



# **POWDER DIFFRACTION FILE**

## **Set 40**

### **Inorganic and Organic**

Compiled by the JCPDS—International Centre for Diffraction Data in cooperation with the American Ceramic Society, American Crystallographic Association, American Society for Testing and Materials, Australian X-Ray Analytical Association, British Crystallographic Association, The Clay Minerals Society, Deutsche Mineralogische Gesellschaft, The Institute of Physics, The Mineralogical Association of Canada, The Mineralogical Society of America, Mineralogical Society of Great Britain and Ireland, and Société Française de Minéralogie et de Cristallographie.

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## **Preface**

The diffraction patterns in Set 40 have been reviewed by use of NBS \*AIDS83, a program for crystallographic data evaluation. This program is also used to build a computer readable data base from which the card images in Set 40 have been produced by photocomposition. For further information see INORGANIC PHASES—ALPHABETICAL INDEXES.

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# EXPLANATION OF THE DATA CARD FORMAT\*

1				8						
<div style="display: flex; justify-content: space-between;"> <span>2</span> <span>3</span> </div> <div style="display: flex; justify-content: space-between;"> <div>Rad. Cut off Ref.</div> <div><math>\lambda</math> nm.</div> <div>Filter</div> <div>d-sp <math>V_{max}</math></div> </div> <div style="text-align: center;">4</div> <div> <div>Syn. a Ref.</div> <div>b <math>\beta</math></div> <div>c <math>\gamma</math></div> <div>S.G.</div> <div>A Z</div> <div>C mp</div> </div> <div> <div><math>D_1</math></div> <div><math>D_2</math></div> <div>SS/FOM</div> </div> <div> <div>ra Ref.</div> <div><math>\alpha\beta</math></div> <div><math>\epsilon\gamma</math></div> <div>6</div> <div>Sign</div> <div>2V</div> </div> <div style="text-align: center;">7</div>				d Å	Int	hkl	d Å	Int	hkl	

The data card shown above has spaces numbered from 1 to 9 inclusive. An explanation of the symbols in the various spaces is given below. Data added by the Editor are enclosed in square brackets.

**Space 1**—The location of the identification number of the card, referred to as the PDF (Powder Diffraction File) number. Should a pattern require two cards, the second card is indicated with a lower case letter "a" following the PDF number.

**Space 2**—Chemical formula and name of the specimen. The nomenclature follows, in general, the 1957 IUPAC *Nomenclature of Inorganic Chemistry* (J. Am. Chem. Soc. 82, 5523 (1960)). Specifically, for the names and formulas of compounds, cations are arranged in order of increasing valence (IUPAC Sect. 6.321) and, within a valence group, are arranged in alphabetical order (compare Sect. 6.322). Anions are placed in the following order:  $O^{2-}$ , single elements, multiple elements  $H^-$ ,  $OH^-$ . The following rules of nomenclature apply to all sets from and including Set 20, plus all future revision sets and to all indexes.

1. The names for monatomic anions shall consist of the name of the element with the termination -ide.

$H^-$  hydride  
 $D^-$  deuteride  
 $F^-$  fluoride  
 $Cl^-$  chloride  
 $Br^-$  bromide  
 $I^-$  iodide  
 $O^{2-}$  oxide  
 $S^{2-}$  sulfide

$Se^{2-}$  selenide  
 $Te^{2-}$  telluride  
 $N^{3-}$  nitride  
 $P^{3-}$  phosphide  
 $As^{3-}$  arsenide  
 $C^4$  carbide  
 $Si^4$  silicide  
 $B^{3-}$  boride

**\*Note:** This explanation corresponds to cards in Sets 34 and above whose format has been revised from the format of earlier sets.

2. The names of certain polyatomic anions have names ending in -ide.

OH<sup>-</sup> hydroxide  
N<sub>3</sub><sup>-</sup> azide  
NH<sub>2</sub><sup>-</sup> imide  
NH<sub>2</sub><sup>-</sup> amide  
N<sub>2</sub>H<sub>3</sub><sup>-</sup> hydrazide  
CN<sup>-</sup> cyanide  
C<sub>2</sub><sup>2-</sup> acetylide  
CN<sub>2</sub><sup>2-</sup> cyanamide  
O<sub>3</sub><sup>-</sup> ozonide

3. No prefixes indicating proportions shall be used.

4. The suffix -ate will be applied to negatively charged complexes formed from B, C, N, O, F, Si, P, S, Cl, As, Se, Br, Te, I, or At with oxygen. The suffix -ite will be used in the following cases only.

