

(200)

TL67W

no-830

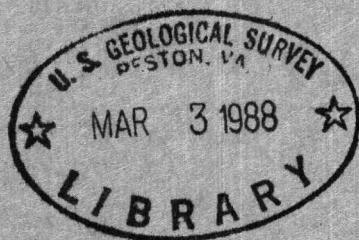
Copy 4

TEI-830

X - R A Y   C R Y S T A L L O G R A P H I C   D A T A  
F O R   M I N E R A L S

By Richard A. Robie, Philip M. Bethke,  
Martha S. Toulmin and Jerry L. Edwards

---



UNITED STATES DEPARTMENT OF THE INTERIOR  
GEOLOGICAL SURVEY

UNITED STATES DEPARTMENT OF THE INTERIOR  
GEOLOGICAL SURVEY

X-RAY CRYSTALLOGRAPHIC DATA FOR MINERALS\*

By

Richard A. Robie, Philip M. Bethke,  
Martha S. Toulmin and Jerry L. Edwards

February 1963

Report TEI-830

This report is preliminary  
and has not been edited for  
conformity with Geological  
Survey format.

\*Prepared on behalf of the  
U. S. Atomic Energy Commission.

USGS - TEI-830

| <u>Distribution</u>   | <u>No. of copies</u> |
|---|----------------------|
| Division of Reactor Development (W. G. Belter) . . . . .  | 5                    |
| Division of Research (D. R. Miller) . . . . .   | 1                    |
| Division of Raw Materials (R. D. Nininger) . . . . .  | 1                    |
| Division of Peaceful Nuclear Explosives (R. Hamburger) . . . . .                                    | 1                    |
| Hanford Operations Office (C. L. Robinson) . . . . .  | 1                    |
| Grand Junction Operations Office . . . . .  | 1                    |
| Idaho Operations Office (John Horan) . . . . .  | 1                    |
| Oak Ridge Operations Office (H. M. Roth) . . . . .  | 1                    |
| Savannah River Operations Office (Karl Herde) . . . . .   | 1                    |
| Division of Technical Information Extension, Oak Ridge . . . . .                                    | 6                    |
| Nevada Operations Office . . . . .  | 2                    |
| U. S. Naval Radiological Defense Lab., San Francisco . . . . .                                      | 1                    |
| Health Physics Division, Oak Ridge National Laboratory<br>(F. L. Parker; E. G. Struxness) . . . . . | 1                    |
| Chemistry Division, Argonne National Lab. (W. M. Manning) . . . . .                                 | 1                    |
| Chemical Tech. Div., Oak Ridge National Lab. (W. E. Clark) . . . . .                                | 1                    |
| U. S. Bureau of Mines, Bartlesville, Oklahoma (J. W. Watkins) . . . . .                             | 1                    |
| Los Alamos Scientific Laboratory (J. H. Hall) . . . . .   | 1                    |
| Los Alamos Scientific Laboratory (C. W. Christenson) . . . . .                                      | 1                    |
| Earth Sciences Division, NAS-NRC (Linn Hoover) . . . . .  | 10                   |
| University of Texas, Austin (E. F. Gloyna) . . . . .  | 1                    |
| General Electric Company, Richland, Washington (E. R. Irish) . . . . .                              | 2                    |
| University of California (W. J. Kaufman) . . . . .  | 1                    |
| E. I. DuPont deNemours & Company (C. M. Patterson) . . . . .  | 1                    |
| Lawrence Radiation Laboratory, Technical Information<br>Division (Clovis G. Craig) . . . . .        | 1                    |
| Lawrence Radiation Laboratory, Livermore (Director) . . . . .                                       | 25                   |
| Headquarters Library, USAEC . . . . .   | 1                    |
|   | <hr/> 70             |
| U. S. Geological Survey:  |                      |
| Geologic Division . . . . .   | 97                   |
| Water Resources Division . . . . .  | 20                   |
|   | <hr/> 187            |

Geologic Division distributionNo. of copies

|  |    |
|--|----|
| Engineering Geology. . . . .                         | 3  |
| Geochemical Exploration and Minor Elements . . . . . | 1  |
| Organic Fuels. . . . .                               | 1  |
| New England. . . . .                                 | 1  |
| Eastern States . . . . .                             | 1  |
| Regional Geology . . . . .                           | 1  |
| Southern Rocky Mountains . . . . .                   | 2  |
| Southwestern Branch. . . . .                         | 1  |
| Pacific Coast States . . . . .                       | 1  |
| Alaskan. . . . .                                     | 1  |
| Regional Geophysics. . . . .                         | 4  |
| Experimental Geochemistry and Mineralogy . . . . .   | 1  |
| Theoretical Geophysics . . . . .                     | 50 |
| Isotope Geology. . . . .                             | 1  |
| Field Geochemistry and Petrology . . . . .           | 2  |
| Analytical Laboratories. . . . .                     | 1  |
| Foreign Geology. . . . .                             | 1  |
| Military Geology . . . . .                           | 1  |
| Library. . . . .                                     | 3  |
| Special Projects . . . . .                           | 3  |
| Geologic Division. . . . .                           | 17 |

---

97



# X-RAY CRYSTALLOGRAPHIC DATA FOR MINERALS

By

Richard A. Robie, Philip M. Bethke,

Martha S. Toulmin and Jerry L. Edwards

X-ray crystallographic data are of particular importance to the mineralogist. Beyond the considerations of structural chemistry they provide one of the most accurate methods for phase and/or compositional determination and for obtaining the molar volumes and densities of minerals (Robie and Bethke, 1962).

Selected data for approximately 300 minerals are tabulated. These data are taken from the recent literature or from unpublished sources. With minor exceptions we have restricted ourselves to the inclusion of data for chemically and physically well-defined phases for which the unit cell parameters are known with an accuracy of the order of 0.2 percent or better.

The data are presented by mineral groups following Dana's System. Within a group, however, the order may be alphabetical, structural, or for the sulfides, approximately by increasing sulfur-metal ratio.

Temperatures at which the measurements were made are given in the second column from the right. The letter r indicates the data were obtained at an unspecified room temperature and may be taken as  $25^{\circ} \pm 5^{\circ}\text{C}$ . The number of gram formula weights per unit cell is given in the column labeled Z.

Compounds denoted by an asterisk indicate the measurements were made on natural specimens which may have deviated slightly from

the listed formula. Substances of rhombohedral symmetry are denoted by the symbol hex-R to distinguish them from materials of true hexagonal symmetry. The space group is given along with its number in the 1952 International Tables for X-ray Crystallography (Henry and Lonsdale, 1952).

All cell dimensions are given in Angstrom units,  $10^{-8}$  centimeters. Where necessary, older data have been converted from kX units to Angstroms using the conversion factor  $1.00204 \pm 0.000014$  of Cohen, Crowe, and DuMond (1957).

Most natural minerals are intermediate members of multicomponent solid solutions. For this reason data have been included for several phases, not known as minerals but which form the end member of a solid solution. We have also included cell parameters, based on the linear extrapolation of data for incomplete solutions, for several hypothetical compounds.

The uncertainties listed are not necessarily those of the original investigator but represent our attempt to evaluate the true accuracy of the data. In this connection it is worthwhile to restate the results of a recent cooperative investigation by the International Union of Crystallography, (Parrish, 1960) involving more than twenty laboratories which has shown that although the reproducibility (that is, precision) of an individual may be a few thousandths of a percent, different investigators working on the same sample showed agreement with one another of only 0.005 percent to 0.015 percent. Data claiming an accuracy of better than 0.01 percent should be considered with these limitations in mind.

For more extensive summaries of X-ray data the reader is referred to the works cited below:

Berry, L. G., and Thompson, R. M., 1962, X-ray powder data for the ore minerals: The Peacock Atlas: Geological Society of America Memoir 85.

Donnay, J. D. H., and Nowacki, W., 1954, Crystal data: Geological Society of America Memoir 60.

International Union of Crystallography, Structure reports: volume 8 through 16 summarize data published from 1940 to 1952.

Pearson, W. B., 1958, Handbook of lattice spacing and structure of alloys: New York, Pergamon Press.

Reference cited

Cohen, E. R., Crowe, K. M., and DuMond, J. W. M., 1957, Fundamental constants of physics: New York, Interscience Publisher.

Henry, N. F. M., and Lonsdale, K., eds., 1952, International tables for X-ray crystallography, v. 1, Symmetry groups: Internat. Union Crystallography, Birmingham, England, Kynoch Press.

Parrish, William, 1960, Results of the International Union of Crystallography precision lattice parameter project: Acta Cryst., v. 13, p. 833.

Robie, R. A., and Bethke, P. M., 1962, Molar volumes and densities of minerals: U. S. Geol. Survey open-file report TEI-822.

## ELEMENTS

| Formula | Name     | Cry.<br>Sys. | Space<br>Group             | Structure<br>Type                | Z   | a <sub>o</sub>     | b <sub>o</sub>   | c <sub>o</sub>    | α <sub>o</sub> | β <sub>o</sub>  | γ <sub>o</sub> | Temp<br>°C | Ref.           |
|---------|----------|--------------|----------------------------|----------------------------------|-----|--------------------|------------------|-------------------|----------------|-----------------|----------------|------------|----------------|
| Ag      | Silver   | cub          | Fm3m (225)                 | f.c.c. <sup>1/</sup>             | 4   | 4.0862<br>±.0002   |                  |                   |                |                 |                | 25         | 146            |
| Au      | Gold     | cub          | Fm3m (225)                 | f.c.c.                           | 4   | 4.0786<br>±.0002   |                  |                   |                |                 |                | 25         | 146            |
| C *     | Diamond  | cub          | Fd3m (227)                 | diamond                          | 8   | 3.56688<br>±.00009 |                  |                   |                |                 |                | 25         | 131            |
| C *     | Graphite | hex          | C6/mmc (194)               | graphite                         | 4   | 2.4612<br>±.0001   |                  | 6.7079<br>±.0007  |                |                 |                | 14.6       | 99             |
| Cu      | Copper   | cub          | Fm3m (225)                 | f.c.c.                           | 4   | 3.6150<br>±.0003   |                  |                   |                |                 |                | 25         | 146            |
| Fe      | α-Iron   | cub          | Im3m (229)                 | b.c.c. <sup>2/</sup>             | 2   | 2.8664<br>±.0005   |                  |                   |                |                 |                | 25         | 149            |
| Ni      | Nickel   | cub          | Fm3m (225)                 | f.c.c.                           | 4   | 3.5238<br>±.0005   |                  |                   |                |                 |                | 25         | 146            |
| Pt      | Platinum | cub          | Fm3m (225)                 | f.c.c.                           | 4   | 3.9231<br>±.0005   |                  |                   |                |                 |                | 25         | 146            |
| S       | α-Sulfur | orth         | Fddd (70)                  | S <sub>8</sub> ring<br>molecules | 128 | 10.4646<br>±.001   | 12.8660<br>±.001 | 24.4860<br>±.002  |                |                 |                | 24.7       | 178, 21        |
| S       | β-Sulfur | mon          | P2 <sub>1</sub> /c (14)    | S <sub>8</sub> ring<br>molecules | 48  | 11.04<br>±.03      | 10.98<br>±.03    | 10.92<br>±.03     |                | 96° 44'<br>±30' |                | 103        | 32             |
| Pb      | Lead     | cub          | Fm3m (225)                 | f.c.c.                           | 4   | 4.9505<br>±.0005   |                  |                   |                |                 |                | 25         | 146            |
| Sn      | β-Tin    | tet          | I4 <sub>1</sub> /amd (141) |                                  | 4   | 5.83146<br>±.0005  |                  | 3.18129<br>±.0007 |                |                 |                | 26         | 69             |
| Sb      | Antimony | hex-R        | R3m (166)                  | Arsenic                          | 6   | 4.307<br>±.001     |                  | 11.273<br>±.001   |                |                 |                | 26         | 148, 126       |
| As      | Arsenic  | hex-R        | R3m (166)                  | Arsenic                          | 6   | 3.760<br>±.002     |                  | 10.548<br>±.004   |                |                 |                | 26         | 148            |
| Bi      | Bismuth  | hex-R        | R3m (166)                  | Arsenic                          | 6   | 4.5459<br>±.0002   |                  | 11.8622<br>±.0005 |                |                 |                | 26         | 69, 126<br>148 |

<sup>1/</sup> f.c.c., face-centered cubic.<sup>2/</sup> b.c.c., body-centered cubic.



