2.94		0.10
2.79		0.10
2.62		0.60
2.46		0.10
2.32		0.40
2.21		0.20
2.07		0.40
1.96		0.10
1.83		0.10
1.77		0.10
1.70		0.10
1.63		0.10
1.52		0.10
1.420		0.10
1.350		0.10
518. $Mg(OH)_2$*		
4.75	(40)	0.53
2.35	(75)	1.00
1.79	(30)	0.40
1.57		0.33
1.490		0.17
1.370		0.13
1.306		0.09
1.183		0.07
1.031		0.03
1.005		0.04
0.945		0.04
0.862		0.01
519. $MgI_2.8H_2O$		
7.9		0.12
6.0		0.08
5.0		0.20
4.31	(12.5)	0.25
4.09	(50)	1.00
3.75		0.08
3.50		0.12
3.23		0.12
3.03	(17.5)	0.35
2.80		0.20
2.65		0.02
2.60		0.08
2.50		0.12
2.42		0.16
2.35		0.10
2.29		0.04
2.23		0.04
2.15		0.16
2.05		0.08
2.03		0.08
1.98		0.10
1.89		0.02
1.85		0.04
1.75		0.14
1.67		0.12
1.63		0.12
1.60		0.12
1.57		0.02
1.51		0.02
1.465		0.04
1.432		0.04
520. $Mg(C_2H_3O_2)_2.3H_2O$		
9.5	(12.5)	1.00
5.1	(10)	0.80
4.52		0.24
3.68	(4)	0.32
3.48		0.24
3.00		0.16
2.70		0.08
2.19		0.16
1.96		0.08
1.84		0.08
521. Mg_3Pb*		
3.91	(15)	1.00
3.39		0.20
2.40	(10)	0.66
2.04	(10)	0.66
1.96		0.07
1.69		0.07
1.56		0.26
1.52		0.13
1.387		0.20
1.307		0.20
1.200		0.07
1.148		0.13
1.131		0.07
1.073		0.07
1.035		0.07
0.949		0.07
522. Mg_2Hg		
4.25		0.30
3.75	(20)	1.00
2.98		0.15
2.36	(15)	0.75
2.09	(7)	0.35
2.02		0.25
1.68		0.15
1.55		0.15
1.438		0.10
1.325		0.10
1.265		0.05
1.230		0.05
1.160		0.05
523. $Mg(NO_3)_2.6H_2O$		
11.0		0.05
8.9		0.05
6.2		0.05
5.8		0.20
4.42	(40)	1.00
4.18		0.25
3.57		0.18
3.29	(17.5)	0.44
3.18		0.13
3.10		0.05
2.93	(20)	0.50
2.85		0.10
2.78		0.08
2.69		0.20
2.61		0.10
2.37		0.15
2.31		0.08
2.20		0.05
2.12		0.15
2.07		0.08
2.03		0.04
1.97		0.03
1.92		0.04
1.86		0.03
1.82		0.05
1.77		0.03
1.73		0.03
1.69		0.04
1.65		0.03
524. Mg_3N_2*		
4.08		0.13
2.87		0.20
2.66	(40)	0.27
2.49		0.20
2.12	(62.5)	0.42
1.95		0.03
1.81		0.01
1.76	(150)	1.00
1.61		0.03
1.53		0.03
1.50		0.02
1.471		0.03
1.438		0.02
1.355		0.20
1.265		0.12
1.243		0.01
1.132		0.01
1.111		0.01
1.074		0.02
1.048		0.01
1.027		0.02
1.015		0.02
525. $MgC_2O_4.2H_2O$		
4.90	(30)	1.00
3.20	(15)	0.50
2.61		0.07
2.54		0.07
2.37		0.20
2.07		0.13
2.02	(8)	0.27
1.85		0.27
1.76		0.03
1.59		0.03
1.52		0.13
1.345		0.03
1.230		0.03
526. MgO*		
2.42		0.06
2.10	(100)	1.00
1.485	(75)	0.75
1.266		0.06
1.213	(15)	0.15
1.050		0.04
0.963		0.01
0.940		0.10$_{\alpha_1}$
0.937		0.05$_{\alpha_2}$
0.860		0.04$_{\alpha_1}$
0.854		0.02$_{\alpha_2}$
527. $MgFe_2O_4$*		
2.95	(20)	0.27
2.51	(75)	1.00
2.08		0.13
1.70		0.12
1.60		0.27
1.476	(30)	0.40
1.320		0.03
1.273		0.07
1.114		0.03
1.085		0.07
1.042		0.01
0.963		0.03
528. $(C_3H_4OHSO_2)_2Mg$		
6.1		0.16
5.6		0.08
4.70	(8)	0.64
4.29	(5)	0.40
3.95		0.40
3.50	(12.5)	1.00
3.15		0.16
2.84		0.24
2.57		0.24
2.30		0.08
2.16		0.08
529. $MgHPO_4.3H_2O$		
5.9	(10)	0.40
5.3		0.20
4.70		0.40
4.15		0.24
3.64		0.08
3.45	(25)	1.00
3.05	(20)	0.80
2.80		0.32
2.71		0.24
2.57		0.32
2.39		0.24
2.20		0.12
2.05		0.12
1.97		0.04
1.92		0.16
1.87		0.08
1.79		0.04
1.75		0.04
1.66		0.08
1.59		0.08
1.490		0.04
1.410		0.08
1.380		0.04
1.325		0.04
530. $Mg(H_2PO_4)_2$		
4.95		0.16
4.47		0.60
4.08		0.50
3.75		0.12
3.60		0.20
3.37	(20)	0.80
3.14	(25)	1.00
2.98		0.60
2.64		0.28
2.55		0.24
2.33	(17.5)	0.70
2.24		0.16
2.16		0.04
2.03		0.04
1.94		0.24
1.84		0.04
1.72		0.12
1.64		0.08
1.56		0.12
1.425		0.12
1.355		0.04
1.315		0.08
1.270		0.04
1.195		0.08
1.160		0.08
1.130		0.04
531. $Mg_3(PO_4)_2.4H_2O$		
6.1		0.20
5.2	(4)	0.80
4.10	(5)	1.00
3.23	(4)	0.80
3.09		0.60
2.87		0.40
2.73		0.40
2.65		0.80
2.51		0.40
2.34		0.40
1.91		0.20
1.79		0.20
1.74		0.20
532. $Mg_3(PO_4)_2.8H_2O$		
7.7		0.24
6.7	(12.5)	1.00
3.19		0.08
2.94	(4)	0.32
2.69	(4)	0.32
2.51		0.24
2.40		0.16
2.30		0.08
2.05		0.08
1.96		0.08
1.87		0.08
1.33		0.08

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

533. $MgNH_4PO_4.6H_2O$

d	I/I1
8.9	0.04
6.0	0.28
5.6	0.32
4.70	0.08
4.28	(25) 1.00
3.92	0.16
3.50	0.08
3.30	0.20
3.03	0.08
2.93	(12.5) 0.50
2.81	0.24
2.69	(12.5) 0.50
2.51	0.04
2.40	0.04
2.36	0.08
2.27	0.04
2.18	0.04
2.13	0.08
2.07	0.04
2.02	0.12
1.97	0.04
1.88	0.12
1.81	0.12
1.74	

534. $Mg_2P_2O_7$

d	I/I1
4.14	(10) 0.10
3.85	0.04
3.45	0.05
3.00	(100) 1.00
2.51	0.08
2.40	0.05
2.30	0.01
2.15	0.02
2.09	(15) 0.15
1.85	0.10
1.69	0.08
1.62	0.07
1.57	0.10
1.51	0.01
1.465	0.07
1.380	0.06
1.322	0.07
1.250	0.05
1.206	0.02
1.155	0.01
1.131	0.01
1.073	0.01
1.044	0.03
1.002	0.02

535. $Mg(H_2PO_2)_2.6H_2O$

d	I/I1
6.0	(30) 0.40
5.2	0.08
4.51	0.08
3.84	0.11
3.65	(40) 0.53
3.40	0.01
3.10	0.08
2.98	(75) 1.00
2.59	0.20
2.36	0.20
2.10	0.03
1.99	0.09
1.82	0.20
1.74	0.09
1.64	0.04
1.56	0.01
1.490	0.03
1.440	0.03
1.378	0.05
1.341	0.01
1.212	0.03
1.155	0.01

536. Magnesium Lactophosphate

d	I/I1
11.2	(6) 1.00
9.5	0.66
8.0	0.50
5.8	(6) 1.00
5.3	0.50
4.55	0.66
4.10	0.66
3.65	(5) 0.83
3.41	0.17
2.82	0.17
2.64	0.17
2.48	0.17

537. $MgSiO_3$*

d	I/I1
3.16	(15) 1.00
2.91	0.33
2.72	0.20
2.55	0.27
2.30	0.20
1.97	(7) 0.47
1.71	0.10
1.64	0.13
1.490	(6) 0.40
1.312	0.27
1.264	0.13
1.228	0.13
1.142	0.07
1.053	0.07
0.992	0.07
0.948	0.07
0.872	0.07

538. Mg_2SiO_4*

d	I/I1
5.1	0.11
3.89	(25) 0.40
3.72	0.05
3.49	0.20
2.99	0.13
2.77	(25) 0.40
2.51	0.32
2.45	0.40
2.26	0.40
2.15	0.11
2.02	0.02
1.95	0.02
1.88	0.03
1.81	0.03
1.74	(62.5) 1.00
1.67	0.10
1.62	0.11
1.57	0.08
1.490	0.32
1.395	0.20
1.350	0.28
1.315	0.10

539. $3MgO.2SiO_2.2H_2O$

d	I/I1
7.4	(50) 1.00
4.83	0.06
4.53	0.16
4.11	0.04
3.66	(30) 0.60
2.98	0.08
2.72	0.04
2.61	0.08
2.53	0.30
2.45	0.30
2.37	0.12
2.10	0.20
1.79	0.04
1.74	0.10
1.70	0.06
1.61	0.10
1.57	0.04
1.53	(30) 0.60
1.485	0.14
1.420	0.04
1.375	0.04
1.310	0.20
1.213	0.02
1.092	0.04
1.045	0.04
0.990	0.04

540. Mg_2Si*

d	I/I1
3.69	(40) 0.40
3.19	0.10
2.25	(100) 1.00
1.92	0.15
1.84	0.02
1.59	0.20
1.463	0.06
1.427	0.02
1.301	(40) 0.40
1.227	0.05
1.127	0.08
1.077	0.03
1.007	0.09
0.852	0.06
0.845	0.03
0.752	0.01

541. $MgSO_4$

d	I/I1
4.18	0.04
3.55	(50) 1.00B
3.35	0.02
3.18	0.02
2.64	(15) 0.30
2.45	0.20
2.35	0.04
2.30	(12.5) 0.25
2.15	0.04
2.02	0.04
1.97	0.08
1.81	0.04
1.77	0.12
1.68	0.06
1.55	0.04
1.51	0.02
1.454	0.06
1.409	0.02
1.382	0.02
1.275	0.06

542. $MgSO_4.H_2O$

d	I/I1
4.82	(30) 0.40
3.38	(75) 1.00
3.07	0.20
2.55	(30) 0.40
2.40	0.05
2.33	0.03
2.19	0.05
2.10	0.04
2.05	0.17
1.97	0.05
1.90	0.05
1.81	0.07
1.67	0.17
1.62	0.08
1.58	0.08
1.54	0.03
1.496	0.05
1.446	0.04
1.397	0.01
1.279	0.08
1.253	0.07
1.224	0.03
1.195	0.04

543. $MgSO_4.6H_2O$

d	I/I1
5.5	0.28
5.1	0.24
4.90	0.24
4.40	(25) 1.00
4.04	(8) 0.32
3.61	0.20
3.42	0.16
3.20	0.12
2.92	(15) 0.60
2.77	0.28
2.67	0.24
2.56	0.08
2.50	0.16
2.28	0.24
2.20	0.04
2.05	0.08
2.00	0.20
1.87	0.24
1.80	0.04
1.76	0.04
1.69	0.04
1.62	0.04
1.50	0.04
1.455	0.04
1.415	0.08
1.395	0.08

544. $MgSO_4.7H_2O$*

d	I/I1
5.9	(20) 0.20
5.3	0.20
4.50	0.08
4.22	(100) 1.00
3.76	0.10
3.41	0.12
3.17	0.02
2.96	0.18
2.87	0.20
2.74	0.08
2.66	(40) 0.40
2.48	0.02
2.38	0.05
2.27	0.02
2.21	0.07
2.10	0.06
2.03	0.02
1.96	0.03
1.88	0.04
1.80	0.04
1.72	0.03
1.64	0.04

545. Magnesium Ethyl Sulfate

d	I/I1
14.0	0.13
13.0	0.13
11.6	0.13
10.2	(30) 1.00
9.8	0.58
5.8	0.10
5.2	0.50
4.90	0.33
3.98	0.33
3.53	(30) 1.00
3.30	0.20
2.98	0.27
2.89	(20) 0.66
2.55	0.07
2.33	0.03
2.19	0.03
2.08	0.03
2.01	0.03
1.95	0.20
1.91	0.07
1.86	0.07
1.80	0.10
1.70	0.10
1.55	0.07
1.320	0.03
1.270	0.03

546. MgS*

d	I/I1
2.99	0.05
2.59	(75) 1.00
1.83	(62.5) 0.83
1.499	(30) 0.40
1.299	0.20
1.160	0.40
1.060	0.33
0.920	0.08
0.867	0.13
0.823	0.08
0.784	0.08
0.751	0.01
0.723	0.05
0.696	0.08
0.632	0.03

547. $MgSO_3.6H_2O$*

d	I/I1
5.7	0.04
4.40	(20) 0.80
3.87	(25) 1.00
3.01	0.32
2.90	0.32
2.74	(25) 1.00
2.42	0.60
2.05	0.12
1.91	0.32
1.77	0.70
1.71	0.04
1.66	0.32
1.63	0.04
1.54	0.08
1.460	0.04
1.375	0.12
1.300	0.04
1.267	0.04
1.240	0.04
1.210	0.04
1.120	0.04

548. $MgC_4H_4O_5.5H_2O$

d	I/I1
6.5	0.40
6.0	(6) 0.60
5.3	(10) 1.00
3.73	(5) 0.50
3.21	0.20
3.03	0.10
2.88	0.40
2.76	0.10
2.65	0.50
2.38	0.20
2.28	0.10
2.02	0.20
1.94	0.20
1.87	0.20
1.81	0.10
1.76	0.10
1.65	0.10
1.59	0.10
1.51	0.10

549. $MgS_2O_3.6H_2O$

d	I/I1
4.70	0.10
4.40	(40) 1.00
3.65	0.20
3.37	0.15
3.10	0.03
3.01	0.15
2.95	0.03
2.82	(12.5) 0.31
2.64	(10) 0.25
2.55	0.15
2.40	0.25
2.29	0.03
2.22	0.18
2.12	0.08
2.03	0.10
1.98	0.08
1.93	0.03
1.88	0.10
1.80	0.08
1.71	0.05
1.67	0.03
1.61	0.03
1.390	0.08
1.350	0.05
1.313	0.05
1.260	0.03

550. Mg_2Sn*

d	I/I1
3.90	(125) 1.00
3.38	0.24
2.38	(125) 1.00
2.03	(100) 0.80
1.95	0.08
1.69	0.24
1.55	0.40
1.51	0.12
1.380	0.60
1.300	0.24
1.194	0.10
1.142	0.20
1.125	0.02
1.068	0.16
1.031	0.06
0.975	0.04
0.946	0.08
0.903	0.12
0.880	0.10

551. $MgC_3H_3N_4O_2$

d	I/I1
10.2	0.05
7.2	0.05
5.8	(6) 0.30
5.0	0.05
4.70	0.20
4.35	0.10
3.84	0.25
3.35	(20) 1.00
3.25	0.20
3.09	(6) 0.30
2.86	0.10
2.75	0.20
2.53	0.10
2.44	0.10
2.15	0.05
2.08	0.05
2.00	0.05
1.90	0.05B
1.66	0.10
1.63	0.05

552. Magnesium Vanadate

d	I/I1
7.2	0.50
5.4	0.42
4.79	(20) 0.67
4.17	(30) 1.00
3.98	0.10
3.80	0.03
3.55	(20) 0.67
3.40	0.07
3.28	0.27
3.07	0.20
2.97	0.20
2.84	0.20
2.69	0.07
2.62	0.07
2.52	0.03
2.46	0.10
2.31	0.10
2.18	0.17
2.12	0.03
2.07	0.03
2.01	0.03
1.98	0.03
1.91	0.10
1.78	0.10
1.69	0.03
1.65	0.10
1.52	0.03
1.48	0.03

553. α-Mn*

d	I/I1
2.36	0.02
2.22	0.02
2.09	(62.5) 1.00
1.89	(12.5) 0.20
1.81	0.10
1.74	0.16
1.340	0.02
1.283	0.07
1.258	0.10
1.210	(17.5) 0.28
1.190	0.02
1.130	0.03
1.048	0.06
0.983	0.02
0.960	0.02
0.936	0.03
0.834	0.02
0.820	0.02
0.813	0.02
0.801	0.02
0.793	0.02
0.770	0.02

554. β-Mn*

d	I/I1
2.81	0.07
2.10	(30) 1.00
2.00	(20) 0.66
1.90	0.27
1.68	0.07
1.485	0.03
1.410	0.03
1.237	(9) 0.30
1.170	0.20
1.064	0.03
1.051	0.03

555. $Mn(C_2H_3O_2)_2.4H_2O$

d	I/I1
8.4	(40) 1.00
6.4	(10) 0.25
5.2	0.05
4.45	(4) 0.10
4.00	0.10
3.72	0.05
3.18	0.08
3.07	0.10
2.86	0.05
2.60	0.03
2.52	0.05
2.42	0.03
2.33	0.05
2.13	0.03
2.00	0.03
1.94	0.03
1.87	0.03
1.79	0.03

556. $MnAl_2O_4$*

d	I/I1
2.92	0.17
2.49	(3) 0.50
2.39	(3) 0.50
1.398	(6) 1.00

557. $Mn(C_6H_5COO)_2.3H_2O$

d	I/I1
14.2	(15) 1.00
11.8	(4) 0.27
6.0	(4) 0.27
4.22	0.13
3.80	0.07
3.22	0.07
3.16	0.07
2.88	0.07
2.73	0.07
2.10	0.07

558. Manganese Borate

d	I/I1
7.8	0.24
6.9	0.08
6.1	0.24
5.2	0.08
4.30	(6) 0.48
4.00	0.08
3.58	0.40
3.18	0.16
3.08	(12.5) 1.00
2.82	(10) 0.80
2.17	0.32
2.07	0.48
1.99	0.48
1.85	0.24
1.77	0.16
1.70	0.08
1.62	0.16
1.489	0.08
1.409	0.08
1.372	0.12
1.287	0.08
1.258	0.16
1.150	0.08

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

559. $MnCO_3$*

d		I/I1
3.65	(15)	0.30
2.84	(50)	1.00
2.36		0.14
2.16		0.12
2.00		0.12
1.82		0.02
1.76	(25)	0.50
1.53		0.06
1.452		0.04
1.365		0.04
1.298		0.02

560. $MnCl_2$*

d		I/I1
5.8	(25)	1.00
3.12		0.50
2.89		0.20
2.57	(17.5)	0.70
2.35		0.16
1.84	(20)	0.80
1.76		0.32
1.50		0.16
1.455		0.16
1.290		0.08
1.164		0.12
1.145		0.16
1.063		0.08

561. $MnCl_2.H_2O$

d		I/I1
7.1		0.66
5.7	(30)	1.00
4.45		0.27
3.55		0.50
3.27		0.27
2.93	(30)	1.00
2.78		0.58
2.66		0.03
2.55	(25)	0.83
2.42		0.33
2.36		0.58
2.29		0.50
2.20		0.13
2.11		0.17
2.02		0.17
1.91		0.06
1.83		0.83
1.75		0.03
1.68		0.13
1.62		0.20
1.55		0.13
1.455		0.17
1.410		0.10
1.300		0.10
1.215		0.13
1.160		0.13
1.126		0.06
1.075		0.13
1.038		0.03

562. $MnCl_2.2H_2O$*

d		I/I1
5.6	(30)	1.00
4.39	(20)	0.66
3.22		0.03
2.90		0.33
2.79	(25)	0.83
2.41		0.42
2.35		0.33
2.19		0.33
2.12		0.50
1.82		0.20
1.78		0.07
1.72		0.20
1.68		0.17
1.62		0.23
1.54		0.07
1.460		0.03
1.400		0.23
1.360		0.03
1.240		0.03
1.210		0.07
1.162		0.07
1.076		0.03
1.058		0.03

563. $MnCl_2.4H_2O$

d		I/I1
5.5		0.40
4.91	(15)	0.85
4.37	(17.5)	1.00
4.03		0.06
3.53		0.06
3.24		0.11
3.04		0.46
2.90	(12.5)	0.71
2.74		0.51
2.58		0.46
2.47		0.34
2.39		0.23
2.32		0.11
2.19		0.28
2.12		0.23
2.03		0.23
1.97		0.40
1.88		0.40
1.80		0.23
1.74		0.11
1.70		0.17
1.67		0.17
1.460		0.11
1.430		0.11
1.400		0.06
1.350		0.06

564. MnF_2*

d		I/I1
3.45	(62.5)	1.00
2.74	(30)	0.48
2.42		0.03
2.38		0.20
2.18		0.06
1.82	(50)	0.80
1.72		0.16
1.64		0.08
1.54		0.06
1.490		0.10
1.455		0.20
1.365		0.02
1.250		0.05
1.218		0.02
1.195		0.05
1.150		0.02
1.130		0.02
1.115		0.02
1.090		0.02
0.980		0.03
0.935		0.02
0.912		0.02

565. MnC_2O_4

d		I/I1
5.9	(25)	1.00
5.6		0.32
4.95		0.32
3.58	(15)	0.60
2.95		0.24
2.78	(17.5)	0.70
2.53		0.20
2.30		0.32
2.15		0.16
2.02		0.32
1.92		0.20
1.87		0.20
1.79		0.20
1.74		0.24
1.68		0.12
1.58		0.12
1.50		0.08
1.450		0.20

566. $MnC_2O_4.2^1/_2H_2O$

d		I/I1
4.80	(50)	1.00
3.91		0.20
3.65		0.25
3.00	(30)	0.60
2.67	(25)	0.50
2.29		0.14
2.14		0.10
2.04		0.16
1.92		0.25
1.84		0.20
1.75		0.02
1.69		0.02
1.65		0.06
1.60		0.08
1.55		0.08
1.52		0.06
1.50		0.06
1.470		0.04
1.436		0.04
1.390		0.08
1.338		0.02
1.304		0.04
1.265		0.04
1.245		0.02
1.219		0.02
1.185		0.04

567. MnO*

d		I/I1
2.56	(20)	0.66
2.22	(30)	1.00
1.57	(20)	0.66
1.339		0.23
1.281		0.17
1.110		0.07
1.019		0.07
0.994		0.17
0.906		0.07
0.853		0.03

568. MnO_2*

d		I/I1
3.11	(25)	1.00
2.40	(12.5)	0.50
2.21		0.04
2.12		0.12
1.98		0.04
1.62	(12.5)	0.50
1.56		0.12
1.440		0.08
1.390		0.04
1.303		0.16
1.050		0.04
1.001		0.04

569. Mn_3O_4*

d		I/I1
4.92		0.20
3.08		0.31
2.87		0.08
2.75	(25)	0.63
2.56		0.08
2.48	(40)	1.00
2.36		0.13
2.22		0.31
2.03		0.15
1.79		0.18
1.70		0.05
1.64		0.05
1.57	(20)	0.50
1.54		0.50
1.466		0.03
1.438		0.18
1.384		0.04
1.340		0.08
1.300		0.03
1.277		0.13
1.237		0.04B
1.192		0.05B
1.123		0.04

570. $(Mn, Co)(Mn, Co)_2O_4$; 2Mn:Co

d		I/I1
4.85		0.17
4.38		0.03
3.90		0.07
2.99	(6)	0.20B
2.71	(6)	0.20
2.48	(30)	1.00
2.31		0.03
2.04		0.10
1.75		0.03
1.69		0.13
1.60		0.13
1.57		0.13
1.52		0.17
1.489		0.10
1.438		0.10
1.269		0.10

571. $Mn_3(PO_4)_2.7H_2O$

d		I/I1
3.45	(1)	0.33
2.96		0.33
2.84		0.33
2.61	(3)	1.00
2.38	(2)	0.66
2.12		0.33
1.72		0.33
1.53		0.33
1.48		0.33
1.42		0.33

572. $Mn(H_2PO_2)_2.H_2O$

d		I/I1
7.6		0.06
6.5	(12.5)	0.72B
5.8		0.40
4.72		0.34
4.05		0.11
3.82		0.28
3.45	(17.5)	1.00
3.20	(8)	0.46
3.00		0.34
2.87		0.06
2.78		0.46
2.38		0.17
2.29		0.23
2.00		0.06
1.94		0.11
1.85		0.06
1.79		0.17
1.74		0.06
1.63		0.06
1.60		0.06
1.57		0.11
1.55		0.11
1.425		0.06

573. $MnSO_4(NH_4)_2SO_4.6H_2O$

d		I/I1
6.4		0.05
5.9		0.30
4.60		0.40
4.20	(10)	0.50
3.59	(10)	0.50
3.22	(20)	1.00
2.95		0.05
2.72		0.25
2.62		0.05
2.56		0.40
2.19		0.20
2.10		0.05
1.90		0.05
1.82		0.05
1.77		0.05
1.66		0.15
1.62		0.10
1.56		0.05
1.52		0.05
1.480		0.05
1.390		0.05

574. $MnSO_4.4H_2O$

d		I/I1
4.9		0.40
3.80		0.02
3.51	(50)	1.00
3.36		0.20
3.15	(25)	0.50
2.59	(25)	0.50
2.45		0.04
2.37		0.08
2.25		0.16
2.14		0.06
2.12		0.06
2.02		0.08
1.98		0.04
1.92		0.02
1.88		0.04
1.75		0.03
1.72		0.16
1.68		0.04
1.65		0.06
1.61		0.06
1.57		0.02
1.54		0.04
1.484		0.10
1.430		0.02
1.390		0.02
1.356		0.02
1.305		0.04
1.240		0.02
1.203		0.02

575. MnS*

d		I/I1
3.02		0.11
2.61	(75)	1.00
1.85	(50)	0.67
1.58		0.04
1.51		0.20
1.309		0.08
1.200		0.01
1.170	(17.5)	0.23
1.070		0.11
0.927		0.03
0.873		0.05
0.828		0.03
0.790		0.03
0.728		0.01
0.700		0.03

576. $MnC_4H_6O_4$

d		I/I1
8.6		0.03
7.5		0.13
5.9		0.67
4.63		0.50
4.47	(30)	1.00
3.67		0.42
3.53	(30)	1.00
3.30		0.13
3.08		0.03
2.92		0.03
2.67		0.23
2.58		0.50
2.44	(30)	1.00
2.23		0.20
2.07		0.50
1.93		0.23
1.87		0.07
1.83		0.03
1.76		0.07
1.72		0.20
1.69		0.20
1.64		0.13
1.59		0.13
1.51		0.17
1.470		0.03
1.440		0.03
1.375		0.03
1.305		0.03
1.271		0.10

577. $Hg(C_2H_3O_2)_2$

d		I/I1
10.0	(12.5)	1.00
5.7	(4)	0.32
4.43		0.16
4.30		0.16
4.07	(3)	0.24
3.66		0.24
3.40		0.16
3.24		0.08
3.18		0.08
2.96		0.08
2.75		0.08
2.19		0.08
2.01		0.08

578. $(HgC_2H_3O_2)_2$

d		I/I1
13.0	(50)	1.00
11.5	(50)	1.00
3.86	(25)	0.50
3.49		0.20
3.00		0.18
2.90		0.06
2.81		0.02
2.61		0.08
2.52		0.06
2.42		0.04
2.36		0.02
2.24		0.04
2.12		0.02
2.01		0.04
1.93		0.04
1.88		0.04
1.85		0.04
1.81		0.02
1.78		0.02
1.66		0.04
1.62		0.02
1.60		0.02
1.55		0.02

579. $Hg(C_2H_3COO)_2$

d		I/I1
15.0	(50)	1.00
7.5		0.08
4.90		0.04
4.30	(6)	0.12
3.90		0.06
3.72	(8)	0.16
3.36		0.10
3.19		0.02
2.94		0.04
2.76		0.02
2.64		0.02
2.50		0.04
2.36		0.06
2.29		0.02
2.19		0.04
2.08		0.02
1.98		0.02
1.92		0.02
1.86		0.02
1.80		0.02
1.73		0.02
1.51		0.02
1.291		0.02

580. $HgBr_2$

d		I/I1
6.2	(8)	1.00
4.31		0.13
3.72	(6)	0.75B
2.96		0.13
2.51		0.13
2.31	(3)	0.38
2.17		0.25
2.08		0.13
2.03		0.38
1.93		0.25
1.88		0.13
1.83		0.13
1.70		0.25
1.63		0.13
1.55		0.25
1.490		0.13
1.451		0.13
1.362		0.13
1.290		0.13
1.250		0.13

581. Hg_2Br_2*

d		I/I1
4.30	(12.5)	0.50
3.29	(25)	1.00
2.77		0.20
2.32		0.24
2.12	(10)	0.40
2.05		0.04
2.00		0.16
1.78		0.12
1.64		0.04
1.52		0.08
1.470		0.04
1.420		0.08
1.304		0.04
1.274		0.04
1.198		0.04
1.064		0.04

582. $Hg(ClO_4)_2$

d		I/I1
6.6		0.05
5.9		0.27
5.6		0.20
4.62	(75)	1.00
3.87		0.20
3.70		0.11
3.51		0.11
3.29	(50)	0.67
3.15		0.33
2.93		0.11
2.80		0.03
2.69		0.20
2.60		0.08
2.30		0.04
2.19	(50)	0.67
2.11		0.04
2.01		0.08
1.93		0.11
1.88		0.12
1.80		0.01
1.72		0.17
1.66		0.05
1.59		0.09
1.53		0.09
1.480		0.07
1.445		0.05
1.417		0.03
1.385		0.04
1.341		0.04
1.160		0.01

583. $HgCl_2$*

d		I/I1
4.35	(8)	1.00
4.10		0.25
3.40		0.38
3.20		0.13
3.00	(6)	0.75
2.70	(4)	0.50
2.41		0.25
2.18		0.13
2.12		0.25
2.06		0.25
2.00		0.50
1.94		0.25
1.90		0.13
1.79		0.13
1.67		0.13
1.62		0.13
1.59		0.13
1.54		0.13
1.455		0.13
1.400		0.13
1.340		0.13

584. Hg_3C

d		I/I1
4.16	(50)	
3.17	(50)	
2.83		
2.72		
2.24		
2.06		
1.97	(40)	
1.73		
1.58		
1.478		
1.417		
1.366		
1.260		
1.237		
1.171		
1.127		
1.083		
1.060		
1.038		
1.003		
0.987		
0.942		

585. Merc Ammonium Cl

d		I/I1
5.2	(20)	
4.35		
3.82	(20)	
2.81		
2.65		
2.55		
2.35	(12.5)	
2.21		
2.16		
2.03		
2.00		
1.85		
1.72		
1.67		
1.59		
1.56		
1.53		
1.490		
1.440		
1.393		
1.334		
1.286		
1.259		
1.200		
1.181		
1.160		

586. $HgCl_2$.

d		I/I1
5.9		
3.95	(4)	
3.23		
2.92	(3)	
2.70	(4)	
2.59		

587. Hg(

d		I/I1
5.6	(4)	
4.65		
4.27		
3.60		
3.35	(6)	
3.11		
2.96	(6)	
2.78		
2.64		
2.52		
2.40		
2.35		
2.30		
2.12		
2.03		
1.93		
1.84		
1.77		
1.72		
1.67		
1.61		
1.57		
1.368		

588. Hg

d		I/I1
5.2	(5)	
3.84	(4)	
3.45	(8)	
3.22		
3.08		
2.81		
2.54		
2.37		
2.32		
1.93		
1.84		
1.81		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

584. Hg_2Cl_2*

d		I/I1
4.16	(50)	1.00
3.17	(50)	1.00
2.83		0.08
2.72		0.30
2.24		0.30
2.06		0.60
1.97	(40)	0.80
1.73		0.35
1.58		0.08
1.478		0.40
1.417		0.16
1.366		0.16
1.260		0.20
1.237		0.06
1.171		0.16
1.127		0.02
1.083		0.06
1.060		0.02
1.038		0.14
1.003		0.02
0.987		0.02
0.942		0.02

585. Mercury Ammonium Chloride

d		I/I1
5.2	(20)	1.00
4.35		0.50
3.32	(20)	1.00
2.81		0.50
2.65		0.50
2.55		0.10
2.35	(12.5)	0.63
2.21		0.30
2.16		0.20
2.03		0.30
2.00		0.15
1.85		0.25
1.72		0.30
1.67		0.10
1.59		0.15
1.56		0.10
1.53		0.10
1.490		0.30
1.440		0.20
1.393		0.10
1.334		0.15
1.286		0.15
1.259		0.05
1.200		0.05
1.181		0.10
1.160		0.10

586. $HgCl_2.3HgO$

d		I/I1
5.9		0.25
3.95	(4)	1.00
3.23		0.50
2.92	(3)	0.75
2.70	(4)	1.00
2.59		0.25

587. $HgCrO_4$

d		I/I1
5.6	(4)	0.67
4.65		0.33
4.27		0.67
3.60		0.17
3.35	(6)	1.00
3.11		0.50
2.96	(6)	1.00
2.78		0.67
2.64		0.33
2.52		0.17
2.40		0.17
2.35		0.50
2.30		0.17
2.12		0.17
2.03		0.33
1.93		0.33
1.84		0.33
1.77		0.17
1.72		0.33
1.67		0.33
1.61		0.17
1.57		0.33
1.368		0.17

588. Hg_2CrO_4

d		I/I1
5.2	(5)	0.63
3.84	(4)	0.50
3.45	(8)	1.00
3.22		0.25
3.08		0.13
2.81		0.25
2.54		0.38
2.37		0.13
2.32		0.13
1.93		0.13
1.84		0.13
1.81		0.1

589. $Hg(CN)_2$*

d		I/I1
4.85	(12.5)	0.83
3.72	(15)	1.00
3.42		0.13
3.03		0.10
2.86		0.07
2.58		0.10
2.51	(10)	0.67
2.42		0.13
2.28		0.10
2.22		0.07
2.17		0.13
2.02		0.33
1.90		0.10
1.86		0.07
1.76		0.10
1.68		0.07
1.61		0.10
1.56		0.10
1.487		0.07
1.455		0.07
1.425		0.07
1.399		0.07

590. HgI_2*

d		I/I1
6.2		0.30
4.11	(40)	0.80
3.56	(50)	1.00
3.00		0.30
2.76		0.40
2.18	(50)	1.00
2.05		0.12
1.92		0.14
1.86		0.25
1.76		0.10
1.65		0.06
1.54		0.12
1.50		0.08
1.418		0.06
1.371		0.04
1.346		0.04
1.314		0.04
1.260		0.14

591. Hg_2I_2*

d		I/I1
4.54		0.20
3.49	(50)	1.00
2.90	(12.5)	0.25
2.46		0.25
2.23	(25)	0.50
2.10		0.20
1.88		0.20
1.74		0.12
1.60		0.12
1.56		0.06
1.490		0.10
1.373		0.06
1.333		0.04
1.247		0.10
1.114		0.06

592. $K_2HgI_4.3H_2O$

d		I/I1
13.5		0.20
7.2	(10)	1.00
6.5		0.20
5.6		0.20
4.30		0.50
4.06		0.50
3.70		0.30
3.49	(8)	0.80
3.42	(8)	0.80
3.28		0.50
3.12		0.10
3.00		0.40
2.74		0.50
2.66		0.10
2.49		0.60
2.32		0.10
2.24		0.50
2.15		0.30
2.11		0.60
2.03		0.20
1.97		0.20
1.91		0.10
1.86		0.30
1.81		0.20
1.76		0.20
1.67		0.10
1.61		0.20
1.58		0.20
1.54		0.10

593. $HgNO_3.H_2O$

d		I/I1
6.6		0.17
5.6	(17.5)	1.00
4.75		0.11
4.20		0.11
3.75	(5)	0.29
3.47	(7)	0.40
3.20		0.17
3.10		0.17
2.80		0.23
2.67		0.06
2.50		0.17
2.38		0.17
2.32		0.17
2.24		0.23
2.17		0.06
2.09		0.11
1.96		0.23
1.91		0.06
1.87		0.06
1.82		0.11
1.79		0.11
1.74		0.06
1.68		0.06
1.61		0.11

594. HgC_2O_4

d		I/I1
4.78		0.50
3.99	(40)	1.00
3.42	(40)	1.00
3.07		0.63
2.78		0.63
2.63		0.20
2.53		0.03
2.38		0.15
2.27	(40)	1.00
1.99		1.00
1.89		0.31
1.77		0.38
1.72		0.20
1.68		0.15
1.64		0.15
1.60		0.23
1.54		0.18
1.453		0.05
1.430		0.05
1.390		0.20
1.358		0.05
1.320		0.23
1.280		0.03
1.260		0.08
1.210		0.08
1.190		0.05
1.135		0.18
1.108		0.03
1.084		0.05
1.071		0.05
1.038		0.03
1.023		0.05
1.013		0.05