NO<sub>2</sub><sup>-</sup> nitrite  
N<sub>2</sub>O<sub>2</sub><sup>2-</sup>  
PO<sub>3</sub><sup>3-</sup> phosphite  
P<sub>2</sub>O<sub>5</sub><sup>4-</sup>  
SO<sub>3</sub><sup>2-</sup>  
S<sub>2</sub>O<sub>3</sub><sup>2-</sup> sulfite  
S<sub>2</sub>O<sub>4</sub><sup>2-</sup>  
S<sub>2</sub>O<sub>2</sub><sup>2-</sup>  
As<sub>2</sub>O<sub>3</sub><sup>-</sup> arsenite  
SeO<sub>3</sub><sup>2-</sup> selenite  
ClO<sub>2</sub><sup>-</sup> chlorite—correspondingly with  
ClO<sup>-</sup> other halogens

Prefixes indicating oxidation state (hypo, per, etc.) or water content (meta, pyro . . . , etc.) will not be used.

For polyatomic anions other than those mentioned, the central atom shall be named first, then the atoms and groups attached to it. That is, the apparent positive ion shall be given its name then the attached anions; e.g., SiF<sub>6</sub><sup>2-</sup> Silicon Fluoride. Certain anionic combination names shall be retained, SCN, thiocyanate; CNO, cyanate; CN, cyanogen; and CS<sub>3</sub>, thiocarbonate.

5. Certain radicals containing oxygen have special names ending in -yl and these shall be used as follows:

HO hydroxyl	SeO seleninyl
CO carbonyl	SeO <sub>2</sub> selenonyl
NO nitrosyl	CrO <sub>2</sub> chromyl
NO <sub>2</sub> nitryl	UO <sub>2</sub> uranyl
PO phosphoryl	NpO <sub>2</sub> neptunyl
VO vanadyl	PuO <sub>2</sub> plutonyl similarly for the actinides
SO sulfinyl	ClO chlorosyl
SO <sub>2</sub> sulfonyl	ClO <sub>2</sub> chloryl and similarly for other halogens
S <sub>2</sub> O <sub>5</sub> sulfuryl	



The above mentioned polyatomic radicals always are treated as forming the positive part of the compound.

6. Acids containing more than two elements, one of which is oxygen, will be named hydrogen -ate subject to the rule for applying the suffix -ate mentioned above.

7. Oxonium shall be used for a hydrated proton  $\text{H}_3\text{O}^+$ .

8. Aqua shall be used for water co-ordinately bound to a specific ion.

## **RULES OF ORDER**

1. Alloy names are arranged in alphabetical order of the element, regardless of the order of the elements in the formulae.

2. Cation names, except hydrogen, shall be arranged in order of increasing valence with polyatomic cation names at the end of their appropriate valence group, except ammine or aqua which shall follow the cation with which it is associated.

3. The cation names of each valence group shall be arranged alphabetically except for the polyatomic cations as described above.

4. Anion names shall be arranged in the order:

A. Oxide

B. Other simple anions (containing one element only) alphabetically except hydride

C. Polyatomic inorganic anions, alphabetically

D. Organic, alphabetically

E. Hydride

F. Hydroxide

G. Hydrate

**Space 3**—"Dot" or structural formula for the specimen when available, above the mineralogical name, if any. Mineral nomenclature follows that established by the International Mineralogical Association. [NR] following a mineral name indicates a name which has not been recognized by the International Mineralogical Association.

### **Space 4—EXPERIMENTAL CONDITIONS**

Rad—Source of the x-rays.

$\lambda$ —Wavelength of x-rays used in angstroms.

Filter—Substance used to filter out extraneous wavelengths.

d-sp—Method used to measure interplanar spacings. (Guin. = Guinier; D.S. = Debye-Scherrer; Mono. = Monochromator; Diff. = Diffractometer; S.S. Det. = Solid State Detector)

Cut off—Maximum spacing possible with the apparatus used.

Int.—Method used to measure intensities.

I/I cor.—Ratio of the intensity of the strongest line of the pattern to the intensity of the strongest line of corundum.

Ref.—Source of the data listed in Spaces 4 and 9.

