INDUSTRIAL and ENGINEERING CHEMISTRY

ANALYTICAL EDITION ◆ Harrison E. Howe, Editor

Chemical Analysis by X-Ray Diffraction

Classification and Use of X-Ray Diffraction Patterns

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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

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.

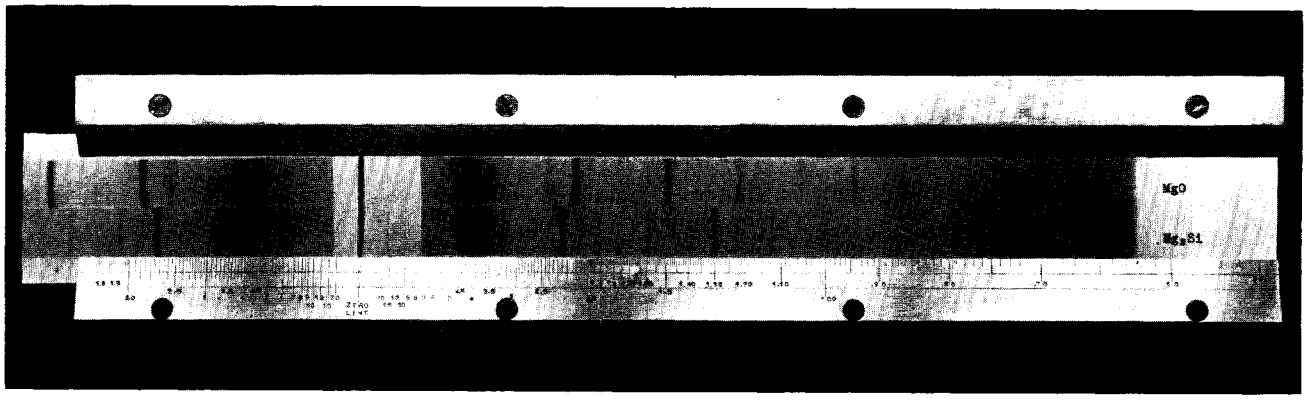

FIGURE 1. ANGSTROM SCALE WITH SYMMETRIC FILM

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		
												743	SiC (Cubic)	1.31	
	8.50– 8.00				4.00–3.90				2.50–2.45						
													1.50–1.45		
	8.00– 7.50				3.90–3.80				2.45–2.40			426	Fe_3O_4	1.62	
												979	$ZnFe_2O_4$	2.97	
	7.50– 7.00				3.80–3.70				2.40–2.35			527	$MgFe_2O_4$	2.95	
	7.00– 6.50				3.70–3.60				2.35–2.30				1.45–1.40		
								372	CuO	1.86					
	6.50– 6.00				3.60–3.50								1.40–1.35		
									2.30–2.25						
	6.00– 5.75				3.50–3.40								1.35–1.30		
									2.25–2.20						
	5.75– 5.50				3.40–3.30								1.30–1.25		
									2.20–2.15						
	5.50– 5.25				3.30–3.20								1.25–1.20		
									2.15–2.10						
	5.25– 5.00				3.20–3.10								1.20–1.15		
108	$Ba(NO_3)_2 \cdot H_2O$	3.48		897	SrO_2	2.00			2.10–2.05						
													1.15–1.10		
	5.00– 4.90				3.10–3.00				2.05–2.00						
													1.10–1.05		
	4.90– 4.80				3.00–2.95				2.00–1.95						
													1.05–1.00		
	4.80– 4.70				2.95–2.90				1.95–1.90						
855	$Na_2SnO_3 \cdot 3H_2O$	1.85											1.00– .90		
					2.90–2.85				1.90–1.85						
	4.70– 4.60												.90– .80		
					2.85–2.80				1.85–1.80						
	4.60– 4.50												.80–		
					2.80–2.75				1.80–1.75						

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	$Ba(NO_3)_2 \cdot H_2O$	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_2	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_2O_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	$FeCl_3$	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_3	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	$FeCl_3$	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	$Na_2C_5H_2O_3N_4.H_2O$	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	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				2.80–2.75				1.90–1.85		
								925	Sn	2.01					
	15.00–12.00				4.30–4.20			178	CaC_2 II	1.95			1.85–1.80		
				818	$NaIO_3$	3.19						779	NaN_3	2.42	
	12.00–10.00								2.75–2.70						
					4.20–4.10			801	Na_2CrO_4	4.09			1.80–1.75		
	10.00– 9.00											396	In_2O_3	1.52	
					4.10–4.00				2.70–2.65						
	9.00– 8.50			465	$Pb_3(PO_4)_2$	3.61							1.75–1.70		
									2.65–2.60						
	8.50– 8.00				4.00–3.90								1.70–1.65		
												303	CsCl	4.11	
	8.00– 7.50				3.90–3.80				2.60–2.55						
								795	$NaHCO_3$	3.48			1.65–1.60		
	7.50– 7.00				3.80–3.70				2.55–2.50						
				152	$CdCO_3$	1.83		918	Th	1.79			1.60–1.55		
	7.00– 6.50														
640	P_2S_5	4.90			3.70–3.60				2.50–2.45				1.55–1.50		
				93	$Ba(ClO_4)_2{\cdot}3H_2O$	2.14		685	$K_2C_2O_4$	2.32					
	6.50– 6.00												1.50–1.45		
600	$HgSO_4{\cdot}2HgO$	5.5			3.60–3.50				2.45–2.40						
													1.45–1.40		
	6.00– 5.75				3.50–3.40				2.40–2.35						
													1.40–1.35		
	5.75– 5.50				3.40–3.30				2.35–2.30						
				715	$C_{16}H_8O_2N_2(SO_3K)_2$	3.00							1.35–1.30		
	5.50– 5.25								2.30–2.25						
877	$Na_2S_2O_3{\cdot}5H_2O$	2.84			3.30–3.20								1.30–1.25		
				797	$NaClO_3$	1.76			2.25–2.20						
	5.25– 5.00												1.25–1.20		
					3.20–3.10				2.20–2.15						
	5.00– 4.90							782	$Na_2B_4O_7{\cdot}5H_2O$	4.40			1.20–1.15		
					3.10–3.00										
	4.90– 4.80								2.15–2.10				1.15–1.10		
					3.00–2.95										
	4.80– 4.70								2.10–2.05				1.10–1.05		
					2.95–2.90										
	4.70– 4.60								2.05–2.00				1.05–1.00		
					2.90–2.85										
	4.60– 4.50								2.00–1.95				1.00– .90		
					2.85–2.80										
	4.50– 4.40								1.95–1.90				.90– .80		
786	$(C_6H_4CO_2)_2$-BONa	3.45													
													.80–		

SUPPLEMENTARY GROUP INDEX 2.95–2.90

No.	Compound	1st line	2nd line	3rd line	No.	Compound	2nd line	1st line	3rd line	No.	Compound	3rd line	1st line	2nd line
640	P_2S_5	2.90	6.7	4.90	532	$Mg_3(PO_4)_2{\cdot}8H_2O$	2.94	6.7	2.69	697	$C_6H_4(CO)_2NK$	2.90	14.5	6.4
600	$HgSO_4{\cdot}2HgO$	2.92	6.2	5.5	561	$MnCl_2{\cdot}1H_2O$	2.93	5.7	2.55	129	$Bi(C_2H_3O_2)_3$	2.90	13.5	3.35
877	$Na_2S_2O_3{\cdot}5$ rd$_2$O	2.93	5.4	2.84	95	$BaCl_2{\cdot}2H_2O$	2.91	4.48	2.54	748	$AgC_2H_3O_2$	2.91	10.0	3.04
786	$(C_6H_4CO_2)_2BONa$	2.94	4.40	3.45	523	$Mg(NO_3)_2{\cdot}6H_2O$	2.93	4.42	3.29	98	$Ba(CN)_2$	2.94	9.4	3.37
818	$NaIO_3$	2.93	4.25	3.19	543	$MgSO_4{\cdot}6H_2O$	2.92	4.40	4.04	927	$SnCl_4{\cdot}5H_2O$	2.94	6.2	5.3
465	$Pb_3(PO_4)_2$	2.91	4.03	3.61	693	KH_2PO_4	2.90	3.72	1.95	326	$CoCl_2{\cdot}6H_2O$	2.94	5.6	4.85
152	$CdCO_3$	2.94	3.77	1.83	991	α-ZnS	2.91	3.29	1.76	377	$CuOH{\cdot}CuPO_4$	2.91	4.81	2.63
93	$Ba(ClO_4)_2{\cdot}3H_2O$	2.90	3.65	2.14	462	PbO	2.93	3.06	2.72	533	$MgNH_4PO_4{\cdot}6H_2O$	2.93	4.28	2.69
715	$C_{16}H_8O_2N_2(SO_3K)_2$	2.90	3.35	3.00	179	CaC_2 III	2.92	2.86	2.05	586	$HgCl_2{\cdot}3HgO$	2.92	3.95	2.70
797	$NaClO_3$	2.94	3.28	1.76	597	Hg_3PO_4	2.94	2.60	3.09	449	$PbHAsO_4$	2.93	3.39	3.17
925	Sn	2.91	2.79	2.01						707	$K_2S_2O_7$	2.90	3.23	3.07
178	CaC_2 II	2.93	2.79	1.95						755	Ag_2CrO_4	2.92	3.14	3.02
801	Na_2CrO_4	2.91	2.73	4.09						701	K_2SeO_3	2.94	3.08	4.35
795	$NaHCO_3$	2.94	2.58	3.49						49	$(NH_4)HC_2O_4{\cdot}H_2O$	2.90	3.00	6.2
918	Th	2.92	2.53	1.79						474	Li_2CO_3	2.91	2.80	4.16
685	$K_2C_2O_4$	2.92	2.46	2.32						853	$Na_2SiO_3{\cdot}9H_2O$	2.92	2.79	3.83
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										

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	I
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.