595. HgO*

d		I/I1
2.96	(40)	1.00
2.83	(30)	0.75
2.75		0.38
2.40	(30)	0.75
1.81		0.63
1.75		0.08
1.64		0.15
1.60		0.10
1.486		0.38
1.440		0.20
1.413		0.08
1.378		0.05
1.200		0.13
1.187		0.10
1.161		0.05
1.148		0.03
1.103		0.05
1.079		0.03
1.050		0.05B
1.026		0.03
0.982		0.03
0.943		0.03

596. $Hg_3(PO_4)_2$

d		I/I1
4.01	(5)	0.71
3.52		0.29
3.19		0.29
3.01	(7)	1.00
2.85	(3)	0.43
2.71		0.14
2.41		0.29
2.12		0.14
2.05		0.14
2.01		0.29

597. Hg_2PO_4

d		I/I1
7.2		0.11
6.3		0.22
5.5		0.22
4.83		0.44
4.40		0.56
3.85		0.44
3.60		0.33
3.48		0.44
3.09	(6)	0.67
2.94	(8)	0.89
2.72		0.22
2.60	(9)	1.00
2.45		0.22
2.28		0.44
2.18		0.17
2.12		0.22
2.01		0.17
1.94		0.22
1.89		0.11
1.86		0.17
1.81		0.17
1.77		0.17
1.66		0.22
1.62		0.11
1.57		0.22
1.52		0.22
1.50		0.22
1.440		0.22
1.384		0.11
1.346		0.11

598. $Hg(CH_3COO)_2$

d		I/I1
7.1	(30)	1.00
6.5		0.03
6.1		0.03
5.6		0.03
4.88		0.13
4.05		0.13
3.80	(5)	0.17
3.62	(15)	0.50
3.47		0.13
3.22		0.07
3.02		0.10
2.81		0.07
2.62		0.07
2.48		0.07
2.37		0.07
2.19		0.07
2.12		0.13
2.03		0.10
1.98		0.05
1.93		0.07
1.88		0.03
1.77		0.03
1.74		0.03
1.67		0.03
1.62		0.03
1.51		0.03
1.404		0.03
1.372		0.03
1.320		0.03
1.272		0.03
1.242		0.03

599. $HgSO_4$

d		I/I1
3.90	(6)	1.00
3.40	(3)	0.50
3.26		0.17
3.01	(2)	0.33
2.81		0.33
2.37		0.33
2.25		0.17
2.13		0.17
2.04		0.33
1.99		0.33
1.93		0.17
1.84		0.17
1.80		0.17
1.64		0.17
1.53		0.17
1.477		0.17
1.381		0.17
1.304		0.17

600. $HgSO_4.2HgO$

d		I/I1
6.2	(8)	0.80
5.5	(8)	0.80
3.33		0.40
2.92	(10)	1.00
2.61		0.40
2.31		0.10
1.93		0.20
1.88		0.10
1.75		0.10
1.66		0.20
1.56		0.10
1.51		0.10
1.470		0.10

601. Hg_2SO_4

d		I/I1
4.42	(12.5)	0.63
4.19	(12.5)	0.63
3.61		0.10
3.47		0.05
3.11		0.10
3.03	(20)	1.00
2.85		0.05
2.73		0.10
2.55		0.25
2.37		0.10
2.20		0.30
2.08		0.30
2.01		0.05
1.96		0.10
1.89		0.25
1.80		0.10
1.73		0.15
1.66		0.05
1.62		0.05
1.52		0.10

602. HgS* (cubic)

d		I/I1
3.37	(50)	1.00
2.92		0.16
2.06	(15)	0.30
1.76	(15)	0.30
1.69		0.04
1.460		0.02
1.340		0.08
1.305		0.06
1.191		0.04
1.124		0.04

603. HgS*

d		I/I1
3.36	(62.5)	0.83
3.16		0.27
2.85	(75)	1.00
2.35		0.08
2.06		0.27
1.97	(25)	0.33
1.89		0.01
1.76		0.11
1.72		0.20
1.67		0.27
1.57		0.08B
1.429		0.09
1.395		0.03
1.340		0.11
1.300		0.13
1.252		0.11
1.179		0.04B
1.121		0.05
1.100		0.05
1.080		0.01
1.027		0.03

604. HgCNS

d		I/I1
6.5	(15)	0.75
5.4	(15)	0.75
4.37		0.75
3.97		0.10
3.80	(20)	1.00
3.32		0.75
2.88		0.05
2.67		0.40
2.56		0.40
2.42		0.50
2.14		0.20
2.02		0.20
1.98		0.20
1.92		0.20
1.89		0.20
1.83		0.20
1.79		0.20
1.70		0.10
1.61		0.05
1.490		0.05
1.445		0.05
1.150		0.05
1.129		0.05

605. Mo*

d		I/I1
2.22	(175)	1.00
1.57	(62.5)	0.36
1.281	(100)	0.57
1.114		0.17
0.995		0.23
0.908		0.07
0.841		0.23
0.787		0.03
0.742		0.14
0.704		0.11
0.672		0.09
0.643		0.05
0.617		0.14

606. H_2MoO_4

d		I/I1
10.9		0.50
8.9		0.63
7.7		0.50
6.6	(40)	1.00
5.9		0.25
5.3		0.15
5.0		0.15
4.71		0.18
4.34		0.05
4.10		0.38
3.47	(40)	1.00
3.30		0.63
3.06	(30)	0.75
2.90		0.38
2.77		0.20
2.63		0.13
2.55		0.25
2.44		0.25
2.37		0.18
2.32		0.20
2.24		0.25
2.19		0.10
2.10		0.10
2.02		0.13
1.95		0.38
1.85		0.05
1.80		0.18
1.69		0.18
1.64		0.05
1.59		0.15
1.53		0.13

607. Mo_2C*

d		I/I1
2.60		0.29
2.36		0.24
2.28	(212.5)	1.00
1.75		0.24
1.50	(75)	0.35
1.350	(75)	0.35
1.300		0.03
1.267		0.35
1.259		0.35
1.182		0.04
1.142		0.06
1.079		0.04
1.005		0.07
0.983		0.03
0.965		0.19
0.930		0.09
0.907		0.05
0.892		0.05
0.872		0.04
0.837		0.08
0.818		0.05

608. Molybdenum Oxalate

d		I/I1
8.4		0.27
5.2	(75)	1.00
4.41	(50)	0.67
4.17		0.17
3.77	(40)	0.53
3.30		0.53
3.09		0.08
2.99		0.12
2.90		0.08
2.77		0.17
2.59		0.11
2.46		0.13
2.17		0.20
2.14		0.20
2.07		0.13
1.91		0.23
1.87		0.08
1.78		0.07
1.74		0.03
1.70		0.08
1.66		0.05
1.63		0.11
1.59		0.12
1.52		0.09
1.485		0.08
1.460		0.03
1.421		0.04
1.388		0.09
1.340		0.09
1.280		0.05
1.235		0.03
1.180		0.03

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

d		*I/I*1
609. MoO_2*		
6.9		0.24
3.80	(75)	0.60
3.46	(50)	0.40
3.25	(125)	1.00
3.00		0.05
2.66		0.32
2.52		0.08
2.30		0.32
2.26		0.08
2.13		0.06
1.97		0.24
1.85		0.24
1.73		0.16
1.70		0.04
1.67		0.12
1.63		0.12
1.60		0.12
1.57		0.14
1.50		0.03
1.475		0.08
1.440		0.20
1.395		0.06
610. Mo_3O_8		
3.42	(125)	1.00
2.42	(100)	0.80
2.22		0.40
2.17		0.03
1.84		0.06
1.71	(100)	0.80
1.57		0.06
1.53		0.16
1.470		0.03
1.405		0.20
1.350		0.02
1.305		0.02
1.285		0.24
1.211		0.16
1.180		0.02
1.141		0.06
1.114		0.06
1.087		0.04
1.032		0.02
1.015		0.01
0.997		0.06
0.976		0.02
0.955		0.02
0.920		0.06
0.880		0.02
0.857		0.05
0.842		0.05
611. $MoSi_2$		
3.91		0.40
2.95	(8)	0.53
2.25	(15)	1.00
1.95		0.27
1.59		0.33
1.478		0.20
1.408		0.20
1.298		0.07
1.253	(8)	0.53
1.311		0.33
1.057		0.20
1.010		0.20
0.980		0.40
612. $NdCl_3$		
6.8		0.20
3.47	(75)	0.75
2.85	(75)	0.75
2.59	(100)	1.00
2.25		0.04
2.18		0.30
2.00		0.50
1.96		0.01
1.92		0.07
1.77		0.25
1.73		0.30
1.59		0.50
1.56		0.15
1.50		0.10
1.453		0.06
1.420		0.13
1.390		0.01
1.353		0.02
1.313		0.07
1.270		0.08
1.248		0.06
1.230		0.10
1.202		0.01
1.190		0.06
1.124		0.04
1.103		0.07
1.080		0.03
1.060		0.07
1.050		0.07

d		*I/I*1
613. $NdCl_3.6H_2O$		
6.5	(20)	1.00
6.0	(12.5)	0.63
5.4		0.50
5.1		0.50
4.85		0.20
4.56		0.30
4.41		0.30
3.98		0.45
3.60		0.35
3.43	(20)	1.00
3.13		0.20
2.88		0.25
2.67		0.05
2.61		0.10
2.54		0.10
2.47		0.05
2.42		0.35
2.36		0.05
2.30		0.25
2.14		0.35
2.07		0.20
2.00		0.05
1.96		0.25
1.92		0.25
1.87		0.05
1.84		0.05
1.78		0.05
1.69		0.10
1.61		0.05
1.55		0.10
1.52		0.10
1.480		0.05
1.439		0.05
1.416		0.05
1.390		0.05
1.358		0.05
1.330		0.05
1.300		0.10
1.272		0.05
1.251		0.05
614. Neodymium Ammonium Nitrate		
9.7		0.03
8.8	(30)	1.00
7.8		0.03
6.9	(30)	1.00
6.2		0.07
5.7		0.27
5.4	(10)	0.33
5.2		0.27
4.44		0.07
4.23		0.30
3.93		0.23
3.56		0.17
3.33		0.17
3.14		0.33
2.94		0.10
2.81		0.33
2.68		0.03
2.63		0.07
2.53		0.10
2.44		0.20
2.38		0.13
2.33		0.03
2.28		0.13
2.21		0.13
2.15		0.23
2.02		0.20
1.90		0.20
1.84		0.03
1.80		0.07
1.76		0.10
1.69		0.10
1.63		0.03
1.59		0.07
1.56		0.03
1.53		0.03
1.51		0.03
1.470		0.07
1.440		0.03
1.410		0.07
1.380		0.03
1.345		0.03
1.295		0.07
615. Ni*		
2.03	(25)	1.00
1.76	(12.5)	0.50
1.244	(8)	0.32
1.061		0.32
1.017		0.04
0.808		0.08
0.788		0.08
0.719		0.08
0.678		0.08

d		*I/I*1
616. $Ni(C_2H_3O_2)_2$		
7.4		0.05
6.9	(40)	1.00
5.9		0.03
4.75	12.5)	0.31
4.48		0.03
4.25		0.08
4.00	(10)	0.25
3.82		0.15
3.57		0.13
3.14		0.25
3.03		0.05
2.95		0.03
2.87		0.15
2.71		0.05
2.50		0.15
2.41		0.05
2.30		0.13
2.18		0.08
2.11		0.10
2.06		0.03
2.01		0.08
1.96		0.03
1.91		0.05
1.86		0.08
1.80		0.04
1.74		0.03
1.70		0.03
1.66		0.04
1.61		0.03
1.58		0.03
1.52		0.03
1.480		0.03
1.440		0.04
1.410		0.03
1.166		0.03
617. $NiAl_2O_4$*		
2.43	(6)	0.75
2.01	(6)	0.75
1.55		0.13
1.421	(8)	1.00
618. $NiCl_2$*		
5.7	(50)	0.67
2.96	(30)	0.40
2.46	(75)	1.00
2.27		0.07
1.91		0.13
1.74		0.40
1.66		0.17
1.495		0.03
1.440		0.01
1.419		0.09
1.390		0.03
1.284		0.03
1.232		0.04
1.131		0.01
1.109		0.01
1.100		0.08
1.030		0.01
1.003		0.04
619. $NiCl_2.2H_2O$*		
5.4	(40)	0.80
4.42	(30)	0.60
3.45		0.06
2.91		0.50
2.74		0.40
2.44	(50)	1.00
2.21		0.40
2.16		0.06
2.11		0.40
1.87		0.25B
1.72		0.50
1.66		0.35
1.63		0.35
1.61		0.35
1.52		0.14
1.465		0.12
1.389		0.06
1.359		0.16
1.317		0.06
1.271		0.10
1.245		0.02
1.219		0.12

d		*I/I*1
620. $NiCl_2.4H_2O$		
5.4		0.31
4.80	(25)	0.63
4.29	(40)	1.00
3.95		0.20
3.63		0.03
3.40		0.03
3.17		0.05
2.94		0.31
2.83	(30)	0.50
2.70		0.38
2.60		0.15
2.52		0.38
2.41		0.18
2.34		0.03
2.27		0.03
2.21		0.03
2.14		0.13
2.09		0.13
2.00		0.31
1.95		0.31
1.83		0.18
1.76		0.44
1.70		0.20
1.65		0.15
1.55		0.13
1.52		0.08
1.470		0.03
1.420		0.05
1.403		0.08
1.355		0.08
1.318		0.08
1.277		0.05
621. $NiCl_2.6H_2O$		
5.5	(50)	1.00
4.85	(50)	1.00
3.53	(25)	0.50
3.08		0.04
2.95		0.50
2.70		0.50
2.54		0.30
2.40		0.50
2.18		0.50
2.05		0.06
2.02		0.06
1.97		0.20
1.90		0.20
1.86		0.14
1.81		0.02
1.77		0.14
1.69		0.20
1.60		0.14
1.54		0.16
1.495		0.02
1.459		0.06
1.390		0.02
1.372		0.04
1.338		0.03
1.304		0.02
1.273		0.04
1.234		0.02
1.195		0.02
1.180		0.02
1.167		0.02
1.129		0.02
1.100		0.02
622. $Ni(CN)_2.4H_2O$		
4.39	(30)	1.00
3.63		0.07
3.53		0.07
2.89		0.13
2.68		0.03
2.54		0.07
2.50	(10)	0.33
2.17	(8)	0.27
2.11		0.03
2.04		0.03
1.93		0.03
1.82		0.03
1.77		0.13
1.72		0.03
1.66		0.03
1.64		0.17
1.58		0.03
1.54		0.03
1.490		0.03
1.450		0.03
1.370		0.03
1.341		0.03
1.291		0.03
1.253		0.03
1.202		0.03
1.178		0.03
1.142		0.03
1.115		0.03
1.017		0.03
0.997		0.03

d		*I/I*1
623. Nickel Fluoride		
4.85	(50)	1.00
4.10	(25)	0.50
3.78		0.04
3.11		0.30
2.98	(25)	0.50
2.75		0.20
2.53		0.12
2.44		0.14
2.31		0.10
2.22		0.12
2.15		0.50
2.00		0.30
1.93		0.16
1.88		0.08
1.78		0.16
1.74		0.25
1.69		0.04
1.65		0.08
1.59		0.08
1.53		0.08
1.487		0.04
1.460		0.10
1.438		0.04
1.400		0.06
1.368		0.08
1.310		0.02
1.260		0.06
1.215		0.06
1.188		0.04
1.160		0.04
1.121		0.02
624. $Ni(CHO_2)_2.2H_2O$		
4.87	(30)	0.75
4.53	(40)	1.00
4.24		0.20
3.93		0.03
3.63		0.03
3.34		0.25
3.12		0.03
3.02		0.03
2.78		0.15
2.70		0.03
2.58	(15)	0.38
2.42		0.15
2.27		0.15
2.18		0.10
2.12		0.08
2.03		0.15
1.91		0.10
1.83		0.08
1.76		0.08
1.68		0.15
1.63		0.08
1.59		0.03
1.56		0.03
1.54		0.03
1.50		0.05
1.460		0.03
1.399		0.03
1.380		0.05
1.355		0.03
1.340		0.03
1.312		0.03
1.279		0.05
1.230		0.03
1.210		0.03
1.166		0.03
1.141		0.03
1.114		0.03
1.087		0.03
1.069		0.03
1.016		0.03
625. $Ni(OH)_2$*		
4.60	(10)	0.67B
2.70	(15)	1.00
2.33	(10)	0.67B
1.75		0.07
1.56		0.53
1.48		0.33
1.348		0.07
1.295		0.07

d		*I/I*1
626. $Ni(NO_3)_2.6H_2O$		
7.2		0.07
5.5	(30)	1.00
5.1		0.23
4.40		0.07
4.14		0.20
3.78	(30)	1.00
3.40		0.33
3.12		0.10
2.90		0.20
2.74	(15)	0.50
2.62		0.03
2.55		0.20
2.37		0.17
2.28		0.10
2.21		0.05
2.16		0.10
2.06		0.03
1.99		0.07
1.89		0.07
1.84		0.10
1.70		0.05
1.65		0.05
1.60		0.03
627. $NiC_2O_4.2H_2O$		
4.72	(20)	1.00
3.90	(4)	0.20
2.96	(4)	0.20
2.52		0.10
2.18		0.05
2.06		0.05
1.91		0.05
1.86		0.05
1.57		0.05
628. NiO*		
2.40	(75)	0.60
2.08	(125)	1.00
1.474	(75)	0.60
1.258		0.24
1.203		0.12
1.042		0.02
0.957		0.04
0.933		0.06
0.852		0.03
0.802		0.02
629. $NiMn_2O_4$*		
4.85		0.12
2.97		0.30
2.53	(50)	1.00
2.41		0.25
2.09	(25)	0.50
1.71		0.08
1.61		0.40
1.480	(30)	0.60
1.280		0.08
1.260		0.12
1.207		0.08
1.119		0.04
1.090		0.10
1.048		0.04
630. $NiSO_4.6H_2O$		
6.4		0.04
4.6	(12.5)	0.25
4.26	(50)	1.00
3.96		0.02
3.77		0.02
3.38		0.12
3.22		0.02
3.18		0.02
2.96		0.18
2.72	(10)	0.20
2.57		0.20
2.34		0.16
2.13		0.20
2.07		0.02
2.02		0.04
1.98		0.02
1.89		0.10
1.85		0.04
1.83		0.02
1.80		0.02
1.75		0.10
1.70		0.08
1.65		0.08
1.59		0.04
1.54		0.02
1.51		0.04
1.470		0.02
1.393		0.02
1.354		0.02
1.301		0.02
1.280		0.02
1.262		0.02
1.250		0.02
1.216		0.02
1.188		0.02
1.164		0.02
1.147		0.02
1.130		0.02
1.112		0.02B
1.035		

d		
631. $NiSO_4$		
8.5		
7.5		
6.0		
5.3		(30)
4.45		
4.20		(50)
3.75		
3.45		
2.96		
2.85		(12.5)
2.75		
2.65		
2.49		
2.36		
2.24		
2.19		
2.09		
2.01		
1.94		
1.90		
1.86		
1.79		
1.72		
1.70		
1.65		
1.61		
632. $NiSO_4.(NH_4)_2SO$		
7.2		
6.2		
5.4		(15)
5.1		
4.16		(40)
3.76		(20)
3.58		
3.39		
3.11		
3.02		
2.78		
2.54		
2.43		
2.21		
2.14		
2.06		
1.98		
1.91		
1.85		
1.80		
1.72		
1.68		
1.62		
1.55		
1.472		
1.432		
633. Nickel Tartrat		
6.4		
5.9		(4)
5.6		
5.2		(8)
4.53		
4.04		
3.70		(3)
3.48		
3.13		
3.01		
2.85		
2.64		
2.31		
2.25		
2.18		
2.12		
2.02		
1.92		
1.86		
1.79		
1.73		
634. Os		
2.36		(8)
2.16		(6)
2.07		(40)
1.59		
1.363		
1.231		
1.178		
1.158		
1.144		
1.082		
1.039		
0.961		
0.915		
0.876		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

631. $NiSO_4.7H_2O$

d	I/I₁
5.5	0.04
7.5	0.04
6.0	0.02
5.3	(30) 0.60
4.45	0.12
4.20	(50) 1.00
3.75	0.16
3.45	0.16
2.96	0.06
2.85	(12.5) 0.25
2.75	0.06
2.65	0.16
2.49	0.04
2.36	0.04
2.24	0.10
2.19	0.12
2.09	0.08
2.01	0.02
1.94	0.06
1.90	0.02
1.86	0.06
1.79	0.02
1.73	0.04
1.70	0.02
1.65	0.04
1.61	

632. $NiSO_4.(NH_4)_2SO_4.6H_2O$

d	I/I₁
7.2	0.05
6.2	0.18B
5.4	(15) 0.38
5.1	0.10
4.16	(40) 1.00
3.76	(20) 0.50
3.58	0.08
3.39	0.18
3.11	0.03
3.02	0.38
2.78	0.20
2.54	0.05
2.43	0.15
2.21	0.08
2.14	0.08
2.06	0.05
1.98	0.03
1.91	0.10
1.85	0.05
1.80	0.08
1.72	0.05
1.68	0.05
1.62	0.03
1.55	0.03
1.472	0.03
1.432	0.03

633. Nickel Tartrate (ous)

d	I/I₁
6.4	0.25
5.9	(4) 0.50
5.6	0.13
5.2	(8) 1.00
4.53	0.13
4.04	0.25
3.70	(3) 0.38
3.48	0.25
3.13	0.25
3.01	0.13
2.85	0.38
2.64	0.13
2.31	0.13
2.25	0.13
2.18	0.13
2.12	0.13
2.02	0.13
1.92	0.13
1.86	0.13
1.79	0.13
1.73	0.13

634. Os*

d	I/I₁
2.36	(8) 0.20
2.16	(6) 0.15
2.07	(40) 1.00
1.59	0.10
1.363	0.13
1.231	0.13
1.178	0.03
1.158	0.10
1.144	0.08
1.082	0.03
1.039	0.03
0.981	0.03
0.915	0.04
0.876	0.05

635. Pd*

d	I/I₁
2.23	(150) 1.00
1.94	(75) 0.50
1.371	(40) 0.27
1.170	0.27
1.120	0.05
0.970	0.01
0.891	0.05
0.869	0.05
0.793	0.02
0.748	0.02

636. $PdCl_2$

d	I/I₁
5.3	(62.5) 1.00
3.29	0.24
3.11	0.28
2.39	(50) 0.80
2.25	0.03
2.02	0.06
1.93	0.03
1.87	0.10
1.82	0.13
1.77	0.24
1.64	(25) 0.40
1.61	0.13
1.57	0.20
1.54	0.03
1.50	0.03
1.430	0.05
1.370	0.02
1.330	0.06
1.308	0.06
1.250	0.03
1.208	0.08
1.124	0.11
1.068	0.02
1.023	0.05
0.960	0.03
0.934	0.05

637. $Pd(NO_3)_2$

d	I/I₁
5.8	(30) 0.48
5.3	0.24
4.85	0.06
4.22	(62.5) 1.00
3.93	0.40
3.58	0.11
3.48	0.11
2.95	0.48
2.80	(40) 0.64
2.65	0.24
2.56	0.16
2.40	0.16
2.30	0.16
2.25	0.02
2.10	0.40
2.06	0.16
1.96	0.08
1.90	0.13
1.82	0.24
1.78	0.13
1.74	0.24
1.69	0.02
1.62	0.13
1.57	0.10
1.54	0.13
1.51	0.10
1.495	0.05
1.440	0.13
1.400	0.11
1.355	0.05
1.329	0.05
1.296	0.05
1.265	0.05

638. PCl_5

d	I/I₁
6.7	0.03
5.8	0.13
4.98	(40) 1.00
4.69	(30) 0.75
3.98	0.20
3.66	0.05
3.47	0.15
2.95	0.50
2.87	0.25
2.78	(40) 1.00
2.44	0.20
2.32	0.10
2.19	0.10
2.08	0.05
2.01	0.15
1.94	0.13
1.86	0.03
1.82	0.03
1.79	0.05
1.67	0.03
1.60	0.13
1.57	0.05
1.472	0.05
1.420	0.05
1.300	0.03
1.212	0.03

639. P_2O_5

d	I/I₁
5.4	(75) 1.00
5.2	(40) 0.53
3.72	0.04
3.39	0.11
3.27	0.33
3.15	0.20
3.02	(40) 0.53
2.57	0.08
2.43	0.17
2.32	0.08
2.24	0.33
2.11	0.03
2.06	0.03
2.00	0.01
1.95	0.23
1.79	0.03
1.75	0.01
1.69	0.01
1.67	0.02
1.63	0.01
1.59	0.01
1.52	0.04
1.485	0.05
1.428	0.03
1.401	0.03
1.357	0.01
1.335	0.03
1.299	0.07
1.266	0.03
1.252	0.03
1.236	0.03
1.210	0.01
1.185	0.03
1.155	0.01
1.140	0.01
1.124	0.02
1.099	0.01
1.084	0.01

640. P_2S_5

d	I/I₁
8.7	0.13
7.4	0.13
6.7	(15) 0.50
6.0	0.23
5.5	0.23
5.1	0.07
4.90	(10) 0.33
4.56	0.13
4.35	0.23
4.05	0.33
3.91	0.27
3.70	0.10
3.45	0.13
3.31	0.13
2.90	(30) 1.00
2.76	0.23
2.65	0.07
2.50	0.13
2.43	0.30
2.33	0.20
2.19	0.20
2.13	0.13
2.06	0.17
2.02	0.17
1.97	0.07
1.90	0.03
1.83	0.10
1.76	0.13
1.73	0.33
1.69	0.10
1.62	0.07
1.56	0.13
1.50	0.07

641. $20MoO_3.2H_3PO_4.48H_2O$

d	I/I₁
11.2	(25) 1.00
9.8	(20) 0.80
5.0	0.20
4.80	0.20
4.35	0.36
3.81	0.28
3.41	0.40
3.21	(20) 0.80
3.10	0.40
2.81	0.16
2.68	0.16
2.55	0.16
2.46	0.24
2.35	0.24
2.18	0.12
2.11	0.12
2.05	0.08
1.96	0.28
1.92	0.24
1.74	0.16
1.69	0.20
1.62	0.12
1.55	0.08
1.490	0.08

642. Pt*

d	I/I₁
2.25	(50) 1.00
1.95	(15) 0.30
1.382	(8) 0.16
1.178	0.16
1.128	0.03
0.897	0.03
0.874	0.02

643. $(NH_4)_2PtCl_6$*

d	I/I₁
5.7	(50) 1.00
4.93	(30) 0.60
3.48	0.20
2.97	(25) 0.50
2.46	0.30
2.26	0.10
2.20	0.20
2.01	0.08
1.89	0.16
1.74	0.14
1.66	0.16
1.64	0.08
1.56	0.03
1.50	0.03
1.421	0.03
1.376	0.06
1.315	0.03
1.282	0.04
1.195	0.03
1.160	0.02
1.140	0.02
1.100	0.03

644. K_2PtCl_6*

d	I/I₁
5.6	(30) 1.00
4.87	(10) 0.33
3.44	(10) 0.33
2.93	0.33
2.43	0.33
2.23	0.13
2.18	0.13
1.99	0.17
1.87	0.17
1.72	0.17
1.65	0.13
1.54	0.03
1.485	0.03
1.404	0.05
1.365	0.07
1.302	0.05
1.268	0.05

645. K_2PtCl_4*

d	I/I₁
7.0	(50) 1.00
4.97	0.12
4.13	0.30
3.54	0.60
3.16	(40) 0.80
2.47	(40) 0.80
2.33	0.02
2.21	0.02
2.12	0.16
2.06	0.08
1.95	0.40
1.76	0.25
1.70	0.04
1.65	0.02
1.61	0.04
1.58	0.12
1.54	0.06
1.410	0.06
1.330	0.08
1.305	0.06
1.263	0.02
1.239	0.04

646. Platinum Sodium Chloride

d	I/I₁
8.0	(15) 1.00
6.5	(10) 0.67
5.8	0.67
5.6	(15) 1.00
4.60	0.67
4.49	0.67
3.99	0.67
3.85	0.47
3.32	0.33
3.12	0.13
2.80	0.27
2.66	0.60
2.51	0.27
2.42	0.27
2.32	0.13
2.25	0.20
2.14	0.13
2.03	0.13
1.95	0.07
1.86	0.10
1.78	0.10
1.72	0.07
1.67	0.07
1.61	0.07

647. $BaPt(CN)_4.4H_2O$

d	I/I₁
9.0	0.53
8.0	0.40
6.9	0.53
5.8	(15) 1.00
4.65	0.27
4.29	0.53
4.10	0.20
3.75	0.27
3.23	(10) 0.67
2.97	0.60
2.89	(10) 0.67
2.78	0.40
2.69	0.40
2.42	0.07
2.34	0.40
2.26	0.27
2.20	0.07
2.14	0.13
2.07	0.13
2.02	0.13
1.96	0.13
1.88	0.13
1.81	0.07
1.69	0.20
1.65	0.27
1.57	0.13
1.485	0.13
1.460	0.13
1.425	0.13
1.389	0.07
1.351	0.13

648. Platinum Magnesium Cyanide

d	I/I₁
9.1	(25) 1.00
8.0	(15) 0.60
5.3	0.60
4.90	0.36
4.65	0.40
4.30	0.16
4.00	0.24
3.51	0.16
3.35	0.16
3.09	(17.5) 0.70
2.90	0.16
2.77	0.04
2.67	0.20
2.58	0.08
2.46	0.08
2.32	0.20
2.24	0.16
2.15	0.08
2.09	0.08
2.02	0.12
1.93	0.12
1.84	0.12
1.78	0.08
1.73	0.08
1.64	0.04
1.55	0.04

649. $K_2Pt(CN)_4.3H_2O$

d	I/I₁
8.0	(30) 1.00
6.7	0.33
4.90	0.20
4.00	(12.5) 0.42
3.60	0.20
3.28	(25) 0.83
3.16	0.33
2.90	0.20
2.69	0.13
2.56	0.13
2.45	0.23
2.37	0.23
2.29	0.03
2.19	0.20
2.12	0.07
2.08	0.07
2.05	0.07
2.01	0.07
1.97	0.07
1.94	0.10
1.89	0.07
1.79	0.10
1.76	0.07
1.70	0.03
1.64	0.10
1.58	0.10
1.491	0.07
1.446	0.07
1.415	0.03
1.385	0.03
1.355	0.07

650. K*

d	I/I₁
3.75	(50) 1.00
2.65	(8) 0.16
2.16	(15) 0.30
1.87	0.04
1.68	0.04
1.52	0.02
1.418	0.02

651. $KC_2H_3O_2$

d	I/I₁
13.6	(17.5) 0.88
10.7	(20) 1.00
9.2	0.75
3.60	0.20
3.47	0.05
3.33	0.10
3.24	(17.5) 0.88B
2.91	0.15B
2.67	0.10B
2.45	0.10B
2.30	0.08
2.17	0.10
2.09	0.05
2.05	0.08
2.00	0.10
1.95	0.08
1.89	0.05
1.84	0.05
1.79	0.10
1.73	0.05
1.70	0.05
1.64	0.05
1.61	0.05
1.56	0.05

652. Potassium Arsenate

d	I/I₁
5.2	(20) 0.67
3.81	(30) 1.00
3.07	0.07
2.98	(20) 0.67
2.69	0.23
2.40	0.03
2.00	0.67
1.91	0.03
1.84	0.03
1.79	0.03
1.74	0.03
1.70	0.13
1.61	0.20
1.490	0.10
1.380	0.13
1.349	0.05
1.308	0.07
1.271	0.03
1.230	0.13
1.208	0.03
1.165	0.03
1.070	0.03
1.059	0.03
1.032	0.07

653. Potassium Arsenite

d	I/I₁
9.7	0.05
7.4	0.08
5.7	0.05
5.0	0.05
4.75	0.10
4.50	0.05
3.98	0.25
3.68	0.20
3.20	0.20
2.99	(20) 1.00
2.87	0.25
2.65	(20) 1.00
2.43	0.20
2.32	0.10
2.19	0.15
2.15	0.35
2.07	0.15
2.00	0.20
1.94	0.20
1.92	0.15
1.85	0.05
1.80	0.15
1.75	0.10
1.70	0.05
1.65	0.25
1.58	(8) 0.40
1.55	0.05
1.50	0.05
1.465	0.20
1.425	0.15
1.380	0.05
1.325	0.20
1.265	0.05
1.248	0.08

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

654. KN_3*

d		I/I1
4.33		0.07
3.05	(25)	0.33
2.75	(75)	1.00
2.55	(10)	0.13
2.32		0.12
2.16		0.13
1.93		0.11
1.85		0.05
1.78		0.07
1.70		0.12
1.65		0.01
1.53		0.08
1.403		0.05
1.370		0.08
1.335		0.07
1.308		0.04
1.270		0.01
1.139		0.04
1.082		0.04
1.009		0.01

655. $K(C_2H_3COO).3H_2O$

d		I/I1
5.7		0.10
5.4		0.10
5.1		0.10
4.64		0.05
4.23		0.05
3.89		0.05
3.75	(10)	0.50
3.55		0.05
3.29		0.20
3.21	(20)	1.00
3.12		0.05
3.00		0.10
2.90		0.05
2.84		0.05
2.73		0.05
2.66		0.05
2.50		0.15
2.38		0.05
2.30		0.10
2.23		0.10
2.12		0.15
1.98	(5)	0.25
1.86		0.05
1.79		0.05
1.73		0.05

656. $K_2B_4O_7.5H_2O$

d		I/I1
5.60	(10)	1.00
3.52	(10)	1.00
3.37	(10)	1.00
2.76		0.30
2.52		0.20
2.38		0.10
2.29		0.10
2.18		0.40
2.11		0.10
1.99		0.10
1.87		0.10
1.60		0.10
1.55		0.10
1.460		0.10

657. $KBrO_3$*

d		I/I1
4.38	(10)	0.50
3.20	(20)	1.00
3.00	(12.5)	0.63
2.72		0.05
2.18		0.50
2.01		0.08
1.89		0.25
1.77		0.25
1.73		0.10
1.60		0.10
1.50		0.10
1.460		0.08
1.412		0.25
1.380		0.05
1.358		0.15
1.235		0.15
1.178		0.10
1.140		0.10
1.100		0.05
1.074		0.05
1.025		0.05
1.004		0.05

658. KBr*

d		I/I1
3.29	(30)	1.00
2.33	(12.5)	0.42
1.89		0.10
1.64		0.07
1.468	(5)	0.17
1.343		0.07
1.164		0.03
1.095		0.03
1.040		0.03

659. K_2CO_3

d		I/I1
7.0		0.02
5.5		0.02
3.39		0.06
2.97	(10)	0.16
2.80	(62.5)	1.00
2.61	(20)	0.32
2.37		0.16
2.31		0.08
2.18		0.06
2.09		0.14
1.99		0.10
1.85		0.08
1.77		0.03
1.70		0.03
1.67		0.02
1.61		0.03
1.55		0.02
1.50		0.02
1.410		0.05
1.345		0.02
1.307		0.02

660. $KHCO_3$

d		I/I1
7.33		0.20
3.68	(8)	0.32
3.10		0.04
2.95		0.28
2.84	(25)	1.00
2.62	(8)	0.32
2.37		0.08
2.28		0.24
2.21		0.16
2.02		0.12
1.96		0.04
1.84		0.12
1.80		0.06
1.75		0.08
1.57		0.04
1.52		0.04
1.421		0.04
1.309		0.04

661. $KClO_3$

d		I/I1
4.40		0.06
3.45	(100)	1.00
3.31		0.10
2.86	(30)	0.30
2.79	(40)	0.40
2.57		0.06
2.32		0.15
2.10		0.30
1.91		0.08
1.81		0.02
1.78		0.02
1.71		0.02
1.67		0.01
1.62		0.04
1.490		0.13
1.421		0.02
1.396		0.01
1.330		0.01

662. $KClO_4$*

d		I/I1
5.6		0.08
4.44		0.30
4.00		0.02
3.78		0.02
3.62		0.20
3.48	(50)	1.00
3.34		0.16
3.13	(50)	1.00
2.88	(40)	0.80
2.81		0.20
2.51		0.50
2.38		0.02
2.26		0.08
2.16		0.50
2.11		0.40
2.05		0.02
1.86		0.08
1.78		0.06B
1.73		0.02
1.68		0.12
1.64		0.20
1.55		0.08

663. KCl*

d		I/I1
3.13	(50)	1.00
2.21	(30)	0.60
1.81	(7)	0.14
1.57		0.06
1.401		0.12
1.280		0.06
1.108		0.02
1.047		0.02
0.991		0.02

664. K_2CrO_4*

d		I/I1
5.2		0.06
4.28	(20)	0.32
3.81		0.13
3.07	(20)	0.32
2.96	(62.5)	1.00
2.57		0.13
2.47		0.11
2.28		0.28
2.14		0.24
1.92		0.06
1.82		0.03
1.72		0.05
1.66		0.02
1.61		0.03
1.475		0.05B
1.390		0.05
1.325		0.02B
1.280		0.02
1.250		0.02
1.203		0.02
1.170		0.02

665. $K_2Cr_2O_7$

d		I/I1
4.83		0.10
3.68		0.50
3.45		0.50
3.29	(20)	1.00
3.02	(15)	0.75
2.85	(12.5)	0.63
2.75		0.05
2.69		0.05
2.62		0.20
2.53		0.15
2.45		0.05
2.38		0.05
2.29		0.05
2.24		0.05
2.18		0.05
2.14		0.05
2.04		0.25
1.90		0.05
1.86		0.05
1.77		0.10
1.70		0.05
1.66		0.05
1.58		0.05
1.450		0.05
1.400		0.05