### **Space 5—PHYSICAL DATA**

Sys.—Crystallographic system to which the sample belongs.

S.G.—The three dimensional space group symbol and, in parentheses, the number of the space group as given in "International Tables for X-ray Crystallography" pp 545-553 (1952).

a, b, and c—Lattice parameters in angstroms.

A = a/b, C = c/b (or c/a for tetragonal, hexagonal or rhombohedral)—Crystal data determinative ratios.

$\alpha$ ,  $\beta$ ,  $\gamma$ —Interaxial angles.

Z—The number of chemical formula units per unit of structure. For chemical elements, Z represents the number of atoms per unit of structure; for compounds, Z represents the number of formula units per unit cell.

mp—melting point.

Ref.—Source of data listed in Space 5.

Dx—Density calculated from x-ray measurements by the NBS-AIDS83 program.

Dm—Measured density.

SS/FOM—Smith-Snyder figure of merit. (For further information, see page xiii.)

#### Space 6—OPTICAL DATA

(Note: If no optical data is given, Space 6 will not appear.)  $\epsilon\alpha$ ,  $\eta\omega\beta$ , and  $\epsilon\gamma$ —Indices of refraction.

Sign—An indicator of the relationship of the intermediate index of refraction to the maximum and minimum indices of refraction.

2V—Angle between optic axes in biaxial crystals.

Ref.—Source of data listed in Space 6.

#### Space 7—GENERAL COMMENTS

Further pertinent information such as color, chemical analysis of the sample, source of the sample, heat treatment, temperature at which pattern was taken, Crystal Data cell (if different from author's cell in Space 5), CAS number, Merck Index number, PSC (Pearson Symbol Code), etc.

**Space 8**—Quality mark assigned to the pattern by the Editor. (Note: Due to the review of the Powder Diffraction File by the use of NBS-AIDS83, the quality of many patterns has been reassessed and may no longer be equivalent to that originally assigned.)

#### Quality Mark Guidelines

In assigning the data quality mark, the editor is assisted by the evaluation provided by NBS-AIDS83. For patterns with more than 20 reflections, the evaluation only considers reflections out to  $90^\circ 2\theta$  whose intensities are greater than or equal to 5. For patterns with a smaller number of reflections, different ranges are used. If there are 10 reflections out to  $120^\circ 2\theta$  whose intensity values are greater than or equal to 2, these reflections are used. Otherwise, all reflections out to  $180^\circ 2\theta$  are considered regardless of intensity.

#### For a '\*' mark:

1. Chemistry well characterized.
2. Intensity must be measured objectively, instrumentally; no visual estimation is allowed.
3. Good range and even spread of intensity.
4. Completeness of a pattern should be sensible when factors such as pseudo symmetry are taken into account. ( $N_{\text{obs}}$  and  $N_{\text{calc}}$  provide one measure of completeness.)
5. Every line with  $d \leq 2.50\text{\AA}$  must retain at least three significant digits after the decimal point. Lines with  $d \leq 1.200\text{\AA}$  must retain at least 4 significant digits after the decimal point.
6. No serious systematic error.
7. No qualifying line may have  $|\Delta 2\theta| \geq 0.05^\circ$ . In the case of multiple indexed reflections, only the minimum  $|\Delta 2\theta|$  will be considered.
8. For qualifying lines the average, absolute delta two-theta value ( $|\overline{\Delta 2\theta}|$ ) must be  $\leq 0.03^\circ$ .
9. No unindexed, space group extinct or impurity lines.

#### For an 'i' mark:

1. Reasonable range and even spread of intensity.
2. Completeness of the pattern should again be sensible.
3. Lines with  $d \leq 2.00\text{\AA}$  must retain at least 3 significant digits after the decimal point.

4. No serious systematic error.
5. No qualifying lines may have  $|\Delta 2\theta| > 0.20^\circ$ . (Note again  $I > I_{lim}$ ,  $2\theta > 2\theta_{lim}$  and the same consideration for multiple reflections.)
6.  $|\Delta 2\theta| \leq 0.06$ .
7. Maximum number of unindexed, space group extinct or impurity lines is  $\leq 2$ , but none of those should pertain to the strongest eight.

**For an 'O' mark:**

This quality mark is assigned by the editor to indicate: (1) data of low precision or, (2) data likely or possibly due to a multiphase mixture or, (3) data from a phase poorly characterized chemically. The 'O' mark is commonly assigned to patterns without a cell unless qualifying information indicates a single phase material. Usually, the editor will insert a comment in space 7 to explain why an 'O' was assigned.