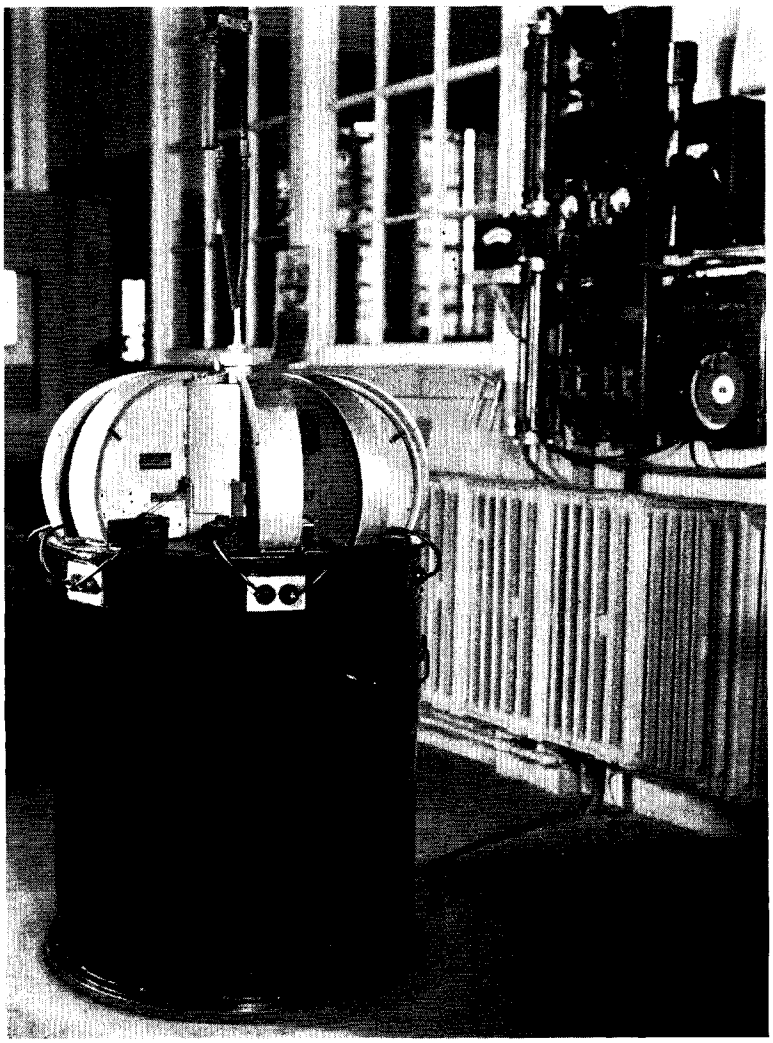

FIGURE 5. DIFFRACTION APPARATUS AND CONTROL BOARD

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.

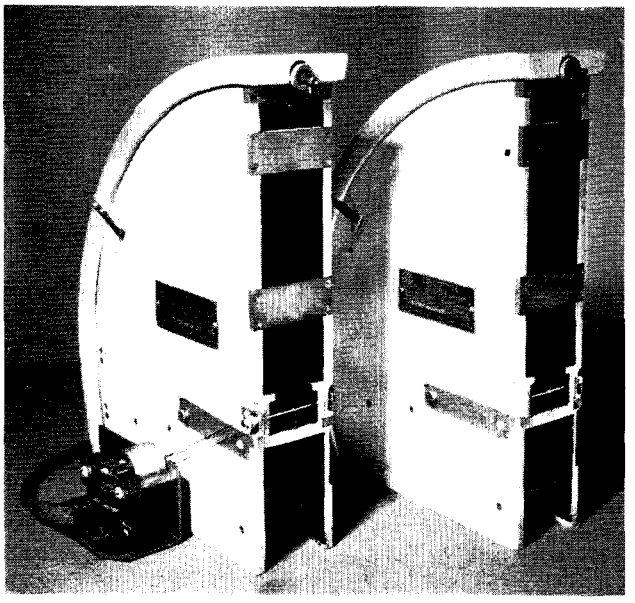

FIGURE 6. FILM CASSETTES WITH SPECIMEN TUBE AND ROTATING DEVICE

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

various ammonium compounds present; but the x-ray patterns showed that as many as six different ammonium compounds are present in the sand after using it awhile, and, by identifying them separately, showed what reactions were taking place and which agents were stable and which effective in inhibiting oxidation. By setting up standard mixtures with a range of concentrations of the various compounds involved—ammonium fluoride, ammonium acid fluoride, ammonium fluosilicate, ammonium borofluoride, ammonium chloride, ammonium sulfate, boric acid, and sulfur—it was possible to make a semiquantitative analysis on the basis of the relative intensities of the diffraction lines. The ability of the x-ray to recognize these compounds separately though mixed together was thus very valuable.

A point in connection with this problem which illustrates the fact that the x-ray pattern serves as a unique identification of a substance was that besides the compounds in the sand which were definitely identified, there occurred a substance giving a pattern which could not be identified. The substance was temporarily called *X*, and it was possible to determine the approximate per cent present in the sand and that it was effective in inhibiting oxidation even before it was isolated and identified by chemical methods. If the file and index of patterns had been available 5 years ago when this problem was investigated, the pattern *X* would have been identified immediately.

2. The analysis is conclusive, even though only minute amounts of material are available. This is especially valuable for corrosion products from small pits or surface attacks. Identification of small deposits and sediments can also be readily accomplished.

3. Substances are analyzed directly in their "as received" state and are not destroyed.

4. Different crystalline phases, states of oxidation or hydration, and physical state are observable. The ability to determine the degree of graphitization of carbon, or to distinguish quartz and cristobalite, or the high- and low-temperature forms of compounds—e. g., dicalcium silicate, etc.—is frequently important. The patterns of the various oxides of an element—e. g., ferrous oxide, ferric oxide, ferrosoferric oxide—are distinct from each other and, of course, from that of the element itself. The state of hydration of calcium chloride as a function of process and also as a function of position in the individual clusters of crystals can be determined, and in other cases the existence of water as water of crystallization can be detected.

5. As has been discussed rather fully in the present article, the process of preparing the specimen and obtaining the x-ray pattern is simple and economical.

6. A permanent record of the original data is always on file in the form of the diffraction pattern.

These features, which have been enumerated, are of obvious importance and would make x-ray diffraction valuable in many analysis problems, even though an easy method of indexing the patterns were not possible. However, the classification system greatly facilitates the use of x-rays in these cases and extends its field of application to include complete unknowns.

At the present stage of development, x-ray diffraction gives a qualitative or semiquantitative analysis. The accuracy possible varies widely in different cases, but in a favorable case allows a determination to within about 5 per cent of the amount present.

Future technical improvements will undoubtedly greatly increase the accuracy attainable as well as the scope of the x-ray diffraction method of analysis.

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RECEIVED March 23, 1938.