666. $K_2C_6H_6O_7.H_2O$

d		I/I1
6.6	(8)	0.40
5.7		0.15
3.90		0.20
3.29	(9)	0.45
3.20		0.30
2.86	(20)	1.00
2.62		0.20
2.50		0.05
2.41		0.20
2.27		0.20
2.13		0.05
2.07		0.10
2.01		0.10
1.86		0.05
1.81		0.05
1.71		0.10
1.50		0.05
1.465		0.05
1.410		0.05
1.325		0.05

667. KCNO*

d		I/I1
4.29		0.14
3.04	(25)	0.50
2.73	(50)	1.00
2.53	(15)	0.30
2.30		0.30
2.14		0.20
1.92		0.25
1.84		0.12
1.77		0.10
1.75		0.10
1.68		0.20
1.63		0.04
1.52		0.12
1.393		0.12
1.358		0.20
1.327		0.12
1.298		0.08
1.268		0.02
1.191		0.02
1.148		0.02
1.129		0.08
1.074		0.06
1.000		0.04

668. KCN*

d		I/I1
3.77		0.10
3.26	(100)	1.00
2.30	(62.5)	0.63
1.96	(12.5)	0.13
1.88		0.10
1.63		0.06
1.493		0.06
1.458		0.09
1.327		0.05
1.252		0.03
1.100		0.01

669. $K_3Fe(CN)_6$*

d		I/I1
6.7		0.03
5.9		0.03
5.2		0.03
4.70		0.02
4.14	(62.5)	1.00
3.99		0.05
3.71		0.02
3.36		0.02
3.21		0.02
3.09	(30)	0.48
2.94	(30)	0.48
2.63		0.48
2.44		0.02
2.31		0.03
2.21		0.06
2.09		0.48
1.99		0.03
1.87		0.08
1.83		0.02
1.79		0.02
1.73		0.02
1.68		0.02
1.64		0.02
1.60		0.02
1.55		0.02
1.51		0.02
1.475		0.16
1.420		0.02
1.316		0.03

670. $K_4Fe(CN)_6$

d		I/I1
6.6		0.20
5.3		0.10
4.91		0.20
4.22		0.20
3.95		0.23
3.60	(25)	0.83
3.47		0.33
3.10		0.67
2.98	(30)	1.00
2.84	(25)	0.83
2.75		0.03
2.39		0.03
2.31		0.03
2.20		0.67
2.12		0.50
2.09		0.27
2.02		0.23
1.94		0.13
1.80		0.33
1.74		0.27
1.66		0.03
1.490		0.20
1.458		0.07
1.422		0.03
1.402		0.03
1.377		0.07

671. $K_4Fe(CN)_6.3H_2O$

d		I/I1
8.5		0.13
6.2		0.10
4.70		0.04
4.20		0.10B
3.90		0.05
3.30		0.07
2.92	(100)	1.00
2.80		0.15
2.60		0.06
2.45		0.01
2.35		0.01
2.22	(30)	0.30
2.15		0.01
2.09	(20)	0.20
2.03		0.06
1.87		0.13
1.83		0.04
1.80		0 04
1.68		0.06
1.48		0.10
1.400		0.01
1.365		0.01
1.316		0.07
1.235		0.03

672. KF*

d		I/I1
3.08	(40)	0.27
2.66	(150)	1.00
1.88	(125)	0.83
1.60		0.10
1.54		0.27
1.333		0.08
1.223		0.04
1.191		0.20
1.089		0.10
1.027		0.01
0.943		0.01
0.901		0.01
0.889		0.02
0.843		0.01

673. $KF.2H_2O$

d		I/I1
4.42	(12.5)	0.63
4.08		0.10
3.37		0.40
3.20		0.35
3.01	(20)	1.00
2.58	(15)	0.75
2.48		0.05
2.22		0.05
2.17		0.20
2.12		0.50
2.03		0.45
1.94		0.40
1.86		0.05
1.81		0.05
1.75		0.08
1.69		0.05
1.59		0.08
1.495		0.05
1.435		0.05
1.409		0.05
1.304		0.05
1.185		0.05

674. K_2SiF_6*

d		I/I1
4.71	(62.5)	0.63
2.88		0.50
2.45		0.01
2.35	(100)	1.00
2.03	(75)	0.75
1.88		0.01
1.82		0.01
1.66		0.20
1.56		0.25
1.438		0.30
1.365		0.08
1.285		0.20
1.225		0.07
1.175		0.06
1.134		0.06
1.087		0.10
1.056		0.01
1.014		0.01
0.996		0.01
0.984		0.01
0.957		0.02
0.936		0.01
0.908		0.02

675. KOH

d		I/I1
4.00		0.17
3.71		0.13
3.13		0.23
2.93	(20)	0.67
2.69	(30)	1.00
2.58		0.13
2.44		0.17
2.30		0.23
1.98	(25)	0.83
1.83		0.17
1.77		0.03
1.73		0.03
1.64		0.10
1.55		0.07
1.460		0.07
1.400		0.07
1.368		0.10
1.340		0.07
1.309		0.07
1.285		0.03
1.240		0.03
1.142		0.07

676. KIO_3*

d		I/I1
4.47	(50)	0.50
3.15	(100)	1.00
2.58		0.03
2.38		0.01
2.23	(30)	0.30
1.99		0.20
1.82		0.30
1.58		0.08
1.53		0.01
1.486		0.05
1.445		0.01
1.410		0.10
1.346		0.02
1.286		0.02
1.236		0.01
1.191		0.07
1.116		0.01
1.081		0.01
1.052		0.02

677. $KIO_3.HIO_3$

d		I/I1
5.6		0.20
5.0		0.14
4.30		0.06
4.00		0.12
3.32	(50)	1.00
3.27	(30)	0.60
2.85		0.16
2.75		0.12
2.49		0.04
2.02	(20)	0.40
1.97		0.02
1.92		0.02
1.88		0.02
1.73		0.30
1.69		0.12
1.66		0.02
1.63		0.02
1.60		0.02
1.440		0.08
1.320		0.06
1.280		0.04
1.175		0.04
1.110		0.02
1.080		0.02
0.964		0.02

678. KIO_4*

d		I/I1
5.2	(50)	0.40
3.40	(125)	1.00
3.14		0.16
2.86		0.16
2.51		0.10
2.31		0.01
2.17		0.03
2.11	(30)	0.24
2.02		0.08
1.86		0.16
1.79		0.06
1.74		0.24
1.70		0.08
1.57		0.05
1.52		0.01
1.470		0.01
1.427		0.01
1.371		0.16
1.317		0.03
1.301		0.01
1.276		0.03
1.240		0.02

679. KI*

d		I/I1
4.08	(25)	0.40
3.53	(62.5)	1.00
2.50	(50)	0.80
2.13		0.24
2.03		0.32
1.76		0.16
1.62		0.08
1.58		0.32
1.442		0.24
1.358		0.05
1.247		0.03
1.194		0.03
1.176		0.08
1.117		0.05
1.095		0.02
1.080		0.02
1.067		0.03
0.990		0.02
0.980		0.02

680. KMn

d		I/I1
5.7		
4.55		
3.89		
3.71		
3.57	(30)	
3.43		
3.22	(50)	
2.95	(40)	
2.86		
2.66		
2.19		
2.03		
1.93		
1.84		
1.74		
1.68		
1.60		
1.54		
1.51		
1.480		
1.450		
1.430		
1.391		

681. K_2M

d		I/I1
5.9		
5.6		
4.70		
3.80		
3.40		
3.17	(40)	
3.03	(20)	
2.92		
2.77		
2.66		
2.26	(25)	
2.03		
1.97		
1.87		
1.79		
1.73		
1.69		
1.58		
1.52		
1.455		
1.385		
1.330		
1.295		
1.265		
1.210		
1.130		

682. KN(

d		I/I1
4.86		
3.77	(25)	
3.03	(9)	
2.77		
2.66	(7)	
2.19		
2.06		
1.96		
1.76		
1.54		
1.395		

683. KN

d		I/I1
4.00		
3.31	(100)	
2.60	(17.5)	
2.20	(15)	
2.12		
2.01		
1.85		
1.71		
1.67		
1.65		
1.61		
1.56		

684. $K_2O_2O_4$

d		I/I1
4.85		
3.95	(15)	
3.04		
2.80	(8)	
2.42		
2.27	(6)	
1.81		
1.66		
1.61		
1.52		
1.483		
1.396		
1.345		
1.250		
1.205		
1.180		
1.110		
0.994		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

680. $KMnO_4$*

d		I/I1
5.7		0.08
4.55		0.50
3.89		0.08
3.71		0.30
3.57	(30)	0.60
3.43		0.04
3.32	(50)	1.00
2.95	(40)	0.80
2.88		0.40
2.66		0.30
2.56		0.60
2.19		0.02
2.03		0.04
1.93		0.20
1.84		0.10
1.74		0.08
1.68		0.06
1.60		0.06
1.54		0.02
1.51		0.02
1.480		0.04
1.450		0.04α1
1.430		0.04
1.391		0.04

681. K_2MoO_4

d		I/I1
6.9		0.15
5.6		0.10
4.70		0.38
3.89		0.18
3.40		0.44
3.17	(40)	1.00
3.03	(20)	0.50
2.92		0.50
2.77		0.03
2.66		0.03
2.26	(25)	0.63
2.03		0.15
1.97		0.31
1.87		0.10
1.79		0.20
1.73		0.15
1.69		0.15
1.58		0.15
1.52		0.10
1.455		0.23
1.385		0.10
1.330		0.10
1.295		0.05
1.265		0.10
1.210		0.05
1.130		0.05

682. KNO_3*

d		I/I1
4.66		0.12
3.77	(25)	1.00
3.03	(9)	0.36
2.77		0.08
2.56	(7)	0.28
2.19		0.24
2.08		0.08
1.98		0.12
1.76		0.04
1.54		0.04
1.365		0.04

683. KNO_2

d		I/I1
4.00		0.02
3.31	(100)	1.00
2.80	(17.5)	0.18
2.20	(15)	0.15
2.12		0.06
2.01		0.08
1.85		0.01
1.71		0.01
1.67		0.01
1.65		0.01
1.61		0.01
1.56		0.01

684. $K_2OsO_4.2H_2O$

d		I/I1
4.85	(15)	1.00
3.95		0.13
3.04	(8)	0.53
2.80		0.27
2.42	(6)	0.40
1.97		0.27
1.81		0.13B
1.66		0.33
1.61		0.07
1.52		0.20
1.465		0.13
1.395		0.07
1.345		0.07
1.250		0.07
1.205		0.07
1.180		0.07
1.110		0.07
0.964		0.13
		0.07

685. $K_2C_2O_4$

d		I/I1
4.95		0.14
4.53		0.03
4.31		0.08
4.05		0.20
3.22		0.02
3.10		0.08
2.92	(50)	1.00
2.80		0.14
2.72		0.04
2.62		0.35
2.46	(30)	0.60
2.32	(30)	0.60
2.24		0.30
2.14		0.12
2.07		0.10
2.02		0.25
1.95		0.04
1.91		0.30
1.82		0.12
1.77		0.06
1.72		0.12
1.66		0.10
1.62		0.02
1.57		0.16
1.53		0.04
1.50		0.02
1.480		0.02
1.451		0.04
1.405		0.06
1.382		0.06
1.330		0.07
1.298		0.02
1.275		0.10
1.238		0.08
1.203		0.02
1.176		0.08
1.135		0.04
1.120		0.04

686. $K_2C_2O_4.H_2O$*

d		I/I1
4.97		0.28
4.33		0.13
4.07		0.16
3.23		0.02
3.08	(20)	0.32
2.95	(20)	0.32
2.81		0.32
2.74		0.13
2.60		0.24
2.45	(62.5)	1.00
2.32		0.06
2.27		0.13
2.16		0.10
2.07		0.13
2.02		0.16
1.93		0.10
1.82		0.10
1.74		0.03
1.69		0.03
1.66		0.03
1.62		0.03
1.57		0.03
1.53		0.10
1.460		0.04
1.370		0.04
1.325		0.04
1.273		0.04

687. $KHC_2O_4.^1/_2H_2O$

d		I/I1
6.1		0.08
4.83		0.12
4.42		0.12
3.91		0.04
3.44		0.03
3.31		0.02
3.12	(50)	1.00
2.96		0.02
2.78	(20)	0.40
2.65		0.02
2.57		0.08
2.43	(10)	0.20
2.35		0.14
2.21		0.08
2.14		0.02
2.06		0.04
2.00		0.04
1.84		0.04
1.80		0.02
1.75		0.02
1.73		0.04
1.64		0.02
1.57		0.04
1.470		0.04
1.379		0.02
1.310		0.02

688. $K(C_6H_4OHSO_3)$

d		I/I1
9.8		0.20
5.2		0.15
4.80		0.23
4.29		0.05
3.83	(40)	1.00
3.38		0.20
3.15	(15)	0.38
2.98	(10)	0.25
2.64		0.15
2.52		0.15
2.40		0.03
2.32		0.03
2.24		0.08
2.13		0.03
2.08		0.05
2.03		0.05
1.91		0.15
1.69		0.03
1.65		0.03
1.57		0.03
1.495		0.03
1.410		0.03
1.320		0.03

689. C_6H_5OK

d		I/I1
20.0		0.20
17.0	(20)	1.00
8.3		0.05
7.8		0.05
7.1		0.15
6.2		0.15
5.3	(10)	0.50
4.51		0.05
4.29	(20)	1.00
4.01		0.05
3.90		0.05
3.80		0.05
3.61		0.05
3.43		0.08
3.27		0.08
2.98		0.50
2.87		0.05
2.80		0.35
2.66		0.40
2.59		0.08
2.55		0.08
2.47		0.05
2.39		0.05
2.30		0.05
2.25		0.05
2.19		0.30

690. K_2PO_4

d		I/I1
5.5		0.30
3.65		0.30
3.44		0.04
3.15		0.30
3.03	(50)	1.00
2.75	(30)	0.60
2.56	(25)	0.50
2.45		0.20
2.39		0.40
2.23		0.16
2.13		0.04
2.07		0.04
2.03		0.02
1.93		0.12
1.89		0.02
1.82		0.20
1.77		0.04
1.73		0.02
1.68		0.02
1.64		0.18
1.58		0.02
1.52		0.02
1.462		0.02
1.435		0.02
1.407		0.06
1.370		0.04

691. K_2HPO_4

d		I/I1
4.26	(10)	0.33
3.80		0.10
3.18		0.07
3.03	(20)	0.67
2.96	(30)	1.00
2.73		0.23
2.54		0.23
2.42		0.17
2.34		0.07
2.24		0.20
2.18		0.07
2.12		0.20
2.01		0.13
1.94		0.03
1.89		0.07
1.84		0.03
1.82		0.03
1.75		0.03
1.71		0.13
1.59		0.07
1.480		0.07
1.440		0.03
1.360		0.03

692. $K_2HPO_4.3H_2O$

d		I/I1
6.9		0.10
6.2		0.13
5.2		0.23
4.85		0.38
3.90		0.04
3.74		0.05
3.43	(40)	1.00
3.08		0.30
2.97		0.05
2.87		0.25
2.73		0.44
2.56	(20)	0.50
2.41	(25)	0.63
2.30		0.20
2.24		0.05
2.14		0.08
2.05		0.20
1.99		0.08
1.91		0.04
1.86		0.03
1.82		0.03
1.78		0.05
1.75		0.04
1.71		0.10
1.67		0.03
1.57		0.04

693. KH_2PO_4*

d		I/I1
5.1		0.10
3.72	(50)	1.00
3.00		0.08
2.90	(50)	1.00
2.63		0.16
2.53		0.06
2.34		0.12
2.22		0.03
1.95	(20)	0.40
1.90		0.02
1.66		0.06
1.57		0.08
1.450		0.04
1.345		0.06
1.318		0.02
1.270		0.04
1.200		0.06
1.175		0.02
1.008		0.02

694. Potassium Ammonium Phosphate

d		I/I1
5.6		0.40
5.0		0.53
3.75	(12.5)	0.83
3.30		0.40
2.91	(15)	1.00
2.65		0.33
2.56		0.53
2.33		0.20
2.10		0.07
1.95	(12.5)	0.83
1.87		0.07
1.69		0.07B
1.57		0.20
1.450		0.13
1.345		0.13
1.270		0.07
1.200		0.13
1.070		0.07

695. $K_4P_2O_7.3H_2O$

d		I/I1
9.3		0.13
5.0		0.13
2.97	(8)	0.53
2.88	(15)	1.00
2.76	(4)	0.27
2.68		0.13
2.50		0.13
2.26		0.13
2.14		0.07
2.10		0.07
1.98		0.13
1.80		0.07
1.72		0.07
1.65		0.07
1.61		0.07
1.51		0.07
1.470		0.07
1.435		0.07

696. KH_2PO_2

d		I/I1
5.0		0.07
3.65	(17.5)	0.58
3.41		0.23
3.26	(30)	1.00
3.10		0.07
2.61	(17.5)	0.58
2.44		0.20
2.30		0.17
2.07		0.23
1.97		0.30
1.93		0.13
1.86		0.20
1.70		0.10
1.61		0.13
1.56		0.07
1.480		0.03
1.445		0.03
1.400		0.03
1.340		0.07
1.290		0.07
1.250		0.03B
1.220		0.10
1.185		0.03
1.130		0.03

697. $C_6H_4(CO)_2NK$

d		I/I1
14.5	(50)	1.00
13.5		0.16
6.4	(12.5)	0.25
5.6		0.02
4.91		0.08
4.35		0.04
3.59		0.04
3.45		0.04
3.30		0.02
3.09		0.16
2.90	(12.5)	0.25
2.67		0.08
2.55		0.04
2.35		0.02
2.17		0.02
2.07		0.02
1.87		0.02
1.77		0.02
1.68		0.02

698. $C_6H_4COOH.COOK$

d		I/I1
13.4	(30)	1.00
4.99	(20)	0.67
4.20		0.23
4.03		0.23
3.70		0.17
3.43		0.05
3.33		0.17
3.14		0.20
2.99	(15)	0.50
2.89		0.17
2.79		0.07
2.70		0.03
2.64		0.20
2.51		0.07
2.39		0.13
2.25		0.10
2.15		0.03
2.06		0.03
2.01		0.03
1.96		0.03
1.88		0.03
1.83		0.03
1.78		0.03

699. $C_6H_4OHCOOK$

d		I/I1
6.4		0.28
5.6	(7)	1.00
4.25		0.14
3.61	(5)	0.71
3.23	(4)	0.57
3.01		0.43
2.85		0.14
2.72		0.28
2.31		0.14
2.23		0.14
2.14		0.14
1.85		0.14

700. K_2SeO_4

d		I/I1
5.2		0.13
4.30	(20)	0.67
3.80		0.27
3.08	(20)	0.67
3.00	(30)	1.00
2.59		0.20
2.47		0.03
2.35		0.03
2.28		0.33
2.15		0.33
1.95		0.13
1.90		0.20
1.82		0.17
1.74		0.27
1.67		0.13
1.61		0.17
1.55		0.13
1.498		0.17
1.460		0.17
1.415		0.03
1.397		0.10
1.348		0.07
1.310		0.03
1.280		0.07
1.252		0.07
1.200		0.07

701. K_2SeO_3

d		I/I1
4.35	(6)	0.40B
4.21		0.07B
3.69		0.07
3.08	(15)	1.00B
2.94	(4)	0.27B
2.85		0.20
2.63		0.13
2.37		0.07
2.30		0.13
2.20		0.13
2.10		0.13
2.03		0.07
1.97		0.07
1.92		0.07
1.84		0.07
1.79		0.07
1.73		0.07
1.67		0.07
1.62		0.07
1.57		0.07
1.53		0.07
1.398		0.07
1.373		0.07
1.341		0.07
1.316		0.07
1.180		0.07

702. KSeCN

d		I/I1
4.97		0.07
4.42		0.17
4.05		0.33
3.70		0.50
3.41		0.23
3.21	(30)	1.00
2.83		0.50
2.75		0.50
2.67		0.13
2.45		0.50
2.38	(20)	0.67
2.28	(20)	0.67
2.12		0.17
2.07		0.07
2.01		0.20
1.93		0.10
1.86		0.27
1.78		0.07
1.72		0.33
1.69		0.17
1.67		0.17
1.61		0.20
1.56		0.13
1.52		0.20
1.490		0.03
1.460		0.13
1.433		0.33
1.400		0.03
1.378		0.17
1.345		0.17
1.310		0.17
1.275		0.13

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

703. $KAlSi_3O_8$

d		I/I1
4.24	(15)	0.38
4.01		0.20
3.85		0.20
3.69		0.20
3.49		0.15
3.35	(10)	0.25
3.25	(40)	1.00
3.03		0.13
2.94		0.25
2.88		0.08
2.76		0.10
2.61		0.15
2.52		0.13
2.43		0.13
2.33		0.08
2.16		0.25
2.10		0.03
2.02		0.03
1.98		0.10
1.92		0.10
1.85		0.03
1.80		0.25
1.73		0.05
1.65		0.03
1.61		0.03
1.57		0.03
1.54		0.03
1.51		0.05
1.468		0.10

704. K_2SO_4*

5.0		0.02
4.19		0.24
3.73		0.08
3.38		0.05
3.00	(100)	0.80
2.88	(125)	1.00
2.66		0.02
2.50		0.12
2.41		0.20
2.21		0.24
2.08	(50)	0.40
2.00		0.05
1.94		0.04
1.88		0.10
1.85		0.04
1.76		0.03
1.68		0.10
1.62		0.04
1.57		0.06
1.440		0.10
1.419		0.03
1.392		0.03
1.350		0.06
1.302		0.05
1.285		0.02
1.245		0.04
1.212		0.01
1.175		0.05
1.141		0.04
1.115		0.01
1.094		0.02
1.048		0.02
1.019		0.02
0.983		0.02
0.965		0.02

705. $KHSO_4$

9.7		0.05
4.92		0.10
3.85	(20)	1.00
3.52		0.63
3.40	(15)	0.75
3.26		0.50
3.14		0.05
3.01	(15)	0.75
2.82		0.10
2.74		0.10
2.66		0.05
2.57		0.05
2.46		0.05
2.37		0.15
2.33		0.05
2.27		0.35
2.19		0.05
2.12		0.10
2.02		0.25
1.93		0.35
1.86		0.10
1.78		0.10
1.71		0.05
1.66		0.15
1.60		0.05
1.56		0.05

706. $K_2S_2O_8$

4.88		0.12
3.72	(30)	0.24
3.45	(30)	0.24
3.24	(125)	1.00
3.03		0.08
2.73		0.12
2.64		0.08
2.55		0.05
2.47		0.20
2.42		0.01
2.29		0.03
2.16		0.02
2.10		0.10
1.99		0.06
1.93		0.10
1.87		0.03
1.81		0.08
1.76		0.01
1.72		0.03
1.62		0.12
1.58		0.06
1.52		0.02
1.427		0.06
1.404		0.01
1.371		0.01
1.336		0.02

707. $K_2S_2O_7$

6.3		0.06
4.80		0.28
4.40		0.04
4.19		0.04
3.85		0.28
3.65		0.28
3.51		0.06
3.40		0.06
3.23	(25)	1.00
3.07	(15)	0.60
2.90	(8)	0.32
2.82		0.12
2.72		0.04
2.61		0.08
2.49		0.06
2.36		0.20
2.27		0.24
2.19		0.12
2.12		0.06
2.09		0.16
2.01		0.16
1.94		0.32
1.89		0.06
1.86		0.04
1.83		0.06
1.76		0.08

708. $KC_2H_3SO_4$

11.7	(62.5)	1.00
6.0		0.08
5.1		0.13
4.42		0.06
4.13		0.05
3.80		0.11
3.36	(20)	0.32
3.14	(15)	0.24
3.00		0.03
2.89		0.24
2.68		0.09
2.56		0.02
2.42		0.06
2.34		0.06
2.21		0.09
2.02		0.06
1.93		0.02
1.84		0.02
1.80		0.05
1.420		0.04
1.380		0.03
1.345		0.03
1.132		0.02

709. $2KCH_3SO_4.H_2O$

9.3	(25)	1.00
5.5		0.08
5.0		0.04
4.59	(10)	0.40
3.85		0.04
3.65		0.04
3.49	(10)	0.40
3.30		0.12
3.15		0.32
3.06		0.08
2.96		0.20
2.80		0.08
2.72		0.08
2.62		0.08
2.42		0.04
2.31		0.16
2.24		0.04
2.17		0.04
2.07		0.08
1.98		0.20
1.81		0.04
1.67		0.04
1.400		0.04
1.370		0.04

710. $K_2SO_3.2H_2O$

4.13		0.20
3.47		0.16
2.96	(50)	1.00
2.87	(40)	0.80
2.40		0.16
2.06	(40)	0.80
1.94		0.04
1.88		0.02
1.69		0.25
1.64		0.12
1.475		0.18
1.440		0.08
1.315		0.10
1.295		0.10
1.200		0.04
1.115		0.08
1.078		0.04
0.985		0.02
0.958		0.02

711. $KHSO_3$

5.1		0.03
4.56		0.07
4.19		0.27
3.90		0.10
3.78		0.07
3.67		0.20
3.50		0.03
3.37		0.03
3.10		0.13
3.00	(30)	1.00
2.89	(30)	1.00
2.65		0.07
2.50		0.17
2.42		0.17
2.28		0.20
2.22		0.20
2.14		0.10
2.07	(10)	0.33
2.03		0.10
1.94		0.03
1.88		0.10
1.78		0.07
1.69		0.07
1.67		0.07
1.62		0.03
1.57		0.07

712. $K_2S_2O_5$

4.75		0.17
4.55		0.17
3.65	(50)	0.67
3.09	(75)	1.00
2.95	(62.5)	0.83
2.83		0.20
2.70		0.01
2.57		0.01
2.45		0.11
2.33		0.08
2.27		0.53
2.13		0.27
2.02		0.27
1.97		0.01
1.92		0.05
1.87		0.05
1.82		0.03
1.78		0.20
1.73		0.07
1.70		0.03
1.67		0.05
1.63		0.03
1.61		0.01
1.54		0.13
1.51		0.01
1.480		0.03
1.439		0.01
1.422		0.01
1.388		0.03
1.352		0.07
1.321		0.04
1.301		0.03
1.278		0.01
1.252		0.02
1.228		0.02
1.190		0.02
1.162		0.05

713. $C_6H_5SO_3K$

15.0	(100)	1.00
5.1	(8)	0.08B
4.15		0.04
3.91	(8)	0.08
3.22		0.01
2.95		0.04
2.65		0.01
2.54		0.01
2.43		0.01
2.24		0.03
2.11		0.02
1.96		0.01
1.71		0.01B

714. Potassium Guaiacol Sulfonate

9.8		0.10
6.7		0.25
5.7	(20)	1.00
4.43		0.35
4.10	(20)	1.00
3.71		0.10
3.42		0.30
3.27	(15)	0.75
3.12		0.20
2.94		0.40
2.68		0.35
2.50		0.30
2.43		0.05
2.38		0.10
2.23		0.15
2.18		0.10
2.12		0.20
2.03		0.10
1.97		0.10
1.92		0.08
1.86		0.10
1.82		0.08
1.79		0.05
1.74		0.05

715. Potassium Indigo Sulfonate

3.35	(6)	0.40
3.00	(6)	0.40
2.90	(15)	1.00
2.51		0.07
2.42		0.07
2.22		0.13
2.07		0.13
1.88		0.07
1.67		0.07
1.430		0.07

716. p-$CH_3C_6H_4SO_3K$

10.3		0.32
5.7		0.70
5.1		0.50
4.60	(20)	0.80
4.29		0.16
4.11	(25)	1.00
3.78		0.24
3.52		0.16
3.43	(20)	0.80
3.30		0.36
3.09		0.24
3.01		0.24
2.91		0.12
2.82		0.50
2.65		0.16
2.54		0.16
2.41		0.04
2.28		0.40
2.21		0.04
2.14		0.04
2.08		0.12
2.02		0.04
2.00		0.08
1.96		0.16
1.89		0.12
1.83		0.04

717. $K_2C_4H_4O_6$

5.5	(3)	1.00
4.70		0.33
3.40	(2)	0.66
3.17	(2)	0.66
2.91		0.66
2.27		0.33
1.97		0.33
1.88		0.33
1.84		0.33
1.79		0.33
1.70		0.33
1.470		0.33B
1.385		0.33

718. $K(NH_4)C_4H_4O_6$

8.0		0.07
6.4		0.07
4.70	(6)	0.40
3.93	(6)	0.40
3.59		0.13
3.10	(15)	1.00
2.66		0.20
2.53		0.27
2.34		0.13
2.24		0.07
2.16		0.07
2.05		0.07
1.97		0.20
1.83		0.07
1.72		0.07

719. $KH(C_4H_4O_6)$

6.3		0.05
5.4		0.05
4.87		0.05
4.36		0.03
4.10		0.03
3.80		0.25
3.64	(30)	0.75
3.22	(30)	0.75
2.87		0.75
2.63		0.15
2.46	(40)	1.00
2.38		0.20
2.34		0.10
2.28		0.03
2.22		0.15
2.17		0.03
2.10		0.20
2.02		0.03
1.98		0.08
1.90		0.10
1.85		0.10
1.78		0.13
1.74		0.03
1.71		0.03
1.68		0.03
1.63		0.03

720. K_2TeO_3

9.7	(8)	0.64
7.0		0.08
5.5		0.08
4.95		0.64
4.50		0.32
3.17	(12.5)	1.00
3.00		0.32
2.75	(10)	0.80
2.59		0.08
2.43		0.08
2.22		0.24
2.01		0.08
1.97		0.08
1.91		0.08
1.82		0.08
1.73		0.08
1.68		0.08
1.63		0.08
1.58		0.08
1.53		0.08
1.485		0.08
1.460		0.08
1.400		0.08

721. K_2CS_3

6.5		0.04
6.1		0.16
5.3		0.20
5.2		0.20
4.87		0.06
4.31		0.40
4.00		0.04
3.69		0.04
3.53	(20)	0.80
3.12	(20)	0.80
3.00	(25)	1.00
2.83		0.32
2.71		0.40
2.63		0.12
2.55		0.16
2.50		0.20
2.43		0.32
2.32		0.04
2.27		0.04
2.16		0.16
2.14		0.16
2.06		0.20
2.02		0.08
1.96		0.08
1.85		0.06

722. $K_2S_2O_3$

5.2		0.38
4.69		0.20
4.30		0.03
4.10		0.03
3.60		0.15
3.40		0.08
3.27	(40)	1.00
2.99	(25)	0.63
2.72		0.05
2.53	(20)	0.50
2.45		0.03
2.38		0.05
2.29		0.03
2.22		0.03
2.17		0.18
2.08		0.13
2.00		0.05
1.96		0.05
1.92		0.05
1.80		0.03
1.75		0.05
1.65		0.18
1.57		0.13
1.53		0.05
1.466		0.05

723. $3K_2S_2O_3.H_2O$

5.1		0.16
4.73	(6)	0.48
4.24		0.32
3.93		0.16
3.73		0.08
3.62		0.08
3.48	(8)	0.64
3.35		0.16
3.19	(12.5)	1.00
3.04		0.48
2.95		0.08
2.83		0.48
2.73		0.48
2.64		0.40
2.57		0.16
2.48		0.16
2.40		0.08
2.37		0.08
2.24		0.08
2.19		0.16
2.15		0.08
2.11		0.16
2.03		0.16
2.00		0.16
1.96		0.16
1.84		0.24

724. KCNS*

3.34		0.35
2.97	(50)	1.00
2.79	(40)	0.80
2.51	(20)	0.40
2.36		0.20
2.23		0.02
1.94		0.25
1.66		0.20
1.61		0.02
1.53		0.16
1.490		0.16
1.460		0.16
1.415		0.12
1.229		0.08
1.181		0.08

725. K_2TiO_3

7.0		0.17
3.46		0.07
3.32		0.03
3.01		0.20
2.76	(30)	1.00
2.32	(7)	0.23
2.18	(7)	0.23
1.87		0.03
1.78		0.07
1.71		0.03
1.64		0.03
1.60		0.03
1.52		0.03
1.480		0.03
1.392		0.03

726. $K_2WO_4.2H_2O$

4.70		0.14
3.92	(10)	0.20
3.60		0.14
3.09	(50)	1.00
2.62		0.08
2.51	(8)	0.16
2.27		0.12
2.17		0.12
2.02		0.04
1.95		0.14
1.89		0.04
1.81		0.08
1.70		0.02B
1.60		0.02
1.54		0.02
1.470		0.04
1.390		0.02
1.305		0.02
1.230		0.02
1.110		0.02

727. K_2UO_4

7.5	(4)	1.00
3.55	(2)	0.50
3.20	(3)	0.75
2.57		0.25
2.02		0.25
1.96		

728. $KHC_5H_3N_4O_3$

4.70	(4)	1.00
3.79	(4)	1.00
3.42	(3)	0.75
3.23		0.50
2.90		0.50
2.55		0.25
2.02		0.25
1.77		0.25
1.70		

729. K

5.3		
3.90		
3.71		
3.11	(62.5)	
2.82	(20)	
2.60	(12.5)	
2.43		
2.30		
1.95		
1.89		
1.77		
1.69		
1.57		
1.50		
1.455		
1.420		
1.310		
1.245		
1.170		
1.087		

730. KS_5C

7.5	(8)	
3.60	(7)	
3.22	(6)	
3.10		
2.95		
2.67		
2.50		
2.41		
2.33		
2.27		
2.19		

731. K

2.38	(10)	
2.22	(6)	
2.10	(30)	
1.62		
1.379		
1.260		
1.170		
1.151		
0.928		
0.884		
0.858		

732. K

2.20	(100	
1.90	(50	
1.345		
1.146	(40	
1.099		
0.952		
0.873		
0.852		
0.777		
0.733		

733. R

3.43	(17.5	
2.42	(10	
1.97		
1.71		
1.53	(5	
1.400		
1.143		

734. R

3.80	(3	
3.29	(17.5	
2.32	(10	
1.98		
1.89		
1.64		
1.50		
1.468		
1.340		
1.095		

735. R

4.24		
3.66	(25)	
2.58	(20)	
2.20		
2.11		
1.83		
1.63	(8)	
1.493		
1.292		
1.220		
1.157		
1.103		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

729. KVO_3

d		I/I1
5.3		0.16
3.90		0.08
3.71		0.06
3.11	(62.5)	1.00
2.82	(20)	0.32
2.60	(12.5)	0.20
2.43		0.11
2.30		0.09
1.95		0.06
1.89		0.02
1.77		0.03
1.69		0.11
1.57		0.05B
1.50		0.02
1.455		0.05
1.420		0.03
1.310		0.03
1.245		0.02
1.170		0.02
1.087		0.02

730. $KS_2COC_2H_5$

d		I/I1
7.5	(8)	1.00
3.60	(7)	0.88
3.22	(6)	0.75
3.10		0.50
2.96		0.13
2.67		0.13B
2.50		0.38
2.41		0.25
2.33		0.13
2.27		0.25
2.19		0.25

731. Re*

d		I/I1
2.38	(10)	0.33
2.22	(6)	0.20
2.10	(30)	1.00
1.62		0.10
1.379		0.17
1.260		0.13
1.170		0.17
1.151		0.17
0.928		0.03
0.884		0.07
0.868		0.03

732. Rh*

d		I/I1
2.20	(100)	1.00
1.90	(50)	0.50
1.345		0.30
1.146	(40)	0.40
1.099		0.13
0.952		0.04
0.873		0.15
0.852		0.15
0.777		0.08
0.733		0.10

733. RbBr*

d		I/I1
3.43	(17.5)	1.00
2.42	(10)	0.57
1.97		0.17
1.71		0.11
1.53	(6)	0.34
1.400		0.23
1.143		0.11

734. RbCl*

d		I/I1
3.80	(3)	0.17
3.29	(17.5)	1.00
2.32	(10)	0.57
1.98		0.11
1.89		0.17
1.64		0.11
1.50		0.06
1.468		0.17
1.340		0.11
1.095		0.06

735. RbI*

d		I/I1
4.24		0.04
3.66	(25)	1.00
2.58	(20)	0.80
2.20		0.04
2.11		0.20
1.83		0.15
1.63	(8)	0.32
1.493		0.16
1.292		0.04
1.220		0.08
1.157		0.04
1.103		0.04

736. $RbNO_3$*

d		I/I1
4.28		0.20
3.85	(7)	0.35
3.29		0.05
3.02	(20)	1.00
2.89		0.20
2.71	(5)	0.25
2.46		0.25
2.35		0.05
2.23		0.15
2.13		0.10
1.98		0.05
1.90		0.25
1.86		0.05
1.82		0.05
1.74		0.20
1.70		0.05
1.51		0.05
1.424		0.10
1.351		0.10
1.320		0.05
1.288		0.10
1.187		0.05
1.145		0.10

737. Rb_2SO_4*

d		I/I1
3.49		0.20
3.26		0.05
3.10	(15)	0.75
2.98	(20)	1.00
2.60		0.10
2.51		0.15
2.45		0.10
2.29		0.15
2.16	(10)	0.50
2.07		0.08
2.00		0.05
1.95		0.10
1.91		0.08
1.83		0.05
1.75		0.15
1.66		0.05
1.63		0.05
1.58		0.05
1.488		0.10
1.440		0.05
1.400		0.10
1.345		0.10