For patterns with a unit cell, the following criteria can be used to suggest the presence of two or more phases:

1. Number of unindexed, space group extinct or impurity lines is 3 or more.
2. One of the three strongest lines is unindexed.

**For a blank mark:**

For patterns which do not meet the criteria for '\*\*', 'i', or 'O'.

**For a 'C' mark:**

The 'C' mark is used to indicate that the powder pattern was calculated from structural parameters. The structure refinement R-factor should be  $< 0.10$ . In addition, the  $F_{calc}$  should be checked against  $F_{obs}$ . Alternatively, a complete check of the bond distances and angles should have been made. If the structure is derived by Rietveld methods, the calculated pattern will be accepted only in unusual cases. The required number of significant digits is also the same as for a '\*\*'.

**Space 9**—Columns of interplanar spacings, relative intensities, and Miller indices. The three strongest reflections will appear in bold face. The following abbreviations may be used in Space 9:

- b—broad, fuzzy or diffuse line
- n—index not permitted by given space group
- x—intensity uncertain due to the presence or overlap of  $\beta$  lines
- +—additional indices possible
- c—calculated by NBS-AIDS83

# Figure of Merit

A figure of merit, when available, is indicated in space 5 of the Powder Diffraction File data card. The figure of merit generally used is that reported by Smith and Snyder (1979) which indicates the completeness and accuracy of measured interplanar spacings.

This figure of merit,  $F_N$ , is defined as:

$$F_N = \left( \frac{1}{|\overline{\Delta 2\theta}|} \right) \left( \frac{N}{N_{\text{poss}}} \right)$$

where  $|\overline{\Delta 2\theta}|$  is the average absolute discrepancy between observed and calculated  $2\theta$  values and  $N_{\text{poss}}$  is the number of independent diffraction lines possible up to the  $N$ th observed line.

Some comments for the counting of possible diffraction lines are:

Systematic absences caused by symmetry elements and lattice type are excluded in the tallying of  $N_{\text{poss}}$ .

Only one plane from the complete set of planes related by crystal symmetry is counted in  $N_{\text{poss}}$ . For example, in the cubic system, the 100 line is counted as one independent line although it is composed of diffracted intensities from all six planes of that crystallographic form.

Some forms, though not related by symmetry, have exactly the same spacing and would give rise to the same line in the powder pattern e.g., (333) and (511) in the cubic system. Forms of this kind are also counted as one independent line. Note that this rule means that the higher-symmetry Laue group of a crystal system is always assumed. When a lower-symmetry Laue group is definitely known from single crystal studies, (e.g. tetragonal, Laue group 4/m) many pairs of lines, not related by symmetry, occur with exactly the same spacings e.g. (420), (240). All these pairs are treated as single lines.

For the case of accidental degeneracy (i.e., nonequivalent forms which have spacings so nearly identical that the individual lines would not be experimentally resolved), all lines in such a cluster are counted as possible independent lines thereby increasing  $N_{\text{poss}}$ . Each author assigned  $hkl$  is used in the calculation of  $|\overline{\Delta 2\theta}|$  even when two or more  $hkl$ 's are assigned to a single observed spacing.

The format used in reporting  $F_N$  is  $F_N = \text{overall value of } F_N (|\overline{\Delta 2\theta}|, N_{\text{poss}})$ , where  $N$ , the number of observed reflections is chosen as thirty, or the maximum number of lines of the pattern if less than thirty.

## References

Smith, G. S. and Snyder, R. J., *J. Appl. Cryst.*, 12, 60 (1979)