[Tables XI and XII follow, pages 467 to 512, inclusive]

TABLE XI. INDEX TO POWDER DIFFRACTION DATA FOR 1000 CHEMICAL SUBSTANCES

Pattern No.	Name	Formula
1	Aluminum	Al
2	bromide	$AlBr_3 \cdot 6H_2O$
3	carbide	Al_4C_3
4	chloride	Al_2Cl_6
5	chloride hexahydrate	$AlCl_3 \cdot 6H_2O$
6	sodium chloride	$AlNaCl_4$
7	fluoride	$AlF_3 \cdot 3\frac{1}{2}H_2O$
8	fluosilicate	$Al_2(SiF_6)_3$
9	iodide	AlI_3
10	nitrate nonahydrate	$Al(NO_3)_3 \cdot 9H_2O$
11	oxide	α-Al_2O_3
12	Diaspore	$AlHO_2$
13	Bauxite	$Al_2O_3 \cdot 2H_2O$
14	β-Alumina	$Na_2O \cdot 11Al_2O_3$
15	Aluminum silicate (sillimanite)	Al_2SiO_5
16	Muscovite (common mica)	$H_2KAl_3(SiO_4)_3$
17	Kaolin	$Al_2Si_2O_5(OH)_4$
18	Bentonite	
19	Aluminum sulfate	$Al_2(SO_4)_3$
20	sulfate octadecahydrate	$Al_2(SO_4)_3 \cdot 18H_2O$
21	ammonium sulfate (alum)	$AlNH_4(SO_4)_2 \cdot 12H_2O$
22	potassium sulfate (alum)	$AlK(SO_4)_2 \cdot 12H_2O$
23	sodium sulfate (alum)	$AlNa(SO_4)_2 \cdot 12H_2O$
24	sulfide	Al_2S_3
25	Ammonium acetate	CH_3COONH_4
26	arsenate trihydrate	$(NH_4)_3AsO_4 \cdot 3H_2O$
27	benzoate	$C_6H_5COONH_4$
28	borate	
29	bromide	NH_4Br
30	Ammonium carbamate	$NH_4CO_2NH_2$
31	carbonate	$(NH_4)_2CO_3 \cdot H_2O$
32	bicarbonate	$(NH_4)HCO_3$
33	perchlorate	NH_4ClO_4
34	chloride	NH_4Cl
35	chromate	$(NH_4)_2CrO_4$
36	bichromate	$(NH_4)_2Cr_2O_7$
37	citrate	$(NH_4)_3HC_6H_5O_7$
38	fluoride	NH_4F
39	borofluoride	NH_4BF_4
40	fluosilicate	$(NH_4)_2SiF_6$
41	formate	$HCOONH_4$
42	iodide	NH_4I
43	paramolybdate	$(NH_4)_6 \cdot Mo_7O_{24} \cdot 4H_2O$
44	phosphomolybdate trihydrate	$(NH_4)_3PO_4 \cdot 12MoO_3 \cdot 3H_2O$
45	nitrate (orthorhombic)	NH_4NO_3
46	nitrite	NH_4NO_2
47	nitrosophenylhydroxylamine	$C_6H_5N \cdot NO \cdot ONH_4$
48	oxalate monohydrate	$(NH_4)_2C_2O_4 \cdot H_2O$
49	oxalate, acid	$(NH_4)HC_2O_4 \cdot H_2O$
50	phenolsulfonate	$C_6H_4(OH)SO_3NH_4$
51	monohydrogen phosphate	$(NH_4)_2HPO_4$
52	dihydrogen phosphate	$(NH_4)H_2PO_4$
53	hypophosphite	$(NH_4)H_2PO_2$
54	picrate monohydrate	$C_6H_2(NO_2)_3 \cdot ONH_4 \cdot H_2O$
55	salicylate	$C_6H_4(OH)COONH_4$
56	succinate	$(CH_2COONH_4)_2$
57	sulfate	$(NH_4)_2SO_4$
58	persulfate	$(NH_4)_2S_2O_8$
59	hydrogen sulfate	NH_4HSO_4

(Continued on succeeding pages)

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	$BiO_2 \cdot C_{10}H_7$
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	hyp phosphite	$Ca(H_2PO_2)_2$
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)	α-Ca_2SiO_4
233	Dicalcium silicate (high)	β-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	$C_6H_3ClNO_2 \cdot NH_2$
257	Cinnamic acid	$C_6H_5CH:CHCOOH$
258	Citric acid	$H_3C_6H_5O_7 \cdot H_2O$

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	$C_{10}H_6OHSO_3H$
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)	$Co_3(AsO_4)_2\cdot 8H_2O$
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)	$Co(NH_3)_6Cl_3$
328	chloride (purpureo)	$Co(NH_3)_5Cl_3$
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)	$(CuOAs_2O_3)_3Cu(C_2H_3O_2)_2$
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)	$CuK_3(CN)_4$
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	$FeAl_3$
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	$Pb_3(SbO_4)_2$
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_3Al_2
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_3Hg
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	$(C_6H_5OHSO_3)_2Mg$
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_3
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	$20MoO_3 \cdot 2H_3PO_4 \cdot 48H_2O$

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	azide	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
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_2HAsO_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	$Na_3(B_3O_6)$
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	

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
1.168		0.07
1.011		0.02
0.928		0.04
0.905		0.04
0.826		0.01
0.778		0.01

2. $AlBr_3.6H_2O$

d		I/I1
7.8		0.29
6.8		0.29
6.2		0.14
4.80		0.14
3.84	(7)	1.00
3.59	(6)	0.86
3.38	(6)	0.86
2.96		0.29
2.63		0.14
2.51		0.14
2.38		0.57
2.29		0.14
2.22		0.43
2.13		0.71
2.01		0.43
1.85		0.43
1.78		0.14
1.69		0.14
1.55		0.29
1.480		0.14
1.440		0.29

3. Al_4C_3*

d		I/I1
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*

d		I/I1
5.8	(40)	0.64
5.1		0.14
2.93		0.40
2.80	(40)	0.64
2.46	(62.5)	1.00
1.92		0.14
1.77		0.20
1.71		0.64
1.64		0.11
1.472		0.32
1.402		0.24
1.279		0.06
1.226		0.10
1.173		0.03
1.110		0.20
1.085		0.16
1.024		0.05
0.993		0.08
0.967		0.10

5. $AlCl_3.6H_2O$

d		I/I1
6.0		0.17
5.2		0.20
3.89		0.13
3.69		0.27
3.41		0.11
3.29	(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
1.380		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. $AlF_3.3\frac{1}{2}H_2O$

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. $Al(NO_3)_3.9H_2O$

d		I/I1
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
1.288		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		0.08
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		0.03
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. $C_5H_5N.NO.ONH_4$

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. $C_6H_4(OH)SO_3NH_4$

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		0.05
2.00		0.27
1.77		0.03
1.68		0.03
1.60		0.05
1.54		0.03
1.473		0.04
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. $(NH_4)H_2PO_2$*

d		I/I1
5.7		0.30
3.97		0.33
3.75		0.33
3.27	(20)	0.67
3.14	(17.5)	0.58
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

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

(Starred patterns were checked with published crystal structure data

57. $(NH_4)_2SO_4$*

d		I/I1
5.2		0.20
4.36	(100)	1.00
3.91		0.20
3.12	(40)	0.40
3.03	(40)	0.40
2.67		0.07
2.51		0.07
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. $(NH_4)_2S_2O_8$*

d		I/I1
5.6	(10)	0.50
5.0		0.50
4.02		0.45
3.52	(15)	0.75
3.35	(20)	1.00
3.13		0.50
3.03		0.05
2.93		0.30
2.85		0.15
2.61		0.05
2.51		0.05
2.47		0.35
2.41		0.10
2.31		0.15
2.21		0.25
2.02		0.20
1.93		0.15
1.86		0.05
1.77		0.05
1.71		0.10
1.65		0.05
1.59		0.05
1.53		0.05

59. NH_4HSO_4

d		I/I1
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. $(NH_4)_2SO_3.H_2O$

d		I/I1
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. $(CHOH)_2(CO_2NH_4)_2$

d		I/I1
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

d		I/I1
9.0		0.10
6.3		0.10
5.3		0.10
4.15		0.60
3.66	(10)	1.00
3.41		0.20
3.31		0.60
3.11	(8)	0.80
2.99	(7)	0.70
2.93		0.70
2.72		0.50
2.60		0.40
2.47		0.10
2.42		0.40
2.33		0.10
2.22		0.10
2.08		0.20
1.99		0.10
1.91		0.10

63 $(NH_4)_2S_2O_3$

d		I/I1
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. $(NH_4)_2WO_4.nH_2O$

d		I/I1
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. $3(NH_4)_2O.P_2O_5.6WO_3.9H_2O$

d		I/I1
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

d		I/I1
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*

d		I/I1
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. $SbAsO_4$

d		I/I1
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

d		I/I1
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		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 $SbBr_3$

d		I/I1
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. $SbCl_3$

d		I/I1
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

d		I/I1
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

d		I/I1
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

d		I/I1
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*

d		I/I1
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_5

d		I/I1
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. $K_2S.Sb_2S_3$

d		I/I1
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. $Sb_2(SO_4)_3$

d		I/I1
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*

d		I/I1
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. $Sb_2(C_4H_4O_6)_3.6H_2O$

d		I/I1
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. $(SbO)KC_4H_4O_6.{}^1/_2H_2O$

d		I/I1
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

d		I/I1
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*

d		I/I1
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*

d		I/I1
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

d		I/I1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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. $Ba(ClO_3)_2$

d		I/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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		0.50
2.74		0.30
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/I_1
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/I_1
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		0.30
1.56		0.30
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		0.10
1.126		0.06
1.085		0.13
1.056		0.20