738. $RbAl(SO_4)_2.12H_2O$*

d		I/I1
5.5		0.27
5.0		0.10
4.34	(30)	1.00
4.09		0.23
3.28	(15)	0.50
3.07		0.33
2.81	(20)	0.67
2.73		0.13
2.62		0.13
2.50		0.23
2.36		0.23
2.26		0.03
2.16		0.03
2.04		0.17
1.99		0.03
1.94		0.33
1.87		0.13
1.70		0.13
1.64		0.27
1.488		0.20
1.448		0.07
1.410		0.03
1.365		0.03
1.332		0.03
1.305		0.03
1.201		0.13

739. Ru*

d		I/I1
2.33	(40)	0.40
2.13	(30)	0.30
2.04	(100)	1.00
1.57		0.25
1.345		0.25
1.213		0.30
1.165		0.04
1.140		0.30
1.128		0.15
1.069		0.03
1.025		0.04
0.971		0.04
0.905		0.10α1
0.884		0.02
0.867		0.20α1
0.839		0.10α1
0.818		0.04α1
0.803		0.06α1
0.790		0.02
0.780		0.04α1
0.751		0.15α1
0.733		0.06α1
0.691		0.04α1
0.682		0.04
0.677		0.04α1

740. Se*

d		I/I1
3.78	(5)	0.33
3.02	(15)	1.00
2.18		0.27
2.07	(6)	0.40
2.00		0.33
1.77		0.27
1.64		0.20
1.51		0.27
1.430		0.20
1.320		0.13
1.239		0.07
1.180		0.07
1.125		0.07
1.084		0.13
1.038		0.07

741. H_2SeO

d		I/I1
8.1		0.29
7.2		0.29
6.3		0.29
4.55	(4)	0.57
4.22		0.29
3.90		0.57
3.60	(7)	1.00
3.39		0.43
2.98	(5)	0.71
2.61		0.29
2.50		0.43
2.45		0.29
2.38		0.29
2.25		0.14
2.12		0.43
2.08		0.14
2.03		0.14
2.00		0.14
1.96		0.43
1.90		0.43
1.86		0.43
1.82		0.43
1.72		0.43
1.63		0.29
1.60		0.14
1.50		0.29

742. Si*

d		I/I1
3.12	(100)	1.00
1.91	(100)	1.00
1.63	(62.5)	0.63
1.354		0.18
1.242		0.25
1.104		0.40
0.958		0.06
0.916		0.13
0.857		0.08
0.826		0.03
0.782		0.01
0.760		0.04α1
0.724		0.06α1
0.705		0.04α1

743. SiC*

d		I/I1
2.51	(100)	1.00
2.17		0.20
1.54	(62.5)	0.63
1.310	(50)	0.50
1.255		0.05
1.087		0.06
0.998		0.18
0.972		0.06
0.887		0.13
0.837		0.10
0.768		0.02
0.735		0.06
0.724		0.02
0.688		0.03
0.663		0.01

744. SiC (commercial)*

d		I/I1
2.63		0.20
2.59		0.06
2.51	(50)	1.00
2.36		0.40
2.17		0.12
2.08		0.02
2.00		0.04
1.83		0.02
1.68		0.04
1.60		0.02
1.54	(40)	0.80
1.420		0.16
1.312	(30)	0.60
1.285		0.04
1.257		0.04
1.220		0.02
1.178		0.02
1.134		0.02
1.110		0.02
1.089		0.06
1.044		0.08
0.999		0.14
0.990		0.04
0.974		0.08
0.958		0.02
0.944		0.04
0.912		0.02
0.901		0.02
0.890		0.16
0.865		0.08
0.839		0.12
0.805		0.02
0.771		0.04
0.738		0.10
0.727		0.02

745. SiO_2* (α-cristobalite)

d		I/I1
4.04	(125)	1.00
3.13		0.16
2.85	(25)	0.20
2.48	(40)	0.32
2.11		0.05
2.02		0.05
1.93		0.12
1.87		0.12
1.69		0.05
1.61		0.12
1.57		0.01
1.53		0.04
1.494		0.06
1.430		0.05
1.400		0.02
1.370		0.03
1.339		0.03
1.300		0.03
1.279		0.03
1.235		0.01
1.203		0.01
1.181		0.02
1.095		0.03

746. SiO_2* (α-quartz)

d		I/I1
4.25	(25)	0.25
3.35	(100)	1.00
2.45		0.15
2.29		0.10
2.23		0.06
2.12		0.09
1.97		0.08
1.82	(25)	0.25
1.66		0.08
1.54		0.20
1.450		0.02
1.375		0.25
1.299		0.04
1.256		0.03
1.228		0.03
1.200		0.06
1.180		0.08
1.155		0.01
1.080		0.04
1.048		0.02
1.035		0.01
1.015		0.01

747. Ag*

d		I/I1
2.36	(75)	1.00
2.04	(40)	0.53
1.445		0.27
1.232	(40)	0.53
1.179		0.05
1.022		0.01
0.938		0.08α1
0.915		0.05α1
0.834		0.03α1
0.786		0.04α1
0.691		0.03α1

748. $AgC_2H_3O_2$

d		I/I1
10.0	(62.5)	1.00
4.11		0.03
3.93		0.03
3.70		0.10
3.31		0.10
3.04	(50)	0.80
2.91	(10)	0.16
2.77		0.08
2.68		0.14
2.59		0.06
2.48		0.06
2.33		0.13
2.21		0.10
2.04		0.06
1.98		0.06
1.85		0.06
1.80		0.03
1.74		0.03
1.69		0.02
1.65		0.03
1.57		0.02
1.53		0.02
1.50		0.02

749. Ag_3AsO_4*

d		I/I1
3.07		0.17
2.74	(75)	1.00
2.50	(50)	0.67
1.94		0.05
1.77		0.13
1.70		0.33
1.63	(40)	0.53
1.53		0.20
1.369		0.13
1.335		0.23
1.305		0.11
1.137		0.20
1.118		0.12
1.082		0.11
1.021		0.07
0.994		0.09
0.915		0.05

750. $AgBrO_3$*

d		I/I1
3.48		0.13
3.04	(20)	0.27
2.95	(75)	1.00
2.70		0.03
2.58		0.01
2.28		0.02
2.22		0.08
2.15		0.20
2.02		0.05
1.92		0.05
1.79		0.07
1.74	(20)	0.27
1.69		0.11
1.65		0.01
1.56		0.03
1.52		0.03
1.490		0.01
1.470		0.03
1.450		0.03
1.411		0.01
1.390		0.01
1.358		0.05

751. AgBr*

d		I/I1
2.88	(50)	1.00
2.03	(30)	0.60
1.66	(10)	0.20
1.441		0.08
1.320		0.02
1.289		0.20
1.178		0.12
1.019		0.02
0.963		0.02α1
0.913		0.02α1
0.871		0.02α1

752. Ag_2CO_3

d		I/I1
4.77		0.20
4.31		0.20
3.05		0.04
2.73	(50)	0.50
2.65	(100)	1.00
2.55		0.02
2.48		0.01
2.42		0.15
2.37		0.03
2.32		0.04
2.27	(30)	0.30
2.20		0.01
2.15		0.08
2.03		0.08
1.92		0.08
1.86		0.04
1.77		0.10
1.67		0.08
1.63		0.10
1.59		0.07
1.53		0.03
1.50		0.02
1.462		0.01
1.440		0.05
1.398		0.04
1.370		0.13
1.328		0.04
1.300		0.02
1.222		0.03
1.133		0.03

753. $AgClO_4.H_2O$

d		I/I1
6.9		0.20
5.2		0.20
4.02		0.50
3.78		0.04
3.50	(50)	1.00
3.39	(40)	0.80
3.11		0.16
2.95		0.02
2.77	(40)	0.80
2.49		0.14
2.42		0.60
2.25		0.02
2.19		0.02
2.10		0.30
2.04		0.12
1.99		0.30
1.95		0.12
1.82		0.02
1.78		0.04
1.76		0.10
1.70		0.04
1.66		0.04
1.61		0.04
1.56		0.10
1.52		0.04
1.422		0.14
1.390		0.12
1.350		0.03

754. AgCl*

d		I/I1
3.20	(40)	0.40
2.77	(100)	1.00
1.96	(75)	0.75
1.67		0.20
1.60		0.25
1.385		0.09
1.270		0.06
1.240		0.20
1.131		0.13
1.065		0.01
0.980		0.01
0.937		0.01
0.924		0.04
0.877		0.01
0.836		0.01

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

755. Ag_2CrO_4

d		I/I1
7.0		0.06
6.5		0.06
6.0		0.06
5.6		0.08
4.97		0.04
4.49		0.04
4.12		0.04
3.84		0.04
3.49		0.08
3.14	(50)	1.00
3.02	(17.5)	0.35
2.92	(15)	0.30
2.85		0.30
2.65		0.30
2.47		0.30
2.31		0.06
2.23		0.08
2.14		0.06
2.07		0.06
1.95		0.30
1.84		0.20
1.79		0.08
1.77		0.08
1.72		0.16
1.66		0.06
1.61		0.08
1.55		0.08
1.53		0.02
1.50		0.02
1.470		0.08
1.430		0.06
1.394		0.06
1.325		0.04
1.268		0.04
1.230		0.04

756. $Ag_2C_2H_2O_4$

d		I/I1
11.4	(50)	1.00
5.9	(25)	0.50
5.4		0.20
4.11		0.40
3.80		0.16
3.50		0.02
3.25		0.12
3.14		0.20
3.07		0.16
2.86	(25)	0.50
2.69		0.08
2.60		0.12
2.52		0.12
2.42		0.04
2.32		0.30
2.17		0.08
2.11		0.08
2.06		0.16
2.00		0.02
1.94		0.20
1.88		0.04
1.83		0.02
1.79		0.04
1.73		0.04
1.66		0.04
1.59		0.08

757. AgCN*

d		I/I1
3.70	(100)	0.80
3.00	(125)	1.00
2.33	(62.5)	0.50
1.84		0.24
1.73		0.12
1.57		0.06
1.50		0.10
1.383		0.02
1.266		0.02
1.230		0.01
1.158		0.01
1.136		0.01

758. Silver Potassium Cyanide

d		I/I1
9.0		0.30
6.2		0.30
4.40	(25)	0.50
3.43	(50)	1.00
3.18	(40)	0.80
3.02		0.02
2.82		0.40
2.61		0.06
2.38		0.40
2.31		0.30
2.21		0.12
2.13		0.02
2.07		0.20
1.99		0.20
1.85		0.16
1.81		0.08
1.76		0.04
1.71		0.40
1.67		0.12
1.59		0.16
1.55		0.08
1.50		0.02
1.465		0.08
1.422		0.12
1.385		0.02
1.190		0.02
1.050		0.02

759. AgI (cubic)*

d		I/I1
3.74	(40)	1.00
2.29	(30)	0.75
1.95	(15)	0.40
1.62		0.05
1.485		0.08
1.321		0.08
1.247		0.05
1.145		0.03
1.096		0.03

760. AgI (cubic and hex.)*

d		I/I1
3.95		0.20
3.74	(62.5)	1.00
3.51		0.10
2.71		0.03
2.29	(50)	0.80
2.19		0.02
2.11		0.06
1.96	(30)	0.48
1.62		0.03
1.55		0.02
1.485		0.06
1.397		0.02
1.321		0.08
1.285		0.02
1.247		0.05
1.148		0.02
1.097		0.03

761. Ag_2MoO_4*

d		I/I1
5.3		0.06
3.28		0.17
2.80	(175)	1.00
2.68		0.17
2.32		0.14
2.12		0.05
1.89		0.06
1.78	(75)	0.43
1.64	(75)	0.43
1.475		0.01
1.422		0.11
1.406		0.11
1.345		0.01
1.245		0.05
1.211		0.17
1.164		0.03
1.097		0.01
1.075		0.09
1.043		0.01
0.978		0.02
0.951		0.05
0.915		0.01

762. $AgNO_3$*

d		I/I1
4.51	(20)	0.50
4.08	(20)	0.50
3.66		0.38
3.00	(40)	1.00
2.80		0.38
2.73		0.44
2.53		0.38
2.29		0.31
2.24		0.25
2.15		0.15
2.11		0.10
2.08		0.50
1.96		0.18
1.90		0.10
1.83		0.25
1.70		0.15
1.66		0.15
1.57		0.05
1.490		0.10
1.420		0.08
1.382		0.05
1.340		0.13
1.310		0.03

763. $AgNO_2$*

d		I/I1
3.95	(50)	0.67
3.06	(75)	1.00
2.90		0.13
2.58		0.40
2.11		0.40
1.97	(50)	0.67
1.90		0.13
1.76		0.07
1.66		0.07
1.60		0.03
1.54		0.07
1.461		0.05
1.385		0.03
1.361		0.07
1.320		0.04
1.292		0.04
1.192		

764. Ag_2O*

d		I/I1
3.35		0.01
2.72	(125)	1.00
2.36	(50)	0.40
1.67	(30)	0.24
1.422		0.16
1.360		0.03
1.179		0.01
1.082		0.02
1.054		0.02
0.960		0.01
0.907		0.01

765. Ag_3PO_4*

d		I/I1
4.25		0.11
3.00		0.17
2.68	(175)	1.00
2.45	(75)	0.43
2.11		0.03
1.89		0.17
1.73		0.29
1.66	(62.5)	0.36
1.60		0.29
1.50		0.11
1.413		0.02
1.376		0.01
1.341		0.06
1.308		0.29
1.278		0.05
1.226		0.02
1.177		0.02
1.113		0.23
1.095		0.05
1.060		0.09
1.029		0.01
1.000		0.02
0.988		0.02
0.973		0.04

766. Ag_2SO_4*

d		I/I1
4.71		0.07
3.98		0.27
3.17	(40)	0.53
2.86	(75)	1.00
2.64	(40)	0.53
2.52		0.11
2.41		0.33
2.35		0.01
2.27		0.08
1.97		0.11
1.91		0.40
1.75		0.03
1.70		0.13
1.66		0.09
1.64		0.07
1.58		0.01
1.56		0.09
1.53		0.09
1.465		0.05
1.447		0.01
1.400		0.07
1.361		0.01
1.330		0.11
1.270		0.04
1.230		0.05
1.187		0.01
1.161		0.04
1.112		0.03
1.091		0.04
1.075		0.03

767. Ag_2S*

d		I/I1
3.94		0.02
3.42		0.12
3.07		0.20
2.80		0.30
2.59	(40)	0.80B
2.43	(50)	1.00
2.37		0.20
2.19		0.30
2.07	(20)	0.40
1.98		0.08
1.96		0.08
1.90		0.08
1.86		0.06
1.81		0.02
1.77		0.02
1.71		0.20
1.58		0.08
1.54		0.06
1.51		0.06
1.470		0.04
1.455		0.10
1.407		0.04
1.336		0.06

768. $Ag_2C_4H_4O_6$

d		I/I1
7.8	(30)	0.60
6.0		0.40
4.01	(50)	1.00
3.70		0.20
3.55		0.08
2.98	(30)	0.60
2.89		0.12
2.61		0.60
2.44		0.08
2.35		0.12
2.26		0.20
2.18		0.20
2.02		0.16
1.96		0.08
1.84		0.50
1.78		0.02
1.73		0.08
1.68		0.08
1.63		0.08
1.55		0.04
1.52		0.04
1.490		0.02
1.455		0.04
1.390		0.04
1.275		0.04
1.230		0.04

769. $Ag_4V_2O_7$

d		I/I1
4.6		0.10
2.88	(150)	1.00
2.77	(150)	1.00
2.56	(30)	0.20
2.49		0.20
2.31		0.13
2.18		0.10
2.03		0.01
1.93		0.01
1.87		0.05
1.78		0.20
1.69		0.13
1.66		0.03
1.63		0.01
1.59		0.01
1.55		0.04
1.495		0.13
1.440		0.10
1.390		0.10
1.278		0.01
1.245		0.01
1.207		0.01
1.170		0.01
1.143		0.01
1.113		0.01
1.085		0.01

770. Na*

d		I/I1
3.02	(40)	1.00
2.13	(6)	0.15
1.75	(8)	0.20
1.51		0.05
1.355		0.05
1.246		0.03
1.145		0.03

771. $NaC_2H_3O_2$

d		I/I1
10.0	(75)	1.00
5.1		0.01
4.47		0.01
3.89	(30)	0.40
3.57		0.01
3.37		0.08
3.21		0.01
2.97	(40)	0.53
2.85		0.11
2.75		0.03
2.62		0.17
2.52		0.17
2.43		0.01
2.35		0.03
2.29		0.01
2.16		0.08
2.09		0.13
2.03		0.08
1.98		0.01
1.92		0.05
1.86		0.01
1.82		0.03
1.76		0.20
1.64		0.11
1.320		0.01
1.292		0.01

772. $NaC_2H_3O_2.3H_2O$

d		I/I1
7.8		0.60
7.0		0.10
5.4		0.30
5.2		0.30
4.65	(9)	0.90
3.93		0.70
3.71		0.10
3.57	(8)	0.80
3.30		0.20
3.17		0.60
3.01	(10)	1.00
2.87		0.30
2.74		0.60
2.66		0.70
2.52		0.40
2.45		0.60
2.40		0.20
2.33		0.10
2.26		0.10
2.21		0.60
2.13		0.20
2.07		0.20
2.03		0.60
1.98		0.15
1.93		0.15
1.87		0.20
1.81		0.30
1.78		0.30
1.72		0.20

773. $Na(UO_2)Zn(C_2H_3O_2)_3$

d		I/I1
7.0	(5)	0.33
6.1	(15)	1.00
4.89		0.20
3.87	(5)	0.33
3.45		0.07
2.60		0.13
2.20		0.07
1.97		0.07

774. $NaNH_2$

d		I/I1
5.7		0.27
5.2	(10)	0.67
3.40		0.07
3.20	(8)	0.53
3.00		0.40
2.85		0.53
2.69		0.13
2.65		0.27
2.35	(15)	1.00
2.24		0.27
2.18		0.13
2.05		0.07
2.02		0.07
1.97		0.40
1.91		0.07
1.83		0.07
1.75		0.13
1.70		0.20
1.66		0.13
1.495		0.07
1.460		0.07

775. $Na_2HAsO_4.7H_2O$

d		I/I1
5.9	(20)	1.00
5.3		0.10
4.62	(9)	0.45
4.08		0.30
3.70		0.25
3.41		0.15
3.21	(20)	1.00
2.98		0.40
2.84		0.40
2.72		0.10
2.64		0.05
2.52		0.30
2.35		0.30
2.26		0.30
2.09		0.05
2.02		0.15
1.98		0.05
1.79		0.15
1.72		0.10B
1.62		0.15
1.56		0.05

776. $CH_3AsO(ONa)_2.6H_2O$

d		I/I1
5.9		0.08
5.6	(8)	0.64
5.2		0.40
4.45	(12.5)	1.00
3.62		0.24
3.30		0.16
3.05	(6)	0.48
2.90		0.48
2.73		0.16
2.57		0.16
2.40		0.08
2.18		0.24
2.05		0.24
1.91		0.08
1.80		0.08
1.70		0.16
1.57		0.08
1.53		0.08
1.375		0.16
1.282		0.08
1.183		0.08

777. Na_2HAsO_3

d		I/I1
5.3		0.13
4.55		0.25
4.20		0.50
3.78		0.50
3.59	(7)	0.88
3.38		0.25
3.10		0.50
2.95	(8)	1.00
2.73	(8)	1.00
2.63		0.13
2.54		0.13
2.46		0.38
2.29		0.13
2.17		0.25
2.06		0.13
1.93		0.13
1.88		0.13
1.80		0.13
1.70		0.13
1.64		0.19
1.60		0.25
1.56		0.13
1.54		0.13
1.50		0.13
1.480		0.13
1.421		0.13

778. Sc Asparag

d		I/I1
5.5		
4.20	(8)	
3.82	(4)	
3.60		
3.09		
2.91		
2.69	(4)	
2.46		
2.26		
2.16		
2.02		

779. N

d		I/I1
3.09		
2.91	(12	
2.42	(2	
2.18		
1.82	(5	
1.78		
1.70		
1.63		
1.54		
1.478		
1.455		
1.400		
1.367		
1.270		
1.240		
1.212		
1.176		
1.140		
1.052		
1.039		
1.029		

780. Sodium B

d		I/I1
8.6	(2	
6.0	(1	
5.4		
4.25	(12	
3.35		
3.13		
2.99		
2.83		
2.66		
2.52		
2.38		
2.22		
2.03		

781. N

d		I/I1
15.6		
7.5	(6)	
4.9		
4.06	(4)	
3.74		
2.95		
2.80		
2.62	(4)	
2.44		
2.33		
2.23		
2.03		
1.85		
1.78		
1.61		
1.58		
1.54		
1.480		
1.310		
1.257		
1.215		
1.053		
1.019		

782. $Na_2B_4O_7$

d		I/I1
5.6		
4.72		
4.40	(9	
3.44		
2.99		
2.94	(15	
2.76		
2.60		
2.40		
2.26		
2.19	(10	
2.01		
1.94		
1.84		
1.80		
1.65		
1.56		
1.495		
1.450		
1.410		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

d		I/I_1
$NaNH_2$		
		0.27
(10)		0.67
		0.07
(8)		0.53
		0.40
		0.53
		0.13
		0.27
(15)		1.00
		0.27
		0.13
		0.07
		0.07
		0.40
		0.07
		0.07
		0.13
		0.20
		0.13
		0.07
		0.07

775. $[AsO_4.7H_2O$

(20)		1.00
		0.10
(9)		0.45
		0.30
		0.25
		0.15
(20)		1.00
		0.40
		0.40
		0.10
		0.05
		0.30
		0.30
		0.30
		0.08
		0.15
		0.05
		0.15
		0.10B
		0.15
		0.05

776. $)(ONa)_3.6H_2O$

		0.08
(8)		0.64
		0.40
(12.5)		1.00
		0.24
		0.16
(6)		0.48
		0.48
		0.16
		0.16
		0.08
		0.24
		0.24
		0.08
		0.08
		0.16
		0.08
		0.08
		0.16
		0.08
		0.08

Na_2HAsO_3

		0.13
		0.25
		0.50
		0.50
(7)		0.88
		0.25
		0.50
(8)		1.00
(7		1.00
		0.13
		0.13
		0.38
		0.13
		0.25
		0.13
		0.13
		0.13
		0.13
		0.19
		0.25
		0.13
		0.13
		0.13
		0.13
		0.13

778. Sodium Asparaginate

5.5		0.25
4.20	(8)	1.00
3.82	(4)	0.50
3.60		0.25
3.09		0.13
2.91		0.25
2.69	(4)	0.50
2.46		0.25
2.26		0.13
2.16		0.13
2.02		0.50

779. NaN_3*

3.09		0.10
2.91	(125)	1.00
2.42	(25)	0.20
2.18		0.16
1.82	(50)	0.40
1.78		0.05
1.70		0.02
1.63		0.02
1.54		0.10
1.478		0.02
1.455		0.02
1.400		0.02
1.367		0.04
1.270		0.02
1.240		0.02
1.212		0.01
1.176		0.06
1.140		0.02
1.052		0.02
1.039		0.02
1.029		0.01

780. Sodium Barbital

8.6	(25)	1.00
6.0	(10)	0.40
5.4		0.32
4.25	(12.5)	0.50
3.35		0.24
3.13		0.16
2.99		0.04
2.83		0.12
2.66		0.04
2.52		0.04
2.38		0.04
2.22		0.04
2.03		0.04

781. $NaBiO_3$

15.6		0.33
7.5	(6)	1.00
4.9		0.33
4.06	(4)	0.67
3.74		0.17
2.95		0.25
2.80		0.33
2.62	(4)	0.67
2.44		0.17
2.33		0.17
2.23		0.25
2.03		0.17
1.85		0.33
1.78		0.17
1.61		0.17
1.58		0.17
1.54		0.17
1.480		0.33
1.310		0.17
1.257		0.17
1.215		0.17
1.053		0.17
1.019		0.17

782. $Na_2B_4O_7.5H_2O$

5.6		0.13
4.72		0.13
4.40	(9)	0.60
3.44		0.53
2.99		0.20
2.94	(15)	1.00
2.76		0.13
2.60		0.33
2.40		0.06
2.26		0.13
2.19	(10)	0.67
2.01		0.33
1.94		0.27
1.84		0.13
1.80		0.40
1.65		0.07
1.56		0.13
1.495		0.07
1.450		0.07
1.410		0.07

783. $Na_2B_4O_7.10H_2O$

9.1		0.07
8.0		0.07
7.1		0.13
5.7		0.20
5.2		0.13
4.86	(7)	0.47
4.45		0.07
3.96		0.40
3.61		0.07
2.97		0.20
2.84	(8)	0.53
2.57	(15)	1.00
2.46		0.07
2.34		0.20
2.20		0.07
2.14		0.07
2.08		0.07
2.02		0.07
1.95		0.07
1.90		0.13
1.85		0.13
1.78		0.07
1.75		0.10
1.70		0.10
1.65		0.07
1.61		0.07

784. $Na_2(B_4O_7)$*

6.9		0.04
6.6		0.08
6.0		0.04
5.3		0.32
4.77	(15)	0.60
4.35		0.04
4.20		0.04
3.72		0.24
3.44		0.40
3.30		0.04
3.00		0.04
2.85	(25)	1.00
2.75		0.08
2.64	(20)	0.80
2.51		0.20
2.38		0.12
2.33		0.32
2.24		0.20
2.18		0.20
2.11		0.04
2.01		0.28
1.88		0.40
1.82		0.16
1.75		0.20
1.66		0.16
1.61		0.24

785. $NaBO_3.2H_2O$

5.4	(8)	1.00
4.70		0.13
3.96		0.13
3.03	(8)	1.00
2.71	(6)	0.75
2.62		0.13
2.49		0.25
2.37		0.13
2.20		0.38
2.13		0.38
2.01		0.13
1.87		0.13
1.81		0.13
1.74		0.13
1.70		0.13
1.64		0.13
1.51		0.13

786. Sodium Borobenzoate

4.40	(5)	0.83
3.92		0.17
3.45	(4)	0.67
2.94	(6)	1.00
2.60		0.17
2.27		0.17
2.18		0.33
2.02		0.17
1.94		0.17
1.79		0.33
1.56		0.17

787. $NaBrO_3$*

4.75		0.40
3.86		0.27
3.34		0.13
2.99	(15)	1.00
2.73	(8)	0.53
2.23		0.20
2.11		0.07
2.01		0.20
1.93		0.07
1.85		0.07
1.78	(12.5)	0.83
1.62		0.07
1.57		0.07
1.53		0.20
1.495		0.07
1.460		0.27
1.313		0.27
1.287		0.07
1.245		0.13
1.220		0.07
1.110		0.07
1.082		0.07
1.042		0.13

788. NaBr*

3.44	(9)	0.45
2.96	(20)	1.00
2.09	(12.5)	0.63
1.79		0.20
1.71		0.20
1.487		0.10
1.362		0.05
1.329		0.35
1.216		0.10
1.145		0.05
1.053		0.05

789. $CH_3CH_2CH_2COONa$

14.5	(62.5)	1.00
5.1		0.02
3.75	(4)	0.06
3.52		0.03
3.10		0.02
3.00		0.02
2.80	(4)	0.06
1.76		0.02

790. $(CH_3)_2AsO_2ONa.3H_2O$

6.0	(7)	0.78
5.5		0.55
5.1		0.33
4.30	(9)	1.00
4.11		0.66
3.57	(8)	0.89
3.22		0.11
3.10		0.33
2.98		0.11
2.84		0.66
2.74		0.11
2.51		0.22
2.39		0.11
2.28		0.11
2.21		0.44
2.14		0.11
2.04		0.33
1.81		0.33
1.73		0.22
1.69		0.11
1.65		0.11
1.61		0.22
1.53		0.11
1.425		0.22
1.355		0.11

791. Na_2CO_3

3.43		0.08
3.22		0.12
2.96	(40)	0.80
2.85		0.02
2.70		0.20
2.60	(30)	0.60
2.54		0.60
2.36	(50)	1.00
2.25		0.40
2.18		0.60
2.11		0.04
2.02		0.14
1.95		0.40
1.88		0.40
1.83		0.02
1.79		0.04
1.71		0.25
1.67		0.12
1.62		0.12B
1.57		0.25B
1.52		0.08
1.482		0.16
1.451		0.06
1.418		0.04
1.388		0.08
1.347		0.04

792. $Na_2CO_3.H_2O$

5.3		0.31
4.15		0.08
2.76	(40)	1.00
2.67	(17.5)	0.44
2.55		0.03
2.47		0.25
2.37	(25)	0.63
2.24		0.20
2.18		0.15
2.12		0.03
2.06		0.18
2.00		0.31
1.91		0.08
1.78		0.08
1.74		0.08
1.67		0.08B
1.65		0.08
1.61		0.25
1.54		0.05
1.470		0.03
1.431		-0.05
1.380		0.03
1.345		0.03
1.315		0.08

793. $Na_2CO_3.2^1/_2H_2O$

10.0		0.15
4.90		0.15
3.17		0.15
3.05	(17.5)	0.88
2.75		0.30
2.64	(20)	1.00
2.48		0.10
2.43	(10)	0.50
2.35		0.10
2.24		0.25
2.02		0.15
1.77		0.05
1.73		0.10
1.65		0.10
1.59		0.10
1.320		0.05

794. $Na_2CO_3.10H_2O$

5.3	(10)	0.57
4.50		0.23
4.03	(6)	0.34
3.52		0.11
3.44		0.11
3.24		0.09
3.17		0.09
3.01		0.23
2.89	(17.5)	1.00
2.80		0.34
2.67		0.17
2.57		0.23
2.43		0.34
2.36		0.06
2.29		0.11
2.22		0.06
2.16		0.06
2.10		0.09
2.05		0.06
1.98		0.17
1.94		0.09
1.91		0.09
1.85		0.06
1.79		0.09
1.75		0.09

795. $NaHCO_3$*

3.49	(2)	0.16
3.04		0.16
2.94	(12.5)	1.00
2.58	(6)	0.48
2.31		0.08
2.22		0.16
2.02		0.16
1.97		0.08
1.91		0.08
1.73		0.08
1.52		0.08

796. $NaKCO_3$

3.07	(30)	0.48
2.72	(62.5)	1.00
2.63		0.16
2.57		0.16
2.48		0.16
2.36		0.08
2.24	(25)	0.40
2.21		0.40
2.14		0.03
1.93		0.14
1.88		0.14
1.81		0.10
1.78		0.10
1.73		0.05
1.59		0.06
1.57		0.13
1.53		0.10
1.362		0.16
1.287		0.02
1.230		0.02
1.211		0.02
1.170		0.02
1.030		0.05

797. $NaClO_3$*

4.65		0.20
3.79		0.33
3.28	(5(	0.67
2.94	(75)	1.00
2.68		0.40
2.32		0.01
2.18		0.33
2.07		0.07
1.98		0.13
1.89		0.01
1.83		0.07
1.76	(50)	0.67
1.64		0.01
1.59		0.11
1.55		0.03
1.51		0.11
1.470		0.03
1.434		0.13
1.404		0.01
1.341		0.01
1.317		0.01
1.289		0.03
1.264		0.05
1.222		0.05
1.200		0.05
1.145		0.03
1.130		0.01
1.114		0.03
1.094		0.01
1.068		0.03
1.042		0.01
1.028		0.08

798. $NaClO_4$*

4.79		0.08
3.97	(40)	0.53
3.53	(75)	1.00
3.25		0.07
2.95	(40)	0.53
2.85		0.17
2.50		0.04
2.39		0.40
2.27		0.17
2.12		0.05
2.07		0.04
1.98		0.07
1.90		0.33
1.77		0.13
1.68		0.20
1.62		0.01
1.58		0.03
1.56		0.11
1.52		0.05

799. $NaClO_4.H_2O$

5.2	(20)	0.40
4.40		0.08
3.65	(40)	0.80
3.44	(50)	1.00
3.19		0.08
2.92		0.02
2.76		0.20
2.66		0.12
2.58		0.02
2.44		0.12
2.20		0.30
2.05		0.08
1.95		0.02
1.88		0.02
1.82		0.14
1.72		0.16
1.70		0.08
1.58		0.02
1.52		0.02
1.415		0.04
1.385		0.03
1.355		0.02
1.330		0.02
1.290		0.03

800. NaCl*

3.25		0.05
2.81	(150)	1.00
1.99	(125)	0.83
1.70		0.02
1.63	(50)	0.33
1.410		0.13
1.293		0.01
1.260		0.33
1.150		0.20
1.080		0.01
0.997		0.30
0.941		$0.05\alpha_1$
0.892		$0.03\alpha_1$
0.852		$0.03\alpha_1$
0.813		0.01
0.782		0.01
0.755		$0.01\alpha_1$

801. Na_2CrO_4*

4.97		0.11
4.09	(30)	0.48
3.88		0.48
3.59		0.32
2.91	(62.5)	1.00
2.73	(40)	0.64
2.48		0.24
2.17		0.10
2.12		0.05
2.03		0.20
1.94		0.16
1.79		0.24
1.71		0.02
1.68		0.03
1.65		0.05
1.62		0.20
1.50		0.20
1.465		0.03
1.417		0.08
1.370		0.06
1.340		0.03
1.270		0.02
1.210		0.10
1.170		0.03

802. $Na_2CrO_4.4H_2O$

6.0		0.33
5.2		0.50
4.50	(30)	1.00
3.70		0.20
3.58	(20)	0.67
3.20	(20)	0.67
2.98		0.58
2.86		0.50
2.71		0.20
2.66		0.33
2.53		0.07
2.44		0.10
2.25		0.20
2.10		0.20
2.03		0.20
1.93		0.23
1.86		0.13
1.79		0.13
1.73		0.07
1.70		0.03
1.65		0.03
1.58		0.20
1.480		0.10
1.395		0.03
1.335		0.03
1.210		0.07

803. $Na_2Cr_2O_7.2H_2O$

5.7		0.20
5.4	(25)	0.84
5.0		0.27
4.25		0.33
3.93	(30)	1.00
3.78		0.07
3.50		0.27
3.32		0.10
3.17		0.07
3.04	(25)	0.84
2.91		0.13
2.82		0.67
2.73		0.23
2.59		0.03
2.42		0.03
2.32		0.07
2.23		0.10B
2.10		0.10
2.01		0.07
1.96		0.07
1.90		0.23
1.86		0.13
1.79		0.13
1.72		0.07
1.68		0.10
1.66		0.13

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TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

804. $C_6H_5CH{:}CHCOONa$

d		I/I1
6.4	(6)	1.00
5.2		0.33
4.35	(6)	1.00
3.50		0.33
2.96	(4)	0.67
2.41		0.16

805. $Na_3C_6H_5O_7.2H_2O$

d		I/I1
7.9	(25)	1.00
5.5	(10)	0.40
5.1		0.40
3.99		0.04
3.70		0.40
3.38		0.04
3.23		0.32
3.13		0.04
2.98		0.32
2.78		0.08
2.73		0.32
2.62		0.08
2.52		0.04
2.43	(15)	0.60
2.34		0.04
2.23		0.08
2.15		0.08
2.06		0.04
2.00		0.32
1.95		0.36
1.87		0.04
1.82		0.08
1.75		0.04
1.70		0.04
1.67		0.08
1.61		0.08

806. $2Na_2C_6H_6O_7.11H_2O$

d		I/I1
6.0	(10)	1.00
5.0	(8)	0.80
4.41		0.50
4.14		0.40
3.95		0.20
3.75		0.20
3.57		0.20
3.47		0.20
3.33		0.10
3.22		0.10
3.01		0.30
2.89	(8)	0.80
2.78		0.40
2.71		0.50
2.58		0.20
2.47		0.20
2.33		0.50
2.28		0.10
2.31		0.60
2.12		0.10
2.07		0.10
2.00		0.10
1.96		0.10
1.92		0.30
1.82		0.30
1.75		0.10

807. NaCN*

d		I/I1
2.94	(75)	1.00
2.07	(40)	0.53
1.77		0.07
1.69	(7)	0.09
1.470		0.05
1.349		0.03
1.315		0.05
1.200		0.01
1.133		0.01

808. C_2H_5ONa

d		I/I1
14.0	(15)	0.50
6.8		0.13
4.90		0.07
4.54		0.23
4.01	(12.5)	0.42
3.15		0.13
2.97		0.20
2.78		0.03
2.52		0.13
2.38	(30)	1.00
2.25		0.07
2.17		0.07
2.05		0.17
1.99		0.10
1.85		0.13
1.74		0.07
1.69		0.42
1.60		0.03
1.57		0.07
1.52		0.03
1.470		0.07
1.393		0.10
1.343		0.10
1.307		0.07
1.195		0.10
1.070		0.07

809. $Na_4Fe(CN)_6$

d		I/I1
5.7	(12.5)	0.13
2.75	(100)	1.00
1.94	(40)	0.40
1.65		0.07
1.58		0.07
1.372		0.03
1.260		0.03
1.229		0.05
1.120		0.01B

810. $Na_4Fe(CN)_6.10H_2O$

d		I/I1
7.4	(12.5)	1.00
6.7		0.08
6.3		0.16
5.8		0.16
4.80		0.12
4.45		0.32
4.21		0.16
4.00		0.48
3.78		0.16
3.51	(9)	0.72
3.09		0.56
2.97		0.32
2.86		0.32
2.74		0.48
2.62		0.24
2.50		0.08
2.42		0.12
2.33		0.08
2.21		0.64
2.12		0.08
2.04	(10)	0.80
1.98		0.12
1.95		0.08
1.90		0.08
1.84		0.32
1.75		0.12