## **Inorganic Section**

**INORGANIC SECTION**

$\text{Ti}_2(\text{CrO}_4)_3$	d Å	Int	hkl	d Å	Int	hkl
Thallium Chromium Oxide	6.38	30	200			
	5.53	70	111			
	4.424	80	211			
	4.313	70	002			
	4.082	10	102			
Rad. $\text{CuK}\alpha_1$ $\lambda$ 1.5405 Filter Beta d-sp D.S. Cut off Int. Visual $I/I_{\text{ref}}$	3.834	10	310			
Ref. Cudenec. Y., Private Communication	3.704	20	112			
	3.580	10	202			
Syn. Orthorhombic S.G. Pbcn (60)	3.517	5	511			
a 12.805 b 8.776 c 8.651 A C	3.324	5	212			
$\alpha$ $\beta$ $\gamma$ Z 4 mp	3.198	10	400			
Ref. Lecert. A. et al. C. R. Seances Acad. Sci., Ser. 2, 296 1047 (1983)	3.038	50	302			
$D_x$ 5.170 $D_m$ 5.060 SS/FOM $F_2 = 61.058.64$	2.988	30	122			
Color Red-brown	2.831	80	411			
Made by reacting $\text{CrO}_3$ and $\text{Ti}(\text{NO}_3)_3 \cdot 3\text{H}_2\text{O}$ at 40 C and washing with acetone. C.D. Cell: a = 8.776, b = 12.805, c = 8.651, a/b = 0.6854, c/b = 0.6756. S.G. = Pbcn (60). PSC. 0P68.	2.672	100	113			
	2.570	20	402			
	2.518	80	213			
	2.486	10	421			
	2.370	50	223, 511			
	2.167	40	004			
	2.137	40	512, 600			
	2.090	10	431			
	2.047	10	204			
	2.016	30	241			

## 40-2

$\text{La}_2\text{MnO}_{4.15}$	d Å	Int	hkl	d Å	Int	hkl
Lanthanum Manganese Oxide	3.779	35	111	1.392	4	208.028
	3.207	15	004	1.341	2	119
	2.905	100	113	1.292	<1	404
	2.821	40	200	1.282	<1	0010
Rad. $\text{CuK}\alpha_1$ $\lambda$ 1.5418 Filter d-sp Cut off 22.1 Int. Visual $I/I_{\text{ref}}$	2.775	30	020	1.277	2	317
Ref. Borlera. M., Abbattista. J. Less-Common Met., 92 55 (1983)	2.545	2	022	1.273	<1	044
	2.153	15	115	1.269	1	137
Syn. Orthorhombic S.G. F	2.138	20	006	1.260	5	333
a 5.642 b 5.550 c 12.83 A C	2.119	15	204	1.258	3	420
$\alpha$ $\beta$ $\gamma$ Z mp	2.100	15	024	1.245	4	228.240
Ref. ibid.	1.980	30	220			
$D_x$ $D_m$ SS/FOM $F_2 = 29(0.28.37)$	1.889	1	222			
Made by heating $\text{LaMnO}_3$ in a reducing atmosphere near 1380 C. C.D. Cell: a = 5.642, b = 12.830, c = 5.550, a/b = 0.4398, c/b = 0.4326. PSC. 0F7.	1.764	2	311			
	1.741	2	131			
	1.703	10	206			
	1.694	12	026			
	1.684	12	224			
	1.663	15	117			
	1.645	20	313			
	1.626	15	133			
	1.604	2	008			
	1.463	2	315			
	1.453	10	226			
	1.450	8	135			
	1.410	2	400			

## 40-3

$\text{Ti}_3\text{SiW}_{12}\text{O}_{40} \cdot 8\text{H}_2\text{O}$	d Å	Int	hkl	d Å	Int	hkl
Thallium Tungsten Silicate Hydrate	8.31	40	110			
	6.76	30	111			
	4.77	60	211			
	3.68	60	310			
Rad. $\text{CuK}\alpha_1$ $\lambda$ 1.5406 Filter Ni d-sp Diff. Cut off Int. Visual $I/I_{\text{ref}}$	3.36	60	222			
Ref. Varfolomeev. M. et al., Russ. J. Inorg. Chem. (Engl. Transl.), 27 1750 (1982)	2.91	100	400			
	2.74	60	411			
Syn. Cubic S.G. $P\bar{4}32$	2.49	40	332			
a 11.65(1) b c A C	2.38	60	422			
$\alpha$ $\beta$ $\gamma$ Z mp	2.29	30	510			
Ref. Ibid.	2.13	40	521			
$D_x$ $D_m$ SS/FOM $F_{15} = 7(0.50.43)$	2.06	40	440			
Made by adding an aqueous solution of $\text{TiNO}_3$ to one of $\text{H}_2\text{SiW}_{12}\text{O}_{40}$ and heating to 80 C. $\text{Cs}_3\text{SiW}_{12}\text{O}_{40} \cdot 8\text{H}_2\text{O}$ type. PSC. cP7.	1.891	40	611			
	1.756	40	622			
	1.649	40	550			