## ELEMENTS continued

| Formula | Name      | Cry.<br>Sys. | Space<br>Group                                       | Structure<br>Type      | Z | a <sub>o</sub>     | b <sub>o</sub> | c <sub>o</sub>   | α <sub>o</sub> | β <sub>o</sub> | γ <sub>o</sub> | Temp<br>°C | Ref. |
|---------|-----------|--------------|--|------------------------|---|--------------------|----------------|------------------|----------------|----------------|----------------|------------|------|
| Zn      | Zinc      | hex          | P6 <sub>3</sub> /mmc(194)                            | h. c. p. <sup>3/</sup> | 2 | 2.665<br>±.001     |                | 4.947<br>±.0007  |                |                |                | 25         | 146  |
| Se      | Selenium  | hex          | P3 <sub>1</sub> 21 (152)<br>P3 <sub>2</sub> 21 (154) | chain                  | 3 | 4.3642<br>±.0005   |                | 4.9588<br>±.0005 |                |                |                | 26         | 143  |
| Te      | Tellurium | hex          | P3 <sub>1</sub> 21 (152)<br>P3 <sub>2</sub> 21 (154) | chain                  | 3 | 4.4570<br>±.0007   |                | 5.9290<br>±.0010 |                |                |                | 25         | 146  |
| Si      | Silicon   | cub          | Fd3m (227)   | diamond                | 8 | 3.56703<br>±.00020 |                |                  |                |                |                | 25         | 183  |

<sup>3/</sup> h. c. p., hexagonal close packed.

## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula  | Name          | Cry.<br>Sys.  | Space<br>Group          | Structure<br>Type            | Z  | a <sub>o</sub>  | b <sub>o</sub>  | c <sub>o</sub>  | α <sub>o</sub> | β <sub>o</sub> | v <sub>o</sub> | Temp<br>°C | Ref     |
|--|---------------|---------------|-------------------------|------------------------------|----|-----------------|-----------------|-----------------|----------------|----------------|----------------|------------|---------|
| β-Ni <sub>3</sub> Pb <sub>2</sub> S <sub>2</sub> * | Shandite      | hex-R         | R $\bar{3}$ m (166)     |                              | 3  | 5.576<br>±.01   |                 | 13.658<br>±.01  |                |                |                | r          | 67, 110 |
| Au <sub>2</sub> Bi                                 | Maldonite     | cub           | Fd3m (227)              | Cu <sub>2</sub> Mg           | 8  | 7.958<br>±.002  |                 |                 |                |                |                | r          | 73      |
| Ag <sub>2</sub> S I                                | Hi-Argentite  | cub           |                         |                              | 4  | 6.269<br>±.020  |                 |                 |                |                |                | 600        | 30      |
| Ag <sub>2</sub> S II                               | Argentite     | cub           |                         |                              | 2  | 4.870<br>±.008  |                 |                 |                |                |                | 189        | 30      |
| Ag <sub>2</sub> S III                              | Acanthite     | mon           | P2 <sub>1</sub> /c (14) |                              | 4  | 4.228<br>±.002  | 6.928<br>±.005  | 7.862<br>±.003  |                |                |                | r          | 30, 155 |
| Ag <sub>2</sub> Se                                 | Hi-Naumannite | cub           |                         |                              |    | 4.993<br>±.016  |                 |                 |                | 99° 35'        |                | 170        | 116     |
| Ag <sub>2</sub> Te I                               |               | cub           |                         |                              | 2  | 5.29<br>±.01    |                 |                 |                |                |                | 825        | 116     |
| Ag <sub>2</sub> Te II                              |               | cub           |                         |                              |    | 6.585<br>±.010  |                 |                 |                |                |                | 250        | 116     |
| Ag <sub>2</sub> Te III *                           | Hessite       | mon           | P2 <sub>1</sub> /c (14) |                              | 4  | 8.09<br>±.02    | 4.48<br>±.01    | 8.96<br>±.02    |                | 123° 20'       |                | r          | 45      |
| Cu <sub>2</sub> S I *                              | Hi-Digenite   | cub           |                         |                              | 4  | 5.725<br>±.010  |                 |                 |                |                |                | 465        | 29, 119 |
| Cu <sub>2</sub> S II *                             | Hi-Chalcocite | hex           |                         |                              |    | 3.961<br>±.004  |                 | 6.722<br>±.007  |                |                |                | 152        | 29, 119 |
| Cu <sub>2</sub> S III *                            | Chalcocite    | orth          | Ab2m (39)               |                              | 96 | 11.881<br>±.004 | 27.323<br>±.008 | 13.491<br>±.004 |                |                |                | r          | 29, 119 |
| Cu <sub>1.79</sub> S (Cu rich<br>side)             | Digenite      | pseudo<br>cub |                         | Deformed<br>CaF <sub>2</sub> | 4  | 5.5695<br>±.001 |                 |                 |                |                |                | 25         | 29, 119 |

## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula                                     | Name          | Cry.<br>Sys.           | Space<br>Group   | Structure<br>Type              | Z  | a <sub>o</sub>  | b <sub>o</sub> | c <sub>o</sub>  | α <sub>o</sub> | β <sub>o</sub> | ν <sub>o</sub> | Temp<br>°C | Ref     |
|---|---------------|------------------------|------------------|--------------------------------|----|-----------------|----------------|-----------------|----------------|----------------|----------------|------------|---------|
| Cu <sub>1.77</sub> S (S rich side)          | Digenite      | pseudo<br>cub          |                  | Deformed<br>CaF <sub>2</sub>   | 4  | 5.5542<br>±.001 |                |                 |                |                |                | 25         | 29, 119 |
| Cu <sub>2</sub> Se                          |               | cub                    |                  |                                | 4  | 5.85<br>±.01    |                |                 |                |                |                | 170        | 119     |
| Ag <sub>1.55</sub> Cu <sub>0.45</sub> S I   |               | cub                    |                  |                                | 4  | 6.110<br>±.010  |                |                 |                |                |                | 300        | 30      |
| Ag <sub>1.55</sub> Cu <sub>0.45</sub> S II  |               | cub                    |                  |                                | 2  | 4.825<br>±.005  |                |                 |                |                |                | 116        | 30      |
| Ag <sub>1.55</sub> Cu <sub>0.45</sub> S III | Jalpaite      | tet                    |                  |                                | 16 | 8.673<br>±.004  |                | 11.756<br>±.006 |                |                |                | r          | 30      |
| Ag <sub>0.93</sub> Cu <sub>1.07</sub> S I   |               | cub                    |                  |                                | 4  | 5.961<br>±.009  |                |                 |                |                |                | 196        | 30      |
| Ag <sub>0.93</sub> Cu <sub>1.07</sub> S II  |               | hex                    |                  |                                | 2  | 4.138<br>±.004  |                | 7.105<br>±.007  |                |                |                | 100        | 30      |
| Ag <sub>0.93</sub> Cu <sub>1.07</sub> S III | Stromeyerite  | orth                   | Cmcn (63)        |                                | 4  | 4.066<br>±.002  | 6.628<br>±.003 | 7.972<br>±.004  |                |                |                | r          | 30      |
| AgCuSe                                      | Eucairite     | orth,<br>pseudo<br>tet | P4/nmm (129)     |                                | 10 | 4.105<br>±.010  | 20.35<br>±.20  | 6.31<br>±.01    |                |                |                |            | 43      |
| Ag <sub>3</sub> AuTe <sub>2</sub> *         | Petzite       | cub                    | I4 32 (214)<br>1 |                                | 8  | 10.38<br>±.02   |                |                 |                |                |                | r          | 44      |
| Cu <sub>3</sub> Se <sub>2</sub> *           | Umangite      | tet                    | P4/mmm (123)     |                                | 2  | 6.402<br>±.01   |                | 4.276<br>±.01   |                |                |                | r          | 8, 36   |
| Ni <sub>3</sub> S <sub>2</sub>              | Heazlewoodite | hex-R                  | R32 (155)        | Ni <sub>3</sub> S <sub>2</sub> | 3  | 5.746<br>±.001  |                | 7.134<br>±.002  |                |                |                |            | 77, 84  |
| Cu <sub>5</sub> FeS <sub>4</sub> *          | Hi-Bornite    | cub                    |                  |                                | 1  | 5.50<br>±.01    |                |                 |                |                |                | 240        | 95      |

## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula  | Name                    | Cry.<br>Sys. | Space<br>Group                                   | Structure<br>Type              | Z  | a <sub>o</sub>   | b <sub>o</sub> | c <sub>o</sub>  | α <sub>o</sub> | β <sub>o</sub> | ν <sub>o</sub> | Temp<br>°C | Ref          |
|--|-------------------------|--------------|--|--------------------------------|----|------------------|----------------|-----------------|----------------|----------------|----------------|------------|--------------|
| Cu <sub>5</sub> FeS <sub>4</sub> <sup>*</sup>  | Metastable Bornite      | cub          |  |                                | 8  | 10.94<br>±.02    |                |                 |                |                |                | r          | 95           |
| Cu <sub>5</sub> FeS <sub>4</sub> <sup>*</sup>  | Lo-Bornite              | tet          | P4 <sub>2</sub> c (144)                          |                                | 16 | 10.94<br>±.02    |                | 21.88<br>±.04   |                |                |                | r          | 95           |
| Ni <sub>11</sub> As <sub>8</sub>   | Maucherite              | tet          | P4 <sub>1</sub> 2 <sub>1</sub> <sup>2</sup> (92) |                                | 4  | 6.870<br>±.001   |                | 21.81<br>±.01   |                |                |                | r          | 176          |
| (Fe, Ni) <sub>9</sub> S <sub>8</sub><br>Fe <sub>5.25</sub> Ni <sub>3.75</sub> S <sub>8</sub> | Pentlandite             | cub          | Fm3m (225)                                       | Co <sub>9</sub> S <sub>8</sub> | 4  | 10.196<br>±.010  |                |                 |                |                |                | r          | 85           |
| (Fe, Ni) <sub>9</sub> S <sub>8</sub><br>Fe <sub>3.75</sub> Ni <sub>5.25</sub> S <sub>8</sub> | Pentlandite             | cub          | Fm3m (225)                                       | Co <sub>9</sub> S <sub>8</sub> | 4  | 10.095           |                |                 |                |                |                | r          | 85           |
| CaS  | Oldhamite               | cub          | Fm3m (225)                                       | NaCl                           | 4  | 5.689<br>±.006   |                |                 |                |                |                | r          | 152, 62, 115 |
| PbS  | Galena                  | cub          | Fm3m (225)                                       | NaCl                           | 4  | 5.9360<br>±.0002 |                |                 |                |                |                | r          | 10, 147, 167 |
| PbSe   | Glausthalite            | cub          | Fm3m (225)                                       | NaCl                           | 4  | 6.1255<br>±.0005 |                |                 |                |                |                | r          | 10           |
| PbTe   | Altaite                 | cub          | Fm3m (225)                                       | NaCl                           | 4  | 6.4606<br>±.0005 |                |                 |                |                |                | r          | 9            |
| MnS  | Albandite               | cub          | Fm3m (225)                                       | NaCl                           | 4  | 5.2234<br>±.0005 |                |                 |                |                |                | r          | 133, 9       |
| MnS  | sphalerite<br>structure | cub          | F43m (216)                                       | sphalerite                     | 4  | 5.611<br>±.002   |                |                 |                |                |                | r          | 132          |
| MnS  | wurtzite<br>structure   | hex          | P6 <sub>3</sub> mc (186)                         | ZnO                            | 2  | 3.9858<br>±.001  |                | 6.4654<br>±.002 |                |                |                | r          | 137          |
| PtS  | Cooperite               | tet          | P4 <sub>2</sub> /mmc (131)                       | PtS                            | 4  | 3.4699<br>±.0006 |                | 6.1098<br>±.001 |                |                |                | r          | 9, 56        |

## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula | Name           | Cry.<br>Sys. | Space<br>Group                                      | Structure<br>Type | Z | a <sub>o</sub>   | b <sub>o</sub> | c <sub>o</sub>   | α <sub>o</sub> | β <sub>o</sub> | v <sub>o</sub> | Temp<br>°C | Ref                 |
|---------|----------------|--------------|---|-------------------|---|------------------|----------------|------------------|----------------|----------------|----------------|------------|---------------------|
| CdS     | Greenockite    | hex          | P6 <sub>3</sub> mc (186)                            | ZnO               | 2 | 4.1354<br>±.0008 |                | 6.7120<br>±.0007 |                |                |                | r          | 137                 |
| CdS     | Hawleyite      | cub          | F43m (216)  | Sphalerite        | 4 | 5.833<br>±.002   |                |                  |                |                |                | r          | 132, 9, 48<br>164   |
| CdS     | (hypothetical) | cub          | Fm3m (225)  | NaCl              | 4 | 5.516<br>±.001   |                |                  |                |                |                | r          | 10                  |
| ZnS     | Sphalerite     | cub          | F43m (216)  | Sphalerite        | 4 | 5.4093<br>±.0002 |                |                  |                |                |                | r          | 10, 132, 135<br>136 |
| ZnS     | Wurtzite       | hex          | P6 <sub>3</sub> mc (186)                            | ZnO               | 2 | 3.8230<br>±.0010 |                | 6.2565<br>±.0010 |                |                |                | r          | 135, 137            |
| ZnSe    | Stilleite      | cub          | F43m (216)  | Sphalerite        | 4 | 5.6685<br>±.0004 |                |                  |                |                |                | r          | 10, 54              |
| ZnTe    |                | cub          | F43m (216)  | Sphalerite        | 4 | 6.1020<br>±.0005 |                |                  |                |                |                | r          | 9                   |
| HgS     | Cinnabar       | hex          | P3 <sub>2</sub> 1 (152)<br>P3 <sub>2</sub> 21 (154) | Cinnabar          | 3 | 4.149<br>±.001   |                | 9.495<br>±.002   |                |                |                | r          | 9, 149              |
| HgS     | Metacinnabar   | cub          | F43m (216)  | Sphalerite        | 4 | 5.8517<br>±.0010 |                |                  |                |                |                | r          | 9, 149              |
| HgSe    | Tiemannite     | cub          | F43m (216)  | Sphalerite        | 4 | 6.0853<br>±.0005 |                |                  |                |                |                | r          | 9, 152              |
| HgTe    | Coloradoite    | cub          | F43m (216)  | Sphalerite        | 4 | 6.4600<br>±.0005 |                |                  |                |                |                | r          | 9                   |
| FeS     | (hypothetical) | cub          | F43m (216)  | Sphalerite        | 4 | 5.455<br>±.001   |                |                  |                |                |                | r          | 132, 136            |



## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula                                     | Name           | Cry.<br>Sys. | Space<br>Group             | Structure<br>Type | Z  | a <sub>o</sub>    | b <sub>o</sub> | c <sub>o</sub>   | α <sub>o</sub> | β <sub>o</sub> | γ <sub>o</sub> | Temp<br>°C | Ref     |
|---|----------------|--------------|----------------------------|-------------------|----|-------------------|----------------|------------------|----------------|----------------|----------------|------------|---------|
| FeS   | (hypothetical) | hex          | P6 <sub>3</sub> mc (186)   | ZnO               | 2  | 3.872<br>±.001    |                | 6.345<br>±.002   |                |                |                | r          | 137     |
| CoS   | (hypothetical) | cub          | F43m (216)                 | Sphalerite        | 4  | 5.339<br>±.001    |                |                  |                |                |                | r          | 63      |
| CdSe  | Cadmoselite    | hex          | P6 <sub>3</sub> mc (186)   | ZnO               | 2  | 4.2977<br>±.0004  |                | 7.0021<br>±.0008 |                |                |                | r          | 9       |
| CdTe  |                | cub          | F43m (216)                 | Sphalerite        | 4  | 6.4805<br>±.0004  |                |                  |                |                |                | r          | 9       |
| CuFeS <sub>2</sub><br>CuFeS <sub>1.90</sub> | Chalcopyrite   | tet          | I42d (122)                 |                   | 4  | 5.2988<br>±.001   |                | 10.434<br>±.005  |                |                |                | r          | 9       |
| CuFeS <sub>2</sub> S <sub>3</sub> *         | Cubanite       | orth         | Pcmm (62)                  | Cubanite          | 4  | 6.46<br>±.01      | 11.12<br>±.01  | 6.23<br>±.01     |                |                |                | r          | 17      |
| AgFe <sub>2</sub> S <sub>3</sub> *          | Sternbergite   | orth         | Ccmm (63)                  |                   | 8  | 11.60<br>±.02     | 12.675<br>±.02 | 6.63<br>±.01     |                |                |                | r          | 109     |
| AgFe <sub>2</sub> S <sub>3</sub> *          | Argentopyrite  | orth         | Pmmm (47)                  |                   | 4  | 6.64<br>±.01      | 11.47<br>±.02  | 6.45<br>±.02     |                |                |                | r          | 98      |
| NiAs  | Niccolite      | hex          | P6 <sub>3</sub> /mmc (194) | NiAs              | 2  | 3.618<br>±.001    |                | 5.034<br>±.001   |                |                |                | r          | 176     |
| NiSb  | Breithauptite  | hex          | P6 <sub>3</sub> /mmc (194) | NiAs              | 2  | 3.942<br>±.001    |                | 5.155<br>±.001   |                |                |                | r          | 66      |
| CuS   | Covellite      | hex          | P6 <sub>3</sub> /mmc (194) | CuS               | 6  | 3.792<br>±.001    |                | 16.34<br>±.01    |                |                |                | r          | 149     |
| CuSe  | Klockmannite   | hex          |                            | Deformed<br>CuS   | 78 | √13x3.94<br>±.001 |                | 17.25<br>±.05    |                |                |                | r          | 35, 157 |

## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula                          | Name              | Cry.<br>Sys. | Space<br>Group          | Structure<br>Type                 | Z  | a <sub>o</sub>   | b <sub>o</sub>  | c <sub>o</sub>   | α <sub>o</sub> | β <sub>o</sub> | ν <sub>o</sub> | Temp<br>°C | Ref              |
|----------------------------------|-------------------|--------------|-------------------------|-----------------------------------|----|------------------|-----------------|------------------|----------------|----------------|----------------|------------|------------------|
| SnS                              | Herzenbergite     | orth         | Pbnm (62)               | GeS                               | 4  | 4.328<br>±.002   | 11.190<br>±.004 | 3.978<br>±.001   |                |                |                | r          | 96               |
| PbSnS <sub>2</sub>               | Teallite          | orth         | Pbnm (62)               | GeS                               | 2  | 4.266<br>±.003   | 11.419<br>±.007 | 4.090<br>±.002   |                |                |                | r          | 96               |
| AsS*                             | Realgar           | mon          | P2 <sub>1</sub> /m (11) |                                   | 16 | 9.29<br>±.05     | 13.53<br>±.05   | 6.57<br>±.03     |                | 106°33'        |                | r          | 13, 181          |
| NiS                              | Millerite         | hex-R        | R3m (160)               | Millerite                         | 9  | 9.616<br>±.001   |                 | 3.152<br>±.001   |                |                |                | r          | 9, 156<br>77, 84 |
| Sb <sub>2</sub> S <sub>3</sub>   | Stibnite          | orth         | Pbnm (62)               | Sb <sub>2</sub> S <sub>3</sub>    | 4  | 11.229<br>±.004  | 11.310<br>±.004 | 3.8389<br>±.0010 |                |                |                | 25         | 150              |
| Bi <sub>2</sub> S <sub>3</sub>   | Bismuthinite      | orth         | Pbnm                    | Sb <sub>2</sub> S <sub>3</sub>    | 4  | 11.150<br>±.004  | 11.300<br>±.004 | 3.981<br>±.001   |                |                |                | 26         | 149              |
| Bi <sub>2</sub> Te <sub>3</sub>  | Tellurobismuthite | hex-R        | R3m (166)               | Bi <sub>2</sub> Te <sub>2</sub> S | 3  | 4.3835<br>±.0005 |                 | 30.487<br>±.001  |                |                |                | r          | 41, 168          |
| As <sub>2</sub> S <sub>3</sub>   | Orpiment          | mon          | P2 <sub>1</sub> /n (14) | As <sub>2</sub> S <sub>3</sub>    | 4  | 11.49<br>±.02    | 9.59<br>±.02    | 4.25<br>±.01     |                | 90° 27'        |                | r          | 16               |
| Co <sub>3</sub> S <sub>4</sub>   | Linnaeite         | cub          | Fd3m (227)              | Cu <sub>3</sub> S <sub>4</sub>    | 8  | 9.401<br>±.005   |                 |                  |                |                |                | r          | 87               |
| Ni <sub>3</sub> S <sub>4</sub>   | Polydymite        | cub          | Fd3m (227)              | Ni <sub>3</sub> S <sub>4</sub>    | 8  | 9.480<br>±.001   |                 |                  |                |                |                | r          | 77               |
| FeNi <sub>2</sub> S <sub>4</sub> | Violarite         | cub          | Fd3m (227)              | Spinel                            | 8  | 9.464<br>±.005   |                 |                  |                |                |                | r          | 86               |
| FeCr <sub>2</sub> S <sub>4</sub> | Daubreeite        | cub          | Fd3m (227)              | Spinel                            | 8  | 9.966<br>±.005   |                 |                  |                |                |                | r          | 83               |

## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula                        | Name        | Cry.<br>Sys. | Space<br>Group             | Structure<br>Type | Z | a <sub>o</sub>   | b <sub>o</sub> | c <sub>o</sub>   | α <sub>o</sub> | β <sub>o</sub> | ν <sub>o</sub> | Temp<br>•C | Ref          |
|--------------------------------|-------------|--------------|----------------------------|-------------------|---|------------------|----------------|------------------|----------------|----------------|----------------|------------|--------------|
| FeS <sub>2</sub>               | Pyrite      | cub          | Pa3 (205)                  | Pyrite            | 4 | 5.4175<br>±.0005 |                |                  |                |                |                | r          | 133, 81, 53  |
| FeS                            | Troilite    | hex          | P6 <sub>3</sub> /mmc (194) | NiAs              | 2 | 3.446<br>±.003   |                | 5.877<br>±.001   |                |                |                | 28 ± 2     | 162          |
| Fe <sub>.980</sub> S           | Pyrrhotite  | hex          | P6 <sub>3</sub> /mmc (194) | defect NiAs       | 2 | 3.4461<br>±.001  |                | 5.8479<br>±.002  |                |                |                | 28 ± 2     | 162          |
| Fe <sub>.885</sub> S           | Pyrrhotite  | hex          | P6 <sub>3</sub> /mmc (194) | defect NiAs       | 2 | 3.4401<br>±.001  |                | 5.7090<br>±.003  |                |                |                | 28 ± 2     | 162          |
| FeS <sub>2</sub> <sup>*</sup>  | Marcasite   | orth         | Pnnm (58)                  | Marcasite         | 2 | 4.443<br>±.002   | 5.423<br>±.002 | 3.3876<br>±.0015 |                |                |                | 25         | 133, 14      |
| FeSe <sub>2</sub>              | Ferroselite | orth         | Pnnm (58)                  | Marcasite         | 2 | 4.801<br>±.005   | 5.778<br>±.005 | 3.587<br>±.004   |                |                |                | r          | 60, 8        |
| FeTe <sub>2</sub>              | Frobergite  | orth         | Pnnm (58)                  | Marcasite         | 2 | 5.265<br>±.005   | 6.265<br>±.005 | 3.869<br>±.002   |                |                |                | r          | 57           |
| CoS <sub>2</sub>               | Cattierite  | cub          | Pa3 (205)                  | Pyrite            | 4 | 5.535<br>±.005   |                |                  |                |                |                | r          | 87           |
| CoSe <sub>2</sub>              | Trogtalite  | cub          | Pa3 (205)                  | Pyrite            | 4 | 5.8588<br>±.001  |                |                  |                |                |                | r          | 20           |
| NiS <sub>2</sub>               | Vaesite     | cub          | Pa3 (205)                  | Pyrite            | 4 | 5.6873<br>±.0005 |                |                  |                |                |                | r          | 9, 77,<br>84 |
| NiSe <sub>2</sub>              |             | cub          | Pa3 (205)                  | Pyrite            | 4 | 5.9604<br>±.001  |                |                  |                |                |                | 20         | 58           |
| NiTe <sub>2</sub>              | Melonite    | hex          | P3m1 (164)                 | CdI <sub>2</sub>  | 1 | 3.869<br>±.01    |                | 5.308<br>±.01    |                |                |                | 84         | 158          |
| MnS <sub>2</sub>               | Hauerite    | cub          | Pa3 (205)                  | Pyrite            | 4 | 6.1014<br>±.0006 |                |                  |                |                |                | 28         | 133          |
| PtAs <sub>2</sub> <sup>*</sup> | Sperrylite  | cub          | Pa3 (205)                  | Pyrite            | 4 | 5.968<br>±.005   |                |                  |                |                |                | r          | 53, 159      |

## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula  | Name                    | Cry.<br>Sys. | Space<br>Group                     | Structure<br>Type     | Z  | a <sub>o</sub>   | b <sub>o</sub> | c <sub>o</sub>  | α <sub>o</sub> | β <sub>o</sub> | γ <sub>o</sub> | Temp<br>•C | Ref           |
|--|-------------------------|--------------|------------------------------------|-----------------------|----|------------------|----------------|-----------------|----------------|----------------|----------------|------------|---------------|
| RuS <sub>2</sub>   | Laurite                 | cub          | Pa3 (205)                          | Pyrite                | 4  | 5.60<br>±.02     |                |                 |                |                |                | r          | 7, 8, 28, 101 |
| NiAs <sub>2</sub>  | Rammelsbergite          | ortho        | Pnnm (58)                          | Marcasite             | 2  | 4.757<br>±.002   | 5.797<br>±.004 | 3.542<br>±.002  |                |                |                | 26         | 119, 155, 176 |
| NiAs <sub>2</sub>  | Pararammels-<br>bergite | ortho        | Pbca (61)                          |                       | 8  | 5.75<br>±.01     | 5.82<br>±.01   | 11.428<br>±.02  |                |                |                | r          | 107, 76       |
| FeAs <sub>2</sub>  | Loellingite             | ortho        | Pa3 (205)                          | Marcasite             | 2  | 5.300<br>±.002   | 5.981<br>±.002 | 2.882<br>±.001  |                |                |                | 26         | 119, 155      |
| CoAs <sub>2</sub>  | Co-safflorite           | mono         |                                    | Deformed<br>Marcasite | 2  | 5.049<br>±.002   | 5.872<br>±.002 | 3.127<br>±.001  |                | 90° 27'        |                | 26         | 119, 155      |
| (Co, Fe)As <sub>2</sub><br>Co <sub>0.5</sub> Fe <sub>0.5</sub> As <sub>2</sub> | Safflorite              | ortho        | Pnnm (58)                          | Marcasite             | 2  | 5.231<br>±.002   | 5.953<br>±.002 | 2.962<br>±.005  |                |                |                | 26         | 119, 155      |
| MoS <sub>2</sub>   | Molybdenite             | hex          | P6 <sub>3</sub> /mmc (194)         | MoS <sub>2</sub>      | 2  | 3.1604<br>±.0005 |                | 12.295<br>±.002 |                |                |                | 26         | 150           |
| WS <sub>2</sub>  | Tungstenite             | hex          | P6 <sub>3</sub> /mmc (194)         | MoS <sub>2</sub>      | 2  | 3.154<br>±.001   |                | 12.362<br>±.004 |                |                |                | 26         | 153           |
| FeAsS*   | Arsenopyrite            | tri          | P $\bar{1}$ (2)                    |                       | 4  | 5.760<br>±.010   | 5.690<br>±.005 | 5.785<br>±.005  | 90°            | 112° 14'       | 90°            | r          | 94            |
| FeSbS*   | Gudmundite              | mono         | B2 <sub>1</sub> /d (14)            |                       | 8  | 10.00<br>±.05    | 5.93<br>±.03   | 6.73<br>±.03    |                | ~90°           |                | r          | 15            |
| (Co, Fe)AsS*   | Glaucodot               | ortho        | Cmmm (65)                          |                       | 24 | 6.64<br>±.05     | 28.39<br>±.10  | 5.64<br>±.05    |                |                |                | r          | 8             |
| CoAsS*   | Cobaltite               | cub          | P2 <sub>1</sub> <sup>3</sup> (198) | NiSbS                 | 4  | 5.60<br>±.05     |                |                 |                |                |                | r          | 8             |

## SULFIDES, TELLURIDES, SELENIDES, AND ARSENIDES

| Formula                                     | Name                            | Cry.<br>Sys. | Space<br>Group          | Structure<br>Type | Z | a <sub>o</sub>    | b <sub>o</sub> | c <sub>o</sub>   | α <sub>o</sub> | β <sub>o</sub> | ν <sub>o</sub> | Temp<br>°C | Ref     |
|---|---------------------------------|--------------|-------------------------|-------------------|---|-------------------|----------------|------------------|----------------|----------------|----------------|------------|---------|
| NiAsS                                       | Gersdorffite                    | cub          | P2 <sub>1</sub> 3 (198) | NiAsS             | 4 | 5.693<br>±.001    |                |                  |                |                |                | 26         | 156     |
| FeAs <sub>3-x</sub><br>FeAs <sub>2.95</sub> | Fe-Skutterudite<br>hypothetical | cub          | Im3 (204)               | CoAs <sub>3</sub> | 8 | 8.1814<br>±.0009  |                |                  |                |                |                | r          | 118     |
| CoAs <sub>3-x</sub><br>CoAs <sub>2.95</sub> | Co-Skutterudite                 | cub          | Im3 (204)               | CoAs <sub>3</sub> | 8 | 8.2060<br>±.0009  |                |                  |                |                |                | r          | 118     |
| NiAs <sub>3-x</sub><br>NiAs <sub>2.95</sub> | Ni-Skutterudite<br>hypothetical | cub          | Im3 (204)               | CoAs <sub>3</sub> | 8 | 8.3300<br>±.0009  |                |                  |                |                |                | r          | 118     |
| Cu <sub>3</sub> AsS <sub>3</sub>            | Tennantite                      | cub          | I $\bar{4}$ 3m (217)    |                   | 8 | 10.190<br>±.004   |                |                  |                |                |                | 26         | 133     |
| Cu <sub>3</sub> SbS <sub>3</sub>            | Tetrahedrite                    | cub          | I $\bar{4}$ 3m (217)    |                   | 8 | 10.327<br>±.004   |                |                  |                |                |                | 26         | 133     |
| Cu <sub>3</sub> AsS <sub>4</sub>            | Enargite                        | orth         | Pnn2 (34)               |                   | 2 | 6.426             | 7.422          | 6.144            |                |                |                | 26         | 133     |
| Cu <sub>3</sub> AsS <sub>4</sub>            | Luzonite                        | tet          | I $\bar{4}$ 2m (121)    |                   | 2 | 5.289             |                | 10.440           |                |                |                | 26         | 133, 47 |
| Cu <sub>3</sub> SbS <sub>4</sub>            | Famatinite                      | tet          | I $\bar{4}$ 2m (121)    |                   | 2 | 5.384             |                | 10.770           |                |                |                | 26         | 133, 47 |
| Ag <sub>3</sub> AsS <sub>3</sub>            | Proustite                       | hex-R        | R3c (161)               |                   | 6 | 10.8160<br>±.0010 |                | 8.6948<br>±.0013 |                |                |                | 26         | 162     |
| Ag <sub>3</sub> SbS <sub>3</sub>            | Pyrargyrite                     | hex-R        | R3c (161)               |                   | 6 | 11.0520<br>±.0015 |                | 8.7177<br>±.0016 |                |                |                | 26         | 162     |



## OXIDES AND HYDROXIDES

| Formula                        | Name        | Cry.<br>Sys. | Space<br>Group           | Structure<br>Type                | Z  | a <sub>o</sub>   | b <sub>o</sub>   | c <sub>o</sub>   | α <sub>o</sub> | β <sub>o</sub>   | γ <sub>o</sub> | Temp<br>°C | Ref.    |
|--------------------------------|-------------|--------------|--------------------------|----------------------------------|----|------------------|------------------|------------------|----------------|------------------|----------------|------------|---------|
| Al <sub>2</sub> O <sub>3</sub> | Corundum    | hex-R        | R $\bar{3}$ c (167)      | α-Al <sub>2</sub> O <sub>3</sub> | 6  | 4.7591<br>±.0004 |                  | 12.9894<br>±.003 |                |                  |                | 25         | 70, 179 |
| AlO(OH)                        | Boehmite    | orth         | Cmcm (63)                | γ-FeO(OH)                        | 4  | 2.868<br>±.003   | 12.227<br>±.003  | 3.700<br>±.003   |                |                  |                | 26         | 148     |
| AlO(OH)*                       | Diaspore    | orth         | Pbnm (62)                |                                  | 4  | 4.401<br>±.005   | 2.421<br>±.005   | 2.845<br>±.002   |                |                  |                | r          | 19, 148 |
| Al(OH) <sub>3</sub>            | Gibbsite    | mon          | P2 <sub>1</sub> /n (14)  |                                  | 8  | 9.719<br>±.002   | 5.0705<br>±.0010 | 8.6412<br>±.0010 |                | 94° 34'<br>± 15' |                | r          | 32      |
| As <sub>2</sub> O <sub>3</sub> | Arsenolite  | cub          | Fd3m (227)               | diamond                          | 16 | 11.074<br>±.005  |                  |                  |                |                  |                | 25         | 146     |
| BeO                            | Bromellite  | hex          | P6 <sub>3</sub> mc (186) |                                  | 2  | 2.698<br>±.005   |                  | 4.380<br>±.005   |                |                  |                | 26         | 146     |
| CaO                            | Lime        | cub          | Fm3m (225)               | NaCl                             | 4  | 4.8108<br>±.0005 |                  |                  |                |                  |                | 26         | 12, 146 |
| Ca(OH) <sub>2</sub>            | Portlandite | hex          | P $\bar{3}$ m1 (164)     | CdI <sub>2</sub>                 | 1  | 3.5933<br>±.0005 |                  | 4.9086<br>±.002  |                |                  |                | 26         | 12, 146 |
| CdO                            |             | cub          | Fm3m (225)               | NaCl                             | 4  | 4.6953<br>±.001  |                  |                  |                |                  |                | 27         | 147     |
| CeO <sub>2</sub>               | Cerianite   | cub          | Fm3m (225)               | CaF <sub>2</sub>                 | 4  | 5.4110<br>±.002  |                  |                  |                |                  |                | 26         | 146     |
| CoO                            |             | cub          | Fm3m (225)               | NaCl                             | 4  | 4.260<br>±.002   |                  |                  |                |                  |                | 26         | 154     |
| Cr <sub>2</sub> O <sub>3</sub> | Eskolaite   | hex-R        | R $\bar{3}$ c (167)      | α-Al <sub>2</sub> O <sub>3</sub> | 6  | 4.954<br>±.002   |                  | 13.584<br>±.002  |                |                  |                | 26         | 150     |
| CuO                            | Tenorite    | mon          | C2/c (15)                |                                  | 4  | 4.684<br>±.005   | 3.425<br>±.005   | 5.129<br>±.005   |                | 99° 28'<br>±10'  |                | 26         | 146     |
| Cu <sub>2</sub> O              | Cuprite     | cub          | Pn3m (224)               | Cu <sub>2</sub> O                | 2  | 4.2696<br>±.001  |                  |                  |                |                  |                | 26         | 147     |
| Fe <sub>.953</sub> O           | Wustite     | cub          | Fm3m (225)               | NaCl(defect)                     | 4  | 4.3088<br>±.0003 |                  |                  |                |                  |                | 17         | 170     |