811. $Na_2Fe(CN)_5NO.2H_2O$

d		I/I1
7.8		0.50
5.8		0.50
4.75	(20)	1.00
4.16	(20)	1.00
3.92		0.10
3.31		0.15
2.95		0.05
2.89	(20)	1.00
2.79		0.05
2.71		0.25
2.60		0.25
2.54		0.50
2.42		0.05
2.38		0.30
2.15		0.40
2.03		0.15
1.98		0.05
1.93		0.15
1.88		0.15
1.72		0.05
1.69		0.10
1.65		0.05
1.61		0.10
1.440		0.10
1.381		0.05
1.350		0.05

812. NaF*

d		I/I1
2.32	(125)	1.00
1.64	(75)	0.60
1.336	(20)	0.16
1.158		0.03
1.035		$0.08\alpha_1$
0.946		$0.03\alpha_1$
0.821		0.01
0.774		0.01

813. Na_3AlF_6

d		I/I1
4.51		0.20
3.88		0.20
3.49		0.03
3.33		0.03
2.75	(50)	0.67
2.43		0.05
2.33		0.40
2.27		0.04
2.22		0.03
2.15		0.13
2.08		0.13
1.94	(75)	1.00
1.89		0.05
1.72		0.13
1.68		0.09
1.60		0.20
1.57	(40)	0.53
1.490		0.04
1.455		0.03
1.425		0.03
1.398		0.01
1.375		0.13
1.350		0.03
1.315		0.08
1.229		0.05

814. Na_2SiF_6

d		I/I1
5.1		0.08
4.42	(40)	0.80
4.21		0.80
3.32		0.80
3.04		0.50
2.89		0.02
2.50		0.04
2.27	(50)	1.00
2.20		0.02
2.10		0.02
2.02		0.04
1.96		0.02
1.89		0.10
1.79	(50)	1.00
1.66		0.25
1.62		0.08
1.58		0.25
1.53		0.02
1.470		0.20
1.449		0.20
1.391		0.16
1.325		0.02
1.257		0.04
1.226		0.04
1.210		0.04
1.181		0.02

815. $NaHCO_2$

d		I/I1
4.34	(30)	0.75
3.39	(30)	0.75
2.95		0.44
2.79	(40)	1.00
2.30		0.63
2.14		0.25
2.08		0.38
2.03		0.13
1.98		0.50
1.96		0.15
1.85		0.23
1.81		0.20
1.72		0.44
1.64		0.20
1.62		0.10
1.54		0.15
1.475		0.15
1.395		0.10
1.350		0.05
1.315		0.05
1.285		0.10
1.160		0.03
1.130		0.03
1.070		0.05

816. Sodium Hippurate

d		I/I1
19.0	(30)	1.00
10.8	(6)	0.20
9.0		0.17
6.8		0.03
6.5		0.03
4.55		0.03
4.20	(8)	0.27
3.97		0.07
3.84		0.07
3.62		0.10
3.40		0.03
3.23		0.03
2.90		0.13

817. NaOH

d		I/I1
5.8		0.13
2.85		0.20
2.35	(100)	1.00
2.03		0.10
1.90		0.08
1.70	(30)	0.30
1.65	(25)	0.25
1.460		0.10
1.346		0.02
1.266		0.05
1.201		0.05
1.178		0.01
1.108		0.02
1.071		0.07
1.019		0.02
0.973		0.04

818. $NaIO_3$*

d		I/I1
4.25	(50)	0.50
4.04		0.20
3.19	(30)	0.30
2.93	(100)	1.00
2.86		0.09
2.50		0.25
2.33		0.09
2.12		0.20
2.02		0.07
1.98		0.05
1.88		0.10
1.82		0.13
1.78		0.25
1.70		0.10
1.66		0.30
1.60		0.01
1.467		0.10
1.429		0.08
1.390		0.04
1.345		0.08
1.308		0.04
1.281		0.06
1.245		0.06
1.187		0.03
1.167		0.02
1.145		0.03
1.118		0.02
1.099		0.01
1.087		0.02

819. $Na_2H_3IO_6$

d		I/I1
4.95	(6)	0.12
4.45	(50)	1.00
3.33		0.12
2.94		0.06
2.74	(15)	0.30
2.59		0.12
2.52		0.02
2.46		0.12
2.21		0.10
2.08		0.12
1.94		0.04
1.89		0.04
1.84		0.04
1.79		0.04
1.74		0.04
1.70		0.06
1.65		0.12
1.62		0.02
1.59		0.04
1.55		0.04
1.473		0.02
1.445		0.04
1.401		0.03
1.375		0.04
1.298		0.03
1.257		0.03

820. NaI*

d		I/I1
3.74	(25)	0.83
3.22	(30)	1.00
2.29	(25)	0.83
1.95		0.58
1.87		0.42
1.61		0.17
1.481		0.23
1.445		0.42
1.320		0.23
1.244		0.13
1.144		0.07
1.094		0.07
1.079		0.07
1.020		0.03
0.974		0.03

821. $NaMnO_4.3H_2O$

d		I/I1
5.2	(25)	0.83
4.38		0.27
4.08		0.07
3.87		0.07
3.67	(25)	0.83
3.48	(30)	1.00
3.18		0.03
3.00		0.07
2.90		0.07
2.82		0.50
2.70		0.07
2.60		0.10
2.48		0.33
2.22		0.20
2.10		0.03
1.99		0.13
1.92		0.03
1.86		0.07
1.79		0.03
1.73		0.13
1.61		0.03
1.57		0.03
1.50		0.03
1.414		0.03
1.365		0.03
1.310		0.03

822. $Na_2MoO_4.2H_2O$

d		I/I1
6.9	(62.5)	1.00
6.0		0.02
5.2		0.02
4.79		0.02
4.22		0.16
3.75		0.05
3.62		0.16
3.32		0.16
3.17	(12.5)	0.20
3.07		0.16
2.98	(15)	0.24
2.88		0.02
2.68		0.16
2.60		0.02
2.34		0.05
2.17		0.05
2.03		0.06
1.98		0.02
1.88		0.06
1.67		0.06
1.59		0.02
1.51		0.02
1.480		0.02
1.415		0.02
1.350		0.02
1.260		0.02

823. Sodium Phosphomolybdate

d		I/I1
8.2		0.23
6.9	(30)	1.00
6.0		0.03
5.3		0.03
4.20	(12.5)	0.42
3.60		0.33
3.40		0.10
3.30		0.17
3.16	(15)	0.50
3.05		0.13
2.98		0.20
2.90		0.13
2.76		0.03
2.66		0.33
2.48		0.07
2.36		0.07
2.18		0.16
2.02		0.16
1.88		0.20
1.81		0.07
1.67		0.23
1.63		0.07
1.59		0.07
1.52		0.07
1.470		0.10
1.410		0.03

824. Sodium Naphthionate

d		I/I1
18.5	(17.5)	1.00
5.5	(17.5)	1.00
4.87		0.28
3.85	(6)	0.34
3.61		0.23
3.07		0.23
2.70		0.11
2.55		0.06
2.45		0.06
2.36		0.06
1.73		0.06
1.68		0.06

825. $NaNO_3$*

d		I/I1
3.90		0.02
3.03	(100)	1.00
2.80		0.06
2.53		0.06
2.31	(30)	0.30
2.11		0.08
1.94		0.02
1.89	(25)	0.25
1.65		0.07
1.63		0.04
1.54		0.03
1.50		0.01
1.490		0.03
1.461		0.06
1.400		0.02
1.367		0.02
1.332		0.01
1.300		0.02
1.265		0.01
1.224		0.01
1.170		0.04

826. Sodium Cobaltic Nitrate

d		I/I1
6.1	(12.5)	1.00
5.0	(10)	0.80
3.91		0.86
3.08		0.80
2.50		0.80
2.41		0.80
2.10	(12.5)	1.00
1.95		0.40
1.80		0.24
1.67		0.08
1.54		0.16
1.50		0.16
1.475		0.16
1.405		0.08
1.325		0.08
1.305		0.08
1.263		0.08

827. $NaNO_2$*

d		I/I1
2.97	(75)	1.00
2.78	(30)	0.40
2.02	(30)	0.40
2.00		0.23
1.93		0.11
1.78		0.12
1.70		0.08
1.64		0.03
1.497		0.05
1.398		0.01
1.389		0.04
1.343		0.02
1.310		0.02
1.290		0.01
1.258		0.01
1.233		0.04
1.211		0.01
1.160		0.01
1.066		0.01
1.048		0.01
1.030		0.01
1.015		0.01

828. $Na_2C_2O_4$

d		I/I1
5.1		0.04
3.45		0.04
2.81	(50)	1.00
2.59	(25)	0.50
2.46		0.08
2.32	(25)	0.50
2.17		0.20
2.13		0.04
2.02		0.25
1.96		0.08
1.92		0.20
1.82		0.12
1.77		0.08
1.73		0.20
1.65		0.25
1.62		0.06
1.56		0.06
1.51		0.04
1.450		0.04
1.420		0.04
1.228		0.02
1.190		0.02
1.162		0.02
1.044		0.02

829. $NaHC_2O_4.H_2O$

d		I/I1
5.4		0.09
4.90		0.13
4.30		0.09
4.11		0.03
3.90		0.09
3.20		0.06
2.97	(62.5)	1.00
2.81		0.02
2.67	(10)	0.16
2.45	(12.5)	0.20
2.13		0.14
1.94		0.06
1.77		0.02
1.72		0.16
1.485		0.03
1.302		0.02

830. N

d	
9.0	
7.8	
5.6	
5.0	
3.75	
3.43	
3.09	
2.87	
2.76	
2.55	(50)
2.47	
2.42	
2.35	(7)
2.30	
2.24	
2.03	
1.96	
1.89	
1.86	
1.80	(25)
1.71	
1.65	
1.56	
1.50	
1.466	
1.438	
1.400	
1.345	
1.275	

831. p-$C_6H_4OHSO_3H.2H_2O$

d	
11.9	
6.1	
5.5	
5.0	
4.72	
4.23	(10
3.99	
3.81	(17.5
3.62	
3.41	
3.21	
3.06	(17.5
2.90	
2.67	
2.52	
2.40	
2.31	
2.23	
2.09	
2.02	
1.96	
1.91	
1.85	
1.79	
1.74	
1.66	

832. So Nitrophen

d	
6.1	(17.5
4.23	
3.45	(10
3.25	(4
3.00	
2.81	
2.60	
2.35	
2.29	
1.72	
1.62	

833. So Dinitrophe

d	
5.8	(15)
3.77	(10)
3.40	(15)
3.15	
3.02	
2.97	
2.75	
2.49	
2.37	
2.28	
2.17	
2.11	
2.01	
1.94	
1.84	
1.77	
1.59	

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

d	I/I1
i. Sodium altic Nitrate	
(12.5)	1.00
(10)	0.80
	0.56
	0.80
	0.80
(12.5)	1.00
	0.40
	0.24
	0.08
	0.16
	0.16
	0.16
	0.08
	0.08
	0.08
	0.08
. $NaNO_2$*	
(75)	1.00
(30)	0.40
(30)	0.40
	0.23
	0.11
	0.12
	0.08
	0.03
	0.05
	0.01
	0.04
	0.02
	0.02
	0.01
	0.01
	0.04
	0.01
	0.01
	0.01
	0.01
	0.01
. $Na_2C_2O_4$	
	0.04
	0.04
(50)	1.00
(25)	0.50
	0.08
(25)	0.50
	0.20
	0.04
	0.25
	0.08
	0.20
	0.12
	0.08
	0.20
	0.25
	0.06
	0.06
	0.04
	0.04
	0.04
	0.02
	0.02
	0.02
	0.02
$NaHC_7O_4.H_2O$	
	0.09
	0.13
	0.09
	0.03
	0.09
	0.06
(62.5)	1.00
	0.02
	0.16
(1	0.20
	0.14
	0.06
	0.02
	0.16
	0.03
	0.02

830. Na_2O_2

d	I/I1
9.0	0.02
7.8	0.02
5.6	0.04
5.0	0.04
3.75	0.02
3.43	0.04
3.09	0.10
2.87	0.04
2.76	0.02
2.55 (50)	1.00
2.47	0.02
2.42	0.04
2.35 (7)	0.14
2.30	0.12
2.24	0.04
2.03	0.10
1.96	0.02
1.89	0.02
1.86	0.04
1.80 (25)	0.50B
1.71	0.04
1.65	0.04
1.56	0.02
1.50	0.04
1.466	0.12
1.438	0.04
1.400	0.04
1.345	0.12
1.275	0.08

831. $p\text{-}C_6H_4OHSO_3Na.2H_2O$

d	I/I1
11.9	0.34
6.1	0.29
5.5	0.06
5.0	0.40
4.72	0.23
4.23 (10)	0.57
3.99	0.11
3.81 (17.5)	1.00
3.62	0.23
3.41	0.06
3.21	0.23
3.06 (17.5)	1.00
2.90	0.11
2.67	0.11
2.52	0.11
2.40	0.06
2.31	0.06
2.23	0.09
2.09	0.11
2.02	0.11
1.96	0.11
1.91	0.06
1.85	0.06
1.79	0.11
1.74	0.06
1.66	0.06

832. Sodium Nitrophenylate

d	I/I1
6.1 (17.5)	1.00
4.23	0.17
3.45 (10)	0.57
3.25	0.17
3.00 (4)	0.23
2.81	0.06
2.60	0.06
2.35	0.06
2.29	0.11
1.72	0.06
1.52	0.06

833. Sodium Dinitrophenylate

d	I/I1
5.8 (15)	1.00
3.77 (10)	0.66
3.40 (15)	1.00
3.15	0.53
3.02	0.40
2.97	0.53
2.75	0.26
2.49	0.20
2.37	0.07
2.28	0.20
2.17	0.20
2.11	0.20
2.01	0.07
1.94	0.07
1.84	0.07
1.77	0.07
1.59	0.07

834. Na_3PO_4

d	I/I1
4.25 (30)	0.48
3.95	0.13
3.84	0.20
3.45	0.06
3.11	0.11
2.70 (30)	0.48
2.55 (62.5)	1.00
2.43	0.10
2.25	0.20
2.15	0.06
2.05	0.20
1.91	0.48
1.81	0.08
1.72	0.11
1.66	0.02
1.57	0.06
1.53	0.24
1.450	0.11
1.400	0.03
1.355	0.06
1.316	0.06
1.275	0.05
1.245	0.03
1.207	0.06
1.193	0.08
1.157	0.03

835. Na_2HPO_4

d	I/I1
4.90	0.04
4.66	0.03
3.99 (30)	0.40
3.81 (30)	0.40
3.41	0.20
2.87	0.17
2.80 (75)	1.00
2.71	0.40
2.64	0.08
2.53	0.11
2.44	0.20
2.30	0.13
2.20	0.20
2.12	0.03
2.05	0.08
1.99	0.20
1.92	0.20
1.81	0.08
1.75	0.27
1.71	0.20
1.63	0.13
1.59	0.27
1.470	0.03
1.445	0.13
1.400	0.08
1.344	0.07

836. $Na_2HPO_4.2H_2O$

d	I/I1
5.2 (25)	1.00
4.61 (25)	1.00
3.95	0.24
3.63	0.16
3.34 (20)	0.80
3.24	0.60
2.88	0.60
2.73	0.50
2.59	0.24
2.47	0.60
2.25	0.28
2.19	0.24
2.06	0.24
2.00	0.16
1.96	0.20
1.90	0.28
1.80	0.04
1.73	0.12
1.64	0.12
1.59	0.12
1.51	0.04
1.468	0.16
1.410	0.12
1.370	0.08
1.089	0.08
1.064	0.04

837. $Na_2HPO_4.12H_2O$

d	I/I1
7.7	0.10
6.2	0.10
5.4 (20)	1.00
4.51	0.05
4.35	0.40
4.00	0.40
3.73	0.20
3.47	0.30
3.30	0.05
3.15	0.05
2.94 (17.5)	0.88B
2.83	0.40
2.71 (12.5)	0.63
2.58	0.05
2.46	0.30
2.40	0.05
2.33	0.15
2.25	0.10
2.18	0.05
2.11	0.15
2.02	0.10
1.95	0.15
1.91	0.25
1.82	0.20
1.70	0.35
1.65	0.10

838. NaH_2PO_4

d	I/I1
4.98	0.08
4.07	0.40
3.94 (25)	1.00
3.38	0.40
3.18 (25)	1.00
3.06	0.08
2.95	0.16
2.85	0.04
2.72 (12.5)	0.50
2.58	0.04
2.48	0.08
2.38	0.16
2.29	0.12
2.23	0.16
2.15	0.16
2.08	0.04
1.97	0.12
1.88	0.08
1.84	0.16
1.73	0.16
1.69	0.04
1.64	0.16
1.51	0.08
1.465	0.08
1.435	0.04
1.395	0.04

839. $NaH_2PO_4.H_2O$

d	I/I1
5.4 (20)	1.00
4.40	0.50
4.18	0.05
3.91	0.10
3.77	0.15
3.68	0.25
3.50	0.20
3.39 (20)	1.00
3.15 (17.5)	0.88
3.05	0.50
2.86	0.05
2.73	0.05
2.65	0.50
2.55	0.50
2.48	0.05
2.42	0.05
2.35	0.30
2.25	0.15
2.20	0.25
2.13	0.05
2.06	0.25
2.02	0.20
1.84	0.30
1.78	0.05
1.74	0.10
1.71	0.15

840. $Na_4P_2O_7.10H_2O$

d	I/I1
7.7	0.15
5.3	0.38
4.90 (25)	0.63
4.10	0.08
3.82 (40)	1.00
3.25	0.15
2.97 (25)	0.63
2.67	0.63
2.45	0.20
2.40	0.38
2.33	0.20
2.04	0.05
1.98	0.15
1.86	0.03
1.77	0.15
1.68	0.05
1.63	0.13
1.59	0.15
1.475	0.08
1.370	0.03
1.335	0.03
1.160	0.03
1.120	0.03
1.050	0.03

841. $NaPO_3$

d	I/I1
6.7	0.15
5.3	0.10
5.0 (12.5)	0.31
3.82	0.20
3.50	0.15
3.39	0.18
3.29	0.15
3.09 (25)	0.63
2.87 (40)	1.00
2.73	0.15
2.53	0.15
2.42	0.15
2.28	0.23
2.15	0.10
2.00	0.03
1.85	0.10
1.74	0.25
1.68	0.10
1.490	0.03
1.470	0.08
1.430	0.05
1.400	0.03
1.370	0.10
1.280	0.03
1.190	0.03
1.100	0.05

842. $Na_4P_2O_7$

d	I/I1
4.40 (40)	1.00
3.38	0.25
2.72 (30)	0.75
2.53	0.03
2.42	0.03
2.33	0.23
2.06	0.10
2.02	0.05
1.91 (12.5)	0.31
1.75	0.10
1.67	0.03
1.55	0.23
1.475	0.13
1.424	0.15
1.342	0.08
1.293	0.05
1.206	0.05
1.165	0.03
1.140	0.05
1.070	0.03
1.013	0.05

843. $Na_4P_2O_7.10H_2O$

d	I/I1
6.5	0.25
5.4	0.40
4.35 (20)	1.00
3.68 (10)	0.50
3.45	0.30
3.05	0.25
2.78 (15)	0.75
2.69	0.10
2.60	0.50
2.52	0.45
2.44	0.40
2.25	0.35
2.00	0.15
1.95	0.10
1.90	0.10
1.79	0.05
1.75	0.10
1.72	0.25
1.67	0.15
1.59	0.15
1.395	0.10
1.333	0.10
1.220	0.05
1.150	0.05

844. $NaNH_4HPO_4.4H_2O$

d	I/I1
10.1	0.45
6.6 (20)	1.00
5.8	0.10
4.6 (10)	0.50
4.23	0.45
3.67	0.30
3.45	0.30
3.27	0.40
3.16	0.05
3.02	0.05
2.89 (20)	1.00
2.67	0.15
2.48	0.10
2.40	0.10
2.32	0.10
2.19	0.15
2.00	0.10
1.91	0.10
1.82	0.10
1.77	0.10
1.73	0.05

845. Sodium Calcium Glycerophosphate

d	I/I1
9.9	0.29
3.98 (7)	1.00
2.73 (3)	0.43
1.97 (3)	0.43
1.78	0.14
1.490	0.14
1.375	0.14

846. $Na_2HPO_4.5H_2O$

d	I/I1
7.0	0.08
6.1	0.04
5.7	0.04
5.4	0.06
4.56	0.12
4.23	0.20
3.95	0.14
3.50	0.12
3.39	0.10
3.17	0.02
3.07	0.02
2.91	0.18
2.81	0.02
2.75	0.02
2.67 (50)	1.00
2.54	0.06
2.44	0.02
2.40	0.02
2.32	0.02
2.26	0.02
2.12	0.02
2.08	0.08
2.02	0.02
1.97	0.02
1.93	0.02
1.89 (12.5)	0.25
1.84	0.02
1.79	0.02
1.74	0.02
1.66	0.02
1.59	0.02
1.54 (12.5)	0.25
1.480	0.02
1.440	0.02
1.405	0.02
1.361	0.02
1.337	0.08
1.193	0.06
1.129	0.02
1.087	0.02
1.010	0.03

847. $NaH_2PO_2.H_2O$

d	I/I1
8.6	0.67
7.8	0.67
6.4	0.40
6.0	0.40
4.65	0.07
4.16 (12.5)	0.83
3.85 (15)	1.00
3.70	0.13
3.53	0.83
3.37	0.13
3.29	0.13
3.12	0.67
3.00	0.40
2.87 (15)	1.00
2.75	0.47
2.64	0.60
2.57	0.07
2.51	0.27
2.42	0.13
2.34	0.13
2.26	0.13
2.18	0.27
2.12	0.33
2.02	0.20
1.99	0.07
1.94	0.27
1.86	0.07
1.84	0.07
1.78	0.40
1.71	0.33
1.67	0.13

848. $Na_2PbO_3.3H_2O$

d	I/I1
4.80 (4)	1.00
4.62 (4)	1.00
4.15	0.25
3.00	0.25
2.90	0.25
2.53 (4)	1.00
1.85	0.75
1.73	0.25
1.62	0.25
1.420	0.25
1.393	0.25
1.260	0.25

849. $Na(C_6H_4OHCOO)$

d	I/I1
14.7 (25)	1.00
6.4 (12.5)	0.50
5.0	0.04
4.70	0.04
3.35 (15)	0.60
3.20	0.08
3.02	0.16
2.84	0.08
2.45	0.08
2.25	0.04
1.79	0.04
1.73	0.04
1.68	0.08

850. Na_2SeO_4

d	I/I1
4.82 (30)	1.00
3.92	0.27
3.27	0.33
3.14	0.20
2.87 (25)	0.83
2.73 (15)	0.50
2.41	0.23
2.00	0.03
1.96	0.03
1.91	0.33
1.86	0.13
1.72	0.33
1.60	0.07
1.53	0.07
1.475	0.07
1.425	0.07
1.365	0.03
1.338	0.13
1.310	0.03
1.200	0.03
1.108	0.03

851. Na_2SeO_3

d	I/I1
4.40	0.40
4.05 (8)	0.80
3.70 (8)	0.80
3.43	0.40
2.98	0.10
2.81	0.30
2.75	0.60
2.44	0.60
2.38 (10)	1.00
2.00	0.10
1.71	0.30
1.56	0.10
1.52	0.10
1.465	0.10
1.425	0.20
1.375	0.10
1.340	0.10
1.285	0.10

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

852. Na_2SiO_3

d		I/I1
5.3		0.20
3.56		0.20
3.04	(62.5)	1.00
2.57	(30)	0.48
2.40	(40)	0.64
1.98		0.09
1.88		0.28
1.83		0.09
1.75		0.40
1.53		0.05
1.445		0.09
1.418		0.40
1.145		0.03
1.114		0.09
1.032		0.02
0.990		0.02
0.932		0.02

853. $Na_2SiO_3.9H_2O$

d		I/I1
8.7		0.10
5.9		0.10
5.3		0.05
5.0		0.10
4.75		0.15
3.83	(6)	0.30
3.16		0.10
2.92	(4)	0.20
2.79	(20)	1.00
2.68		0.05
2.53		0.05
2.33		0.05
2.19		0.10
2.12		0.08
2.02		0.15
1.92		0.05
1.82		0.10
1.71		0.05
1.61		0.08
1.54		0.05
1.51		0.05
1.450		0.05
1.428		0.05
1.418		0.05
1.399		0.05
1.351		0.05

854. $NaAlSi_2O_6$

d		I/I1
6.4		0.08
4.05	(17.5)	0.35
3.80		0.16
3.66	(12.5)	0.25
3.20	(50)	1.00
2.96		0.25
2.65		0.02
2.56		0.12
2.44		0.14
2.32		0.12
2.18		0.06
2.13		0.12
1.99		0.08
1.90		0.12
1.83		0.18
1.80		0.08
1.73		0.08
1.67		0.06
1.58		0.12
1.50		0.08
1.460		0.16
1.425		0.16
1.380		0.08
1.350		0.14
1.270		0.14
1.223		0.12
1.200		0.04
1.169		0.08
1.137		0.06
1.050		0.04
1.005		0.02
0.958		0.04
0.910		0.02
0.895		0.02
0.877		0.02

855. $Na_2SnO_3.3H_2O$

d		I/I1
5.4		0.16
4.75	(40)	0.80
4.17		0.16
2.96		0.30
2.72		0.12
2.60		0.04
2.51	(50)	1.00
2.43		0.02
2.36		0.02
2.29		0.35
2.19		0.02
2.10		0.02
2.00		0.02
1.93		0.02
1.85	(20)	0.40
1.78		0.02
1.72		0.20
1.65		0.04
1.61		0.16
1.53		0.04
1.482		0.04
1.420		0.14
1.390		0.12
1.310		0.04
1.259		0.06
1.161		0.02
1.143		0.02
1.125		0.02
1.095		0.06
1.079		0.02
1.058		0.02
1.035		0.02
1.014		0.04
0.993		0.02
0.973		0.02

856. $Na(C_{17}H_{35}COO)$

d		I/I1
4.59	(2)	0.20
4.16	(10)	1.00
3.90	(2)	0.20
3.73		0.15
3.53		0.10

857. $(CH_2COONa)_2.6H_2O$

d		I/I1
5.1		0.48
4.39	(8)	0.64
3.90		0.48
3.58		0.08
3.22		0.24
3.05	(8)	0.64
2.79	(12.5)	1.00
2.68		0.08
2.55		0.40
2.48		0.08
2.40		0.16
2.17		0.32
2.09		0.40
2.03		0.08
1.96		0.08
1.88		0.24
1.81		0.08
1.72		0.16
1.39		0.08

858. Na_2SO_4*

d		I/I1
4.66	(30)	0.40
3.84		0.13
3.18		0.33
3.08		0.27
2.78	(75)	1.00
2.64		0.40
2.33		0.27
2.22		0.03
1.87	(40)	0.53
1.79		0.05
1.67		0.17
1.60		0.05
1.55		0.20
1.50		0.08
1.428		0.11
1.385		0.05
1.320		0.04
1.295		0.16
1.280		0.08
1.213		0.03
1.164		0.01
1.133		0.05
1.100		0.01
1.075		0.05
1.063		0.10
1.042		0.04
0.984		0.03
0.966		0.04
0.930		0.01

859. Na_2SO_4 (heated)

d		I/I1
4.75		0.02
4.22		0.01
3.92	(30)	0.30
3.76		0.20
3.51		0 18
2.80	(100)	1.00
2.63	(50)	0.50
2.37		0.18
2.24		0.01
2.13		0.02
2.08		0.02
1.96		0.25
1.88		0.10
1.74		0.25
1.69		0.01
1.61		0.02
1.57		0.13
1.53		0.01
1.490		0.01
1.455		0.08
1.397		0.03
1.380		0.01
1.335		0.01
1.319		0.01
1.298		0.02
1.233		0.01
1.172		0.05
1.130		0.04
1.090		0.01
1.052		0.03
1.010		0.01

860. $Na_2SO_4.10H_2O$

d		I/I1
6.3		0.03
5.5	(30)	1.00
4.80		0.42
4.33		0.13
3.82		0.27
3.60		0.07
3.40		0.07
3.22	(15)	0.50
3.10	(15)	0.50
2.93		0.07
2.80		0.27
2.70		0.10
2.56		0.07
2.52		0.27
2.44		0.10
2.37		0.07
2.29		0.07
2.19		0.07
2.10		0.20
2.03		0.07
1.97		0.07
1.92		0.17
1.83		0.03
1.79		0.10
1.74		0.07
1.71		0.07
1.66		0.10
1.55		0.03
1.460		0.03
1.370		0.07
1.311		0.07
1.262		0.03

861. $NaHSO_4$

d		I/I1
4.48		0.32
4.09		0.28
3.70		0.12
3.40	(25)	1.00
3.17		0.16
2.98	(15)	0.60
2.77	(10)	0.40
2.58		0.04
2.51		0.12
2.27		0.12
2.22		0.08
2.17		0.08
2.05		0.04
1.95		0.08
1.90		0.04
1.85		0.08
1.74		0.08
1.71		0.04
1.67		0.04
1.63		0.04
1.59		0.04
1.56		0.04

862. $NaHSO_4.H_2O$

d		I/I1
5.2	(15)	0.60
4.37		0.04
4.00		0.08
3.92		0.08
3.55	(25)	1.00
3.43	(25)	1.00
2.76		0.40
2.64		0.16
2.55		0.08
2.42		0.28
2.20		0.28
2.17		0.20
2.10		0.04
2.05		0.04
2.00		0.08
1.88		0.20
1.82		0.04
1.78		0.08
1.73		0.04
1.69		0.20
1.62		0.04
1.59		0.04
1.56		0.04
1.51		0.04
1.475		0.04
1.450		0.04
1.418		0.06
1.382		0.08
1.350		0.08
1.295		0.04

863. $Na_2S_2O_8$

d		I/I1
4.56	(50)	0.80
4.23		0.03
3.90		0.02
3.55		0.13
3.32	(62.5)	1.00
3.19	(50)	0.80
2.89		0.10
2.80		0.05
2.71		0.14
2.63		0.02
2.37		0.24
2.27		0.32
2.20		0.02
2.08		0.06
1.97		0.10
1.87		0.05
1.78		0.11
1.72		0.10
1.66		0.06
1.58		0.05
1.51		0.03
1.455		0.03
1.433		0.02
1.407		0.02
1.377		0.02
1.328		0.02
1.304		0.02
1.278		0.05
1.254		0.02
1.238		0.03
1.186		0.02
1.164		0.02
1.131		0.02
1.103		0.05

864. $Na_2S.9H_2O$

d		I/I1
3.80	(4)	0.66
3.17		0.16
2.70	(5)	0.83
2.62	(6)	1.00
2.38		0.16
2.19		0.16
1.89		0.32
1.55		0.16

865. Na_2SO_3

d		I/I1
4.71		0.03
3.72		0.67
3.07		0.27
2.72	(75)	1.00
2.57	(75)	1.00
2.48		0.20
2.35		0.11
2.20		0.20
2.02		0.03
1.87	(75)	1.00
1.78		0.11
1.71		0.01
1.63		0.03
1.57		0.40
1.54		0.53
1.460		0.17
1.360		0.27
1.282		0.13
1.245		0.01
1.201		0.20
1.161		0.20
1.100		0.08
1.030		0.08
1.021		0.13
0.996		0.05
0.960		0.07

866. $Na_2SO_3.7H_2O$

d		I/I1
8.9		0.05
7.9		0.05
7.3		0.05
6.2		0.20
5.7		0.10
4.95		0.05
4.70		0.10
4.26	(6)	0.30
4.00		0.20
3.80		0.05
3.50		0.10
3.31		0.05
3.13		0.15
3.04		0.10
2.87	(20)	1.00
2.66	(10)	0.50
2.47		0.20
2.39		0.10
2.28		0.10
2.17		0.15
2.07		0.30
2.02		0.05
1.94		0.08
1.90		0.08
1.82		0.10
1.72		0.10
1.56		0.05
1.52		0.05
1.464		0.05
1.450		0.05

867. $Na_2S_2O_4.2H_2O$

d		I/I1
5.6		0.16
4.28	(20)	0.40
3.39		0.02
3.27	(30)	0.60
2.93		0.12
2.82	(50)	1.00
2.56		0.02
2.30		0.14
2.15		0.12
2.04		0.14
2.02		0.14
1.80		0.30
1.75		0.12
1.72		0.02
1.64		0.04
1.62		0.12
1.59		0.02
1.57		0.06
1.53		0.02
1.50		0.02
1.462		0.03
1.412		0.12
1.304		0.03
1.290		0.03
1.250		0.02
1.212		0.02

868. $Na_2S_2O_5$

d		I/I1
4.44	(30)	0.75
4.33		0.03
4.06	(30)	0.75
3.78		0.18
3.40		0.38
3.23		0.03
3.09		0.38
2.99		0.15
2.75		0.20
2.60	(40)	1.00
2.42		0.18
2.32		0.03
2.24		0.05
2.15		0.03
2.08		0.04
2.02		0.08
1.95		0.10
1.88		0.10
1.82		0.05
1.77		0.03
1.72		0.05
1.67		0.04
1.64		0.05
1 59		0.05
1.55		0.08
1.51		0.10
1.450		0.04
1.418		0.05
1.390		0.05
1.360		0.05
1.307		0.03
1.297		0.03
1.203		0.05
1.182		0.03
1.161		0.05
1.115		0.05

869. $C_{14}H_7O_3SO_2Na$

d		I/I1
5.6		0.30
5.3	(7)	0.35
4.41	(7)	0.35
4.15		0.20
3.89		0.30
3.49	(20)	1.00
3.35		0.05
3.10		0.20
3.01		0.05
2.93		0.05
2.81		0.05
2.72		0.15
2.65		0.05
2.57		0.05
2.42		0.05
2.37		0.05
2.19		0.10
2.11		0.05
2.03		0.05
2.01		0.05
1.94		0.05
1.89		0.05
1.84		0.05
1.79		0.05
1.75		0.05
1.69		0.05

870. $C_{12}H_7SO_3Na$

d		I/I1
5.4	(12.5)	1.00
4.96		0.32
4.78		0.32
4.39		0.08
4.15		0.24
3.82	(6)	0.48
3.57	(6)	0.48
3.03		0.32
2.86		0.08
2.82		0.08
2.71		0.08
2.60		0.08
2.48		0.08
2.41		0.08
2.28		0.08
2.24		0.08
2.18		0.08
2.11		0.08
2.08		0.08
2.05		0.08
2.02		0.08
2.00		0.08

871. $C_{25}H_9(SO_3Na)_2$

d		I/I1
11.9	(12.5)	1.00
4.85	(12.5)	1.00
4.38	(4)	0.32
4.18		0.32
3.39		0.24
3.02		0.24
2.84		0.08
2.61		0.08
2.49		0.16
2.04		0.08
1.93		0.08
1.78		0.08

872. $Na_2C_4H_4O_6.2H_2O$

d		I/I1
9.2	(20)	1.00
4.65		0.20
4.54		0.20
3.62		0.30
3.50		0.10
3.35		0.10
2.95		0.05
2.85	(8)	0.40
2.80	(8)	0.40
2.63		0.20
2.48		0.35
2.32		0.20
2.16		0.15
2.06		0.15
1.91		0.05
1.86		0.05
1.80		0.05

873. $NaHC_4H_4O_6.H_2O$

d		I/I1
4.50	(8)	0.64
4.30	(12.5)	1.00
4.00		0.48
3.34	(10)	0.80
3.15		0.08
2.96		0.08
2.65		0.32
2.52		0.16
2.38		0.16
2.26		0.08
2.15		0.08
2.07		0.08

874. Na

d	
6.0	(25
5.0	
4.45	
4.27	(1.
4.10	
3.75	
3.42	
3.23	
3.09	
2.97	
2.82	(12.1
2.46	
2.42	
2.35	
2.29	
2.23	
2.16	
2.01	
1.94	
1.79	
1.75	
1.72	
1.61	
1.56	
1.53	
1.470	
1.410	

875. Na

d		
8.1		
6.7		
6.0		
5.3		
4.61		
4.30		
3.49	(40)	
3.32		
3.20	(75)	
2.96	(40)	
2.86		
2.75		
2.65		
2.57		
2.48		
2.40		
2.28		
2.19		
2.13		
2.04		
1.95		
1.90		
1.85		
1.80		
1.75		
1.70		
1.66		
1.58		
1.55		
1.52		
1.480		
1.470		
1.438		
1.407		
1.381		
1.351		
1.318		
1.270		
1.248		
1.190		
1.159		
1.138		
1.081		

876. Na

d		
5.5	(9)	
4.86		
4.47		
3.70	(7)	
3.50		
3.23	(10)	
2.95		
2.84		
2.72		
2.64		
2.43		
2.30		
2.24		
2.11		
2.02		
1.85		
1.64		
1.60		
1.435		
1.315		

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TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

869. $H_7O_2SO_2Na$

d	I/I₁
5.0	0.30
(7)	0.35
(7)	0.35
	0.20
	0.30
(20)	1.00
	0.05
	0.20
	0.05
	0.05
	0.05
	0.15
	0.05
	0.05
	0.05
	0.05
	0.05
	0.10
	0.05
	0.05
	0.05
	0.05
	0.05
	0.05

$C_{12}H_7SO_2Na$

d	I/I₁
(12.5)	1.00
	0.32
	0.32
	0.08
	0.24
(6)	0.48
(6)	0.48
	0.32
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08
	0.08

$C_{12}H_8(SO_2Na)_2$

d	I/I₁
(12.5)	1.00
(12.5)	1.00
(4)	0.32
	0.32
	0.24
	0.24
	0.08
	0.08
	0.16
	0.08
	0.08
	0.08