$\text{Th}_2\text{SiW}_{12}\text{O}_{40}$				d Å	Int	hkl	d Å	Int	hkl
Thallium Tungsten Silicate				8.36	40	110			
				6.83	30	111			
				4.83	60	211			
				3.73	60	310			
				3.40	100	222			
Rad. $\text{CuK}\alpha$	$\lambda$ 1.5418	Filter Mono.	d-sp Guinier	2.95	60	400			
Cut off	Int. Visual		$I/I_{\text{cor}}$	2.77	30	411			
Ref. Varfolomeev, M. et al., <i>Russ. J. Inorg. Chem. (Engl. Transl.)</i> , 27:1750 (1982)				2.51	40	332			
Sys. Cubic				2.40	30	422			
a 11.78	b	c	S.G. $P\bar{4}32$	2.31	40	510			
$\alpha$	$\beta$	$\gamma$	A	2.14	40	(521)			
Ref. Ibid.				2.08	40	440			
				1.906	40	611			
$D_1$ $D_2$ SS/FOM $F_{12} = 0.065(33)$									
Pattern at 450 C. Made by heating $\text{Th}_2\text{SiW}_{12}\text{O}_{40} \cdot 8\text{H}_2\text{O}$ at 450 C. $\text{Cs}_2\text{SiW}_{12}\text{O}_{40}$ type. PSC: cP?									

## 40-5

$\text{Th}_2\text{W}_6\text{O}_{19}$				d Å	Int	hkl	d Å	Int	hkl
Thallium Tungsten Oxide				6.45	60	110			
				3.84	80	002			
				3.30	90	022, 112			
				3.25	60	040			
				3.20	100	220			
Rad. $\text{CuK}\alpha$	$\lambda$ 1.5418	Filter Mono.	d-sp Guinier	2.68	40	132			
Cut off	Int. Visual		$I/I_{\text{cor}}$	2.66	60	202			
Ref. Varfolomeev, M. et al., <i>Russ. J. Inorg. Chem. (Engl. Transl.)</i> , 27:1750 (1982)				2.483	40	042			
Sys. Orthorhombic				2.460	60	222			
a 7.38(2)	b 12.99(3)	c 7.68(2)	S.G. C	2.060	40	331, 242			
$\alpha$	$\beta$	$\gamma$	A	1.921	60	004			
Ref. Ibid.				1.869	60	260			
				1.839	60	114			
$D_1$ $D_2$ SS/FOM $F_{13} = 8(0.035, 47)$									
Pattern at 760 C. $\text{K}_2\text{W}_6\text{O}_{19}$ type. C.D. Cell: a = 7.680, b = 12.990, c = 7.380, a/b = 0.5912, c/b = 0.5681, S.G. = A. PSC: oC?									

## 40-6

$\text{AgLaSb}_2\text{O}_7$				d Å	Int	hkl	d Å	Int	hkl
Silver Lanthanum Antimony Oxide				5.19	4	002			
				3.076	100	022			
				3.003	95	202			
				2.665	47	220			
				2.570	20	[004]			
Rad. $\text{CuK}\alpha$	$\lambda$ 1.5418	Filter	d-sp Diff.	2.394	2	301			
Cut off	Int. Diffractometer		$I/I_{\text{cor}}$	2.353	2	131*			
Ref. Lopatin, S. et al., <i>Russ. J. Inorg. Chem. (Engl. Transl.)</i> , 27:1559 (1982)				2.049	3	033			
Sys. Orthorhombic				1.919	11	040			
a 7.391	b 7.679	c 10.271	S.G. $\text{I}2\text{mm}$ (44)	1.850	60	224			
$\alpha$	$\beta$	$\gamma$	A	1.616	20	242			
Ref. Ibid.				1.584	20	422			
				1.563	9	026			
$D_1$ 6.862 $D_2$ SS/FOM $F_{21} = 5(0.036, 129)$				1.554	9	206			
Color Yellow				1.537	8	044			
Made by heating $\text{AgSbO}_3$ and $\text{LaSbO}_3$ for 7 hours at 900 C and at 1000-1150 C in air. Weberite, $\text{AlF}_7\text{MgNa}_2$ type. C.D. Cell: a = 7.679, b = 10.271, c = 7.391, a/b = 0.7476, c/b = 0.7196, S.G. = $\text{Immm}$ (44).				1.500	8	404			
*Not permitted by space group.				1.330	5	440			
External standard used. PSC: oI44.				1.242	3	062			
				1.207	7	246			
				1.194	7	426			
				1.181	5	444			
				1.173	3	620			