108. $Ba(NO_2)_2.H_2O$

d		I/I_1
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
1.429		0.15
1.385		0.13
1.335		0.13
1.305		0.05
1.278		0.05
1.252		0.10
1.215		0.05
1.180		0.08
1.150		0.05
1.120		0.10
1.096		0.08
1.066		0.05

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

(Starred patterns were checked with published crystal structure data)

109. BaC_2O_4

d		*I/I*1
8.5		0.40
7.7	(15)	0.60
4.81		0.60
4.40		0.16
3.80	(20)	0.80
3.41		0.60
3.20	(25)	1.00
3.10		0.40
2.83		0.04
2.65		0.24
2.53		0.32
2.41		0.24
2.29		0.24
2.20		0.24
2.10		0.32
1.95		0.28
1.87		0.12
1.82		0.08
1.64		9.04
1.54		0.16
1.50		0.08
1.430		0.04
1.380		0.08

110. BaO*

3.20	(20)	1.00
2.75	(17.5)	0.88
1.95	(15)	0.75
1.66		0.50
1.59		0.25
1.380		0.10
1.265		0.20
1.231		0.25
1.128		0.15
1.060		0.05
0.975		0.05
0.933		0.10
0.920		0.05

111. BaO_2*

3.37	(50)	1.00
2.68	(40)	0.80
2.11	(40)	0.80
1.95		0.50
1.89		0.30
1.65		0.80
1.443		0.08
1.360		0.40
1.282		0.16
1.250		0.16
1.200		0.10
1.137		0.16
1.108		0.08
1.063		0.16
1.045		0.08
0.980		0.04
0.958		0.06
0.930		0.02
0.915		0.04
0.879		0.02
0.828		0.02

112. $Ba(C_6H_4OH.SO_3)_2$

18.0	(30)	1.00
11.5	(30)	1.00
9.5		0.13
7.0		0.10
5.4		0.07
4.60		0.13
4.25	(10)	0.33
3.53		0.27
3.33		0.20
3.20		0.20
2.80		0.13
2.65		0.20
2.14		0.13
2.07		0.07
1.98		0.07
1.91		0.03
1.69		0.03

113. $Ba_3(PO_4)_2$

4.45	(17.5)	0.23
3.85		0.09
3.58	(75)	1.00
3.20		0.01
3.00		0.13
2.85		0.20
2.51	(30)	0.40
2.19		0.08
1.99		0.10
1.88		0.03
1.83		0.03
1.76		0.05
1.68		0.05
1.58		0.08
1.490		0.03
1.420		0.04
1.330		0.03
1.150		0.04

114. Barium Phosphite

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)	0.50
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. $Ba(H_2PO_2)_2.H_2O$

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		0.05
1.295		0.05
1.222		0.07
1.193		0.06
1.180		0.06
1.143		0.05
1.130		0.05

116. $BaSO_4$*

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*

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. $BaSO_3$

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. $BaC_4H_4O_6.H_2O$

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. $Ba(CNS)_2.2H_2O$

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. $BaS_2O_3.H_2O$

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

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. $Ba(C_4H_9CO_2)_2$

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*

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*

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. $BeSO_3$

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. $BeSO_4.4H_2O$

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*

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		0.27
1.327		0.13
1.180		0.03
1.135		0.10
1.089		0.07
1.073		0.07
1.045		0.03
1.020		0.03

129. $Bi(C_2H_3O_2)_3$

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. $Bi(C_6H_5COO)_3$

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

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. $Bi_2O_3.CO_2.H_2O$

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

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. $(BiO)_2CrO_4$

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

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. $Bi(OH)_3$

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. $Bi(C_6H_9O_8).7H_2O$

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		0.05
1.95		0.05

138. $BiO_2.C_{10}H_7$

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. $BiO.NO_3.H_2O$

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*/*I*$_1$
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. $Bi_2(C_2O_4)_3$

d		*I*/*I*$_1$
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

d		*I*/*I*$_1$
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. $Bi_2O_4.2H_2O$

d		*I*/*I*$_1$
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. $BiPO_4$

d		*I*/*I*$_1$
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. $Bi_2(C_6H_4OHCOO)_3$

d		*I*/*I*$_1$
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. $Bi_2(SO_4)_3$

d		*I*/*I*$_1$
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

d		*I*/*I*$_1$
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$_4$C

d		*I*/*I*$_1$
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*

d		*I*/*I*$_1$
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		0.10α_1
0.921		0.02α_1
0.863		0.04α_1
0.821		0.02α_1

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

d		*I*/*I*$_1$
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. $Cd(BrO_3)_2.H_2O$

d		*I*/*I*$_1$
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. $CdCO_3$*

d		*I*/*I*$_1$
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. $CdCl_2$*

d		*I*/*I*$_1$
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. $CdCl_2.2\frac{1}{2}H_2O$

d		*I*/*I*$_1$
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. $Cd(OH)_2$*

d		*I*/*I*$_1$
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. $2KI.CdI_2.2H_2O$

d		*I*/*I*$_1$
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. $Cd(NO_3)_2.4H_2O$

d		*I*/*I*$_1$
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*/*I*$_1$
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. $CdC_2O_4.3H_2O$

d		*I*/*I*$_1$
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*

d		*I*/*I*$_1$
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*/*I*$_1$
3.08	(17.5)	0.58
2.62	(30)	1.00
2.52		0.17
2.19		0.07
2.00		0.03
1.78		0.20
1.67	(12.5)	0.42
1.54		0.42
1.489		0.07
1.455		0.07
1.377		0.07
1.329		0.10
1.313		0.10
1.259		0.03
1.165		0.13
1.135		0.17

162. $Cd_3(PO_4)_2$

d		*I*/*I*$_1$
8.5	(4)	0.67
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		0.50

163. $Cd(C_6H_4OHCOO)_2.H_2O$

d		*I*/*I*$_1$
16.0	(75)	1.00
10.0		0.09
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		0.04
3.82	(20)	0.26
3.65		0.20
3.45		0.13
3.24		0.07
3.10		0.07
2.87		0.03
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. $3CdSO_4.8H_2O$

d		*I*/*I*$_1$
4.90	(40)	0.80
3.70		0.20
3.55	(50)	1.00
3.20		0.60
3.10		0.16
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		0.16
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. $CdWO_4$

d		*I*/*I*$_1$
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

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

(Starred patterns were checked with published crystal structure data)