872. $_2H_4O_6.2H_2O$

d	I/I₁
(20)	1.00
	0.20
	0.20
	0.30
	0.10
	0.10
	0.05
(8)	0.40
(8)	0.40
	0.20
	0.35
	0.20
	0.15
	0.15
	0.05
	0.05
	0.05

873. $C_4H_4O_6.H_2O$

d	I/I₁
(8)	0.64
(12.5)	1.00
	0.48
(10)	0.80
	0.08
	0.08
	0.32
	0.16
	0.16
	0.08
	0.08
	0.08

874. Na_2TeO_3

d	I/I₁
(25)	1.00
	0.32
	0.16
(15)	0.60
	0.40
	0.24
	0.40
	0.32
	0.08
	0.16
(12.5)	0.50
	0.24
	0.50
	0.04
	0.28
	0.32
	0.12
	0.12
	0.08
	0.08
	0.04

875. NaCNS

d	I/I₁
8.1	0.01
6.7	0.08
6.0	0.01
5.3	0.01
4.61	0.01
4.30	0.04
3.49 (40)	0.53
3.32	0.20
3.20 (75)	1.00
2.96 (40)	0.53
2.86	0.33
2.75	0.08
2.65	0.11
2.57	0.11
2.48	0.01
2.40	0.33
2.26	0.20
2.19	0.11
2.13	0.01
2.04	0.53
1.95	0.11
1.90	0.08
1.85	0.13
1.80	0.12
1.75	0.07
1.70	0.01
1.66	0.09
1.58	0.11
1.55	0.07
1.52	0.03
1.480	0.03
1.470	0.03
1.438	0.03
1.407	0.03
1.381	0.01
1.351	0.08
1.318	0.04
1.270	0.03
1.248	0.07
1.190	0.05
1.159	0.01
1.138	0.02
1.081	0.02

876. $Na_2S_2O_3$

d	I/I₁
5.5 (9)	0.90
4.86	0.50
4.47	0.20
3.70 (7)	0.70
3.50	0.10B
3.23 (10)	1.00
2.95	0.20
2.84	0.10
2.72	0.10
2.64	0.40
2.43	0.20
2.30	0.30
2.24	0.10
2.11	0.10
2.02	0.10
1.85	0.30
1.64	0.10
1.60	0.10
1.435	0.10
1.315	0.10

877. $Na_2S_2O_3.5H_2O$

d	I/I₁
7.2	0.08
6.1	0.12
5.8	0.32
5.4 (10)	0.80
5.1	0.24
4.51	0.32
4.20	0.32
3.80	0.32
3.66	0.24
3.45	0.16
3.30	0.40
3.13	0.32
2.93 (12.5)	1.00
2.84 (10)	0.80
2.76	0.80
2.60	0.08
2.43	0.64
2.34	0.32
2.26	0.16
2.21	0.08
2.08	0.08
2.02	0.08
1.90	0.12
1.83	0.12
1.79	0.08
1.74	0.12
1.67	0.08
1.62	0.16

878. $Na_2WO_4.2H_2O$

d	I/I₁
6.9 (40)	1.00
6.0	0.18
5.3	0.20
4.80	0.10
4.22 (30)	0.75
3.61	0.25
3.46	0.05
3.30	0.15
3.17 (15)	0.38
3.07	0.05
2.99	0.20
2.89	0.05
2.67	0.31
2.38	0.05
2.17	0.15
2.11	0.05
2.02	0.20
1.98	0.03
1.88	0.20
1.81	0.03
1.76	0.03
1.68	0.15
1.59	0.05
1.52	0.03
1.480	0.05
1.451	0.03
1.420	0.03
1.355	0.03
1.317	0.03
1.268	0.05

879. $Na_2C_4H_2O_3N_4.H_2O$

d	I/I₁
4.72 (2)	0.11
3.17 (17.5)	1.00
2.90	0.06
2.66 (3)	0.17
2.48	0.06
2.02	0.06
1.68	0.06

880. $NaVO_3.H_2O$

d	I/I₁
7.1	0.15
5.0 (40)	1.00
4.25	0.03
3.54	0.20
3.24 (15)	0.38
3.13	0.03
3.01	0.20
2.95 (20)	0.50
2.81	0.08
2.68	0.10
2.53	0.10
2.36	0.03
2.29	0.08
2.23	0.03
2.18	0.03
2.06	0.04
2.00	0.04
1.96	0.15
1.88	0.05
1.82	0.20
1.76	0.05
1.71	0.15
1.67	0.03
1.62	0.03
1.59	0.13
1.55	0.05
1.50	0.04
1.470	0.05
1.431	0.03
1.390	0.04
1.330	0.03
1.312	0.03
1.268	0.03
1.255	0.04
1.198	0.04
1.180	0.03
1.148	0.03

881. $Na_3VO_4.16H_2O$

d	I/I₁
8.5	0.07
8.0	0.07
7.3	0.20
4.63 (30)	1.00
4.21	0.13
4.08	0.13
3.89	0.07
3.69	0.20
3.09 (10)	0.33
2.98	0.07
2.85	0.20
2.75	0.07
2.66 (20)	0.67
2.56	0.03
2.45	0.07
2.38	0.23
2.24	0.03
2.15	0.03
2.07	0.03
1.96	0.03
1.92	0.13
1.78	0.10
1.75	0.17
1.62	0.03

882. Sr*

d	I/I₁
3.50 (5)	1.00
3.03 (3)	0.60
2.14	0.20
1.83 (5)	1.00
1.74	0.20

883. $Sr(C_2H_3O_2)_2.^1/_2H_2O$

d	I/I₁
11.0 (10)	1.00
10.1 (10)	1.00
9.5	0.20
6.5	0.10
4.7	0.10
4.4	0.10
3.99	0.20
3.52 (10)	1.00
3.33	0.40
3.21	0.40
2.97	0.40
2.53	0.10
2.37	0.10
2.10	0.10
2.00	0.10
1.90	0.20

884. $SrBr_2.6H_2O$*

d	I/I₁
4.11 (17.5)	1.00
3.60 (10)	0.57
2.91	0.17
2.70 (8)	0.46
2.36	0.34
2.25	0.46
2.04	0.11
1.85	0.11
1.79	0.23
1.63	0.06
1.56	0.23
1.51	0.11
1.484	0.06
1.462	0.06

885. $SrCO_3$*

d	I/I₁
3.53 (12.5)	1.00
2.56	0.08
2.45 (5)	0.40
2.18	0.08
2.05 (5)	0.40
1.98	0.08
1.90	0.16
1.81	0.32

886. $Sr(ClO_3)_2.8H_2O$

d	I/I₁
6.9	0.16
6.5	0.16
5.7 (6)	0.48
4.00	0.08
3.50	0.32
3.30 (12.5)	1.00
3.21 (8)	0.64
3.14	0.32
2.99	0.08
2.87	0.32
2.65	0.40
2.40	0.24
2.22	0.32
2.14	0.48
2.05	0.16
2.01	0.24
1.97	0.16
1.87	0.24
1.83	0.24
1.74	0.16
1.72	0.40
1.60	0.08
1.58	0.08
1.50	0.32
1.401	0.24
1.352	0.16
1.311	0.08
1.240	0.08
1.200	0.16
1.157	0.08
1.140	0.08
1.124	0.16

887. $SrCl_2.6H_2O$*

d	I/I₁
6.9 (20)	1.00
3.97	0.88
3.54	0.88
2.85	0.40
2.64 (20)	1.00
2.29	0.75
2.20 (20)	1.00
2.06	0.20
1.98	0.40
1.91	0.10
1.83	0.20
1.73	0.45
1.62	0.20
1.59	0.15
1.53	0.20
1.50	0.20
1.475	0.20
1.442	0.05
1.428	0.05
1.405	0.10
1.325	0.10
1.272	0.05

888. $SrCrO_4$

d	I/I₁
7.2	0.10
4.48	0.10
3.61	0.07
3.47	0.07
3.23 (15)	1.00
3.00	0.13
2.84 (10)	0.67
2.65	0.07
2.53	0.07
2.23	0.10
2.13	0.20
2.05	0.07
1.97 (4)	0.27
1.83	0.13
1.71	0.13
1.64	0.10
1.59	0.07
1.410	0.10

889. $Sr(HCO_3)_2$

d	I/I₁
15.0	0.20
10.6	0.40
6.3	0.40
5.4 (10)	1.00
4.60	0.10
4.31	0.10
3.91	0.10
3.65	0.20
3.30 (5)	0.50
3.01 (5)	0.50
2.90	0.20
2.70	0.50
2.50	0.40
2.35	0.30
2.22	0.30
2.12	0.40
2.02	0.50
1.95	0.30
1.88	0.20
1.64	0.10
1.54	0.10
1.457	0.15
1.400	0.10
1.354	0.15

890. $Sr(HCO_3)_2.2H_2O$

d	I/I₁
6.3 (15)	1.00
5.6	0.13
4.68	0.47
4.25	0.13
3.91	0.13
3.67	0.13
3.56	0.13
3.15 (12.5)	0.83
2.85 (10)	0.67
2.61	0.07
2.51	0.13
2.35	0.13
2.27	0.07
2.20	0.47
2.12	0.27
1.99	0.53
1.91	0.20
1.83	0.27
1.79	0.07
1.75	0.07
1.70	0.13
1.67	0.13
1.58	0.07
1.52	0.07

891. SrF_2*

d	I/I₁
3.37 (20)	1.00
2.91	0.05
2.06 (20)	1.00
1.75 (10)	0.50
1.68	0.05
1.455	0.10
1.336	0.15
1.302	0.05
1.189	0.20
1.121	0.15
1.029	0.05
0.979	0.10

892. $Sr(OH)_2.8H_2O$*

d	I/I₁
6.4	0.40
5.8	0.40
4.51	0.40
4.29 (10)	0.67
3.54	0.53
3.19	0.07
2.76 (10)	0.67
2.63	0.20
2.54	0.53
2.43	0.27
2.28	0.27
2.14	0.13
2.08	0.13
2.02 (15)	1.00
1.89	0.13
1.84	0.07
1.76	0.07
1.68	0.07
1.59	0.07
1.53	0.07
1.490	0.07
1.451	0.07

893. $SrI_2.6H_2O$

d	I/I₁
4.34 (17.5)	1.00
3.85 (15)	0.86
3.10	0.34
2.86	0.57
2.48	0.57
2.38 (12.5)	0.71
2.23	0.11
2.15	0.23
1.98	0.29
1.88	0.46
1.83	0.06
1.73	0.11
1.66	0.11
1.63	0.17
1.60	0.11
1.56	0.06
1.54	0.06
1.318	0.06

894. $Sr(C_2H_4O_2)_2.3H_2O$

d	I/I₁
10.0 (17.5)	1.00
5.7	0.17
5.1 (8)	0.46
4.80	0.06
4.30	0.29
4.09 (10)	0.57
3.65	0.17
3.30	0.11
3.07	0.17
2.94	0.06
2.86	0.06
2.76	0.23
2.64	0.17
2.53	0.23
2.45	0.06
2.38	0.17
2.29	0.06
2.23	0.11
2.15	0.07
2.04	0.11
2.00	0.17
1.95	0.11
1.90	0.17
1.80	0.06
1.73	0.06
1.69	0.11
1.66	0.06
1.63	0.06

895. $Sr(NO_3)_2$*

d	I/I₁
4.50 (6)	1.00
3.91	0.33
3.48	0.33
3.18	0.33
2.35 (6)	1.00
2.24 (6)	1.00
1.94	0.17
1.78	0.17
1.75	0.17
1.58	0.17
1.50	0.17
1.376	0.17
1.315	0.17

896. $SrC_2O_4.H_2O$

d	I/I₁
6.1 (20)	1.00
3.76 (12.5)	0.63
3.34	0.05
3.11	0.10
3.04	0.40
2.63	0.10
2.53	0.05
2.47	0.10
2.39	0.10
2.36	0.10
2.27	0.10
2.17	0.05
2.03 (10)	0.50
1.95	0.10
1.87	0.05
1.80	0.05
1.72	0.05
1.66	0.05
1.57	0.05

897. SrO_2*

d	I/I₁
3.30	0.40
3.13 (17.5)	0.88
2.52 (20)	1.00
2.00 (10)	0.50
1.87	0.50
1.78	0.15
1.57	0.30
1.55	0.30
1.375	0.05
1.290	0.35
1.260	0.05
1.210	0.05
1.176	0.10
1.127	0.10
1.066	0.10
1.045	0.05
1.015	0.10

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

898. $SrHPO_4$

d		I/I₁
3.66	(8)	1.00
3.25	(2)	0.25
3.02		0.13
2.87	(4)	0.50
2.60		0.25
2.44		0.13
2.25		0.25
2.02		0.25
1.92		0.13
1.84		0.25
1.76		0.13
1.52		0.13
1.430		0.13
1.320		0.13
1.260		0.13

899. $Sr(C_7H_5O_3)_2.2H_2O$

d		I/I₁
9.7	(15)	1.00
6.1		0.13
5.1	(6)	0.40
4.20		0.27
3.64	(10)	0.67
3.38		0.07
3.13		0.13
3.03		0.20
2.55		0.07
2.39		0.07
2.28		0.07
2.13		0.07
2.08		0.07
2.03		0.07
1.93		0.07
1.83		0.13

900. $SrSO_4$*

d		I/I₁
4.22		0.14
3.42		0.14
3.29		0.29
3.16		0.21
2.97	(7)	1.00
2.70	(5)	0.72
2.37		0.14
2.26		0.14
2.12		0.14
2.03	(3)	0.43
2.00		0.21
1.94		0.14
1.88		0.14
1.84		0.14
1.76		0.14
1.67		0.14
1.59		0.14
1.55		0.14
1.465		0.14
1.415		0.14

901. $SrC_4H_4O_6.4H_2O$

d		I/I₁
7.7		0.25
6.7	(6)	0.75
5.8		0.25
5.3	(6)	0.75
4.80		0.13
4.35		0.25
3.91		0.38
3.56	(8)	1.00
3.40		0.13
3.20		0.75
2.96		0.38
2.86		0.50
2.70		0.50
2.55		0.25
2.38		0.50
2.27		0.38
2.17		0.50
2.10		0.50
2.02		0.50
1.91		0.38
1.73		0.13
1.60		0.63

902. S

d		I/I₁
5.8		0.31
3.85	(40)	1.00
3.45		0.31
3.21	(20)	0.50
3.10	(15)	0.38
2.85		0.38
2.63		0.20
2.50		0.18
2.43		0.20
2.38		0.15
2.30		0.15
2.12		0.25
2.00		0.03
1.90		0.25
1.83		0.18
1.78		0.20
1.73		0.18
1.66		0.10
1.61		0.20
1.54		0.03
1.480		0.03
1.440		0.10
1.425		0.15
1.360		0.13
1.310		0.03
1.235		0.03

903. Ta*

d		I/I₁
2.33	(20)	1.00
1.65	(4)	0.20
1.346	(6)	0.30
1.165		0.05
1.042		0.05
0.881		0.05

904. $KTaF_6$

d		I/I₁
8.5		0.38
7.1		0.25
5.3	(7)	0.88
5.1	(7)	0.88
4.65		0.38
4.45		0.75
4.25		0.88
4.04		0.13
3.65		0.38
3.44	(8)	1.00
3.33		0.38
3.18		0.63
3.05		0.13
2.94		0.50
2.85		0.38
2.65		0.13
2.57		0.25
2.53		0.25
2.42		0.13
2.34		0.25
2.25		0.13
2.20		0.13
2.10		0.38
2.03		0.38
1.99		0.13
1.93		0.25
1.88		0.13
1.83		0.13
1.78		0.13
1.69		0.38
1.64		0.13
1.59		0.13
1.53		0.13

905. Ta_2O_5

d		I/I₁
6.2		0.03
5.7		0.17
4.48		0.03
3.96	(30)	1.00
3.49		0.27
3.23		0.23
3.05		0.33
2.95		0.13
2.81	(17.5)	0.58
2.61		0.23
2.45		0.03
2.29		0.03
2.15		0.03
1.98		0.42
1.87		0.17
1.77	(15)	0.50
1.71		0.07
1.66		0.10
1.62		0.27
1.52		0.03
1.470		0.05
1.400		0.05
1.360		0.05
1.322		0.13

906. Te*

d		I/I₁
5.8		0.19
3.86		0.14
3.24	(62.5)	1.00
2.34	(30)	0.48
2.22	(20)	0.32
2.08		0.14
1.96		0.14
1.83		0.28
1.77		0.10
1.61		0.20
1.470		0.28
1.418		0.13
1.380		0.16
1.309		0.08
1.258		0.05
1.175		0.14
1.119		0.05
1.045		0.05
1.005		0.05
0.968		0.02
0.866		0.02

907. $TeCl_2$

d		I/I₁
8.8		0.13
7.7		0.13
6.3		0.25
5.7		0.13
4.54		0.19
4.29	(3)	0.38
3.90		0.13
3.24	(8)	1.00
3.11		0.13
2.92		0.13
2.69	(8)	1.00
2.60		0.19
2.53		0.13
2.35		0.19
2.23		0.19
2.15		0.13
2.08		0.13
2.00		0.13
1.97		0.13
1.91		0.13
1.87		0.19
1.83		0.13
1.77		0.13
1.71		0.13
1.66		0.13
1.64		0.13
1.61		0.13
1.58		0.13
1.56		0.13
1.54		0.13
1.480		0.13
1.460		0.13
1.423		0.13
1.377		0.13
1.312		0.13
1.261		0.13
1.204		0.13
1.181		0.13
1.120		0.13
1.087		0.13

908. TeO_2

d		I/I₁
6.8	(40)	1.00
4.25		0.13
3.88		0.10
3.41		0.44
3.23		0.50
3.09	(25)	0.63
2.82	(30)	0.75
2.29		0.31
2.17		0.03
2.12		0.05
2.07		0.03
1.93		0.08
1.83		0.20
1.78		0.15
1.73		0.20
1.64		0.08
1.58		0.10
1.55		0.03
1.51		0.13
1.440		0.04
1.407		0.13
1.359		0.03
1.315		0.03
1.281		0.03

909. $4TeO_2.N_2O_5.1^1/_2H_2O$

d		I/I₁
7.6		0.02
7.1		0.02
6.1		0.06
5.8		0.06
5.6		0.06
5.3		0.06
5.0		0.06
4.54		0.02
4.38		0.05
4.07		0.02
3.87		0.05
3.40	(50)	0.80
3.28		0.03
3.00	(62.5)	1.00
2.72		0.03
2.63		0.02
2.55		0.02
2.41		0.32
2.29		0.06
2.13		0.08
2.07		0.03
2.00		0.02
1.87	(50)	0.80
1.72		0.02
1.70		0.03
1.66		0.32
1.59		0.02
1.52		0.13
1.485		0.24
1.443		0.02
1.430		0.02
1.410		0.02
1.387		0.02
1.356		0.03
1.308		0.02
1.292		0.02
1.267		0.20
1.250		0.20
1.227		0.10
1.188		0.14
1.153		0.02
1.133		0.02
1.119		0.05
1.093		0.10
1.075		0.02

910. Tellurium Nitrate (ic)

d		I/I₁
7.3	(15)	0.50
5.7		0.27
4.45		0.20
4.29		0.42
3.81	(17.5)	0.58
3.40		0.20
3.30	(30)	1.00
3.07		0.03
2.73		0.27
2.64		0.20
2.43		0.50
2.30		0.20
2.24		0.13
2.14		0.42
1.99		0.07
1.88		0.33
1.73		0.20
1.64		0.13
1.59		0.23
1.55		0.07
1.53		0.07
1.490		0.03
1.470		0.07
1.430		0.10
1.390		0.03
1.360		0.07
1.295		0.07
1.275		0.03
1.218		0.03

911. H_2TeO_4

d		I/I₁
8.5		0.03
7.3		0.03
4.75	(125)	1.00
4.19	(100)	0.80
3.19		0.05
3.09		0.16
2.71		0.05
2.63	(50)	0.40
2.58		0.40
2.38		0.03
2.30		0.02
2.23		0.03
2.09		0.16
2.03		0.10
1.94		0.10
1.88		0.40
1.81		0.04
1.77		0.16
1.73		0.06
1.67		0.06
1.65		0.06
1.59		0.05
1.53		0.08
1.51		0.08
1.465		0.12
1.406		0.06
1.375		0.03
1.354		0.05
1.318		0.05
1.290		0.05
1.237		0.03
1.199		0.08

912. $Te(OH)_2$*

d		I/I₁
4.74		0.40
4.53	(62.5)	1.00
4.19		0.32
3.92	(30)	0.48
3.20		0.05
3.08		0.05
2.77		0.20
2.65		0.13
2.59		0.13
2.36	(30)	0.48
2.26		0.10
2.09		0.06
2.03		0.10
1.96		0.11
1.88		0.11
1.80		0.28
1.75		0.28
1.60		0.20
1.55		0.02
1.51		0.20
1.465		0.02
1.388		0.02
1.327		0.16
1.307		0.05
1.240		0.06
1.197		0.06
1.182		0.06
1.100		0.03
1.048		0.05
1.022		0.05

913. α-Tl*

d		I/I₁
3.00	(7)	0.40
2.75		0.23
2.62	(17.5)	1.00
2.02		0.23
1.73	(5)	0.29
1.56		0.29
1.460		0.23
1.445		0.17
1.158		0.11
1.105		0.17
1.074		0.06
0.962		0.06

914. TlCl*

d		I/I₁
3.82	(2)	0.40
2.71	(5)	1.00
2.21		0.20
1.91		0.20
1.71		0.20
1.56	(1.5)	0.30
1.355		0.20

915. $Tl(NO_3)_3.3H_2O$

d		I/I₁
4.40	(25)	0.63
4.00		0.25
3.11		0.15
2.95	(40)	1.00
2.44	(17.5)	0.44
2.19		0.20
1.99		0.10
1.93		0.18
1.82		0.18
1.75		0.18
1.68		0.18
1.59		0.03
1.55		0.03
1.53		0.03
1.472		0.13
1.427		0.05
1.398		0.10
1.375		0.08
1.305		0.03
1.270		0.05
1.250		0.03
1.222		0.05
1.176		0.05
1.150		0.04
1.134		0.04
1.099		0.05

916. Tl_2O_3*

d		I/I₁
3.02	(10)	1.00
2.62		0.50
2.06		0.10
1.86	(6)	0.60
1.58	(6)	0.60
1.54		0.10
1.51		0.10
1.200		0.20
1.170		0.10

917. Tl_2SO_4

d		I/I₁
4.35		0.40
3.53	(6)	0.48
3.26		0.16
3.13	(12.5)	1.00
3.03		0.32
2.95		0.40
2.77		0.08
2.63		0.08
2.53		0.32
2.45		0.16
2.37		0.08
2.31		0.24
2.24		0.08
2.17	(6)	0.48
2.10		0.08
2.05		0.16
1.96		0.32
1.92		0.32
1.87		0.08
1.83		0.24
1.78		0.32
1.72		0.16
1.69		0.08
1.56		0.16
1.480		0.16
1.420		0.08
1.388		0.08
1.340		0.08
1.280		0.08
1.196		0.16

918. Th*

d		I/I₁
2.92	(40)	1.00
2.53	(20)	0.50
1.79	(15)	0.38
1.52		0.31
1.460		0.13
1.265		0.08
1.160		0.15
1.133		0.08
1.033		0.05
0.975		0.04
0.895		0.03

919. Thorium

d		I/I₁
9.7	(20)	
8.7	(25)	
7.5		
4.71		
4.31		
4.17	(8)	
3.76		
3.60		
3.48		
3.18		
2.90		
2.78		
2.63		
2.48		
2.34		
2.23		
2.15		
2.09		
2.02		
1.91		
1.87		
1.83		
1.78		
1.73		
1.70		
1.67		
1.63		
1.59		
1.55		
1.490		
1.428		
1.399		
1.355		

920. T

d		I/I₁
9.1		
7.8		
7.2	(10)	
6.5	(8)	
5.8		
5.4		
4.44		
4.12	(4	
3.72		
3.39		
2.94		
2.67		
2.62		
2.52		
2.38		
2.26		
2.18		
2.06		
1.95		
1.89		
1.83		
1.77		
1.73		
1.67		
1.63		
1.59		

921 $Th(NO_3)_4$

d		I/I₁
7.3	(12.	
5.8		
5.4		
5.1		
4.82		
3.92		
3.48		
3.32		
3.20		
3.09		
3.00		
2.84		
2.79		
2.68		
2.62		
2.55		
2.40		
2.33		
2.28		
2.23		
2.17		
2.11		
2.06		
2.02		
1.92		
1.88		
1.83		
1.78		
1.75		
1.71		
1.68		
1.65		
1.60		
1.57		
1.50		
1.450		
1.421		
1.392		
1.361		
1.342		

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

919. Thorium Acetate

d		I/I_1
9.7		0.24
8.7	(20)	0.80
7.5	(25)	1.00
4.71		0.16
4.31		0.08
4.17		0.08
3.76	(8)	0.32
3.60		0.16
3.48		0.20
3.18		0.20
2.90		0.24
2.78		0.08
2.63		0.28
2.48		0.12
2.34		0.08
2.23		0.08
2.15		0.04
2.09		0.04
2.02		0.08
1.91		0.08
1.87		0.08
1.83		0.08
1.78		0.04
1.73		0.04
1.70		0.04
1.67		0.04
1.63		0.04
1.59		0.04
1.55		0.04
1.490		0.04
1.428		0.04
1.399		0.04
1.355		0.04

920. $ThCl_4$

d		I/I_1
9.1		0.10
7.8		0.10
7.2	(10)	1.00
6.5	(8)	0.80
5.8		0.10
5.4		0.10
4.44		0.10
4.12	(4)	0.40
3.72		0.40
3.39		0.30
2.94		0.20
2.67		0.10
2.62		0.20
2.52		0.10
2.38		0.10
2.26		0.10
2.18		0.10
2.06		0.10
1.95		0.10
1.89		0.10
1.83		0.10
1.77		0.10
1.73		0.10
1.67		0.10
1.63		0.10
1.59		0.10

921. $Th(NO_3)_4 \cdot 12H_2O$

d		I/I_1
7.3	(12.5)	1.00
5.8		0.32
5.4	(7)	0.56
5.1		0.48
4.82	(8)	0.64
3.92		0.24
3.48		0.16
3.32		0.08
3.20		0.40
3.09		0.40
3.00		0.08
2.84		0.08
2.79		0.24
2.68		0.08
2.62		0.08
2.55		0.16
2.40		0.48
2.33		0.16
2.28		0.08
2.23		0.08
2.17		0.16
2.11		0.16
2.06		0.24
2.02		0.16
1.92		0.08
1.88		0.08
1.83		0.16
1.78		0.08
1.75		0.08
1.71		0.08
1.68		0.08
1.65		0.08
1.60		0.08
1.57		0.08
1.50		0.08
1.450		0.08
1.421		0.08
1.392		0.08
1.361		0.08
1.342		0.08

922. $Th(C_2O_4)_2$

d		I/I_1
7.9	(15)	0.75
6.5	(20)	1.00
5.0	(15)	0.75
4.60		0.05
3.95		0.50
3.21		0.05
2.98		0.50
2.88		0.20
2.70		0.15
2.28		0.25
2.15		0.15
2.08		0.05
2.03		0.10
1.98		0.15
1.96		0.15
1.82		0.05
1.79		0.05
1.75		0.05
1.73		0.05
1.70		0.05
1.65		0.05
1.61		0.05
1.52		0.05
1.430		0.05
1.414		0.05
1.285		0.05
1.267		0.05

923. ThO_2*

d		I/I_1
3.22	(8)	1.00
2.80		0.38
1.97	(6)	0.75
1.68	(7)	0.88
1.399		0.13
1.280		0.38
1.245		0.25
1.140		0.38
1.074		0.38
0.987		0.13
0.943		0.25
0.931		0.25

924. $Th(SO_4)_2$

d		I/I_1
6.8		0.07
5.9		0.07
4.77	(30)	1.00
4.23		0.03
3.54		0.10
3.30	(8)	0.27
3.03		0.20
2.86		0.20
2.74	(10)	0.33
2.42		0.17
2.36		0.17
2.28		0.17
2.14		0.17
2.08		0.27
2.04		0.27
1.88		0.27
1.79		0.27
1.70		0.20
1.65		0.20
1.57		0.17
1.490		0.13
1.440		0.13
1.419		0.13
1.370		0.07
1.309		0.07
1.285		0.07
1.175		0.07
1.163		0.10

925. Sn*

d		I/I_1
2.91	(62.5)	1.00
2.79	(50)	0.80
2.05		0.32
2.01	(50)	0.80
1.65		0.24
1.480		0.24
1.450		0.20
1.298		0.16
1.200		0.20
1.092		0.11
1.040		0.08
1.022		0.06
0.980		0.03
0.927		0.06
0.885		0.02
0.847		0.03
0.805		0.02

926. SnSb*

d		I/I_1
3.05	(62.5)	1.00
2.16	(50)	0.80
1.76		0.24
1.53		0.13
1.367	(17.5)	0.28
1.250		0.16
1.080		0.03
1.020		0.05
0.967		0.05
0.921		0.03
0.847		0.02
0.816		0.02

927. $SnCl_4 \cdot 5H_2O$

d		I/I_1
6.2	(62.5)	1.00
5.3	(30)	0.48
5.0		0.20
4.21		0.08
3.86		0.20
3.70		0.06
3.49		0.05
3.22		0.11
3.10		0.06
2.94	(17.5)	0.28
2.76		0.16
2.64		0.24
2.52		0.16
2.42		0.05
2.35		0.10
2.18		0.08
2.16		0.06
2.03		0.16
1.97		0.16
1.91		0.05
1.84		0.10
1.76		0.03
1.71		0.06
1.64		0.06
1.55		0.08
1.487		0.03
1.434		0.02
1.402		0.02
1.360		0.02
1.304		0.02
1.254		0.02
1.224		0.02
1.179		0.02
1.166		0.02
1.135		0.02
1.101		0.02
1.075		0.02
1.057		0.02

928. $(NH_4)_2SnCl_6$*

d		I/I_1
5.8	(75)	1.00
5.0	(50)	0.67
3.54		0.20
3.02		0.53
2.89		0.20
2.50	(75)	1.00
2.30		0.13
2.24		0.53
2.04		0.11
1.93		0.33
1.77		0.67
1.69		0.33
1.67		0.27
1.58		0.07
1.53		0.08
1.449		0.17
1.403		0.17
1.340		0.07
1.307		0.13
1.254		0.07
1.217		0.13
1.182		0.05
1.158		0.09
1.121		0.13
1.099		0.11

929. $SnCl_2 \cdot 2H_2O$

d		I/I_1
8.1		0.23
7.2	(12.5)	0.71
5.2		0.11
4.72		0.57
4.33		0.34
4.00	(12.5)	0.71
3.60	(17.5)	1.00
3.23		0.34
3.01		0.40
2.82		0.40
2.73		0.57
2.58		0.71
2.41		0.57
2.24		0.23
2.16		0.40
2.07		0.40
2.01		0.23
1.97		0.17
1.94		0.17
1.89		0.23
1.84		0.23
1.79		0.29
1.73		0.34
1.66		0.23
1.58		0.29
1.490		0.29
1.448		0.23
1.400		0.23
1.358		0.11
1.327		0.11
1.280		0.11
1.240		0.06

930. SnI_4*

d		I/I_1
6.9		0.10
5.5		0.27
5.0		0.10
3.53	(30)	1.00
3.28		0.03
3.05		0.23
2.80		0.03
2.66		0.03
2.27		0.03
2.16	(15)	0.50
1.84	(10)	0.33
1.76		0.03
1.66		0.03
1.56		0.03
1.53		0.05
1.402		0.10
1.368		0.03
1.248		0.07
1.178		0.05

931. SnC_2O_4

d		I/I_1
4.62	(50)	1.00
4.27	(17.5)	0.35
3.99	(25)	0.50
3.37		0.60
3.24		0.40
2.90		0.06
2.81		0.02
2.58		0.30
2.53		0.30
2.42		0.25
2.39		0.25
2.33		0.20
2.12		0.20
2.04		0.04
2.00		0.16
1.94		0.30
1.83		0.02
1.79		0.20
1.74		0.12
1.69		0.06
1.65		0.06
1.61		0.06
1.57		0.02
1.53		0.02
1.51		0.02
1.480		0.02
1.457		0.02
1.410		0.12
1.370		0.12
1.328		0.06
1.302		0.04
1.274		0.02
1.237		0.02
1.213		0.02
1.182		0.02
1.156		0.02
1.132		0.02
1.091		0.02
1.064		0.04
1.032		0.02

932. SnO*

d		I/I_1
4.81	(6)	0.30
2.97	(20)	1.00
2.66		0.25
2.39		0.05
1.89		0.15
1.79		0.30
1.59	(8)	0.40
1.480		0.15
1.332		0.05
1.222		0.05
1.194		0.05
1.165		0.10
1.073		0.05
1.025		0.05

933. SnO_2*

d		I/I_1
3.34	(100)	1.00
2.64	(62.5)	0.63
2.36		0.18
1.75	(62.5)	0.63
1.67		0.10
1.58		0.05
1.492		0.10
1.435		0.10
1.412		0.15
1.315		0.06
1.213		0.10
1.180		0.02
1.150		0.06
1.110		0.03
1.085		0.08
1.057		0.03
1.035		0.02
0.948		0.08
0.929		0.01
0.905		0.04
0.880		0.04
0.845		0.02

934. $Sn_3(PO_4)_2$

d		I/I_1
6.9		0.07
6.1		0.03
4.39		0.33
3.98	(30)	1.00
3.42		0.20
3.11	(30)	1.00
2.78		0.20
2.68		0.27
2.48		0.27
2.39		0.17
2.30		0.20
2.06		0.03
2.01		0.13
1.96		0.17
1.90		0.17
1.77	(10)	0.33
1.71		0.07
1.65		0.07
1.482		0.07
1.445		0.03

935. $Sn(SO_4)_2 \cdot 2H_2O$

d		I/I_1
6.8	(30)	1.00
4.85	(30)	1.00
4.29	(30)	1.00
3.67		0.30
3.51		0.27
3.38		0.33
3.20		0.42
2.98		0.33
2.90		0.20
2.77		0.42
2.70		0.20
2.59		0.42
2.41		0.83
2.31		0.13
2.23		0.07
2.16		0.83
2.11		0.13
1.99		0.17
1.92		0.23
1.83		0.23
1.76		0.50
1.68		0.10
1.61		0.13
1.54		0.13
1.485		0.13
1.450		0.13
1.410		0.20
1.345		0.20
1.290		0.20
1.252		0.20
1.218		0.20
1.200		0.20

936. $SnSO_4$

d		I/I_1
4.35		0.24
3.58		0.24
3.41		0.16
3.08	(62.5)	1.00
2.80		0.16
2.67	(20)	0.32
2.46		0.13
2.28		0.20
2.17		0.28
2.10	(20)	0.32
1.95		0.28
1.75		0.13
1.65		0.28
1.61		0.24
1.460		0.06
1.420		0.06
1.382		0.05
1.355		0.05
1.315		0.02
1.280		0.02
1.250		0.20
1.153		0.02
1.129		0.08
1.080		0.11
1.030		0.06

937. SnS_2*

d		I/I_1
5.9	(50)	0.50
3.14		0.40
2.77	(100)	1.00
2.14	(50)	0.50
1.82		0.50
1.74		0.40
1.66		0.13
1.57		0.06
1.52		0.20
1.469		0.02
1.388		0.13
1.331		0.10
1.299		0.04
1.190		0.04
1.168		0.13
1.144		0.08
1.103		0.10
1.050		0.05
1.035		0.04
1.018		0.04
0.990		0.01
0.927		0.02

938. SnS*

d		I/I_1
4.04		0.16
3.42	(25)	0.40
3.24	(25)	0.40
2.93		0.32
2.83	(62.5)	1.00
2.30		0.32
2.12		0.11
2.02		0.24
1.99		0.24
1.87		0.32
1.78		0.16
1.72		0.16
1.69		0.16
1.62		0.20
1.56		0.03
1.450		0.20
1.399		0.13
1.361		0.13
1.292		0.10
1.262		0.10
1.224		0.10
1.197		0.03

939. $SnC_4H_4O_6$

d		I/I_1
6.4		0.20
5.8		0.03
4.89	(20)	0.50
4.69		0.50
4.34		0.50
3.97		0.44
3.59	(40)	1.00
3.24		0.08
2.95		0.08
2.75	(30)	0.75
2.65		0.05
2.48		0.18
2.37		0.10
2.27		0.10
2.17		0.15
2.11		0.31
2.04		0.13
1.99		0.10
1.91		0.08
1.85		0.20
1.80		0.23
1.74		0.13
1.70		0.05
1.65		0.15
1.55		0.18
1.490		0.10
1.451		0.13
1.408		0.05
1.372		0.05
1.340		0.03
1.305		0.03
1.270		0.03

940. Ti*

d		I/I_1
2.54	(20)	0.27
2.34	(15)	0.20
2.23	(75)	1.00
1.72		0.13
1.470		0.13
1.330		0.13
1.275		0.01
1.248		0.11
1.230		0.05

941. TiC*

d		I/I_1
2.49	(75)	0.75
2.15	(100)	1.00
1.52	(50)	0.50
1.300		0.25
1.245		0.10
1.079		0.03
0.990		0.05
0.965		0.09
0.881		0.05
0.831		0.02