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40-9

$Zn_2SiO_4$				d Å	Int	hkl	d Å	Int	hkl
Zinc Silicate				6.905	10	110			
				4.551	25	200			
				4.162	40	210			
				3.543	40	030			
				3.027	85	300			
Rad. $\lambda$ Filter d-sp									
Cut off Int. Diffractometer $I/I_{002}$									
Ref. Doroshev, A. et al., <i>Neues Jahrb. Mineral. Monatsh.</i> , 1983 277 (1983)				2.978	25	002			
				2.868	40	012			
				2.840	25	102			
				2.732	85	112			
				2.633	100	320			
Sys. Orthorhombic S.G. $P_{2121}$				2.607	10	022			
a 9.085(10) b 10.625(8) c 5.962(4) A 0.8551 C 0.5611				2.553	25	140			
α β γ Z 2 mp				2.529	40	231			
Ref. Ibid.				2.507	85	122			
D <sub>2</sub> D <sub>2h</sub> SS/FOM $F_{011} = 4(041.137)$				2.427	55	212, 041			
Sample was made by treating $Zn_2SiO_4$ and $H_2O$ kbar at 1200 C for 20 minutes and quenching. Called $Zn_2SiO_4$ VI. Silicon used as internal standard. PSC. oP?				2.401	40	321			
				2.122	10	302, 401			
				2.081	70	312			
				2.070	70	150			
				1.702	40	133			
				1.475	25	014			

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$Ca_3(PO_3)_6 \cdot 10H_2O$				d Å	Int	hkl	d Å	Int	hkl
Calcium Phosphate Hydrate				9.02	100	020	2.610	8	052
				8.08	20	110	2.596	10	161
				6.95	9	011			
				6.39	50	120			
				5.79	8	021			
Rad. $CuK\alpha_1$ $\lambda$ 1.5406 Filter d-sp Diff.				5.05	8	101			
Cut off Int. Diffractometer $I/I_{002}$				5.02	10	130			
Ref. El-Horr, N., Durif, C. R. <i>Seances Acad. Sci., Ser. 2</i> , 296 1185 (1983)				4.89	5	111			
Sys. Monoclinic S.G. $P2_1/n$ (14)				4.71	25	031			
a 9.332(7) b 18.13(1) c 7.841(5) A 0.5147 C 0.4325				4.55	50	040			
α β γ Z 2 mp				4.43	18	121			
Ref. Ibid.				3.879	13	041			
D <sub>2</sub> 2.023 D <sub>2h</sub> SS/FOM $F_{111} = 15(025.74)$				3.769	4	141			
Isostructural with the similar Cd and Mn compounds. PSC. mP114.				3.360	35	150			
				3.264	35	051			
				3.209	6	221			
				3.172	3	241			
				3.020	7	060			
				2.961	4	232			
				2.862	95	160			
				2.805	5	061			
				2.796	7	132			
				2.763	5	161			
				2.734	3	241			
				2.670	4	330			

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$Mn_3(PO_3)_6 \cdot 10H_2O$				d Å	Int	hkl	d Å	Int	hkl
Manganese Phosphate Hydrate				8.86	50	020	2.715	6	331
				7.88	65	110	2.668	16	242
				6.74	40	011	2.625	10	330
				6.24	65	111, 120	2.595	30	322
				5.64	35	021	2.547	30	103
Rad. $CuK\alpha_1$ $\lambda$ 1.5418 Filter d-sp Diff.				5.34	17	121	2.521	14	113
Cut off Int. Diffractometer $I/I_{002}$				4.91	25	130	2.519	13	142
Ref. El-Horr, N., Durif, C. R. <i>Seances Acad. Sci., Ser. 2</i> , 296 1185 (1983)				4.59	70	031	2.514	13	341
Sys. Monoclinic S.G. $P2_1/n$ (14)				4.43	95	040, 131			
a 9.219(4) b 17.733(8) c 7.644(3) A 0.5199 C 0.4311				4.40	45	200			
α β γ Z 2 mp				4.27	95	210, 311			
Ref. Ibid.				3.936	12	221			
D <sub>2</sub> 2.280 D <sub>2h</sub> SS/FOM $F_{30} = 34(012.72)$				3.793	35	131			
Isostructural with the Ca and Cd salts. PSC. mP114.				3.648	35	002			
				3.573	60	012			
				3.530	45	230			
				3.341	9	202			
				3.292	35	211			
				3.194	30	132			
				3.130	40	151			
				3.057	13	301			
				3.013	100	311			
				2.893	60	122, 310			
				2.803	25	160			
				2.761	9	250, 251			