d		I/I_1
166. Ca*		
3.21	(40)	1.00
2.80	(12.5)	0.30
1.97	(8)	0.20
1.68		0.20
1.61		0.10
1.28		0.05
1.246		0.03
1.138		0.05
167. $Ca(C_2H_3O_2)_2$		
11.0	(50)	1.00
8.5	(10)	0.20
6.7		0.06
5.9		0.12
5.5		0.10
3.80		0.08
3.58		0.08
3.34	(25)	0.50
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. $Ca(C_2H_3O_2)_2.H_2O$		
10.0	(75)	1.00
6.7		0.11
6.0	(10)	0.13
5.2		0.05
4.10		0.08
3.78		0.08
3.61		0.01
3.28	(40)	0.53
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)		
3.09		0.18
2.83	(30)	0.60
2.70	(50)	1.00
2.42		0.04
2.33		0.02
2.25		0.02
2.18	(30)	0.60
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. $3CaO.Al_2O_3$*		
4.08		0.20
3.30		0.04
2.68	(25)	1.00
2.39		0.04
2.19		0.08
2.03		0.04
1.90	(6)	0.24
1.55	(6)	0.24
1.342		0.12
1.203		0.08
1.015		0.04
171. $5CaO.3Al_2O_3$*		
4.95	(20)	0.67
3.19		0.20
3.01		0.23
2.68	(30)	1.00
2.44	(15)	0.50
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. $Ca_3(AsO_4)_2$		
8.7		0.16
6.0		0.04
5.5		0.04
4.90		0.04
4.01		0.40
3.51	(12.5)	0.50
3.22		0.04
3.05		0.20
2.90	(25)	1.00
2.82	(20)	0.80
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		
9.0		0.48
4.97		0.32
4.49	(8)	0.64
3.54		0.16
3.05	(12.5)	1.00
2.85		0.40
2.65	(7)	0.56
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. $Ca(C_6H_5CO_2)_2.3H_2O$		
6.4		0.07
5.8		0.13
5.3	(7)	0.47
4.41		0.33
4.22	(12.5)	0.83
3.98		0.07
3.48	(15)	1.00
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		
5.8		0.07
3.40	(12.5)	0.42
3.04	(30)	1.00
2.90		0.23
2.76		0.07
2.62		0.33
2.25		0.07
2.14	(12.5)	0.42
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. $CaBr_2.6H_2O$*		
4.03	(25)	1.00
3.49	(12.5)	0.50
2.85		0.50
2.65		0.50
2.34		0.50
2.21	(15)	0.60
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*		
3.32		0.25
3.18	(20)	0.50
2.74	(40)	1.00
2.08	(17.5)	0.44
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*		
3.49		0.20
3.32		0.16
3.17		0.16
2.93	(62.5)	1.00
2.79	(25)	0.40
2.28		0.14
2.09		0.24
2.06		0.16
2.00		0.13
1.95	(17.5)	0.28
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		
3.52		0.60
3.20		0.10
2.92	(8)	0.80
2.86	(10)	1.00
2.27		0.40
2.15		0.20
2.05	(8)	0.80
1.93		0.60
1.78		0.60
180. $CaCO_3$*		
3.86		0.08
3.04	(125)	1.00
2.49		0.20
2.28	(30)	0.24
2.09		0.20
1.92	(40)	0.32
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. $Ca(ClO_3)_2.2H_2O$		
6.0		0.30
5.6		0.12
5.4		0.12
4.68		0.14
4.30	(25)	0.50
3.62		0.06
3.30		0.10
3.05	(30)	0.60
2.94		0.12
2.80	(50)	1.00
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. $CaCl_2$*		
4.49	(25)	1.00
3.46		0.16
3.05	(20)	0.80
2.85		0.32
2.33	(15)	0.60
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. $CaCl_2.H_2O$		
5.9	(10)	0.40
4.38		0.12
3.41		0.12
3.22		0.24
3.03		0.40
2.81		0.24
2.55	(25)	1.00
2.40		0.24
2.26	(15)	0.60
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. $CaCl_2.2H_2O$		
6.1		0.40
4.34		0.50
3.05	(17.5)	0.70
2.82	(25)	1.00
2.68		0.16
2.51		0.20
2.35		0.20
2.26		0.16
2.16		0.24
2.12	(15)	0.60
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. $CaCl_2.4H_2O$		
6.0		0.27
5.2		0.20
4.70	(12.5)	0.42
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	(30)	1.00
2.39		0.42
2.22	(20)	0.67
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. $CaCl_2.6H_2O$		
6.9		0.15
3.93	(30)	0.75
3.41		0.31
2.78	(25)	0.63
2.58		0.50
2.27		0.50
2.16	(40)	1.00
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. $CaCl_2.CaF_2$		
6.8		0.04
3.39		0.08
3.18		0.02
2.75	(25)	0.50
2.56	(50)	1.00
2.14		0.40
1.94	(25)	0.50
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. $Ca(ClO)_2.4H_2O$		
4.95		0.25
3.18	(25)	0.63
2.47		0.05
2.36	(40)	1.00
1.93	(20)	0.50
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. $CaCrO_4$*		
4.80		0.06
3.63	(100)	1.00
2.90		0.15
2.70	(75)	0.75
2.57		0.15
2.39		0.20
2.27		0.08
1.86	(75)	0.75
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. $CaCrO_4.2H_2O$		
8.0	(15)	0.50
4.30	(30)	1.00
4.02		0.07
3.90		0.07
3.66		0.23
3.11	(20)	0.67
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. $CaCr_2O_7$		
7.0	(9)	0.60
6.4		0.07
5.3		0.27
4.98		0.27
4.20		0.07
4.08		0.07
3.90	(15)	1.00
3.73		0.53
3.50	(12.5)	0.83
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. $Ca_3(C_6H_5O_7)_2.4H_2O$		
15.3	(6)	1.00
3.95	(4)	0.67
3.09	(4)	0.67
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. $CaCN_2$		
4.90	(4)	0.40
3.36		0.20
3.03	(10)	1.00
2.62	(8)	0.80
2.50		0.10
2.29		0.10
2.08		0.10
1.92		0.40
1.87		0.10
1.79		0.10
1.68		0.10
1.59		0.10

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/I*₁
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. $CaSiF_6.2H_2O$

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. $Ca(CH_2OHCOO)_2$

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. $Ca(CH_2OHCOO)_2.3H_2O$

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. $Ca(CH_2OHCOO)_2.3^1/_2H_2O$

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		0.10
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. $Ca(IO_3)_2$

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. $Ca(NO_3)_2$*

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. $Ca(NO_2)_2.H_2O$

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*

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

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

(Starred patterns were checked with published crystal structure data)

219. $Ca(H_2PO_4)_2$*

d		I/I1
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
2.96		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/I1
12.0	(15)	0.75
5.6		0.20
4.95		0.40
3.88	(20)	1.00
3.69	(15)	0.75
3.36		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/I1
6.6		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
1.063		0.03
1.038		0.07
1.018		0.05

222. $Ca_3(PO_4)_2.H_2O$

d		I/I1
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/I1
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. $CaO_2.PO.OC_6H_5(OH)_2$

d		I/I1
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/I1
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/I1
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_2P_2

d		I/I1
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
1.450		0.20
1.315		0.05
1.285		0.05
1.110		0.05

228. $Ca_3H_2PO_2$

d		I/I1
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_2NaHPO_4

d		I/I1
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/I1
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/I1
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/I1
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/I1
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/I1
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/I1
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/I1
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. $CaSO_4.\frac{1}{2}H_2O$

d		I/I1
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/I1
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/I1
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. $CaSO_4$

d		I/I1
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. $CaC_4H_4O_6.4H_2O$

d		I/I1
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. $CaC_6H_2O_3N_4$

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. $C_6H_3ClNO_2.NH_2$

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. $H_3C_6H_5O_7.H_2O$

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. $C_9H_8O_2$

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. $(C_6H_5)_2SO$

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. $C_2H_5NH_3Cl$

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_2NH_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. $CH_2OHCOOH$

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		0.13
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_2I_2

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		0.04
1.385		0.08
1.355		0.06
1.326		0.04
1.275		0.06
1.240		0.06
1.200		0.06

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

(Starred patterns were checked with published crystal structure data)

272. C_6H_4IOH

d		*I/I*$_1$
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
4.27		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. $C_{10}H_7OH$

d		*I/I*$_1$
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		0.06
1.84		0.06
1.76		0.06

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		0.13
2.34		0.33
2.24		0.33
2.18		0.13
2.06		0.27
1.95		0.07
1.90		0.13
1.80		0.13
1.74		0.07
1.69		0.20
1.64		0.07

288. $(CH_3)_2C(SO_2C_2H_5)_2$

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. $C_4H_6O_6.H_2O$

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. $C_6H_2Br_4$-(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. $C_6H_2Cl_3.CH_2CN$

d		*I/I*
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. $C_2H_5CH_3C{:}(SO_2C_2H_5)_2$

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. $Ce(NO_3)_3.6H_2O$

d		*I/I*
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
1.450		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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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
1.357		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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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		0.06α;

316. CrO_3*

d		I/I_1
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
1.47[0]		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/I_1
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/I_1
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/I_1
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		0.08
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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/I_1
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. $Co(NH_3)_6Cl_3$

d		I/I_1
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		0.02
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. $Co(NH_3)_5Cl_3$

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. $CoCrO_4$

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. $Co(OH)_2$

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)$_2O_4$; 2Co:Mn*

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. $Co(NO_3)_2.6H_2O$

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*

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. $CoCo_2O_4$*

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. $Co_3(PO_4)_2.8H_2O$

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)

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. $CoSO_4(NH_4)_2SO_4.6H_2O$

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*

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*

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. $(CuOAs_2O_3)_3$-$Cu(C_2H_3O_2)_2$

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. $CuAl_2O_4$*

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. $Cu(C_6H_5COO)_2.2H_2O$

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)

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)

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*

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. $CuBr_2$

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. $2CuCO_3.Cu(OH)_2$

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. $CuCO_3.Cu(OH)_2$

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*

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. $CuCl_2$

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. $CuCl_2.2H_2O$*

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. $CuCl_2.2NH_4Cl.2H_2O$

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. $CuCl_2.2KCl.2H_2O$

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. $CuCrO_4.2CuO.2H_2O$

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)