## OXIDES AND HYDROXIDES continued

| Formula                        | Name          | Cry. Sys. | Space Group                | Structure Type                   | Z  | a <sub>o</sub>                             | b <sub>o</sub>              | c <sub>o</sub>                            | α <sub>o</sub> or α <sub>r</sub> | β <sub>o</sub>  | γ <sub>o</sub> | Temp °C | Ref.     |
|--------------------------------|---------------|-----------|----------------------------|----------------------------------|----|--|-----------------------------|---|----------------------------------|-----------------|----------------|---------|----------|
| Fe <sub>2</sub> O <sub>3</sub> | Hematite      | hex-R     | R $\bar{3}$ c (167)        | α-Al <sub>2</sub> O <sub>3</sub> | 6  | 5.0329<br>±.001<br>a <sub>r</sub> = 5.4266 |                             | 13.749 <sub>2</sub><br>±.001 <sub>2</sub> | 55° 15.4'<br>±5'                 |                 |                | 25      | 59, 169  |
| Fe <sub>3</sub> O <sub>4</sub> | Magnetite     | cub       | Fd3m (227)                 | spinel                           | 8  | 8.3940<br>±.0005                           |                             |   |                                  |                 |                | 22      | 1, 161   |
| α-FeO(OH)*                     | Goethite      | orth      | Pbnm (62)                  |                                  | 4  | 4.596<br>±.05                              | 9.957<br>±.010              | 3.021<br>±.003                            |                                  |                 |                | r       | 108      |
| γ-FeO(OH)*                     | Lepidocrocite | orth      | Amam (63)                  |                                  | 4  | 3.868<br>±.010                             | 12.52 <sub>5</sub><br>±.010 | 3.066<br>±.010                            |                                  |                 |                | r       | 108      |
| H <sub>2</sub> O               | Ice           | hex       | P6 <sub>3</sub> /mmc(194)  |                                  | 4  | 4.5212<br>±.0010                           |                             | 7.3666<br>±.0010                          |                                  |                 |                | 0       | 79       |
| HfO <sub>2</sub>               | Hafnia        | mon       | P2 <sub>1</sub> /c (14)    | ZrO <sub>2</sub>                 | 4  | 5.1156<br>±.001                            | 5.1722<br>±.001             | 5.2948<br>±.001                           |                                  | 99° 11'<br>± 5' |                | r       | 2        |
| HgO                            | Montroydite   | orth      | Pnma (62)                  |                                  | 4  | 6.608<br>±.003                             | 5.518<br>±.003              | 3.519<br>±.003                            |                                  |                 |                | 25      | 154      |
| MgO                            | Periclase     | cub       | Fm3m (225)                 | NaCl                             | 4  | 4.2117<br>±.0005                           |                             |   |                                  |                 |                | 25      | 131, 146 |
| Mg(OH) <sub>2</sub>            | Brucite       | hex       | P $\bar{3}$ ml (164)       | CdI <sub>2</sub>                 | 1  | 3.147<br>±.004                             |                             | 4.769<br>±.004                            |                                  |                 |                | 26      | 151      |
| MnO                            | Manganosite   | cub       | Fm3m (225)                 | NaCl                             | 4  | 4.4448<br>±.0005                           |                             |   |                                  |                 |                | 26      | 150, 49  |
| MnO <sub>2</sub>               | Pyrolusite    | tet       | P4/mnm (136)               | rutile                           | 2  | 4.388<br>±.003                             |                             | 2.865<br>±.002                            |                                  |                 |                | r       | 145, 32  |
| Mn <sub>2</sub> O <sub>3</sub> | Bixbyite      | cub       | Ia3 (206)                  | Tl <sub>2</sub> O <sub>3</sub>   | 16 | 9.411<br>±.005                             |                             |   |                                  |                 |                | 25      | 154      |
| Mn <sub>3</sub> O <sub>4</sub> | Hausmanite    | tet       | I4 <sub>1</sub> /amd (141) |                                  | 4  | 8.136<br>±.005                             |                             | 9.422<br>±.005                            |                                  |                 |                | 20      | 165      |
| MoO <sub>3</sub>               | Molybdite     | orth      | Pbnm (62)                  |                                  | 4  | 3.962<br>±.002                             | 13.858<br>±.005             | 3.697<br>±.004                            |                                  |                 |                | 26      | 148      |

## OXIDES AND HYDROXIDES continued

| Formula                        | Name           | Cry.<br>Sys. | Space<br>Group   | Structure<br>Type    | Z  | a <sub>o</sub>    | b <sub>o</sub>  | c <sub>o</sub>    | α <sub>o</sub> | β <sub>o</sub>   | γ <sub>o</sub> | Temp<br>°C | Ref.     |
|--------------------------------|----------------|--------------|--|----------------------|----|-------------------|-----------------|-------------------|----------------|------------------|----------------|------------|----------|
| NiO                            | Bunsenite      | cub          | Fm3m (225)   | NaCl                 | 4  | 4.177<br>±.002    |                 |                   |                |                  |                | 26         | 146      |
| PbO                            | Litharge       | tet          | P4/nmm (129)   |                      | 2  | 3.9759<br>±.004   |                 | 5.023<br>±.004    |                |                  |                | 27         | 147      |
| PbO                            | Massicot       | orth         | Pb2a (32)  |                      | 4  | 5.489<br>±.003    | 4.755<br>±.004  | 5.891<br>±.004    |                |                  |                | 27         | 147      |
| Sb <sub>2</sub> O <sub>3</sub> | Senarmontite   | cub          | Fm3m (225)   | arsenic<br>trioxide  | 16 | 11.152<br>±.003   |                 |                   |                |                  |                | 26         | 148      |
| Sb <sub>2</sub> O <sub>3</sub> | Valentinite    | orth         | Pccn (56)  | antimony<br>trioxide | 4  | 4.914<br>±.002    | 12.468<br>±.005 | 5.421<br>±.004    |                |                  |                | 25         | 155      |
| SiO <sub>2</sub> *             | α-Quartz       | hex          | P3 <sub>1</sub> 21 (152)<br>P3 <sub>2</sub> 21 (154)                           |                      | 3  | 4.91355<br>±.0001 |                 | 5.40512<br>±.0001 |                |                  |                | 25         | 42, 179  |
| SiO <sub>2</sub> *             | β-Quartz       | hex          | P6 <sub>4</sub> 22 (181)<br>P6 <sub>2</sub> 22 (180)                           |                      | 3  | 4.9990<br>±.0005  |                 | 5.4592<br>±.0005  |                |                  |                | 575        | 42, 71   |
| SiO <sub>2</sub>               | α-Cristobalite | tet          | P4 <sub>1</sub> 2 <sub>1</sub> 2 (92)<br>P4 <sub>3</sub> 2 <sub>1</sub> 2 (96) |                      | 4  | 4.971<br>±.003    |                 | 6.918<br>±.003    |                |                  |                | 25         | 155      |
| SiO <sub>2</sub>               | β-Cristobalite | cub          | Fd3m (227)   |                      | 8  | 7.1382<br>±.0010  |                 |                   |                |                  |                | 405        | 139      |
| SiO <sub>2</sub>               | Keatite        | tet          | P4 <sub>1</sub> 2 <sub>1</sub> 2 (92)<br>P4 <sub>3</sub> 2 <sub>1</sub> 2 (96) |                      | 12 | 7.456<br>±.003    |                 | 8.604<br>±.005    |                |                  |                | r          | 129, 182 |
| SiO <sub>2</sub>               | β-Tridymite    | hex          | P6 <sub>2</sub> c (172)<br>P6 <sub>3</sub> /mmd (194)                          |                      | 4  | 5.0463<br>±.0020  |                 | 8.2563<br>±.0030  |                |                  |                | 405        | 139      |
| SiO <sub>2</sub> *             | Coesite        | mon          | B2/b (15)  |                      | 16 | 7.152<br>±.001    | 12.379<br>±.002 | 7.152<br>±.001    |                | 120° 00'<br>±10' |                | 25         | 133      |
| SiO <sub>2</sub> *             | Stishovite     | tet          | P4/mnm (136)   | rutile               | 2  | 4.1790<br>±.001   |                 | 2.6649<br>±.001   |                |                  |                | r          | 23       |
| SiO <sub>2</sub> *             | Melanophlogite | cub          | P4 <sub>2</sub> 32 (208)   |                      | 48 | 13.402<br>±.004   |                 |                   |                |                  |                | r          | 180      |
| SnO <sub>2</sub>               | Cassiterite    | tet          | P4/mnm (136)   | rutile               | 2  | 4.738<br>±.003    |                 | 3.188<br>±.003    |                |                  |                | 26         | 146      |

## OXIDES AND HYDROXIDES continued

-10-

| Formula                       | Name           | Cry.<br>Sys. | Space<br>Group   | Structure<br>Type | Z | a <sub>o</sub>    | b <sub>o</sub>  | c <sub>o</sub>               | α <sub>o</sub> | β <sub>o</sub> | γ <sub>o</sub> | Temp<br>°C | Ref.            |
|-------------------------------|----------------|--------------|--|-------------------|---|-------------------|-----------------|------------------------------|----------------|----------------|----------------|------------|-----------------|
| TeO <sub>2</sub> <sup>*</sup> | Tellurite      | orth         | Pbca (61)  | tellurite         | 8 | 5.607<br>±.003    | 12.034<br>±.005 | 5.463<br>±.003               |                |                |                | 25         | 154             |
| TeO <sub>2</sub>              | Para-tellurite | tet          | P4 <sub>1</sub> 2 <sub>1</sub> 2 (92)<br>P4 <sub>3</sub> 2 <sub>1</sub> 2 (96) |                   | 4 | 4.810<br>±.002    |                 | 7.613<br>±.002               |                |                |                | 25         | 155             |
| ThO <sub>2</sub>              | Thorianite     | cub          | Fm3m (225)   | CaF <sub>2</sub>  | 4 | 5.59525<br>±.0005 |                 |                              |                |                |                | 25         | 131, 146        |
| TiO <sub>2</sub>              | Rutile         | tet          | P4/mnm (136)   | rutile            | 2 | 4.59374<br>±.0005 |                 | 2.9617 <sub>7</sub><br>±.002 |                |                |                | 25         | 144, 27,<br>146 |
| TiO <sub>2</sub>              | Anatase        | tet          | I4 <sub>1</sub> /amd (141)   |                   | 4 | 3.785<br>±.002    |                 | 9.514<br>±.006               |                |                |                | r          | 27, 146         |
| TiO <sub>2</sub> <sup>*</sup> | Brookite       | orth         | Pcab (61)  |                   | 8 | 5.447<br>±.010    | 9.185<br>±.010  | 5.145<br>±.010               |                |                |                | r          | 32              |
| UO <sub>2</sub>               | Uraninite      | cub          | Fm3m (225)   | CaF <sub>2</sub>  | 4 | 5.4682<br>±.001   |                 |                              |                |                |                | 26         | 147             |
| ZnO                           | Zincite        | hex          | P6 <sub>3</sub> mc (186)   | ZnO               | 2 | 3.2495<br>±.0005  |                 | 5.2069<br>±.0005             |                |                |                | 25         | 64              |
| ZrO <sub>2</sub>              | Baddeleyite    | mon          | P2 <sub>1</sub> /c (14)  | ZrO <sub>2</sub>  | 4 | 5.1454<br>±.001   | 5.2075<br>±.001 | 5.3107<br>±.001              |                | 99° 14'<br>±5' |                | r          | 2               |