942. TiF_4

d		I/I_1
6.5		0.10
5.4		0.03
4.75		0.02
4.35		0.02
3.80	(100)	1.00
3.56		0.02
3.40		0.02
3.22		0.20
2.68		0.13
2.35		0.03
2.18		0.06
1.90	(40)	0.40
1.70	(40)	0.40
1.61		0.04
1.55		0.06
1.485		0.01
1.345		0.13
1.266		0.10
1.098		0.02
1.054		0.02
1.015		0.02
0.921		0.02

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

943. $K_2TiF_6.H_2O$

d		I/I1
4.95	(12.5)	0.19
4.65		0.09
3.39	(40)	0.59
2.85		0.26
2.47		0.08
2.34		0.15
2.18	(67.5)	1.00
2.10		0.14
1.73		0.10
1.69		0.19
1.65		0.05
1.460		0.09
1.430		0.12
1.362		0.08
1.318		0.08
1.196		0.03
1.135		0.05

944. TiO_2* (anatase)

d		I/I1
3.52	(62.5)	1.00
2.37		0.24
1.88	(25)	0.40
1.70	(17.5)	0.28
1.66		0.24
1.480		0.24
1.362		0.08
1.335		0.08
1.262		0.11
1.164		0.06
1.045		0.03
0.950		0.02
0.913		0.02
0.894		0.02

945. TiO_2* (rutile)

d		I/I1
3.24	(40)	0.80
2.49	(30)	0.60
2.29		0.04
2.19		0.30
2.05		0.12
1.69	(50)	1.00
1.62		0.30
1.485		0.20
1.449		0.20
1.355		0.30
1.245		0.04
1.170		0.08
1.147		0.04
1.091		0.08
1.040		0.08
0.964		0.04
0.903		0.02
0.890		0.08
0.875		0.04
0.843		0.02
0.832		0.04
0.822		0.04

946. W*

d		I/I1
2.23	(17.5)	1.00
1.58		0.29
1.290	(12.5)	0.71
1.117		0.17
1.000		0.29
0.913		0.06
0.846	(6)	0.34
0.745		0.11
0.707		0.06
0.674		0.06
0.622		0.06

947. $H_2W_4O_{13}$

d		I/I1
5.3	(20)	0.50
3.48	(40)	1.00
2.93		0.08
2.69		0.05
2.60		0.10
2.55	(10)	0.25
2.37		0.10
2.31		0.08
2.23		0.03
2.10		0.03
1.97		0.08
1.84		0.20
1.73		0.15
1.69		0.03
1.63		0.13
1.60		0.08
1.50		0.05
1.470		0.05
1.410		0.05
1.305		0.03
1.276		0.03
1.245		0.03
1.215		0.03
1.189		0.03
1.157		0.05

948. WO_3

d		I/I1
3.81	(30)	1.00
3.65	(12.5)	0.42
3.34		0.13
3.15		0.23
2.65	(17.5)	0.58
2.52		0.03
2.44		0.10
2.16		0.23
2.02		0.07
1.92		0.07
1.82		0.27
1.70		0.13
1.65		0.27
1.59		0.03
1.54		0.07
1.490		0.13
1.389		0.03
1.309		0.03
1.240		0.13
1.179		0.03
1.160		0.03
1.121		0.03

949. $UO_2(C_2H_3O_2)_2.2H_2O$

d		I/I1
8.1	(7)	0.78
6.3	(8)	0.89
5.9		0.67
5.2		0.45
4.59	(9)	1.00
4.44		0.44
3.91		0.44
3.72		0.44
3.44		0.56
3.13		0.17
2.95		0.33
2.72		0.44
2.52		0.33
2.41		0.22
2.24		0.33
2.11		0.11
2.02		0.17
1.97		0.11
1.90		0.11
1.80		0.22
1.74		0.11
1.64		0.11
1.60		0.11
1.53		0.11
1.483		0.11
1.445		0.11
1.310		0.11

950. $UO_2(NO_3)_2.6H_2O$*

d		I/I1
6.6	(10)	0.80
5.7	(12.5)	1.00
4.33	(12.5)	1.00
3.63		0.08
3.29		0.56
2.93		0.08
2.85		0.08
2.62		0.16
2.54		0.12
2.46		0.24
2.37		0.12
2.28		0.24
2.17		0.16
2.11		0.16
1.98		0.08
1.89		0.48
1.84		0.08
1.78		0.08
1.71		0.12
1.64		0.12
1.59		0.12
1.54		0.08

951. V*

d		I/I1
2.14	(100)	1.00
1.51	(7)	0.07
1.236	(20)	0.20
1.072		0.03
0.958		0.03
0.875		0.01
0.810		0.03
0.759		0.01
0.714		0.01

952. VC*

d		I/I1
2.40	(40)	1.00
2.07	(40)	1.00
1.469	(20)	0.50
1.251		0.25
1.199		0.10
1.039		0.05
0.952		0.05
0.929		0.10
0.849		0.05
0.800		0.03

953. Vanadium Chloride

d		I/I1
11.4	(40)	1.00
5.6	(40)	1.00
5.2		0.05
4.30		0.25
4.00		0.18
3.68		0.05
3.50		0.10
3.30		0.08
3.11		0.03
3.01		0.03
2.78	(30)	0.75
2.63		0.25
2.52		0.25
2.42		0.03
2.34		0.03
2.24		0.08
2.15		0.08
2.00		0.10
1.93		0.05
1.82		0.15
1.67		0.10
1.63		0.10
1.55		0.03
1.51		0.08
1.440		0.03
1.390		0.03
1.330		0.03
1.260		0.03

954. V_2O_3*

d		I/I1
3.65	(30)	0.60
2.70	(40)	0.80
2.47		0.60
2.32		0.02
2.18		0.20
2.03		0.02
1.83		0.25
1.69	(50)	1.00
1.61		0.02
1.57		0.03
1.470		0.25
1.429		0.30
1.330		0.10
1.235		0.04
1.218		0.02
1.193		0.02
1.170		0.06
1.125		0.03
1.093		0.06
1.057		0.06

955. V_2O_5*

d		I/I1
5.7		0.33
4.38	(15)	1.00
4.09		0.13
3.39	(12.5)	0.83
2.87	(8)	0.53
2.76		0.13
2.68		0.07
2.61		0.13
2.18		0.07
1.99		0.07
1.92		0.13
1.86		0.07
1.77		0.10
1.65		0.07
1.56		0.07
1.51		0.07
1.490		0.07
1.452		0.07
1.305		0.07

956. $(VO)_2(SO_4)_3.16H_2O$

d		I/I1
6.3		0.32
5.8		0.32
5.4		0.32
5.1		0.08
4.55	(25)	1.00
4.35	(12.5)	0.50
3.90		0.24
3.70		0.16
3.51	(12.5)	0.50
3.30		0.28
3.16		0.16
3.04		0.28
2.82		0.28
2.70		0.24
2.64		0.28
2.47		0.12
2.34		0.20
2.18		0.20
2.03		0.08
1.98		0.08
1.92		0.20
1.88		0.08
1.75		0.04
1.64		0.04
1.55		0.04
1.450		0.08

957. $Y(NO_3)_3.6H_2O$

d		I/I1
8.4	(10)	1.00
5.7	(6)	0.60
5.3	(8)	0.80
4.65		0.20
4.24		0.20
3.91		0.20
3.23		0.30
3.04		0.15
2.98		0.20
2.92		0.20
2.79		0.15
2.61		0.20
2.53		0.30
2.39		0.20
2.30		0.20
2.22		0.10
2.12		0.60
2.05		0.15
1.98		0.20
1.95		0.10
1.92		0.20
1.89		0.10
1.86		0.10
1.83		0.10
1.79		0.15
1.76		0.15
1.70		0.15
1.65		0.10
1.61		0.10
1.54		0.10

958. Y_2O_3*

d		I/I1
4.29		0.02
3.05	(50)	1.00
2.64		0.16
2.50		0.03
2.37		0.02
2.26		0.03
2.07		0.04
1.93		0.02
1.87	(20)	0.40
1.81		0.02
1.71		0.02
1.64		0.02
1.60	(15)	0.30
1.56		0.02
1.52		0.02
1.343		0.02
1.322		0.02
1.215		0.04
1.186		0.03
1.141		0.02
1.116		0.02
1.081		0.02

959. Zn*

d		I/I1
2.46	(12.5)	0.25
2.30	(10)	0.20
2.08	(50)	1.00
1.68		0.14
1.330		0.18
1.169		0.12
1.120		0.08
1.040		0.02
0.941		0.02
0.905		0.02

960. $Zn(C_2H_3O_2)_2$

d		I/I1
7.5	(50)	1.00
4.55	(30)	0.60
4.22		0.12
4.02		0.12
3.68	(17.5)	0.35
3.46		0.10
3.28		0.08
3.12		0.08
2.90		0.02
2.80		0.02
2.72		0.04
2.60		0.02
2.50		0.08
2.39		0.04
2.29		0.10
2.20		0.10
2.12		0.04
2.06		0.08
2.01		0.04
1.97		0.02
1.90		0.02
1.79		0.04
1.72		0.04
1.67		0.02
1.62		0.06
1.56		0.04
1.485		0.04
1.440		0.02
1.405		0.02
1.374		0.02

961. $Zn(C_2H_3O_2)_2.2H_2O$

d		I/I1
6.8	(10)	0.33
5.4	(30)	1.00
5.0		0.03
4.7		0.27
4.45	(25)	0.83
4.00		0.20
3.80		0.33
3.58		0.27
3.28		0.27
3.20		0.27
3.01		0.03
2.85		0.13
2.70		0.17
2.40		0.17
2.30		0.03
2.14		0.07
2.04		0.07
2.00		0.03
1.96		0.07
1.80		0.03
1.76		0.03
1.68		0.05
1.60		0.03
1.58		0.03
1.50		0.03

962. $ZnAl_2O_4$*

d		I/I1
2.85	(8)	0.53
2.44	(15)	1.00
2.02		0.07
1.91		0.07
1.85		0.07B
1.65		0.13
1.55		0.33
1.480		0.07
1.431	(6)	0.40
1.232		0.07

963. $Zn_3(AsO_4)_2.8H_2O$

d		I/I1
7.9	(10)	0.80
6.2		0.24
5.5		0.32
4.90		0.24
4.60		0.72
4.25		0.12
3.60		0.16
3.25	(12.5)	1.00
2.98		0.48
2.79	(10)	0.80
2.70		0.40
2.62		0.32
2.53		0.08
2.45		0.32
2.16		0.48
2.05		0.08
1.98		0.16
1.83		0.40
1.67		0.08
1.62		0.40
1.58		0.16
1.51		0.24
1.485		0.32
1.400		0.08

964. Zinc Arsenite

d		I/I1
4.00	(8)	0.53
3.40		0.20
3.15	(15)	1.00
2.95	(5)	0.33
2.63		0.33
2.40		0.13
2.18		0.13
2.01		0.07
1.95		0.07
1.83		0.07
1.68		0.13
1.55		0.13
1.435		0.20
1.380		0.07

965. $Zn(C_2H_3COO)_2$

d		I/I1
11.0	(12.5)	1.00
9.8	(6)	0.48
8.4		0.16
7.5		0.48
5.3		0.32
4.90		0.40
4.51		0.24
4.27	(8)	0.64
4.10		0.16
3.92		0.08
3.55		0.16
3.33		0.12
3.13		0.08
3.05		0.08
2.90		0.12
2.71		0.08
2.61		0.08
2.46		0.08
2.23		0.08

966. $Zn(ClO_4)_2.6H_2O$

d		I/I1
6.9	(50)	1.00
6.0		0.04
4.79		0.30
4.45		0.02
4.22		0.10
4.05	(10)	0.20
3.82		0.10
3.60		0.12
3.18	(12.5)	0.25
3.05		0.08
2.90		0.20
2.71		0.08
2.52		0.12
2.41		0.04
2.30		0.12
2.20		0.06
2.13		0.06
2.08		0.02
2.02		0.08
1.97		0.04
1.91		0.04
1.87		0.10
1.80		0.04
1.74		0.04
1.67		0.06
1.58		0.04
1.480		0.02
1.445		0.02
1.405		0.02

967. Zinc Chloride (fused)

d		I/I1
4.79	(20)	0.67
3.06	(30)	1.00
2.90		0.17
2.34		0.20
1.97		0.10
1.91		0.10
1.86	(10)	0.33
1.62		0.10
1.57		0.10

968. $ZnCrO_4$

d		I/I1
9.5	(15)	0.38
4.67		0.38
3.10		0.23
2.67	(40)	1.00
2.53		0.03
2.44		0.15
2.34		0.03
2.24		0.13
2.14	(17.5)	0.43
1.95		0.05
1.85		0.06
1.75		0.03
1.60		0.13
1.57		0.25
1.480		0.03
1.466		0.20
1.398		0.05
1.350		0.05
1.294		0.03
1.265		0.03
1.195		0.03
1.145		0.03
1.123		0.03
1.100		0.05
1.070		0.03
1.020		0.03

969. $Zn(CN)_2$

d		I/I1
4.19	(75)	1.00
3.40		0.13
2.95		0.04
2.40	(30)	0.40
2.08	(20)	0.27
1.86		0.11
1.70		0.01
1.57		0.20
1.470		0.01
1.390		0.07
1.315		0.03
1.256		0.01
1.202		0.01
1.157		0.03

970. Zinc Potassium Cyanide

d		I/I1
4.44	(15)	0.37
3.79	(40)	1.00
3.14		0.10
2.57		0.05
2.42		0.15
2.22	(10)	0.25
1.98		0.02
1.92		0.05
1.68		0.05
1.63		0.05
1.480		0.02
1.458		0.02

971. $Zn_2Fe(CN)_6$

d		I/I1
5.4	(17.5)	
4.51		
4.08	(20)	
3.64	(8)	
3.11		
3.00		
2.70		
2.54		
2.37		
2.32		
2.20		
2.08		
2.03		
1.95		
1.89		
1.80		
1.69		
1.56		
1.480		

972. Zr

d		I/I1
3.33	(62.5	
2.60	(50	
2.35		
2.27		
2.10		
1.75	(50	
1.67		
1.56		
1.490		
1.405		
1.300		
1.250		
1.205		
1.177		
1.135		
1.112		
1.075		

973. ZnF

d		I/I1
4.87	(3	
4.10	(12.	
3.78		
3.57		
3.33		
3.15		
2.99	(	
2.76		
2.60		
2.44		
2.31		
2.24		
2.17		
2.02		
1.95		
1.88		
1.79		
1.74		
1.66		
1.61		
1.410		

974.

d		I/I1
6.5	(7)	
5.7		
4.5		
3.98		
3.49	(25)	
3.06		
2.93		
2.75		
2.17		
2.11	(7	
1.84		
1.79		
1.74		
1.53		
1.378		
1.242		

97. $Zn(C_2H_5C$

d		I/I1
9.1	(3	
6.8		
4.43	(	
4.12		
3.32		
3.19		
2.98		
2.72	(	
2.58		
2.24		
2.03		
1.69		
1.58		

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TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Continued*)

(Starred patterns were checked with published crystal structure data)

971. $Zn_2Fe(CN)_6.3H_2O$

d	I/I1
5.4	0.88
4.61	0.35
4.08	1.00
3.64	0.40
3.11	0.30
3.00	0.05
2.70	0.20
2.64	0.20
2.37	0.10
2.32	0.05
2.20	0.10
2.08	0.05
2.03	0.05
1.95	0.05
1.89	0.05
1.80	0.05
1.69	0.05
1.58	0.05
1.480	0.05

(17.5) (20) (8)

972. ZnF_2*

d	I/I1
3.33	1.00
2.60	0.80
2.35	0.06
2.27	0.20
2.10	0.05
1.75	0.80
1.67	0.20
1.56	0.08
1.490	0.11
1.405	0.32
1.300	0.03
1.250	0.02
1.205	0.06
1.177	0.02
1.135	0.06
1.112	0.02
1.075	0.06

(62.5) (50)

973. $ZnF_2.4H_2O$

d	I/I1
4.87	1.00
4.10	0.42
3.78	0.03
3.57	0.03
3.33	0.20
3.15	0.20
2.99	0.30
2.76	0.10
2.60	0.10
2.44	0.03
2.31	0.03
2.24	0.03
2.17	0.17
2.02	0.10
1.95	0.05
1.88	0.05
1.79	0.05
1.74	0.20
1.66	0.03
1.61	0.03
1.410	0.03

(30) (12.5) (9)

974. ZnI_2

d	I/I1
6.5	0.28B
5.7	0.20B
4.5	0.12
3.98	0.12
3.49	1.00
3.06	0.08
2.93	0.04
2.75	0.04
2.17	0.16
2.11	0.28
1.84	0.20
1.79	0.08
1.74	0.04
1.53	0.04
1.378	0.04
1.242	0.04

(25) (7)

975. $Zn(C_6H_5O_2)_2.3H_2O$

d	I/I1
9.1	1.00
6.8	0.03
4.43	0.07
4.12	0.03
3.32	0.03
3.19	0.07
2.98	0.03
2.72	0.10
2.58	0.03
2.24	0.07
2.03	0.03
1.69	0.03
1.58	0.03

(30) (2) (3)

976. $ZnC_2O_4.2H_2O$

d	I/I1
4.73	1.00
3.93	0.17
3.58	0.17
2.95	0.33
2.66	0.13
2.55	0.11
2.23	0.11
2.15	0.03
2.08	0.05
2.03	0.04
1.99	0.01
1.92	0.07
1.88	0.07
1.80	0.05
1.76	0.05
1.69	0.01
1.65	0.01
1.59	0.01
1.55	0.01
1.52	0.01
1.480	0.01
1.427	0.01
1.367	0.01
1.245	0.01

(75) (12.5) 25)

977. ZnO*

d	I/I1
2.81	0.50
2.61	0.30
2.46	1.00
1.91	0.16
1.61	0.30
1.474	0.30
1.402	0.02
1.378	0.20
1.355	0.08
1.302	0.02
1.236	0.02
1.179	0.02
1.093	0.04
1.063	0.02
1.042	0.04
1.016	0.02
0.977	0.02
0.955	0.02
0.937	0.02
0.906	0.02

(25) (15) (50)

978. $ZnCo_2O_4$

d	I/I1
4.65	0.08
2.84	0.40
2.43	1.00
2.32	0.07
2.01	0.17
1.65	0.11
1.55	0.40
1.425	0.40
1.378	0.07
1.357	0.03
1.280	0.07
1.230	0.13
1.215	0.03
1.161	0.01
1.078	0.01
1.050	0.09
1.008	0.03

(30) (75) (30)

979. $ZnFe_2O_4$*

d	I/I1
2.97	0.25
2.53	1.00
2.42	0.02
2.10	0.12
1.71	0.08
1.61	0.25
1.484	0.30
1.327	0.02
1.282	0.02
1.122	0.02
1.003	0.08
1.049	0.02
0.969	0.04

(12.5) (50) (15)

980. $Zn(MnO_4)_2.6H_2O$

d	I/I1
5.2	0.05
4.16	0.67
3.93	1.00
3.15	0.03
2.85	0.67
2.63	0.05
2.44	0.07
2.31	0.10
2.26	0.05
2.07	0.13
2.01	0.03
1.96	0.17
1.88	0.03
1.84	0.17
1.78	0.13
1.69	0.03
1.62	0.03
1.55	0.03
1.53	0.03
1.490	0.07
1.425	0.03
1.389	0.03
1.309	0.05

(20) (30) (20)

981. $Zn(C_6H_4OHSO_2)_2.8H_2O$

d	I/I1
13.7	0.50
12.3	0.10
5.7	0.30
5.3	0.20
5.1	0.20
4.80	1.00
4.66	1.00
4.31	0.40
3.98	0.75
3.54	0.75
3.35	0.10
3.15	0.30
3.05	0.05
2.85	0.30
2.70	0.05
2.58	0.30
2.46	0.05
2.31	0.10
2.23	0.10
2.06	0.05
1.98	0.10
1.91	0.10
1.84	0.05
1.81	0.05
1.77	0.10
1.69	0.05
1.450	0.05

(20) (20) (15)

982. Zinc Phosphate

d	I/I1
13.4	0.32
7.7	0.64
6.7	0.16
5.8	0.32
4.34	0.32
3.81	0.40
3.61	0.64
3.45	0.08
3.32	0.08
3.20	0.08
3.11	0.16
2.85	1.00
2.68	0.16
2.62	0.32
2.43	0.08
2.35	0.16
2.15	0.16
2.07	0.16
1.99	0.16
1.94	0.16
1.87	0.08
1.81	0.16
1.76	0.32
1.69	0.08
1.62	0.08
1.58	0.08
1.495	0.24
1.421	0.08
1.391	0.08

(8) (8)

983. $Zn_3(PO_4)_2.4H_2O$

d	I/I1
9.1	0.40
5.3	0.08
5.1	0.08
4.86	0.12
4.59	0.25
4.40	0.25
4.01	0.20
3.65	0.08
3.47	0.40
3.40	0.40
3.13	0.08
2.85	1.00
2.75	0.04
2.63	0.40
2.52	0.40
2.42	0.20
2.33	0.10
2.27	0.20
2.20	0.08
2.15	0.10
2.09	0.14
2.03	0.04
2.00	0.20
1.94	0.35
1.82	0.30
1.78	0.04
1.73	0.08
1.70	0.10
1.67	0.04
1.63	0.04
1.59	0.06
1.56	0.12
1.52	0.14
1.51	0.14
1.480	0.02
1.440	0.08
1.410	0.08
1.385	0.04
1.353	0.08
1.324	0.04
1.296	0.04
1.270	0.06
1.237	0.10

(50)

984. $ZnHPO_3.2^1/_2H_2O$

d	I/I1
7.7	0.20
6.3	0.13
5.9	0.13
5.3	0.20
4.38	0.25
4.18	1.00
3.77	0.63
3.60	0.13
3.39	0.13
3.11	0.10
3.01	0.25
2.88	0.13
2.80	0.20
2.70	0.10
2.54	0.10
2.43	0.25
2.20	0.15
2.15	0.18
2.07	0.10
1.98	0.05
1.90	0.15
1.86	0.03
1.81	0.13
1.75	0.05
1.72	0.03
1.68	0.05

(10) (40) (25)

985. $Zn(H_2PO_2)_2.H_2O$

d	I/I1
7.5	1.00
6.7	0.04
6.0	0.40
5.3	0.40
5.0	0.36
4.70	0.16
4.30	0.28
4.00	0.20
3.70	0.24
3.47	0.36
3.25	0.32
3.05	0.32
2.94	0.16
2.89	0.12
2.77	0.20
2.67	0.50
2.60	0.50
2.50	0.16
2.36	0.04
2.26	0.28
2.20	0.08
2.06	0.28
1.99	0.24
1.87	0.20
1.81	0.12
1.75	0.16
1.76	0.16
1.71	0.04
1.66	0.12
1.62	0.16
1.58	0.12
1.53	0.04
1.455	0.08
1.385	0.12

(25) (12.5) (12.5)

986. $Zn(C_6H_4OHCOO)_2.3H_2O$

d	I/I1
9.3	1.00
7.8	0.20
5.78	1.00
5.1	0.16
4.48	0.60
4.08	0.24
3.89	0.24
3.68	0.08
3.43	1.00
2.95	0.04
2.83	0.08
2.66	0.12
2.61	0.16
2.37	0.08
2.19	0.12
2.07	0.08
2.01	0.08
1.96	0.16
1.92	0.08
1.85	0.08
1.83	0.08
1.75	0.08
1.69	0.08
1.62	0.04
1.56	0.08
1.51	0.08

(25)

987. $ZnSO_4.H_2O$

d	I/I1
4.80	0.64
3.80	0.11
3.40	1.00
3.06	0.40
2.52	0.40
2.40	0.06
2.34	0.11
2.19	0.14
2.10	0.10
2.05	0.05
1.97	0.13
1.91	0.08
1.81	0.08
1.70	0.03
1.67	0.11
1.62	0.08
1.58	0.08
1.53	0.02
1.50	0.05
1.444	0.05
1.405	0.02
1.360	0.02
1.325	0.02
1.280	0.03
1.260	0.03

(40) (62.5) (25)

988. $ZnSO_4.7H_2O$

d	I/I1
5.3	0.60
4.50	0.16
4.20	1.00
3.92	0.12
3.76	0.20
3.44	0.30
3.30	0.04
3.14	0.02
2.99	0.12
2.87	0.30
2.75	0.10
2.66	0.25
2.50	0.12
2.37	0.08
2.25	0.20
2.20	0.25
2.12	0.20
2.08	0.20
2.02	0.06
1.95	0.12
1.87	0.12
1.80	0.10
1.74	0.06
1.71	0.08
1.63	0.14
1.58	0.04
1.52	0.02
1.495	0.08
1.468	0.08
1.438	0.02
1.385	0.04
1.360	0.04
1.325	0.02

(30) (50) (15)

989. $ZnSO_4(NH_4)_2SO_4.6H_2O$

d	I/I1
8.8	0.03
7.8	0.07
6.1	0.13
5.4	0.20
5.1	0.03
4.20	1.00
3.78	0.67
3.62	0.03
3.41	0.13
3.13	0.03
3.03	0.33
2.89	0.03
2.79	0.13
2.69	0.03
2.55	0.03
2.44	0.07
2.22	0.03
2.15	0.05
2.07	0.03
1.98	0.03
1.91	0.03
1.85	0.03
1.81	0.03
1.76	0.03
1.62	0.03
1.56	0.03
1.480	0.03
1.440	0.03

(30) (20) (10)

990. $ZnSO_4.K_2SO_4.6H_2O$

d	I/I1
7.1	0.03
6.2	0.20
5.4	0.10
5.2	0.07
4.4	0.13
4.14	1.00
3.68	1.00
3.31	0.20
3.15	0.03
3.06	0.27
2.97	0.33
2.82	0.27
2.74	0.03
2.65	0.03
2.51	0.10
2.37	0.50
2.25	0.03
2.20	0.27
2.13	0.07
2.06	0.20
1.99	0.07
1.93	0.03
1.87	0.07
1.83	0.07
1.77	0.07
1.73	0.07
1.68	0.07
1.62	0.03
1.57	0.03
1.51	0.03
1.460	0.03
1.432	0.03
1.400	0.03
1.360	0.03
1.321	0.03
1.300	0.03
1.282	0.03
1.260	0.03
1.206	0.03
1.191	0.03
1.142	0.03
1.121	0.03

(15)

991. α-ZnS*

d	I/I1
3.29	1.00
3.11	0.47
2.91	1.00
2.27	0.47
1.90	0.83
1.76	1.00
1.62	0.67
1.59	0.33
1.459	0.27
1.292	0.40
1.249	0.13
1.224	0.27
1.168	0.33
1.099	0.20
1.070	0.47
1.039	0.13
0.997	0.07
0.955	0.07
0.914	0.20
0.883	0.20

(15) (15)

992. β-ZnS*

d	I/I1
3.12	1.00
2.69	0.05
1.91	0.75
1.63	0.50
1.353	0.05
1.242	0.18
1.211	0.03
1.104	0.15
1.044	0.05
0.957	0.03
0.913	0.04

(40) (30) (20)

993. $ZnSO_4.2^1/_2H_2O$

d	I/I1
7.7	1.00
5.8	0.25
4.78	0.10
4.55	0.10
4.25	0.03
3.81	0.20
3.50	0.20
3.26	0.20
3.14	0.18
2.91	0.15
2.80	0.15
2.70	0.10
2.35	0.03
2.28	0.10
2.20	0.08
2.16	0.10
2.13	0.10
2.09	0.10
2.00	0.10
1.94	0.10
1.89	0.10
1.75	0.15
1.70	0.05
1.62	0.03
1.58	0.03
1.56	0.05

(8) (8)

TABLE XII. POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES (*Concluded*)

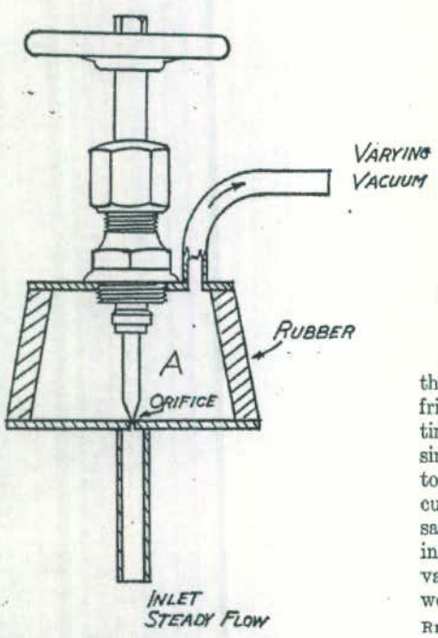
(Starred patterns were checked with published crystal structure data)

d		I/I_1	d		I/I_1	d		I/I_1	d		I/I_1	d		I/I_1	d		I/I_1
994. $(CH_3CH_2CH_2-CH_3COO)_2Zn.2H_2O$			995. Zr*			997. $Zr(NO_3)_4.5H_2O$			998. ZrO_2* (Monoclinic)			999. $ZrSiO_4$*			1000. Zirconyl Sulfate		
12.5	(62.5)	1.00	2.78	(12.5)	0.31	9.6	(40)	1.00				4.43		0.50	6.5	(8)	0.40
7.2		0.03	2.56	(8)	0.20	6.9	(40)	1.00	5.1		0.05	3.29	(100)	1.00	4.92		0.20
6.3		0.06	2.44	(40)	1.00	6.1		0.05	3.69		0.24	2.64		0.04	4.35	(20)	1.00
5.5		0.10	1.88		0.18	5.2		0.10	3.19	(125)	1.00	2.51	(100)	1.00	3.47		0.25
4.85	(30)	0.48	1.61		0.18	4.73	(20)	0.50	2.85	(100)	0.80	2.33		0.13	2.98	(17.5)	0.88
4.55	(15)	0.24	1.460		0.18	4.21		0.18	2.63		0.32	2.21		0.15	2.90		0.10
4.25		0.08	1.360		0.15	3.64		0.20	2.55		0.16	2.05		0.30	2.70		0.05
3.78		0.24	1.343		0.10	3.49		0.15	2.34		0.08	1.90		0.25	2.51		0.05
3.57		0.10	1.282		0.05	3.25		0.38	2.21		0.24	1.74		0.15	2.33		0.30
3.10		0.08	1.220		0.03B	3.03		0.10	2.01		0.16	1.71	(75)	0.75	2.13		0.15
2.98		0.03	1.180		0.03B	2.56		0.18	1.85		0.32	1.64		0.25	1.98		0.20
2.87		0.02	1.082		0.05	2.43		0.15	1.81	(50)	0.40	1.54		0.03	1.89		0.10
2.70		0.06	1.038		0.08	2.33		0.15	1.70		0.20	1.479		0.15	1.82		0.05
2.57		0.05	1.003		0.03	2.17		0.15	1.66		0.24	1.380		0.20	1.77		0.10
2.48		0.02	0.977		0.03	2.13		0.15	1.62		0.05	1.360		0.15	1.72		0.05
2.35		0.06	0.898		0.03	2.07		0.13	1.59		0.06	1.285		0.06	1.69		0.08
2.30		0.03	0.877		0.03	1.98		0.13	1.55		0.24	1.255		0.20	1.64		0.10
2.24		0.02				1.91		0.08	1.51		0.08	1.210		0.02	1.59		0.10
2.19		0.03	996. $ZrOCl_2.8H_2O$			1.81		0.10	1.486		0.16	1.185		0.18	1.52		0.05
2.12		0.03	12.8	(15)	1.00	1.74		0.08	1.426		0.16	1.163		0.03	1.460		0.05
2.07		0.06	10.6		0.27	1.70		0.05	1.363		0.05	1.098		0.15	1.392		0.05
2.02		0.05	7.9		0.20	1.64		0.10	1.330		0.08	1.057		0.08	1.358		0.05
1.96		0.05	6.9	(10)	0.67	1.59		0.03	1.307		0.03	1.046		0.13	1.280		0.05
1.88		0.06	4.80		0.13	1.55		0.05	1.270		0.12	0.999		0.04	1.250		0.05
1.81		0.03	4.12		0.27	1.51		0.03	1.219		0.05	0.972		0.10	1.090		0.05
1.76		0.03	3.82		0.20	1.476		0.03	1.167		0.06				1.053		0.05
1.69		0.05	3.60	(12.5)	0.83	1.390		0.03	1.113		0.06						
1.60		0.03	3.24		0.40	1.360		0.05	1.036		0.04						
1.490		0.03	2.96		0.07	1.295		0.03	1.001		0.06						
			2.74		0.07	1.228		0.03									
			2.55		0.07												
			2.39		0.07												
			2.22		0.13												
			2.15		0.20												
			2.07		0.13												
			2.00		0.07												
			1.91		0.13												
			1.81		0.13												
			1.71		0.13												
			1.62		0.13												
			1.57		0.07												
			1.51		0.07												
			1.460		0.07												
			1.423		0.07												

A Compact Self-Regulating Valve

L. WILLIAMS AND A. H. WILSON BUSBY

Consolidated Mining & Smelting Company of Canada, Ltd., Trail, B. C.



IN CONNECTION with collecting air samples by means of an evacuated chamber, a constant rate of flow of the sample was required as the vacuum in the chamber dropped. The controlling device had to be compact, light, and sufficiently strong to stand a lot of abuse. The volume of the chamber was approximately 1 cubic foot, and it was desired to sample this volume in about 3 minutes.

The valve as illustrated was made from materials at hand and performed well. A No. 10 rubber stopper was cut out to leave a 0.19-inch wall and two 0.063-inch brass plates were vulcanized over the open ends. In the center of one plate was drilled a 0.047-inch orifice and a copper connecting tube was soldered on. In the center of the other plate was soldered a 0.125-inch valve stem and packing gland. The original valve needle had been cut away and a smaller long needle set in its place. This end plate also contained the 0.25-inch vacuum connection.

As the vacuum in chamber *A* varies, the end plates move accordingly and the orifice adjusts the flow to an approximately constant value. There is no friction involved in the movement and the adjustment takes place without any time lag. With the full vacuum applied, the needle was screwed in until the desired rate of flow was attained, and it was found that the flow remained constant to within 10 per cent for a variation of vacuum from 28 down to 2 inches of mercury, below which the flow fell off at a rate depending on the friction in the sampling system. The steadiness of flow may be improved by suitably shaping the point of the needle valve. By a reverse arrangement of the needle, the valve may be adapted for governing air flow from a pressure source. The valve worked surprisingly well and can be refined and adapted to other purposes.

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Application No.: 11 838 195.3

The application and the invention to which it relates seem to meet the requirements of the EPC. Upon presence of a valid request for examination and consideration by the examining division, a communication under Rule 71(3) EPC may be issued.

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Polymorphism in Molecular Crystals

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McCrone (1957, 1965) has also given detailed descriptions of the microscopic examinations and phenomena that can be used to distinguish polymorphism from other phenomena that sometimes have been mistakenly labelled as pseudopolymorphism: mesomorphism (i.e. liquid crystals), grain growth (boundary migration and recrystallization), and lattice strain.

1.2.3 *Conventions for naming polymorphs*

Part of the difficulty encountered in searching and interpreting the literature on polymorphic behaviour of materials is due to the inconsistent labelling of polymorphs. In many cases, the inconsistency arises from lack of an accepted standard notation. However, often, and perhaps more important, it is due to the lack of various authors' awareness of previous work or lack of attempts to reconcile their own work with earlier studies (see, for instance, Bar and Bernstein 1985). While many polymorphic minerals and inorganic compounds actually have different names (e.g. calcite, aragonite and vaterite for calcium carbonate or rutile, brookite, and anatase for titanium dioxide) this has not been the practice for molecular crystals, which have been labelled with Arabic (1, 2, 3, ...) or Roman (I, II, III, ...) numerals, lower or upper case Latin (a, b, c, ... or A, B, C, ...) or lower case Greek (α, β, γ, ...) letters, or by names descriptive of properties (red form, low-temperature polymorph, metastable modification, etc.).

As Threlfall (1995) and Whitaker (1995) have commented, arbitrary systems for naming polymorphs should be discouraged to avoid confusion surrounding the number and identity of polymorphs for any compound. Relative stability and/or order of melting point, as well as a specification of the monotropic or enantiotropic nature of the polymorphic form (see Section 2.2.4) have also been suggested as a basis for labelling (Herbstein 2001), but these do not allow for the discovery of forms with intermediate values, in addition to the fact that small differences in stability or melting point might lead to different order and different labelling by different workers. McCrone (1965) proposed using Roman numerals for the polymorphs in the order of their discovery, with the numeral I specifying the most stable form at room temperature. By Ostwald's Rule (Ostwald 1897) (Section 2.3) the order of discovery should in general follow the order of stability the least stable appearing first. McCrone also supported the suggestion by the Koflers (Kofler and Kofler, 1954) that the Roman numeral be followed by the melting point in parentheses. In fact, the successors of the Koflers at the Innsbruck school have very much followed this practice (Kuhnert-Brandstätter 1971), although in general it has not been adopted by others. The use of melting points is complicated by the fact that while this datum has a clear thermodynamic definition, a number of techniques are employed to determine the melting point (or melting point range, in many cases) so that real or apparent inconsistencies may arise from such a designation (see Sections 4.2 and 4.3).

In view of the body of literature already extant and the questions surrounding the definition of a polymorph it does not appear to be practical to define hard and fast rules for labelling polymorphs. The Kofler method has clear advantages, since the melting point designation may eliminate some questions of identity; hence its use should be

encouraged. For those studying (and naming) polymorphic systems it is important to be fully aware of previous work, to try to identify the correspondence between their own polymorphic discoveries and those of earlier workers, and to avoid flippancy in the use of nomenclature in the naming of truly new polymorphs.