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. $2Cu_2C_6H_5O_7.5H_2O$

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
1.78		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. $Cu(NO_3)_2.3H_2O$

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. $CuFeS_2$*

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/I*1
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/I*1
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/I*1
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/I*1
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
4.36		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/I*1
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/I*1
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/I*1
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/I*1
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/I*1
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/I*1
2.72	(62.5)	1.00
2.46		0.25
2.29	(25)	0.40
1.68	(20)	0.30
1.62		0.15
1.462		0.20
1.395		0.30
1.355		0.15
1.144		0.02
1.088		0.10
1.055		0.02
1.040		0.02
1.025		0.02
0.980		0.02
0.948		0.06
0.905		0.02
0.888		0.02

395. $InCl_3$

d		*I/I*1
5.8	(62.5)	1.00
5.3		0.13
5.0		0.20
4.50		0.24
4.01		0.24
3.82		0.06
3.58		0.32
3.41		0.10
3.00	(25)	0.40
2.84		0.32
2.68		0.10
2.55	(30)	0.48
2.44		0.10
2.32		0.24
2.23		0.13
2.10		0.03
2.05		0.16
2.00		0.13
1.92		0.10
1.84		0.24
1.76		0.08
1.63		0.11
1.59		0.03
1.51		0.03
1.475		0.03
1.445		0.06
1.390		0.06
1.328		0.06

396. In_2O_3*

d		*I/I*1
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/I*1
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/I*1
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/I*1
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/I*1
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/I*1
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/I*1
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/I*1
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_5

d		*I/I*1
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. $Fe_3(AsO_4)_2.6H_2O$

d		*I/I*1
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. $Fe[(CH_3)_2AsO_2]_3$

d		*I/I*1
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		0.07

407. $FeCl_3$

d		*I/I*1
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. $FeCl_3.6H_2O$

d		*I/I*1
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. $FeCl_2.2H_2O$

d		*I/I*1
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
1.76		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. $Fe(HCO_2)_3.H_2O$

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. $Fe(C_3H_5O_3)_2.3H_2O$

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. $Fe(NO_2)_3.9H_2O$

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. $(NH_4)_3Fe(C_2O_4)_3$

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. $K_3Fe(C_2O_4)_3.3H_2O$

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. $2Na_3Fe(C_2O_4)_3.9H_2O$

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. $(C_6H_7OHSO_3)_3.Fe$

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		0.08
1.208		0.17
1.102		0.11
1.070		0.06
1.043		0.11

430. $Fe(H_2PO_2)_3$

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)	0.67
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		0.03
1.480		0.07
1.441		0.07
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. $FeC_4H_3O_6$

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

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

(Starred patterns were checked with published crystal structure data)

483. LiI.3H$_2$O*

d		*I*/*I*$_1$
6.4		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$_3$H$_5$O$_3$

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$_3$*

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$_2$C$_2$O$_4$

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$_6$H$_4$OH.COO)

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$_2$SO$_4$*

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$_2$SO$_4$.H$_2$O*

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$_2$C$_4$H$_4$O$_6$.H$_2$O

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$_4$H$_4$O$_6$

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*

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		0.03
1.225		0.03
1.180		0.03
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$_2$H$_3$O$_2$)$_2$

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		0.05
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$_2$H$_3$O$_2$)$_2$.4H$_2$O

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$_2$Al$_3$

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
1.030		0.03
0.972		0.03
0.928		0.01

496. Mg$_3$Al$_2$*

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$_2$O$_4$*

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
1.158		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$_2$O

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$_6$H$_5$COO)$_2$.3H$_2$O

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

7.7		0.12
6.1		0.16
5.3		0.08
4.29		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$_2$O

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$_2$Ca

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$_2$C$_3$*

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$_2$O*

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$_2$O*

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$_3$*

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
1.468		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)

507. $Mg(ClO_4)_2$

d		I/I1
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. $Mg(ClO_4)_2.3H_2O$

d		I/I1
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. $Mg(ClO_4)_2.6H_2O$

d		I/I1
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. $MgCl_2$*

d		I/I1
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. $MgCl_2.6H_2O$*

d		I/I1
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. $MgCl_2.NH_4Cl.6H_2O$

d		I/I1
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. $MgCrO_4.7H_2O$

d		I/I1
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. $Mg_3(C_6H_5O_7)_2.14H_2O$

d		I/I1
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*

d		I/I1
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. $MgSiF_6.6H_2O$

d		I/I1
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. $Mg(CHO_2)_2.2H_2O$

d		I/I1
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. $Mg(OH)_2$*

d		I/I1
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. $MgI_2.8H_2O$

d		I/I1
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. $Mg(C_3H_3O_3)_2.3H_2O$

d		I/I1
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_2Pb*

d		I/I1
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_3Hg

d		I/I1
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. $Mg(NO_3)_2.6H_2O$

d		I/I1
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*

d		I/I1
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. $MgC_2O_4.2H_2O$

d		I/I1
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
1.280		0.03

526. MgO*

d		I/I1
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. $MgFe_2O_4$*

d		I/I1
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. $(C_6H_{11}OHSO_3)_2Mg$

d		I/I1
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. $MgHPO_4.3H_2O$

d		I/I1
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. $Mg(H_2PO_4)_2$

d		I/I1
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. $Mg_3(PO_4)_2.4H_2O$

d		I/I1
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. $Mg_3(PO_4)_2.8H_2O$

d		I/I1
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
2.20		0.08
2.05		0.08
1.66		0.08
1.57		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/I*$_1$
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		0.04
2.07		0.08
2.02		0.04
1.97		0.12
1.88		0.04
1.81		0.12
1.74		0.12

534. $Mg_2P_2O_7$

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. $Mg(H_2PO_2)_2.6H_2O$

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

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. $MgSiO_3$*

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*

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. $3MgO.2SiO_2.2H_2O$

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		0.08
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*

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		0.05
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. $MgSO_3$

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. $MgSO_4.H_2O$

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. $MgSO_4.6H_2O$

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. $MgSO_4.7H_2O$*

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

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*

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. $MgSO_3.6H_2O$*

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. $MgC_4H_2O_4.5H_2O$

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. $MgS_2O_3.6H_2O$

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*

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. $MgC_5H_2N_4O_3$

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

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*

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*

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. $Mn(C_2H_3O_2)_2.4H_2O$

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. $MnAl_2O_4$*

2.92		0.17
2.49	(3)	0.50
2.39	(3)	0.50
1.398	(6)	1.00

557. $Mn(C_5H_8COO)_2.3H_2O$

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

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		0.66
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. $MnC_4H_4O_6$

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. $Hg(C_6H_5COO)_2$

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

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_3PO_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
4.38		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		0.06
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)

609. MoO_3*

d		I/I1
6.9		0.24
3.80	(75)	0.60
3.46	(50)	0.40
3.25	(125)	1.00
3.00		0.06
2.66		0.32
2.52		0.08
2.30		0.32
2.26		0.06
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_2O_3

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
2.26	(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

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
4.28		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

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

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	(20)	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
1.91		0.18
1.88		0.44
1.76		0.20
1.70		0.15
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

623. Nickel Fluoride

4.85	(50)	1.00
3.78	(25)	0.50
3.11		0.04
2.98	(25)	0.30
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

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		0.03
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		0.02
1.035		0.02B

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/I*₁
8.5		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
1.72		0.04
1.70		0.02
1.65		0.02
1.61		0.04

632. $NiSO_4.(NH_4)_2SO_4.6H_2O$

d		*I/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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
1.56		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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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/I*₁
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. $K(C_6H_5COO).3H_2O$

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. $K_3C_6H_5O_7.H_2O$

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
1.86		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		0.02
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

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
3.22	(50)	1.00
2.95	(40)	0.80
2.86		0.40
2.56		0.30
2.19		0.60
2.03		0.02
1.93		0.04
1.84		0.20
1.74		0.10
1.68		0.08
1.60		0.06
1.54		0.02
1.51		0.02
1.480		0.04
1.450		0.04α_1
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
3.80		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
2.66	(7)	0.28
2.19		0.24
2.06		0.08
1.96		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
2.50	(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		0.13
0.964		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*

d		I/I1
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. $KHSO_4$

d		I/I1
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. $K_2S_2O_8$

d		I/I1
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. $K_2S_2O_7$

d		I/I1
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. $KC_2H_5SO_4$

d		I/I1
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. $2KCH_3SO_4.H_2O$

d		I/I1
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. $K_2SO_3.2H_2O$

d		I/I1
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. $KHSO_3$

d		I/I1
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. $K_2S_2O_5$

d		I/I1
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. $C_6H_5SO_3K$

d		I/I1
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

d		I/I1
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

d		I/I1
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-$CH_3C_6H_4SO_3K$

d		I/I1
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. $K_2C_4H_4O_6$

d		I/I1
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. $K(NH_4)C_4H_4O_6$

d		I/I1
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. $KH(C_4H_4O_6)$

d		I/I1
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

d		I/I1
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

d		I/I1
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. $K_2S_2O_3$

d		I/I1
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. $3K_2S_2O_3.H_2O$

d		I/I1
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*

d		I/I1
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

d		I/I1
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. $K_2WO_4.2H_2O$

d		I/I1
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		0.06
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

d		I/I1
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		0.25

728. $KHC_5H_2N_4O_3$

d		I/I1
4.70	(4)	1.00
3.79	(4)	1.00
3.42	(3)	0.75
3.23		0.75
2.90		0.50
2.55		0.50
2.02		0.25
1.77		0.25
1.70		0.25