## SPINELS, ALUMINATES AND TITINATES

| Formula                          | Name          | Cry.<br>Sys. | Space<br>Group    | Structure<br>Type | Z | a <sub>o</sub>   | b <sub>o</sub>   | c <sub>o</sub>   | α <sub>o</sub> | β <sub>o</sub> | γ <sub>o</sub> | Temp<br>°C | Ref.   |
|----------------------------------|---------------|--------------|-------------------|-------------------|---|------------------|------------------|------------------|----------------|----------------|----------------|------------|--------|
| BeAl <sub>2</sub> O <sub>4</sub> | Chrysoberyl   | orth         | Pnma (62)         | olivine           | 4 | 9.4041<br>±.003  | 5.4756<br>±.002  | 4.4267<br>±.002  |                |                |                | 25         | 154    |
| MgAl <sub>2</sub> O <sub>4</sub> | Spinel        | cub          | Fd3m (227)        | spinel            | 8 | 8.0800<br>±.002  |                  |                  |                |                |                | 26         | 147    |
| FeAl <sub>2</sub> O <sub>4</sub> | Hercynite     | cub          | Fd3m (227)        | spinel            | 8 | 8.154<br>±.003   |                  |                  |                |                |                | 25         | 163    |
| MnAl <sub>2</sub> O <sub>4</sub> | Galaxite      | cub          | Fd3m (227)        | spinel            | 8 | 8.258<br>±.002   |                  |                  |                |                |                | 25         | 154    |
| ZnAl <sub>2</sub> O <sub>4</sub> | Gahnite       | cub          | Fd3m (227)        | spinel            | 8 | 8.0848<br>±.002  |                  |                  |                |                |                | 26         | 147    |
| FeFe <sub>2</sub> O <sub>4</sub> | Magnetite     | cub          | Fd3m (227)        | spinel            | 8 | 8.3940<br>±.0005 |                  |                  |                |                |                | 22         | 1, 161 |
| MnFe <sub>2</sub> O <sub>4</sub> | Jacobsite     | cub          | Fd3m (227)        | spinel            | 8 | 8.499<br>±.005   |                  |                  |                |                |                | 25         | 154    |
| NiFe <sub>2</sub> O <sub>4</sub> | Trevorite     | cub          | Fd3m (227)        | spinel            | 8 | 8.339<br>±.005   |                  |                  |                |                |                | 25         | 155    |
| MgCr <sub>2</sub> O <sub>4</sub> | Picrochromite | cub          | Fd3m (227)        | spinel            | 8 | 8.333<br>±.005   |                  |                  |                |                |                | 26         | 154    |
| CaTiO <sub>3</sub>               | Perovskite    | orth         | Pcmn (62)         | perovskite        | 4 | 5.3670<br>±.0001 | 7.6438<br>±.0001 | 5.4439<br>±.0001 |                |                |                | r          | 74     |
| FeTiO <sub>3</sub> *             | Ilmenite      | hex-R        | R $\bar{3}$ (148) | ilmenite          | 6 | 5.018<br>±.005   |                  | 14.055<br>±.010  |                |                |                | r          | 104    |
| MgTiO <sub>3</sub>               | Geikielite    | hex-R        | R $\bar{3}$ (148) | ilmenite          | 6 | 5.054<br>±.005   |                  | 13.898<br>±.005  |                |                |                | 26         | 150    |



HALIDES

| Formula                            | Name        | Cry.<br>Sys. | Space<br>Group           | Structure<br>Type | Z | a <sub>o</sub>                         | b <sub>o</sub>                         | c <sub>o</sub>                         | α <sub>o</sub> | β <sub>o</sub>  | γ <sub>o</sub> | Temp<br>°C | Ref.    |
|------------------------------------|-------------|--------------|--------------------------|-------------------|---|--|--|--|----------------|-----------------|----------------|------------|---------|
| NaCl                               | Halite      | cub          | Fm3m (225)               | NaCl              | 4 | 5.6402<br>±.0002                       |  |  |                |                 |                | 26         | 147     |
| KCl                                | Sylvite     | cub          | Fm3m (225)               | NaCl              | 4 | 6.2931<br>±.0002                       |  |  |                |                 |                | 25         | 146     |
| NaF                                | Villiaumite | cub          | Fm3m (225)               | NaCl              | 4 | 4.6342<br>±.0005                       |  |  |                |                 |                | 25         | 146     |
| AgBr                               | Bromyrite   | cub          | Fm3m (225)               | NaCl              | 4 | 5.7745<br>±.0005                       |  |  |                |                 |                | 26         | 149     |
| AgCl                               | Cerargyrite | cub          | Fm3m (225)               | NaCl              | 4 | 5.5491<br>±.0005                       |  |  |                |                 |                | 26         | 149     |
| AgI                                | Iodyrite    | hex          | P6 <sub>3</sub> mc (186) | ZnO               | 2 | 4.5922<br>±.002                        |  | 7.510<br>±.005                         |                |                 |                | 25         | 153     |
| AgI                                | Miersite    | cub          | F43m (216)               | Sphalerite        | 4 | 6.495<br>±.005                         |  |  |                |                 |                | r          | 166     |
| CaF <sub>2</sub>                   | Fluorite    | cub          | Fm3m (225)               | CaF <sub>2</sub>  | 4 | 5.4626<br>±.0003                       |  |  |                |                 |                | 25         | 146, 4  |
| MgF <sub>2</sub>                   | Sellaite    | tet          | P4 <sub>2</sub> /mm(136) | Cassiterite       | 2 | 4.621<br>±.001                         |  | 3.050<br>±.001                         |                |                 |                | 18         | 34, 149 |
| HgCl                               | Calomel     | tet          | I4/mm (139)              |                   | 4 | 4.478<br>±.005                         |  | 10.91<br>±.005                         |                |                 |                | 26         | 146     |
| Na <sub>3</sub> AlF <sub>6</sub> * | Cryolite    | mon          | P2 <sub>1</sub> /n (14)  |                   | 2 | 5.40 <sub>0</sub><br>±.01 <sup>0</sup> | 5.60 <sub>1</sub><br>±.01 <sup>1</sup> | 7.77 <sub>6</sub><br>±.01 <sup>6</sup> |                | 90° 11'<br>+15' |                | r          | 104     |
| NaMgF <sub>3</sub>                 | Neighborite | orth         | Pcmn (62)                | Perovskite        | 4 | 5.363<br>±.001                         | 7.676<br>±.001                         | 5.503<br>±.001                         |                |                 |                | 18         | 22      |

## CARBONATES AND NITRATES

| Formula  | Name           | Cry<br>Sys. | Space<br>Group      | Structure<br>Type | Z | a <sub>o</sub>                              | b <sub>o</sub> | c <sub>o</sub>  | α <sub>o</sub> or α <sub>r</sub> | β <sub>o</sub> | γ <sub>o</sub> | Temp<br>°C | Ref. |
|--|----------------|-------------|---------------------|-------------------|---|---|----------------|-----------------|----------------------------------|----------------|----------------|------------|------|
| BaMg(CO <sub>3</sub> ) <sub>2</sub> <sup>*</sup>               | Norsethite     | hex-R       | R32 (155)           | calcite           | 3 | 5.020<br>±.005<br>a <sub>r</sub> = 6.29     |                | 16.75<br>±.02   | ±05'<br>47° 02'                  |                |                | r          | 97   |
| CaCO <sub>3</sub>  | Calcite        | hex-R       | R $\bar{3}$ c (167) | calcite           | 6 | 4.9899<br>±.0002<br>a <sub>r</sub> = 6.3760 |                | 17.064<br>±.001 |                                  |                |                | 26±3       | 55   |
| CaMg(CO <sub>3</sub> ) <sub>2</sub> <sup>*</sup>               | Dolomite       | hex-R       | R $\bar{3}$ (148)   | calcite           | 3 | 4.8079<br>±.0010<br>a <sub>r</sub> = 6.0154 |                | 16.010<br>±.003 |                                  |                |                | 26±3       | 55   |
| CdCO <sub>3</sub>  | Otavite        | hex-R       | R $\bar{3}$ c (167) | calcite           | 6 | 4.9204<br>±.0005<br>a <sub>r</sub> = 6.1306 |                | 16.298<br>±.003 |                                  |                |                | 26±3       | 55   |
| CoCO <sub>3</sub>  | Cobalticalcite | hex-R       | R $\bar{3}$ c (167) | calcite           | 6 | 4.6581<br>±.0005<br>a <sub>r</sub> = 5.6650 |                | 14.958<br>±.002 |                                  |                |                | 26±3       | 55   |
| FeCO <sub>3</sub>  | Siderite       | hex-R       | R $\bar{3}$ c (167) | calcite           | 6 | 4.6887<br>±.0004<br>a <sub>r</sub> = 5.7954 |                | 15.373<br>±.004 |                                  |                |                | 26±3       | 55   |
| MgCO <sub>3</sub>  | Magnesite      | hex-R       | R $\bar{3}$ c (167) | calcite           | 6 | 4.6330<br>±.0003<br>a <sub>r</sub> = 5.6752 |                | 15.016<br>±.002 |                                  |                |                | 26±3       | 55   |
| Mg <sub>3</sub> Ca(CO <sub>3</sub> ) <sub>4</sub> <sup>*</sup> | Huntite        | hex-R       | R32 (155)           | calcite           | 3 | 9.5062<br>±.003<br>a <sub>r</sub> = 6.0762  |                | 7.8219<br>±.004 |                                  |                |                | 26±3       | 55   |
| MnCO <sub>3</sub>  | Rhodochrosite  | hex-R       | R $\bar{3}$ c (167) | calcite           | 6 | 4.7771<br>±.0003<br>a <sub>r</sub> = 5.9050 |                | 15.664<br>±.003 |                                  |                |                | 26±3       | 55   |
| NiCO <sub>3</sub>  |                | hex-R       | R $\bar{3}$ c (167) | calcite           | 6 | 4.5975<br>±.0005<br>a <sub>r</sub> = 5.5795 |                | 14.723<br>±.002 |                                  |                |                | 26±3       | 55   |

## CARBONATES AND NITRATES continued

| Formula   | Name         | Cry.<br>Sys | Space<br>Group   | Structure<br>Type | Z | a <sub>o</sub>                              | b <sub>o</sub>  | c <sub>o</sub>  | α <sub>o</sub> or α <sub>r</sub> | β <sub>o</sub>  | γ <sub>o</sub> | Temp<br>°C | Ref. |
|---|--------------|-------------|--|-------------------|---|---|-----------------|-----------------|----------------------------------|-----------------|----------------|------------|------|
| ZnCO <sub>3</sub>   | Smithsonite  | hex-R       | R $\bar{3}$ c (167)  | calcite           | 6 | 4.6528<br>±.0003<br>a <sub>r</sub> = 5.6833 |                 | 15.025<br>±.003 | 48° 19.6'                        |                 |                | 26±3       | 55   |
| BaCO <sub>3</sub>   | Witherite    | orth        | Pmcn (62)  | aragonite         | 4 | 5.314<br>±.005                              | 8.904<br>±.005  | 6.430<br>±.005  |                                  |                 |                | 26         | 147  |
| CaCO <sub>3</sub>   | Aragonite    | orth        | Pmcn (62)  | aragonite         | 4 | 4.959<br>±.005                              | 7.968<br>±.005  | 5.741<br>±.005  |                                  |                 |                | 26         | 148  |
| PbCO <sub>3</sub>   | Cerussite    | orth        | Pmcn (62)  | aragonite         | 4 | 5.195<br>±.005                              | 8.436<br>±.005  | 6.152<br>±.005  |                                  |                 |                | 26         | 147  |
| SrCO <sub>3</sub>   | Strontianite | orth        | Pmcn (62)  | aragonite         | 4 | 5.107<br>±.005                              | 8.414<br>±.005  | 6.029<br>±.005  |                                  |                 |                | 26         | 148  |
| <sup>-23</sup> Cu <sub>2</sub> (OH) <sub>2</sub> CO <sub>3</sub>  | Malachite    | mon         | P2 <sub>1</sub> /a (14)  | complex           | 4 | 9.502<br>±.007                              | 11.974<br>±.007 | 3.240<br>±.003  |                                  | 98° 45'<br>±15' |                | 25         | 155  |
| Cu <sub>3</sub> (OH) <sub>2</sub> (CO <sub>3</sub> ) <sub>2</sub> | Azurite      | mon         | P2 <sub>1</sub> /c (14)  | complex           | 2 | 5.008<br>±.005                              | 5.844<br>±.005  | 10.336<br>±.005 |                                  | 92° 27'<br>±15' |                | 25         | 155  |
| CaCO <sub>3</sub>   | Vaterite     | hex         |  |                   | 6 | 7.135<br>±.005                              |                 | 8.524<br>±.007  |                                  |                 |                | r          | 88   |
| KNO <sub>3</sub>  | Niter        | orth        | Pmcn (62)  | aragonite         | 4 | 5.414<br>±.005                              | 9.164<br>±.005  | 6.431<br>±.005  |                                  |                 |                | 26         | 148  |
| NaNO <sub>3</sub>   | Soda Niter   | hex-R       | R $\bar{3}$ c (167)  | calcite           | 6 | 5.0696<br>±.0010<br>a <sub>r</sub> = 6.3273 |                 | 16.829<br>±.005 | 47° 9.8'                         |                 |                | 25         | 151  |
| Cu <sub>2</sub> (NO <sub>3</sub> )(OH) <sub>3</sub>               | Gerhardite   | orth        | P2 <sub>1</sub> <sup>2</sup> <sub>1</sub> <sup>2</sup> <sub>1</sub> (41) |                   | 4 | 5.592<br>±.004                              | 6.075<br>±.004  | 13.812<br>±.008 |                                  |                 |                | r          | 111  |