1.3 Is this material polymorphic?

1.3.1 *Occurrence of polymorphism*

Perhaps the most well-known statement about the occurrence of polymorphism is that of McCrone (1965): 'It is at least this author's opinion that every compound has different polymorphic forms and that, in general, the number of forms known for a given compound is proportional to the time and money spent in research on that compound.' As a corollary to this rather sweeping, even provocative, statement, McCrone noted that 'all the common compounds (and elements) show polymorphism', and he cited many common organic and inorganic examples.

These echo similar statements by Findlay (1951) p. 35, '[polymorphism] is now recognized as a very frequent occurrence indeed', Buerger and Bloom (1937), 'polymorphism is an inherent property of the solid state and that it fails to appear only under special conditions', and Sirota (1982), '[polymorphism] is now believed to be characteristic of all substances, its actual non-occurrence arising from the fact that a polymorphic transition lies above the melting point of the substance or in the area of yet unattainable values of external equilibrium factors or other conditions providing for the transition.'

Such statements tend to give the impression that polymorphism is the rule rather than the exception. The body of literature in fact indicates that caution should be exercised in making them. It appears to be true that instances of polymorphism are not uncommon in those industries where the preparation and characterization of solid materials are integral aspects of the development and manufacturing of products (i.e. those on which a great deal of time and money is spent): silica, iron, calcium silicate, sulphur, soap, pharmaceutical products, dyes, and explosives. Such materials, unlike the vast majority of compounds that are isolated, are prepared not just once, but repeatedly, under conditions that may vary slightly (even unintentionally) from time to time. Similarly, in the attempt to grow crystals of biomolecular compounds, much time and effort is invested in attempts to crystallize proteins under carefully controlled and slightly varying conditions, and polymorphism is frequently observed (Bernstein *et al.* 1977; McPherson 1982). Even with the growing awareness and economic importance of polymorphism, most documented cases have been discovered by serendipity rather than through systematic searches. Some very common materials, such as sucrose and naphthalene, which certainly have been crystallized innumerable times, have not been reported to be polymorphic. The *possibility* of polymorphism may exist for any particular compound, but the conditions required to prepare as yet unknown polymorphs are by no means obvious. There are as yet no comprehensive systematic methods for feasibly determining those conditions. Moreover, we are almost totally ignorant about the properties to be expected from any new polymorphs that might be obtained.

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The Predictably Elusive Form II of Aspirin

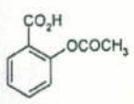
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Polymorphism, the existence of more than one crystalline form of a compound, is an intensely studied phenomenon, yet it remains poorly understood and controlled.[1] Polymorphism in active pharmaceutical ingredients, API's, is critical from both regulatory and intellectual property perspectives[1a] since polymorphs can exhibit different physical and/or chemical properties. However, the very nature of API's, which typically exhibit exterior hydrogen bonding sites and/or conformational flexibility, makes them ideal candidates for polymorphism control using additives or templates.[2] Furthermore, whereas API's have traditionally been limited to polymorphs, solvates, and salts,[3] in recent years, an alternative form, pharmaceutical co-crystals, has been targeted.[4] In this context, aspirin is somewhat of an enigma. Aspirin was first synthesized in 1853[5] and had by the turn of the 19th century become the world's best-selling drug.[6] In the 1960s and 1970s, aspirin was subjected to a series of studies[7] to determine whether it exhibits polymorphism, and there were indications that there could be a metastable form.[7d] However, these studies were inconclusive. In the end, differences in physical properties were attributed to salicylic acid impurities.[8] Most recently, computational studies have addressed polymorphism in aspirin.[9]

In this contribution, we report the results of a series of studies concerning pharmaceutical co-crystals of aspirin, resulting in isolation and structural characterization of the elusive form II of aspirin as well as a pharmaceutical co-crystal involving aspirin and another API, carbamazepine.



Aspirin

The crystal structure of aspirin form I has been studied by both X-ray[10] and neutron diffraction.[11] Herein we shall use as a reference point Wilson's 100 K structure[11] (CSD refcode: ACSALA02) to compare with form II since our data were also collected at 100 K. Form I consists of centrosymmetric carboxylic acid dimer moieties (O···O: 2.635 Å, 177.7°) that are, in turn, linked via centrosymmetric methyl C−H···O (C···O: 3.553 Å, 164.0°)[12] contacts of acetyl groups, thereby forming 1D chains (Figure 1a).

Aspirin form II was repeatedly obtained during attempted 1:1 co-crystallization of aspirin and levetiracetam from hot acetonitrile and was subsequently also observed in the presence of a molar equivalent of acetamide. Small plate-like crystals form in approximately 3 days, and one was mounted on a diffractometer directly from the viscous mother liquor to avoid conversion into form I. In addition to single crystal structure determination, form II was also characterized by melting point, IR, DSC, and HPLC

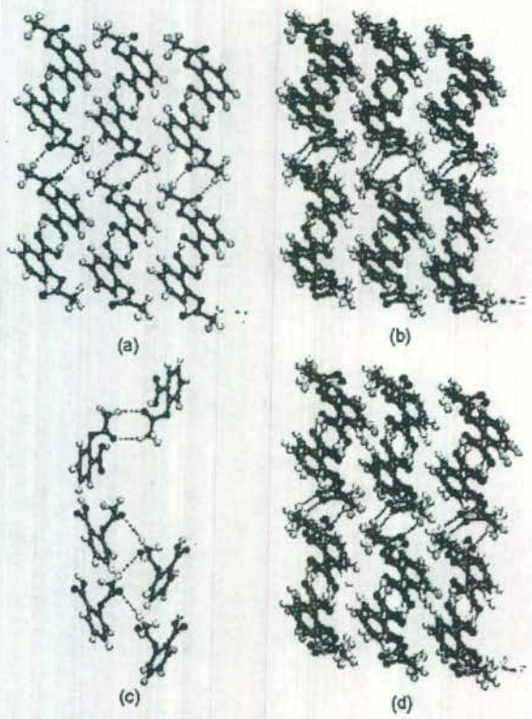


Figure 1. Crystal packing of aspirin forms I, II, and S. L. Price predicted form II. (a) Form I: 1D chains sustained by alternating carboxylic acid and acetyl group centrosymmetric dimers. (b) Form II: acid dimers are connected via catemeric methyl C−H···O and phenyl C−H···O (not shown) hydrogen bonds. (c) Acetyl group C−H···O dimers in form I and catemers in form II. (d) S. L. Price predicted form II. Note the similarity with the crystal packing of form II (b).

(see Supporting Information). Crystals of form II convert to form I under ambient conditions; however, they are relatively stable at 100 K. DSC thermograms reveal an endothermic peak at 135.5 °C for form II versus a melting transition at 143.9 °C for form I. The chemical composition of bulk samples of form II aspirin was determined by HPLC to be consistent with those of form I, salicylic acid content of 0.5−3.0% in form I versus 1.7% in a form II sample.

There are clear differences between the unit cell parameters: form I ($P2_1/c$): $a = 11.233(3)$ Å, $b = 6.544(1)$ Å, $c = 11.231(3)$ Å, $\beta = 95.89(2)°$, $V = 821.218$ Å^3; form II ($P2_1/c$):[13] $a = 12.095(7)$ Å, $b = 6.491(4)$ Å, $c = 11.323(6)$ Å, $\beta = 111.509(9)°$, $V = 827.1(8)$ Å^3. The molecular geometry of aspirin molecules in form II is slightly different in terms of the torsion angle defined by the carboxylic acid and acetyl groups, although the centrosymmetric carboxylic acid dimer remains intact [O···O: 2.632(14) Å, 173.1°].

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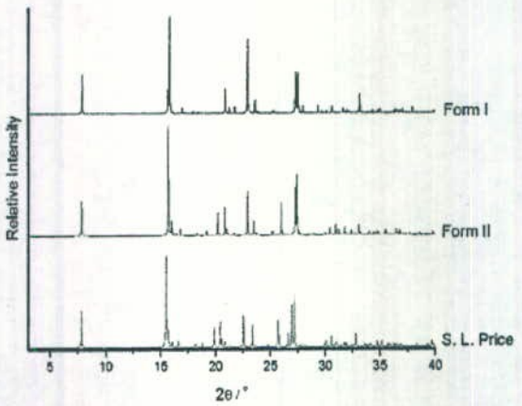


Figure 2. Simulated powder X-ray diffraction (PXRD) patterns of aspirin form I, II, and S. L. Price predicted form II crystal structures. See the noticeable additional peaks in form II and S. L. Price predicted form II compared to form I near 2θ: 20 and 26°.

However, the crystal packing of adjacent dimers is different; methyl groups form catemeric C−H···O [C···O: 3.85(2) Å, 164.0°] hydrogen bonds with the carbonyl oxygen (graph set C(4)) of the acetyl group versus centrosymmetric dimers (graph set $R^2_2(8)$) in form I (Figure 1). The existence of competing catemer/dimer motifs is well documented in polymorphs of carboxylic acids and primary amides.[1u,4,14] Simulated powder X-ray diffraction patterns also exhibit significant differences (Figure 2). It is interesting to note that a computational study concerning polymorphism in aspirin predicted a low energy polymorph with a low shear elastic constant, implying a low barrier to transformation. This calculated structure is consistent with that of form II.[9a]

The discovery of a new form of aspirin through attempted co-crystallization of amides and acids is perhaps unexpected when one considers that acids and amides are known to form reliable supramolecular heterosynthons.[15] Indeed, attempted co-crystallization of carbamazepine and aspirin resulted in the expected[4b] 1:1 co-crystal, the structure of which is illustrated in Supporting Information (Figure S3). This crystal structure[16] reveals that aspirin molecules form acid−amide supramolecular heterosynthons to carbamazepine molecules through O−H···O [O···O: 2.564(2) Å, 167.5°] and N−H_s···O [N···O: 2.914(3) Å, 168.4°] hydrogen bonds.

The salient feature of this study is not just the identification of aspirin form II, it is also the manner in which it was prepared. That crystallization of aspirin form II can occur in the presence of certain amides, whereas a co-crystal with carbamazepine can also occur and might appear to be counterintuitive. However, these observations are consistent with studies that have demonstrated how tailor-made additives can disrupt nucleation and induce polymorphism.[2] Supramolecular heterosynthons, therefore, seem to have implications for control of polymorphism.

To summarize, we have obtained and characterized a new polymorph and a new co-crystal of aspirin. In our opinion, the most salient features of the results reported herein are the method by which the once elusive form II of aspirin was isolated and the fact that it had been hitherto predicted.

Supporting Information Available: X-ray crystallographic information in CIF format, IR, DSC, HPLC, aspirin and carbamazepine 1:1 co-crystal packing diagram, torsional angle, and hydrogen bond tables. This material is available free of charge via the Internet at http://pubs.acs.org.

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(13) Crystal data of form II: chemical formula $C_9H_8O_4$, formula weight 180.15, monoclinic, space group $P2_1/c$, a = 12.095(7) Å, b = 6.491(4) Å, c = 11.323(6) Å, β = 111.509(9)°, V = 827.1(8) Å^3, Z = 4, ρ_{calc} = 1.447 Mg m^{-3}, T = 100 K, μ = 0.115 mm^{-1}, 1780 reflections measured, 748 unique reflections, 648 observed reflections [$I > 2\sigma(I)$], $R1_{obs}$ = 0.162, $wR2_{obs}$ = 0.308. Crystal size: 0.25 × 0.15 × 0.005 mm. All atoms were refined isotropically because of the relatively weak data.

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Polymorphism

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On the Polymorphism of Aspirin: Crystalline Aspirin as Intergrowths of Two "Polymorphic" Domains**

Andrew D. Bond, Roland Boese,* and Gautam R. Desiraju**

In the preceding paper, we highlighted the ambiguity that exists in the literature concerning the nature of crystalline aspirin.[1] In 2004, Ouvrard and Price demonstrated computationally that the long-established aspirin crystal structure[2–4] was amongst those predicted to be most stable, but they identified a slightly more stable structure as the thermodynamic minimum.[5] At the time, it was unclear whether the predicted minimum-energy structure was a remnant of inadequate energy assessment,[6] or whether it was a plausible structure that awaited discovery. This issue appeared to be resolved in 2005, when Peterson, Zaworotko, and co-workers (hereafter referred to as PZ) claimed to have obtained the predicted second polymorph,[7] following X-ray analysis of aspirin crystals obtained from hot acetonitrile solution in the presence of either levetiracetam or acetamide. The proposed new polymorph was labelled aspirin "form II", and the long-established aspirin crystal structure was thereby designated "form I".

The distinction between the proposed aspirin polymorphs is subtle. They contain identical arrangements of O–H···O hydrogen-bonded dimers lying in layers, but these layers are arranged differently with respect to each other in the two forms (Figure 1). In form I, the layers are arranged so that C–H···O interactions form centrosymmetric dimers (arrangement **A**, Figure 1). In the proposed form II, adjacent layers are arranged so that C–H···O interactions generate catemers (arrangement **B**, Figure 1). Both interlayer arrangements are reasonable and acceptable in terms of the C–H···O interactions. Taken with the accord between the experimental and computational findings,[5] the PZ description of aspirin polymorphism appeared superficially to be plausible.[7] However, there are serious problems with their structure refinement. For the proposed form II, their crystallographic *R*-factors are unacceptable ($R1 = 0.162$, $wR2 = 0.327$), and several refined displacement parameters are close to or equal to zero, with anisotropic refinement being impossible. Combined with very close metric similarity between the unit cells of the form I and form II structures, this caused us to raise the question of whether the proposed form II might actually be an experimental artifact originating from erroneous handling of diffraction data collected from a form I crystal.[1] Indeed, we showed that form II of aspirin as reported by PZ may be derived, to the accuracy and precision reported by those workers, from experimental diffraction data collected on an aspirin crystal that was most certainly form I. Thus, we stressed that the PZ report did not establish the existence of aspirin form II to any acceptable level of scientific rigor.[1] In this report, we are able to resolve the issue fully. Aspirin exhibits a tendency to crystallize with an

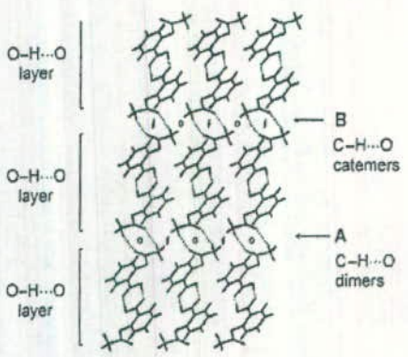


Figure 1. Illustration of the two interlayer arrangements within a representative aspirin crystal. Arrangement A, comprising centrosymmetric C–H···O dimers, exists between the layers that are colored red. Arrangement B, comprising C–H···O catemers extending along 2_1 screw axes, exists between the layers that are colored blue. The change in color within the central layer is for illustration only; all O–H···O hydrogen-bonded layers are identical.

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Supporting information for this article is available on the WWW under http://www.angewandte.org or from the author.

InterScience
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intergrowth structure, in which layers of O–H···O hydrogen-bonded dimers form domains with arrangement **A** and domains with arrangement **B**, within the same single crystal. The distribution and total ratio of the domains is variable but appears to be limited. Aspirin form I, which comprises 100% arrangement **A**, is commonplace, but pure form II, which would comprise 100% arrangement **B**, has not been realized.

The crucial experimental result was first obtained after we freshly synthesized aspirin from salicylic acid (see the Supporting Information) and prepared single crystals by rapidly cooling a solution in hot acetonitrile (Table 1). Single-crystal X-ray diffraction analysis of these crystals (denoted **1a**, laths of typical dimension $0.20 \times 0.10 \times 0.05$ mm) proceeded apparently routinely to provide the form II structure, with $R1 = 0.071$ and $wR2 = 0.197$, against data measured to $2\theta = 50°$ ($Mo_{K\alpha}$).[8] Unlike the PZ report, our refinement was anisotropic and entirely satisfactory, although we noted that our R-factors were a little higher than expected. These crystals were obtained without addition of levetiracetam or acetamide, demonstrating that the additive is not a significant factor. We obtained similar results by slow evaporation of an acetonitrile solution, indicating that the rapid cooling procedure also is not important. Powder X-ray diffraction seemed to confirm that the single crystal **1a** was representative of the bulk sample,[9] and the polymorphism of aspirin might therefore appear to be clear-cut. However, reconstruction of precession photographs in the a^*c^* planes of our experimental data (Figure 2a) revealed numerous additional reflections lying halfway between those of the principal form II lattice in the odd l rows, together with diffuse streaks along a^* between the Bragg reflections. In physical terms, the diffraction pattern demonstrates that aspirin crystals contain layers of O–H···O hydrogen-bonded dimers that are consistent (Figure 1), but that these layers form domains in which they adopt arrangement **A** (form I) and domains in which they adopt arrangement **B** (form II). The existence of the form I and form II domains is shown by the two sets of Bragg reflections, while the streaks indicate some degree of stacking disorder.

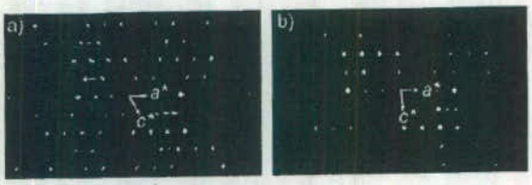


Figure 2. Reconstructed ($h-1\,l$) precession photographs for crystals **1a** and **2**. a) Crystal **1a** exhibits sharp Bragg reflections corresponding to the form II lattice (reciprocal lattice vectors shown), broader maxima halfway between these reflections in the odd l rows, and diffuse streaks along a^*. This indicates extended form II domains, smaller domains of form I, and regions in which there is a disordered distribution. b) For crystal **2**, the most intense Bragg reflections correspond to the form I lattice (reciprocal lattice vectors shown), and Bragg reflections of comparable profile exist for the form II lattice. This indicates a relatively more ordered structure than in **1a** (a) with extended form I and form II domains.

From analyses of numerous crystals obtained under various experimental conditions, including crystallization in the presence of acetamide[10] (Table 1), we find that both the relative intensities of the two sets of Bragg reflections and the extent of the streaking are variable. In crystal **2** (Figure 2b), for example, all Bragg reflections are relatively sharp, and there are no obvious streaks, consistent with extended well-ordered domains of form I and form II. In crystals **1a** and **1b**, sharp Bragg reflections for the form II lattice indicate extended form II domains, while the broader Bragg reflections between these lattice points indicate smaller domains of form I. The diffuse streaks also indicate regions with a less ordered pattern of interlayer arrangements **A** and **B**. Thus, both the sizes and distribution of the form I and form II domains are variable.

The interpretation of one-dimensionally diffuse diffraction data has a long history[11] and has been summarized

Table 1: Summary of crystallization conditions and single-crystal refinements.

Crystallization conditions	No.	Conventional refinement of single-crystal data[b]			Single-crystal refinement with batch scaling factors			Refined batch scaling factors[c]
		form	$R1$	$wR2$	form	$R1$	$wR2$	
rapid cooling of solution in hot MeCN	**1a**[a]	I	0.344	0.658	I	0.075	0.202	0.132(1)
		II	0.071	0.197	II	0.054	0.132	0.747(2)
	1b[a]	I	0.544	0.846	I	0.076	0.220	0.038(1)
		II	0.041	0.116	II	0.034	0.080	0.858(2)
rapid cooling of solution in hot MeCN in the presence of 1 equiv acetamide	**2**	I	0.059	0.175	I	0.056	0.140	0.803(3)
		II	0.305	0.631	II	0.076	0.288	0.146(1)
as synthesized (see the Supporting Information)	**3**[d]	I	0.033	0.089	I	0.033	0.089	0.982(4)
		II	unstable		II	0.076	0.141	0.003(1)

[a] Crystals **1a** and **1b** are different single crystals from the same crystallization batch. [b] Based on data sets obtained from two separate standard integrations of the CCD frames, considering only Bragg peaks. Refinements are performed against all F^2 data to $2\theta_{max} = 50°$ ($Mo_{K\alpha}$). $R1$ is quoted for data with $I > 2\sigma(I)$, $wR2$ is quoted for all data. [c] The high precision refers to that obtained from the least-squares refinement. See the text for discussion of the approximations and limitations of the approach. [d] A pure form I crystal. For form I refinement, the batch scale factor refines to be essentially unity. Conventional form II refinement against all F^2 data is unstable. For batch refinement, the scale factor refines to zero, effectively omitting all odd l reflections, thereby emulating a data set that contains only the even l reflections. This is exactly the situation that we noted in our previous manuscript.[1]

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recently for molecular crystals.[12] The literature includes examples in which layered structures exhibit only one kind of interlayer arrangement, that is, structures for which there are alternative positions of adjacent layers that have exactly equivalent interatomic/intermolecular contacts (as for the close packing of spheres, for example).[13] The aspirin case is apparently the first of its kind in that it exhibits two distinctly different interlayer arrangements (**A** and **B**), both of which are physically and chemically reasonable. The accidental energetic degeneracy of the two possibilities,[5,6] combined with the specific metric relation between the form I and form II lattices, is the reason for the unusual crystallographic observations, since it allows aspirin diffraction patterns to be processed in two different ways to provide two different structures, both of which are physically reasonable. The metric transformation [1 0 ½ 0 −1 0 0 0 −1] that relates the form I and form II unit cells causes all Bragg reflections *hkl* with even *l* to overlay but places the odd *l* reflections of form II halfway between those of form I.[14] Thus, the Bragg reflections arising from the two types of domain appear to a first approximation as a weighted overlay of the form I and form II diffraction patterns, with the distribution dependent on the relative domain ratio. If such a diffraction pattern is indexed in the usual way to one or other of the form I or form II unit cells, standard integration (that is, considering only Bragg reflections, and discounting any other features),[15] will provide a data set in which the even *l* reflections are of the correct intensity, but the odd *l* reflections are systematically weak. This is the path that was followed by PZ.[7] The extent to which the odd *l* reflections are in error reflects the ratio of the form I and form II domains.

On the basis of our description, a practical procedure to obtain an estimate of the total domain ratio is to introduce a batch scale factor into the crystallographic refinements, applied only to reflections with odd *l*. The refined value of this scale factor gives the relative weights of the form I and form II reciprocal lattices and therefore a direct estimate of the crystal composition. This estimate will be good for crystals that exhibit only sharp Bragg peaks and no diffuse streaks, while it will be more approximate when the streaking is more significant. Thus, the approach would be exact for two perfectly ordered domains with a single domain boundary, but it becomes progressively more approximate for real aspirin crystals as the extent of the domain disorder increases. The procedure gives a total composition estimate but no direct information concerning the sizes of the form I and form II domains or their distribution. For crystal **1a**, such a refinement against the form II data set[16] gives $R1 = 0.054$ and $wR2 = 0.132$, a significant improvement on the standard refinement, and the refined batch scale factor indicates that roughly 75% of the crystal comprises form II domains. The practical effectiveness of the process is illustrated more dramatically by batch refinement of the form I data set obtained from the same crystal. While standard treatment of the form I structure gives $R1 = 0.344$, $wR2 = 0.658$ and does not permit anisotropic refinement, introduction of the batch scale factor allows routine refinement with all non-H atoms anisotropic to give $R1 = 0.075$, $wR2 = 0.202$. In this instance, the refined batch scale factor indicates approximately 15% form I domains. The discrepancy between the two indications of the crystal composition (in other words, that they do not sum to 100%) reflects principally the failure to account for the diffuse features of the diffraction pattern.[17] With this procedure, the refined crystal structure will be either pure form I (100% arrangement **A**) or pure form II (100% arrangement **B**) if the batch scale factor should refine to unity. This is the case for crystal **3** (Table 1), which is pure form I. In all other cases, the intergrowth structure is present, and a more complex analysis of the entire diffraction pattern, including diffuse features, is necessary to extract further information regarding domain size and distribution.[12]

Using our straightforward approach, a general correlation can be derived between approximate domain ratio and the expected crystallographic *R*-values for a conventional treatment of the X-ray data.[18] Figure 3 provides a guide for assessment of the total domain ratio in any aspirin crystal using the *R*-values obtained from F^2 refinement on the basis of either the pure form I or the (hypothetical) pure form II structure if standard data reduction and refinement procedures should be followed. Using the correlation shown in Figure 3, the *R*-factors reported by PZ[7] show that their crystal actually comprised approximately equal proportions of domains with interlayer arrangement **A** and domains with interlayer arrangement **B**.

Chemically speaking, it is reasonable (albeit realized in hindsight) that aspirin crystals should provide intergrowth

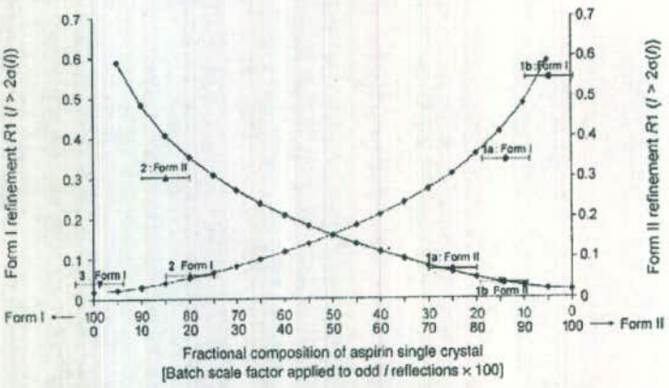


Figure 3. Correlation between total domain ratio and expected crystallographic *R*1 value, obtained for conventional refinement against all F^2 data. The correlation is derived from experimental data for crystal **3** (see the Supporting Information for full details). The red and blue curves refer to standard data reduction and refinement on the basis of the form I and form II structures, respectively, for an aspirin crystal with domain ratio indicated by the horizontal axis. The experimental points correspond to the *R* values obtained for the crystals listed in Table 1. For these, the composition estimate is taken from the batch scale factor refinement, with error bars indicating ±5% composition. For example, conventional refinement of crystal **1a** as form II gives $R1 = 0.071$. The separate batch scale factor refinement indicates 75% form II domains. The same crystal **1a** refined conventionally as form I gives $R1 = 0.344$, with the separate batch scale factor refinement indicating 15% form I domains.

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structures in this way. The strongest interactions (O–H···O, herringbone) occur within the layers parallel to the (100) planes, which constitute the persistent building blocks within aspirin crystals. These are presumably the most robust growth units[19] in the system. Shearing of these layers relative to each other along [001], which is in effect the movement that transforms arrangement **A** into arrangement **B**, involves rupture and creation of weak C–H···O interactions. The energy difference between the **A** and **B** arrangements is clearly very small,[5,6] and together with the consistent layer surface at (100), this permits facile turnover between the two possibilities in the composite crystal. If the energy difference were significantly greater, individual crystals of one pure polymorph (either form I or form II) would be accordingly more stable. Ouvrard and Price[5] noted that form II should have "a low shear elastic constant, implying that it is so readily deformed that there may be problems in its growth". In the course of our present study, we have frequently observed crystals of pure form I (at least to the limits of detection possible for single-crystal and powder X-ray diffraction[20]), but the maximum proportion of form II domains that we have observed is approximately 85%. Thus, aspirin form II has not been documented in a pure form so far. Whether this means that arrangement **A** is inherently more stable than arrangement **B**, contrary to the calculations,[5] is a matter that remains to be firmly established. If it were, form II might be a metastable kinetic product[21] which could still potentially be observed, but which might transform to the more stable form I. However, we have not observed any such transformation, at least for single crystals standing in air over a period of two months.[22] It is also possible that arrangement **B** is indeed more stable than arrangement **A**,[5] but that the growth problems associated with arrangement **B** prevent the isolation of a pure aspirin form II. In this case, approximately 85% arrangement **B** may be the most that we can expect. Clearly, much future work remains to clarify completely the thermodynamic and kinetic aspects of crystalline aspirin.

Finally, the case of aspirin raises issues with regard to nomenclature. As for any evolving scientific area, crystal engineering is presently subject to lively and ongoing debate pertaining to the naming of concepts and phenomena. Terms such as "co-crystal" and "pseudopolymorph" have been discussed recently in this context.[23] The term "polymorph" has so far stayed above such controversies and is used to signify a situation where the same substance exhibits different crystal packing arrangements.[24] For crystallographers, this definition might be considered to encompass only crystals for which long-range translational order is dominant; in other words, it is appropriate only at one end of a continuum that ranges from perfect crystals to systems without long-range translational order. To chemists, the accepted distinction is rather more clear. Polymorphism implies that a molecule may adopt one or other type of packing arrangement in the crystalline state, and different polymorphs are distinct entities that display different physical and chemical properties. A single crystal of a given chemical substance is either one polymorph or another. In this context, one might ask how many polymorphs of aspirin actually exist. The domains with interlayer arrangements **A** (form I) and **B** (form II) certainly represent two different crystal structures that serve as reference points. However, considering that aspirin crystals display both arrangements within a single crystal, should aspirin really be described as polymorphic? What is certain is that the PZ description of their crystal as a polymorph distinct from form I is not justifiable. The PZ crystal, like several other aspirin crystals described in this paper, is an intergrowth of two "polymorphic" domains. We emphasize that the intergrowth crystals are exactly that: they are not simply mixtures of form I and form II, and they are not twins. Each aspirin crystal is an integral whole in which the domains are intimately connected with each other, with possibly many turnovers of domain within a single crystal. Further, it seems that the ratio of the domains in aspirin crystals is likely to be constant in any particular batch prepared under the same conditions.

This issue has implications beyond nomenclature. Should individual form I/form II compositions qualify for separate patent protection? Should patents be granted only for ranges of form I and form II domain ratios and not for specific compositions?[25] Is (pure) form II entitled to patent protection considering that it has not been realized as yet? Could this problem be solved by calling these crystals "polytypes", considering the voluminous literature on this topic in inorganic solid-state chemistry?[26] If so, would different polytypes then be entitled to patent protection? These and other issues suggest that one keeps an open mind with regard to definitions in crystal engineering, including that of the term "polymorph".[27] In an evolving subject, no definition should be carved in stone.

The Supporting Information includes details of the synthesis and crystallization procedures, powder X-ray diffraction data, reconstructed precession photographs for single crystals **1a**, **1b**, **2**, and **3**, a description of the geometry and intensities of the Bragg reflections in aspirin diffraction patterns, and details regarding the correlation between *R*-factors and the total domain ratio. The results of all refinements referred to in Table 1 are available in CIF format, with the corresponding *hkl* data available in SHELXL HKLF-4 format. All CCD frames (Bruker APEX2 format) can be obtained from the authors on request.

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[6] The minimum-energy structure was just 0.2 kJ mol^{-1} lower in energy than the established crystal structure, and in our opinion this value is so small that the order of energies might just as easily have been reversed.

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[8] The highest form II domain ratio observed from 15 single-crystal data collections is in crystal **1b**. For this crystal, conventional refinement of the form II structure gives: $C_9H_8O_4$, $M_r = 180.15$, monoclinic, space group $P2_1/c$, $a = 12.1515(10)$, $b = 6.5064(5)$, $c = 11.3677(9)$ Å, $\beta = 111.574(3)°$, $V = 835.79(12)$ Å^3, $T = 180(2)$ K, $\mu(Mo_{K\alpha}) = 0.114$ mm^{-1}, $2\theta_{max} = 50°$, 9778 reflections measured, 1474 unique reflections ($R_{int} = 0.029$), 1149 observed reflections, $R1(I > 2\sigma(I)) = 0.041$, $wR2$(all data) = 0.116, $S = 1.02$. CCDC-617840 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

[9] Compared to the powder X-ray diffraction pattern of pure form I, the principal features that reveal the presence of form II domains are peaks at $2\theta \approx 20.9$ and 26.0° (at 295 K, see the Supporting Information).

[10] With extremely rapid cooling of a hot equimolar solution of aspirin and acetamide in acetonitrile (that is, by plunging the flask directly into liquid N_2 or dry ice/2-propanol), we obtained a 1:1 molecular complex of aspirin and acetamide, which contains the expected acid–amide heterosynthon. This would argue in favor of acetamide acting as a growth inhibitor at the (200) faces of aspirin, leading to platelike crystals that cannot grow easily along [100]. It is likely that levetiracetam would behave in a similar way, and this is the morphology reported by PZ for their aspirin crystal. Crystal data for the aspirin/acetamide (1:1) co-crystal: $(C_9H_8O_4)(C_2H_5NO)$, $M_r = 239.22$, orthorhombic, space group $Pbca$, $a = 9.5268(4)$, $b = 8.7495(3)$, $c = 28.4520(11)$ Å, $V = 2371.61(16)$ Å^3, $T = 203(2)$ K, $\mu(Mo_{K\alpha}) = 0.107$ mm^{-1}, 68487 reflections measured, 3074 unique reflections ($R_{int} = 0.059$), 2586 observed reflections, $R1(I > 2\sigma(I)) = 0.042$, $wR2$(all data) = 0.119, $S = 1.04$. CCDC-618012 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

[11] a) H. Jagodzinski, *Acta Crystallogr.* **1949**, *2*, 201; b) H. Jagodzinski, *Acta Crystallogr.* **1949**, *2*, 208; c) "Disorder Diffuse Scattering of X-rays and Neutrons": H. Jagodzinski, F. Frey in *International Tables for Crystallography, Vol. B* (Ed.: U. Shmueli), International Union of Crystallography and Kluwer Academic Publishers, Dordrecht, **2001**.

[12] H.-B. Bürgi, M. Hostettler, H. Birkedal, D. Schwarzenbach, *Z. Kristallogr.* **2005**, *220*, 1066.

[13] a) K. Dornberger-Schiff, H. Grell-Niemann, *Acta Crystallogr.* **1961**, *14*, 167; b) K. Dornberger-Schiff, J. D. Dunitz, *Acta Crystallogr.* **1965**, *19*, 471; c) K. Dornberger-Schiff, *Acta Crystallogr. Sect. A* **1982**, *38*, 483; d) D. Schwarzenbach, K. Kirschbaum, A. A. Pinkerton, *Acta Crystallogr. Sect. B* **2006**, *62*, 944.

[14] In crystallographic parlance, the Bragg reflections with even l are referred to as "family reflections" and are common to both the form I and form II structures. The family reflections alone define a "superposition structure", which in the case of aspirin comprises two O–H···O dimers overlaid in a unit cell with c dimension half that of the true c dimension. The distribution of the intensities along the odd l rows contains the information to decompose the superposition structure into chemically reasonable arrangements, that is, the information regarding the particular sequence of the O–H···O layers. See Ref. [12].

[15] Neglecting any diffuse scattering is clearly a simplification. However, the procedures that we describe have the advantage that they are standard (that is, they are based only on procedures used for routine crystallographic analyses), require no specialist knowledge, and can be applied in any crystallographic laboratory.

[16] The term "form II data set" refers to the list of intensities (the *hkl* file) that is obtained when the diffraction data are indexed on the basis of the form II unit cell and integrated using standard procedures. The additional Bragg reflections that could be described on the basis of the form I unit cell and any diffuse features are ignored. The term "form I data set" refers to the opposite situation.

[17] In particular, there may be problems associated with assessment of the background intensity in the presence of diffuse streaks in the vicinity of the Bragg reflections.

[18] The correlation is derived from the experimental form I data set (crystal **3**), with a suitable fractional scale factor applied to the odd l reflections (see the Supporting Information for full details). The batch refinement must be based on all F^2 data. The Figure provides an immediate approximate guide, based on standard refinement procedures. Application of the batch refinement procedure will provide an improved estimate.

[19] R. J. Davey, K. Allen, N. Blagden, W. I. Cross, H. F. Lieberman, M. J. Quayle, S. Righini, L. Seton, G. J. T. Tiddy, *CrystEngComm* **2002**, *4*, 257.

[20] Since interlayer arrangements **A** and **B** are structurally and energetically so finely balanced, disorder is thermodynamically inherent in the aspirin system. All aspirin crystals should contain some of arrangements **A** and **B** at real temperatures. They are detectable by X-ray diffraction only when their number becomes significant.

[21] In general, for any system of hydrogen bonds (O–H···O or C–H···O) wherein the dimer and catemer alternatives are well matched, there is a consensus that the catemer is kinetically favored since it is a higher dimensional pattern than the dimer. See: D. Das, G. R. Desiraju, *Chem. Asian J.* **2006**, *1*, 231.

[22] PZ have reported that "form II" transforms into form I at 100 K. Our assessment of the stability of the form II domains is based on re-collection of single-crystal data for **1b** after the crystal had stood in air for two months.

[23] Co-crystal: a) G. R. Desiraju, *CrystEngComm* **2003**, *5*, 466; b) J. D. Dunitz, *CrystEngComm* **2003**, *5*, 468. Pseudopolymorph: c) K. R. Seddon, *Cryst. Growth Des.* **2004**, *4*, 1088; d) G. R. Desiraju, *Cryst. Growth Des.* **2004**, *4*, 1089; e) J. Bernstein, *Cryst. Growth Des.* **2005**, *5*, 1661; f) A. Nangia, *Cryst. Growth Des.* **2006**, *6*, 1.

[24] However, one of us has argued (in Ref. [23d]) that difficulties in the use of the word "pseudopolymorph" might have arisen because the definition of the term "polymorph" is too rigid with respect to identity of chemical composition among substances that are deemed to qualify for the polymorph epithet.

[25] To some extent, this situation parallels that of isomorphous crystalline solvates, for which patents have been granted for ranges of solvent content. However, while variable solvent content is a common occurrence, it is not clear how common the aspirin situation will be.

[26] A. R. Verma, P. Krishna, *Polymorphism and Polytypism in Crystals*, Wiley, New York, **1966**.

[27] G. Coquerel *Chem. Eng. Proc.* **2006**, *45*, 857

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