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
2.95		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		0.10α_1
0.884		0.02
0.867		0.20α_1
0.839		0.10α_1
0.818		0.04α_1
0.803		0.06α_1
0.790		0.02
0.780		0.04α_1
0.751		0.15α_1
0.733		0.06α_1
0.691		0.04α_1
0.682		0.04
0.677		0.04α_1

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		0.04α_1
0.724		0.06α_1
0.705		0.04α_1

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		0.08α_1
0.915		0.05α_1
0.834		0.03α_1
0.786		0.04α_1
0.691		0.03α_1

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		0.02α_1
0.913		0.02α_1
0.871		0.02α_1

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. $Ag_3C_6H_6O_7$

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		0.03
1.461		0.07
1.385		0.05
1.361		0.03
1.320		0.07
1.292		0.04
1.192		0.04

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

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

(Starred patterns were checked with published crystal structure data)

778. Sodium Asparaginate

d		*I/I*1
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		0.03
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. $Na_3(B_3O_6)$*

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. $(CH_3)_2AsO.ONa.3H_2O$

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. $NaClO_3.H_2O$

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
2.75		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

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. $2Na_2C_6H_5O_7.-11H_2O$

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
2.21		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. $NaHCO_3$

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		0.03
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		0.56
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

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

(Starred patterns were checked with published crystal structure data)

830. Na_2O_2

d		*I/I*₁
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-$C_6H_4OHSO_3Na.2H_2O$

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

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

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

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

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. $Na_2HPO_4.2H_2O$

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. $Na_2HPO_4.12H_2O$

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		0.25
1.82		0.20
1.70		0.35
1.65		0.10

838. NaH_2PO_4

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. $NaH_2PO_4.H_2O$

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. $Na_4P_2O_6.10H_2O$

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. $NaPO_3$

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. $Na_4P_2O_7$

4.40	(40)	1.00
3.88		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. $Na_4P_2O_7.10H_2O$

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. $NaNH_4HPO_4.4H_2O$

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

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. $Na_2HPO_4.5H_2O$

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. $NaH_2PO_2.H_2O$

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. $Na_2PbO_2.3H_2O$

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. $Na(C_6H_4OHCOO)$

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

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
2.42		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

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. $NaAlSi_3O_8$

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		0.08
1.82		0.20
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
1.76		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. $C_{14}H_7O_2SO_3Na$

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. $C_{10}H_7SO_3Na$

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. $C_{10}H_6(SO_3Na)_2$

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

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

(Starred patterns were checked with published crystal structure data)

874. Na_2TeO_3

d		*I/I*₁
6.0	(25)	1.00
5.0		0.32
4.45		0.16
4.27	(15)	0.60
4.10		0.40
3.75		0.24
3.42		0.40
3.23		0.32
3.09		0.08
2.97		0.16
2.82	(12.5)	0.50
2.46		0.24
2.42		0.50
2.35		0.04
2.29		0.04
2.23		0.04
2.16		0.08
2.01		0.12
1.94		0.08
1.79		0.04
1.75		0.28
1.72		0.32
1.61		0.12
1.56		0.12
1.53		0.08
1.470		0.08
1.410		0.04

875. NaCNS

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
2.28		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. $Na_2S_2O_3$

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. $Na_2S_2O_3.5H_2O$

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. $Na_2WO_4.2H_2O$

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. $Na_2C_6H_2O_3N_4.H_2O$

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. $NaVO_3.H_2O$

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. $Na_3VO_4.16H_2O$

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*

3.50	(5)	1.00
3.03	(3)	0.60
2.14		0.20
1.83	(5)	1.00
1.74		0.20

883. $Sr(C_2H_3O_2)_2.1/2H_2O$

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. $SrBr_2.6H_2O$*

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		0.05

885. $SrCO_3$*

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. $Sr(ClO_3)_2.8H_2O$

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. $SrCl_2.6H_2O$*

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. $SrCrO_4$

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. $Sr(HCO_2)_2$

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. $Sr(HCO_2)_2.2H_2O$

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*

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. $Sr(OH)_2.8H_2O$*

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. $SrI_2.6H_2O$

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. $Sr(C_3H_5O_3)_2.3H_2O$

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. $Sr(NO_3)_2$*

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. $SrC_2O_4.H_2O$

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*

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/I*₁
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. $Sr(C_7H_5O_3)_2.2H_2O$

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. $SrSO_4$*

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. $SrC_4H_4O_6.4H_2O$

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

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*

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. $KTaF_6$

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

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*

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. $TeCl_2$

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

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. $4TeO_2.N_2O_5.1\frac{1}{2}H_2O$

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
1.259		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)

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

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. $Te(OH)_6$*

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*

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*

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. $Tl(NO_3)_3.3H_2O$

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*

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

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*

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

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. $ThCl_4$

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. $Th(NO_3)_4.12H_2O$

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. $Th(C_2O_4)_2$

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*

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. $Th(SO_4)_2$

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*

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*

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. $SnCl_4.5H_2O$

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. $(NH_4)_2SnCl_6$*

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. $SnCl_2.2H_2O$

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*

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

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*

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*

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. $Sn_3(PO_4)_2$

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. $Sn(SO_4)_2.2H_2O$

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. $SnSO_4$

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*

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*

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. $SnC_4H_4O_6$

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*

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*

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

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)

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)

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*

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. $H_2W_4O_{13}$

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

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. $UO_2(C_2H_3O_2)_2.2H_2O$

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. $UO_2(NO_3)_2.6H_2O$*

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*

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*

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

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*

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_3*

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. $(VO)_2(SO_4)_2.16H_2O$

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		0.03

957. $Y(NO_3)_3.6H_2O$

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*

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*

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. $Zn(C_2H_3O_2)_2$

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. $Zn(C_2H_3O_2)_2.2H_2O$

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. $ZnAl_2O_4$*

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. $Zn_3(AsO_4)_2.8H_2O$

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

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. $Zn(C_6H_5COO)_2$

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. $Zn(ClO_4)_2.6H_2O$

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)

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. $ZnCrO_4$

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		0.05
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. $Zn(CN)_2$

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

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

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/I*1
5.4	(17.5)	0.88
4.51		0.35
4.08	(20)	1.00
3.64	(8)	0.40
3.11		0.30
3.00		0.05
2.70		0.20
2.54		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
1.56		0.05
1.480		0.05

972. ZnF_2*

3.33	(62.5)	1.00
2.60	(50)	0.80
2.35		0.06
2.27		0.20
2.10		0.05
1.75	(50)	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		0.05
1.112		0.02
1.075		0.06

973. $ZnF_2.4H_2O$

4.87	(30)	1.00
4.10	(12.5)	0.42
3.78		0.03
3.57		0.03
3.33		0.20
3.15		0.20
2.99	(9)	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

974. ZnI_2

6.5	(7)	0.28B
5.7		0.20B
4.5		0.12
3.98		0.12
3.49	(25)	1.00
3.06		0.08
2.93		0.04
2.75		0.04
2.17		0.16
2.11	(7)	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

975. $Zn(C_3H_5O_3)_2.3H_2O$

9.1	(30)	1.00
6.8		0.03
4.43	(2)	0.07
4.12		0.03
3.32		0.03
3.19		0.07
2.98		0.03
2.72	(3)	0.10
2.58		0.03
2.24		0.07
2.03		0.03
1.69		0.03
1.58		0.03

976. $ZnC_2O_4.2H_2O$

4.73	(75)	1.00
3.93	(12.5)	0.17
3.58		0.17
2.95	25)	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

977. ZnO*

2.81	(25)	0.50
2.61	(15)	0.30
2.46	(50)	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

978. $ZnCo_2O_4$

4.65		0.08
2.84	(30)	0.40
2.43	(75)	1.00
2.32		0.07
2.01		0.17
1.65		0.11
1.55	(30)	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