## SULFATES AND BORATES

| Formula  | Name         | Cry.<br>Sys. | Space<br>Group   | Structure<br>Type               | Z | a <sub>o</sub>                           | b <sub>o</sub>  | c <sub>o</sub>            | α <sub>o</sub>  | β <sub>o</sub>   | γ <sub>o</sub>  | Temp<br>°C | Ref. |
|--|--------------|--------------|--|---------------------------------|---|--|-----------------|---------------------------|-----------------|------------------|-----------------|------------|------|
| BaSO <sub>4</sub>  | Barite       | orth         | Pnma (62)  | BaSO <sub>4</sub>               | 4 | 8.878<br>±.005                           | 5.450<br>±.005  | 7.152<br>±.003            |                 |                  |                 | 26         | 148  |
| CaSO <sub>4</sub>  | Anhydrite    | orth         | Ccmm (63)<br>Bbmm  | CaSO <sub>4</sub>               | 4 | 6.238<br>±.005                           | 6.991<br>±.005  | 6.996<br>±.005            |                 |                  |                 | 26         | 149  |
| PbSO <sub>4</sub>  | Anglesite    | orth         | Pnma (62)  | BaSO <sub>4</sub>               | 4 | 8.480<br>±.005                           | 5.398<br>±.005  | 6.958<br>±.003            |                 |                  |                 | 25         | 148  |
| SrSO <sub>4</sub>  | Celestite    | orth         | Pnma (62)  | BaSO <sub>4</sub>               | 4 | 8.359<br>±.005                           | 5.352<br>±.005  | 6.866<br>±.005            |                 |                  |                 | 26         | 147  |
| ZnSO <sub>4</sub>  | Zinkosite    | orth         | Pnma (62)  | BaSO <sub>4</sub>               | 4 | 8.588<br>±.008                           | 6.740<br>±.006  | 4.770<br>±.005            |                 |                  |                 | 25         | 152  |
| K <sub>2</sub> SO <sub>4</sub>                                       | Arcanite     | orth         | Pnma (62)  | K <sub>2</sub> SO <sub>4</sub>  | 4 | 5.772<br>±.005                           | 10.072<br>±.005 | 7.483<br>±.004            |                 |                  |                 | 25         | 148  |
| Na <sub>2</sub> SO <sub>4</sub>                                      | Thenardite   | orth         | Fddd (70)  | Na <sub>2</sub> SO <sub>4</sub> | 8 | 5.863<br>±.005                           | 12.304<br>±.005 | 9.821<br>±.005            |                 |                  |                 | 25         | 147  |
| CaSO <sub>4</sub> ·2H <sub>2</sub> O*                                | Gypsum       | mon          | C2/c (15)  |                                 | 4 | 6.58<br>±.010                            | 15.18<br>±.010  | 6.29<br>±.010             |                 | 113° 50'<br>±15' |                 | r          | 104  |
| MgSO <sub>4</sub> ·7H <sub>2</sub> O                                 | Epsomite     | orth         | P2 <sub>1</sub> <sup>2</sup> <sub>1</sub> <sup>2</sup> <sub>1</sub> (41) |                                 | 4 | 11.964<br>±.01                           | 12.054<br>±.01  | 6.879<br>±.01             |                 |                  |                 | 25         | 104  |
| Na <sub>2</sub> SO <sub>4</sub> ·10H <sub>2</sub> O                  | Mirabilite   | mon          | P2 <sub>1</sub> /c (14)  |                                 | 4 | 11.51<br>±.01                            | 10.38<br>±.01   | 12.83<br>±.01             |                 | 107° 45'<br>±10' |                 | 24         | 121  |
| CuSO <sub>4</sub> ·5H <sub>2</sub> O                                 | Chalcanthite | tri          | P $\bar{1}$ (2)  |                                 | 2 | 6.104 <sub>5</sub><br>±.005 <sub>5</sub> | 10.72<br>±.01   | 5.949<br>±.007            | 97° 34'<br>±10' | 107° 17'<br>±10' | 77° 26'<br>±10' | r          | 39   |
| Cu <sub>4</sub> SO <sub>4</sub> (OH) <sub>6</sub> *                  | Brochantite  | mon          | P2 <sub>1</sub> /c (14)  |                                 | 4 | 13.06 <sub>6</sub><br>±.01               | 9.85<br>±.01    | 6.02 <sub>2</sub><br>±.01 |                 | 103° 16'<br>±15' |                 | r          | 32   |
| K <sub>2</sub> Ca(SO <sub>4</sub> ) <sub>2</sub> ·H <sub>2</sub> O   | Syngenite    | mon          | P2 <sub>1</sub> /m (11)  |                                 | 2 | 9.775<br>±.005                           | 7.156<br>±.005  | 6.251<br>±.005            |                 | 104° 00'<br>±15' |                 | r          | 6    |
| CaB <sub>3</sub> O <sub>4</sub> (OH) <sub>3</sub> ·H <sub>2</sub> O* | Colemanite   | mon          | P2 <sub>1</sub> /a (14)  |                                 |   | 8.743<br>±.004                           | 11.264<br>±.002 | 6.102<br>±.003            |                 | 110° 7'<br>±5'   |                 | r          | 24   |
| Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> ·10H <sub>2</sub> O    | Borax        | mon          | C2/c (15)  |                                 | 4 | 11.858<br>±.005                          | 10.674<br>±.005 | 12.197<br>±.005           |                 | 106° 41'<br>±2'  |                 | r          | 92   |

## SULFATES AND BORATES

| Formula   | Name         | Cry.<br>Sys. | Space<br>Group          | Structure<br>Type | Z | a <sub>o</sub> | b <sub>o</sub> | c <sub>o</sub>  | α <sub>o</sub> | β <sub>o</sub>    | γ <sub>o</sub> | Temp.<br>°C | Ref.    |
|---|--------------|--------------|-------------------------|-------------------|---|----------------|----------------|-----------------|----------------|-------------------|----------------|-------------|---------|
| Na <sub>2</sub> B <sub>4</sub> O <sub>7</sub> ·4H <sub>2</sub> O    | Kernite      | mon          | P2 <sub>1</sub> /c (14) |                   | 4 | 7.022<br>±.003 | 9.151<br>±.004 | 15.676<br>±.008 |                | 108° 50'<br>± 15' |                | r           | 120     |
| KAl <sub>3</sub> (SO <sub>4</sub> ) <sub>2</sub> (OH) <sub>6</sub>  | Alunite      | hex-R        | R3m (160)               |                   | 3 | 6.982<br>±.005 |                | 17.32<br>±.01   |                |                   |                | r           | 11, 105 |
| NaAl <sub>3</sub> (SO <sub>4</sub> ) <sub>2</sub> (OH) <sub>6</sub> | Natroalunite | hex-R        | R3m (160)               |                   | 3 | 6.974<br>±.005 |                | 16.69<br>±.01   |                |                   |                | r           | 105     |

PHOSPHATES, MOLYBDATES AND TUNGSTATES

| Formula  | Name            | Cry.<br>Sys. | Space<br>Group   | Structure<br>Type    | Z | a <sub>o</sub>   | b <sub>o</sub> | c <sub>o</sub>  | α <sub>o</sub> | β <sub>o</sub>  | γ <sub>o</sub> | Temp<br>°C | Ref. |
|--|-----------------|--------------|--|----------------------|---|------------------|----------------|-----------------|----------------|-----------------|----------------|------------|------|
| AlPO <sub>4</sub>                                  | Berlinite       | hex          | P3 <sub>1</sub> 21 (152)<br>or P3 <sub>2</sub> 21(154) | α-quartz             | 3 | 4.942<br>±.005   |                | 10.97<br>±.007  |                |                 |                | 25         | 155  |
| Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> OH | Hydroxylapatite | hex          | P6 <sub>3</sub> /m (176)                               | apatite              | 2 | 9.432<br>±.005   |                | 6.881<br>±.005  |                |                 |                | r          | 114  |
| YPO <sub>4</sub>                                   | Xenotime        | tet          | I4 <sub>1</sub> /amd (141)                             | zircon               | 4 | 6.885<br>±.005   |                | 5.982<br>±.005  |                |                 |                | 26         | 153  |
| CaMoO <sub>4</sub>                                 | Powellite       | tet          | I4 <sub>1</sub> /a (100)                               | calcium<br>tungstate | 4 | 5.226<br>±.005   |                | 11.43<br>±.007  |                |                 |                | 25         | 151  |
| PbMoO <sub>4</sub>                                 | Wulfenite       | tet          | I4 <sub>1</sub> /a (100)                               | calcium<br>tungstate | 4 | 5.435<br>±.007   |                | 12.11<br>±.007  |                |                 |                | 25         | 152  |
| CaWO <sub>4</sub>                                  | Seheelite       | tet          | I4 <sub>1</sub> /a (100)                               | calcium<br>tungstate | 4 | 5.242<br>±.005   |                | 11.372<br>±.005 |                |                 |                | 25         | 151  |
| PbWO <sub>4</sub>                                  | Stolzite        | tet          | I4 <sub>1</sub> /a (100)                               | calcium<br>tungstate | 4 | 5.4616<br>±.0020 |                | 12.046<br>±.002 |                |                 |                | 25         | 152  |
| FeWO <sub>4</sub>                                  | Ferberite       | mon          | P2/c (13)  | wolframite           | 2 | 4.732<br>±.004   | 5.708<br>±.003 | 4.965<br>±.004  |                | 90° 00'<br>±03' |                | r          | 127  |
| MnWO <sub>4</sub>                                  | Huebnerite      | mon          | P2/c (13)  | wolframite           | 2 | 4.834<br>±.004   | 5.758<br>±.003 | 4.999<br>±.004  |                | 91° 11'<br>±03' |                | r          | 127  |
| Fe <sub>5</sub> Mn <sub>5</sub> WO <sub>4</sub>    | Wolframite      | mon          | P2/c (13)  | wolframite           | 2 | 4.782<br>±.004   | 5.731<br>±.003 | 4.982<br>±.004  |                | 90° 34'<br>±03' |                | r          | 127  |
| Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> F  | Fluorapatite    | hex          | P6 <sub>3</sub> /m (176)                               | apatite              | 2 | 9.369<br>±.005   |                | 6.884<br>±.003  |                |                 |                | r          | 89   |
| Ca <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> Cl | Chlorapatite    | hex          | P6 <sub>3</sub> /m (176)                               | apatite              | 2 | 9.629<br>±.005   |                | 6.777<br>±.003  |                |                 |                | r          | 89   |