$\text{Ca}_3(\text{Mn}(\text{OH})_6)_2$				d Å	Int	hkl	d Å	Int	hkl
Calcium Manganese Hydroxide				5.077	20	211			
				4.397	50	220			
				<b>3.109</b>	85	400			
				2.781	60	420			
				<b>2.539</b>	100	422			
Rad. CuK $\alpha$ $\lambda$ 1.5418 Filter Ni d-sp Diff.				2.439	30	431			
Cut off Int. Diffractometer $V_{\text{rec}}$				2.271	45	521			
Ref. Ivanov-Emin. B. et al., <i>Russ. J. Inorg. Chem. (Engl. Transl.)</i> , 27 1755 (1982)				2.018	60	611			
Sys. Cubic S.G. Ia3d (230)				1.966	10	620			
a 12.437(5) b c A C				1.919	25	541			
Ref. Ibid.				1.795	15	444			
				1.725	25	640			
D <sub>4</sub> 2.998 D <sub>m</sub> SS/FOM $F_{12} = 110(007.21)$				1.692	10	721			
Made by reaction of manganese acetate, $\text{CaCl}_2$ , in NaOH solution. Hydrogarnet type. PSC: c1232.				<b>1.662</b>	85	642			
				1.554	10	800			



$\text{Sr}_3(\text{Mn}(\text{OH})_6)_2$				d Å	Int	hkl	d Å	Int	hkl
Strontium Manganese Hydroxide				5.26	40	211			
				3.443	40	321			
				3.220	35	400			
				<b>2.881</b>	100	420			
				<b>2.630</b>	60	422			
Rad. CuK $\alpha$ $\lambda$ 1.5418 Filter Ni d-sp Diff.				2.350	35	(521)			
Cut off Int. Diffractometer $V_{\text{rec}}$				2.090	35	611			
Ref. Ivanov-Emin. B. et al., <i>Russ. J. Inorg. Chem. (Engl. Transl.)</i> , 27 1755 (1982)				1.786	25	640			
Sys. Cubic S.G. Ia3d (230)				1.753	10	721			
a 12.382(5) b c A C				1.722	35	642			
Ref. Ibid.									
D <sub>4</sub> 3.585 D <sub>m</sub> SS/FOM $F_{12} = 58(009.19)$									
Color Brown									
Made by reaction of manganese acetate with $\text{SrCl}_2$ in NaOH solution. Hydrogarnet type. PSC: c1232.									



$\alpha\text{-CaSr}_2\text{WO}_6$				d Å	Int	hkl	d Å	Int	hkl
Calcium Strontium Tungsten Oxide				4.755	25	101			
				4.729	25	110			
				4.111	6	011,200			
				3.672	2	111			
				<b>2.9224</b>	30	002			
Rad. CoK $\alpha$ $\lambda$ 1.7902 Filter d-sp Diff.				<b>2.9014</b>	100	211			
Cut off Int. Diffractometer $V_{\text{rec}}$				2.8818	25	020			
Ref. Zherngmin. F. et al., <i>Sci. Sin. (Engl. Ed.)</i> , 26 835 (1983)				2.7516	2	102			
Sys. Orthorhombic S.G. Pmm2 (25)				2.6190	1	012			
a 8.2033 b 5.7676 c 5.8489 A C				2.4822	11	112			
Ref. Ibid.				2.4674	19	301,310			
D <sub>4</sub> 5.943 D <sub>m</sub> 5.981 SS/FOM $F_{12} = 9(056.23)$				2.3830	1	202			
Low temperature form, $\text{CaSr}_2\text{WO}_6$ is cubic above 860 C. C.D. Cell: a = 5.849, b = 8.203, c = 5.768, a/b = 0.7130, c/b = 0.7031. S.G. = P2mm (25). PSC: oP20.									