979. $ZnFe_2O_4$*

2.97	(12.5)	0.25
2.53	(50)	1.00
2.42		0.02
2.10		0.12
1.71		0.08
1.61		0.25
1.484	(15)	0.30
1.327		0.02
1.282		0.02
1.122		0.02
1.093		0.08
1.049		0.02
0.969		0.04

980. $Zn(MnO_4)_2.6H_2O$

5.2		0.05
4.16	(20)	0.67
3.93	(30)	1.00
3.15		0.03
2.85	(20)	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

981. $Zn(C_6H_4OHSO_3)_2.8H_2O$

13.7		0.50
12.3		0.10
5.7		0.30
5.3		0.20
5.1		0.20
4.80	(20)	1.00
4.66	(20)	1.00
4.31		0.40
3.98	(15)	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

982. Zinc Phosphate

13.4		0.32
7.7	(8)	0.64
6.7		0.16
5.8		0.32
4.34		0.32
3.81		0.40
3.61	(8)	0.64
3.45		0.08
3.32		0.08
3.20		0.08
3.11		0.16
2.85	(12.5)	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

983. $Zn_3(PO_4)_2.4H_2O$

9.1	(20)	0.40
5.3		0.08
5.1		0.06
4.86		0.12
4.59		0.25
4.40		0.25
4.01		0.20
3.65		0.08
3.47	(20)	0.40
3.40		0.40
3.13		0.08
2.85	(50)	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

984. $ZnHPO_3.2^1/_2H_2O$

7.7		0.20
6.3		0.13
5.9		0.13
5.3		0.20
4.38	(10)	0.25
4.18	(40)	1.00
3.77	(25)	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

985. $Zn(H_2PO_2)_2.H_2O$

7.5	(25)	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	(12.5)	0.50
2.60	(12.5)	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
1.78		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

986. $Zn(C_6H_4OHCOO)_2.3H_2O$

9.3	(25)	1.00
7.8		0.20
5.78	(25)	1.00
5.1		0.16
4.48		0.60
4.08		0.24
3.89		0.24
3.68		0.08
3.43	(25)	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

987. $ZnSO_4.H_2O$

4.80	(40)	0.64
3.80		0.11
3.40	(62.5)	1.00
3.06	(25)	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

988. $ZnSO_4.7H_2O$

5.3	(30)	0.60
4.50		0.16
4.20	(50)	1.00
3.92		0.12
3.76		0.20
3.44	(15)	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

989. $ZnSO_4(NH_4)_2SO_4.6H_2O$

8.8		0.03
7.8		0.07
6.1		0.13
5.4		0.20
5.1		0.03
4.20	(30)	1.00
3.78	(20)	0.67
3.62		0.03
3.41		0.13
3.13		0.03
3.03	(10)	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

990. $ZnSO_4.K_2SO_4.6H_2O$

7.1		0.03
6.2		0.20
5.4		0.10
5.2		0.07
4.4		0.13
4.14	(30)	1.00
3.68	(30)	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	15)	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

991. α-ZnS*

3.29	(15)	1.00
3.11		0.47
2.91	(15)	1.00
2.27		0.47
1.90		0.83
1.76	(15)	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

992. β-ZnS*

3.12	(40)	1.00
2.69		0.05
1.91	(30)	0.75
1.63	(20)	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

993. $ZnSO_3.2^1/_2H_2O$

7.7	(40)	1.00
5.8		0.25
4.78		0.10
4.55		0.10
4.25		0.03
3.81	(8)	0.20
3.50	(8)	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

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

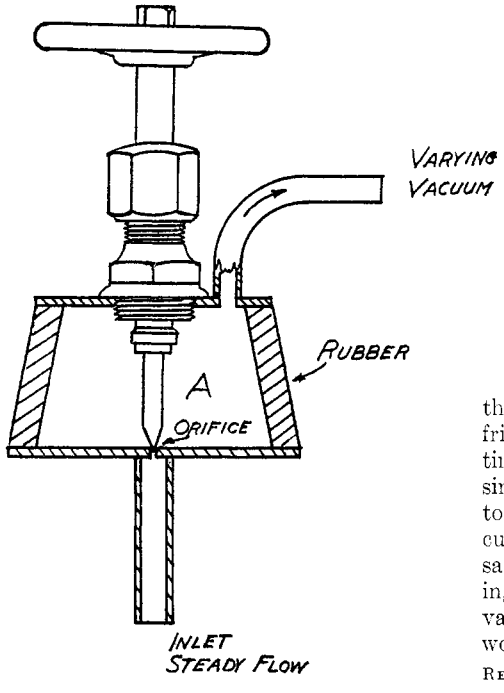
(Starred patterns were checked with published crystal structure data)

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. $(CH_3CH_2CH_2-CH_2COO)_2Zn.2H_2O$				**995. Zr***		**997. $Zr(NO_3)_4.5H_2O$**			**998. ZrO_2* (Monoclinic)**			**999. $ZrSiO_4$***			**1000. Zirconyl Sulfate**		
			2.78	(12.5)	0.31	9.6	(40)	1.00				4.43		0.50	6.5	(8)	0.40
12.5	(62.5)	1.00	2.56	(8)	0.20	6.9	(40)	1.00	5.1		0.05	3.29	(100)	1.00	4.92		0.20
7.2		0.03	2.44	(40)	1.00	6.1		0.05	3.69		0.24	2.64		0.04	4.35	(20)	1.00
6.3		0.06	1.88		0.18	5.2		0.10	3.19	(125)	1.00	2.51	(100)	1.00	3.47		0.25
5.5		0.10	1.61		0.18	4.73	(20)	0.50	2.85	(100)	0.80	2.33		0.13	2.98	(17.5)	0.88
4.85	(30)	0.48	1.460		0.18	4.21		0.18	2.63		0.32	2.21		0.15	2.90		0.10
4.55	(15)	0.24	1.360		0.15	3.64		0.20	2.55		0.16	2.05		0.30	2.70		0.05
4.25		0.08	1.343		0.10	3.49		0.15	2.34		0.08	1.90		0.25	2.51		0.05
3.78		0.24	1.282		0.05	3.25		0.38	2.21		0.24	1.74		0.15	2.33		0.30
3.57		0.10	1.220		0.03B	3.03		0.10	2.01		0.16	1.71	(75)	0.75	2.13		0.15
3.10		0.08	1.180		0.03B	2.56		0.18	1.85		0.32	1.64		0.25	1.98		0.20
2.98		0.03	1.082		0.05	2.43		0.15	1.81	(50)	0.40	1.54		0.03	1.89		0.10
2.87		0.02	1.038		0.08	2.33		0.15	1.70		0.20	1.479		0.15	1.82		0.05
2.70		0.06	1.003		0.03	2.17		0.15	1.66		0.24	1.380		0.20	1.77		0.10
2.57		0.05	0.977		0.03	2.13		0.15	1.62		0.05	1.360		0.15	1.72		0.05
2.48		0.02	0.898		0.03	2.07		0.13	1.59		0.06	1.285		0.06	1.69		0.08
2.35		0.06	0.877		0.03	1.98		0.13	1.55		0.24	1.255		0.20	1.64		0.10
2.30		0.03				1.91		0.08	1.51		0.08	1.210		0.02	1.59		0.10
2.24		0.02		**996. $ZrOCl_2.8H_2O$**		1.81		0.10	1.486		0.16	1.185		0.18	1.52		0.05
2.19		0.03				1.74		0.08	1.426		0.16	1.163		0.03	1.460		0.05
2.12		0.03	12.8	(15)	1.00	1.70		0.05	1.363		0.05	1.098		0.15	1.392		0.05
2.07		0.06	10.6		0.27	1.64		0.10	1.330		0.08	1.057		0.08	1.358		0.05
2.02		0.05	7.9		0.20	1.59		0.03	1.307		0.03	1.046		0.13	1.280		0.05
1.96		0.05	6.9	(10)	0.67	1.55		0.05	1.270		0.12	0.999		0.04	1.250		0.05
1.88		0.06	4.80		0.13	1.51		0.03	1.219		0.05	0.972		0.10	1.090		0.05
1.81		0.03	4.12		0.27	1.476		0.03	1.167		0.06				1.053		0.05
1.76		0.03	3.82		0.20	1.390		0.03	1.113		0.06						
1.69		0.05	3.60	(12.5)	0.83	1.360		0.05	1.036		0.04						
1.60		0.03	3.24		0.40	1.295		0.03	1.001		0.06						
1.490		0.03	2.96		0.07	1.228		0.03									
			2.74		0.07												
			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.

RECEIVED August 22, 1938.