## SILICATES

| Formula  | Name           | Cry.<br>Sys. | Space<br>Group          | Structure<br>Type | Z | a <sub>o</sub>             | b <sub>o</sub>              | c <sub>o</sub>             | α <sub>o</sub>  | β <sub>o</sub>   | γ <sub>o</sub>   | Temp<br>°C | Ref. |
|--|----------------|--------------|-------------------------|-------------------|---|----------------------------|-----------------------------|----------------------------|-----------------|------------------|------------------|------------|------|
| Al <sub>2</sub> SiO <sub>5</sub> *                                   | Andalusite     | orth         | Pnnm (58)               |                   | 4 | 7.7959<br>±.005            | 7.8983<br>±.002             | 5.5583<br>±.002            |                 |                  |                  | 25         | 134  |
| Al <sub>2</sub> SiO <sub>5</sub> *                                   | Kyanite        | tri          | P $\bar{1}$ (2)         |                   | 4 | 7.123<br>±.001             | 7.848<br>±.002              | 5.564<br>±.008             | 89° 55'<br>±09' | 101° 15'<br>±05' | 105° 58'<br>±05' | 25         | 134  |
| Al <sub>2</sub> SiO <sub>5</sub> *                                   | Sillimanite    | orth         | Pbnm<br>Pnma (62)       |                   | 4 | 7.4843<br>±.003            | 7.6730<br>±.003             | 5.7711<br>±.004            |                 |                  |                  | 25         | 134  |
| Ca <sub>3</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>      | Grossularite   | cub          | Ia3d (230)              | garnet            | 8 | 11.851<br>±.001            |                             |                            |                 |                  |                  | 25         | 130  |
| Ca <sub>3</sub> Cr <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>      | Uvarovite      | cub          | Ia3d (230)              | garnet            | 8 | 11.999<br>±.002            |                             |                            |                 |                  |                  | 26         | 155  |
| Ca <sub>3</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>      | Andradite      | cub          | Ia3d (230)              | garnet            | 8 | 12.048<br>±.001            |                             |                            |                 |                  |                  | 25         | 130  |
| -27- Fe <sub>3</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>12</sub> | Almandite      | cub          | Ia3d (230)              | garnet            | 8 | 12.526<br>±.001            |                             |                            |                 |                  |                  | 25         | 130  |
| Mg <sub>3</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>      | Pyrope         | cub          | Ia3d (230)              | garnet            | 8 | 11.459<br>±.001            |                             |                            |                 |                  |                  | 25         | 130  |
| Mn <sub>3</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>      | Spessartite    | cub          | Ia3d (230)              | garnet            | 8 | 11.621<br>±.001            |                             |                            |                 |                  |                  | 25         | 130  |
| γ-Ca <sub>2</sub> SiO <sub>4</sub> *                                 | Lime Olivine   | orth         | Pbnm (62)               | olivine           | 4 | 5.07 <sub>0</sub><br>±.020 | 11.30 <sub>3</sub><br>±.020 | 6.79 <sub>4</sub><br>±.020 |                 |                  |                  | r          | 102  |
| Fe <sub>2</sub> SiO <sub>4</sub>                                     | Fayalite       | orth         | Pbnm (62)               | olivine           | 4 | 4.817<br>±.005             | 10.477<br>±.005             | 6.105<br>±.010             |                 |                  |                  | r          | 175  |
| Mg <sub>2</sub> SiO <sub>4</sub>                                     | Forsterite     | orth         | Pbnm (62)               | olivine           | 4 | 4.758<br>±.002             | 10.214<br>±.003             | 5.984<br>±.002             |                 |                  |                  | 25         | 133  |
| Mn <sub>2</sub> SiO <sub>4</sub> *                                   | Tephroite      | orth         | Pbnm (62)               | olivine           | 4 | 4.871<br>±.005             | 10.636<br>±.005             | 6.232<br>±.005             |                 |                  |                  | r          | 68   |
| CaMgSiO <sub>4</sub> *   | Monticellite   | orth         | Pbnm (62)               | olivine           | 4 | 4.827<br>±.005             | 11.084<br>±.005             | 6.376<br>±.005             |                 |                  |                  | r          | 124  |
| CaFeSiO <sub>4</sub>   | Kirschsteinite | orth         | Pbnm (62)               | olivine           | 4 | 4.886<br>±.005             | 11.146<br>±.005             | 6.434<br>±.010             |                 |                  |                  | r          | 124  |
| β-Ca <sub>2</sub> SiO <sub>4</sub> *                                 | Larnite        | mon          | P2 <sub>1</sub> /n (14) |                   | 4 | 5.48<br>±.02               | 6.76<br>±.02                | 9.28<br>±.02               |                 | 94° 33'<br>±20'  |                  | r          | 91   |

SILICATES continued

| Formula  | Name             | Cry.<br>Sys. | Space<br>Group    | Structure<br>Type | Z  | a <sub>o</sub>   | b <sub>o</sub> | c <sub>o</sub>                 | α <sub>o</sub> or α <sub>r</sub> | β <sub>o</sub>    | γ <sub>o</sub>   | Temp<br>°C | Ref.    |
|--|------------------|--------------|-------------------|-------------------|----|--|----------------|--------------------------------|----------------------------------|-------------------|------------------|------------|---------|
| Be <sub>2</sub> SiO <sub>4</sub> *                                       | Phenacite        | hex-R        | R $\bar{3}$ (148) | phenacite         | 18 | 12.472<br>±.005<br>a <sub>r</sub> = 7.708 <sub>2</sub> |                | 8.252<br>±.005                 | 108° 0.42'                       |                   |                  | 25         | 153     |
| Zn <sub>2</sub> SiO <sub>4</sub>   | Willemite        | hex-R        | R $\bar{3}$ (148) | phenacite         | 18 | 13.94<br>±.01<br>a <sub>r</sub> = 8.123                |                | 3.309<br>±.003                 | 118° 11'                         |                   |                  | 25         | 152     |
| ThSiO <sub>4</sub>   | Thorite          | tet          | I4/amd (141)      | zircon            | 4  | 7.143<br>±.004   |                | 6.327<br>±.003                 |                                  |                   |                  | r          | 46      |
| ZrSiO <sub>4</sub>   | Zircon           | tet          | I4/amd (141)      | zircon            | 4  | 6.604<br>±.005   |                | 5.979<br>±.005                 |                                  |                   |                  | 25         | 149     |
| USiO <sub>4</sub>  | Coffinite        | tet          | I4/amd (141)      | zircon            | 4  | 6.995<br>±.004   |                | 6.263<br>±.005<br>7.07<br>±.01 |                                  |                   |                  | r          | 46      |
| KAl <sub>2</sub> (AlSi <sub>3</sub> O <sub>10</sub> )(OH) <sub>2</sub> * | Muscovite        | mon          | C2/c (15)         | mica (2M)         | 4  | 5.203<br>±.005   | 8.995<br>±.007 | 20.030<br>±.005                |                                  | 94° 28'<br>±30'   |                  | 27         | 174, 40 |
| KMg <sub>3</sub> (AlSi <sub>3</sub> O <sub>10</sub> )(OH) <sub>2</sub> * | Phlogopite       | mon          | Cm (8)            | mica (1M)         | 2  | 5.314<br>±.01  | 9.204<br>±.02  | 10.314<br>±.005                |                                  | 99° 54'<br>±10'   |                  | r          | 173     |
| KMg <sub>3</sub> (AlSi <sub>3</sub> O <sub>10</sub> )F <sub>2</sub>      | Fluor-Phlogopite | mon          | Cm (8)            | mica (1M)         | 2  | 5.299<br>±.004   | 9.188<br>±.002 | 10.135<br>±.002                |                                  | 99° 55'<br>±3'    |                  | r          | 75      |
| KFe <sub>3</sub> (AlSi <sub>3</sub> O <sub>10</sub> )(OH) <sub>2</sub>   | Annite           | mon          | Cm (8)            | mica (1M)         | 2  | 5.391<br>±.01  | 9.350<br>±.004 | 10.313<br>±.02                 |                                  | 99° 42'<br>±15'   |                  | 26         | 172     |
| Al <sub>2</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub> *      | Pyrophyllite     | mon          | C2/c (15)         | sheet             | 4  | 5.14<br>±.02   | 8.90<br>±.02   | 18.55<br>±.03                  |                                  | 99° 55'<br>±5'    |                  | r          | 61      |
| Mg <sub>3</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub> *      | Talc             | mon          | C2/c (15)         | sheet             | 4  | 5.287<br>±.007   | 9.158<br>±.008 | 18.95<br>±.01                  |                                  | 99° 30'           |                  | r          | 142     |
| Al <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> (OH) <sub>4</sub> *       | Kaolinite        | tri          |                   |                   |    | 5.155<br>±.007   | 8.959<br>±.010 | 7.407<br>±.008                 | 91° 41'<br>± 20'                 | 104° 52'<br>± 20' | 89° 56'<br>± 20' | r          | 52      |
| Al <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> (OH) <sub>4</sub> *       | Dickite          | mon          | Cc (9)            | sheet             | 4  | 5.150<br>±.002   | 8.940<br>±.003 | 14.424<br>±.005                |                                  | 96° 44'<br>±5'    |                  | r          | 100     |

## SILICATES continued

| Formula   | Name               | Cry.<br>Sys. | Space<br>Group  | Structure<br>Type | Z  | a <sub>o</sub>  | b <sub>o</sub>  | c <sub>o</sub>  | α <sub>o</sub>   | β <sub>o</sub>   | γ <sub>o</sub>   | Temp<br>°C | Ref      |
|---|--------------------|--------------|-----------------|-------------------|----|-----------------|-----------------|-----------------|------------------|------------------|------------------|------------|----------|
| CaSiO <sub>3</sub> <sup>*</sup>   | Parawollastonite   | mon          | P2 <sub>1</sub> | (4)               | 12 | 15.417<br>±.004 | 7.321<br>±.002  | 7.066<br>±.002  |                  | 95° 24'<br>±3'   |                  | r          | 160, 106 |
| CaSiO <sub>3</sub> <sup>*</sup>   | Pseudowollastonite | tri<br>(mon) |                 |                   | 24 | 6.90<br>±.02    | 11.78<br>±.02   | 19.65<br>±.02   |                  | 90° 48'<br>±15'  |                  | r          | 72       |
| Ca <sub>2</sub> NaHSi <sub>3</sub> O <sub>9</sub> <sup>*</sup>                                    | Pectolite          | tri          | P $\bar{1}$     | (2) wollastonite  | 2  | 7.99<br>±.01    | 7.04<br>±.01    | 7.02<br>±.01    | 90° 03'<br>±15'  | 95° 17'<br>±15'  | 102° 28'<br>±15' | r          | 18       |
| CaSiO <sub>3</sub> <sup>*</sup>   | Wollastonite       | tri          | P $\bar{1}$     | (2) wollastonite  | 6  | 7.94<br>±.01    | 7.32<br>±.01    | 7.07<br>±.01    | 90°02'<br>± 15'  | 95°22'<br>± 15'  | 103°26'<br>± 15' | r          | 18, 106  |
| MgSiO <sub>3</sub> <sup>*</sup>   | Clino-Enstatite    | mon          | C2/c            | (15) diopside     | 8  | 9.618<br>±.005  | 8.825<br>±.005  | 5.186<br>±.005  |                  | 108° 21'<br>±5'  |                  | r          | 93       |
| MgSiO <sub>3</sub> <sup>*</sup>   | Enstatite          | orth         | Pcab            | (61)              | 16 | 8.829<br>±.01   | 18.22<br>±.01   | 5.192<br>±.01   |                  |                  |                  | 26         | 151, 65  |
| MnSiO <sub>3</sub> <sup>*</sup>   | Rhodonite          | tri          | P $\bar{1}$     | (2) wollastonite  | 10 | 6.68<br>±.02    | 7.66<br>±.03    | 12.20<br>±.04   | 111° 06'<br>±20' | 86° 00'<br>±20'  | 93° 12'<br>±20'  | r          | 82       |
| CaMg(SiO <sub>3</sub> ) <sub>2</sub>  | Diopside           | mon          | C2/c            | (15) diopside     | 4  | 9.743<br>±.005  | 8.923<br>±.005  | 5.251<br>±.005  |                  | 74° 04'<br>±15'  |                  | r          | 125      |
| CaFe(SiO <sub>3</sub> ) <sub>2</sub> <sup>*</sup>   | Hedenbergite       | mon          | C2/c            | (15) diopside     | 4  | 9.854<br>±.010  | 9.024<br>±.010  | 5.263<br>±.010  |                  | 75° 46'<br>±20'  |                  | r          | 78       |
| NaAlSi <sub>2</sub> O <sub>6</sub> <sup>*</sup>   | Jadeite            | mon          | C2/c            | (15) diopside     | 4  | 9.499<br>±.020  | 8.608<br>±.010  | 5.241<br>±.020  |                  | 107° 26'<br>±15' |                  | r          | 171      |
| Ca <sub>2</sub> Mg <sub>5</sub> Si <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub> <sup>*</sup>    | Tremolite          | mon          | C2/m            | (12) tremolite    | 2  | 9.840<br>±.006  | 18.052<br>±.005 | 5.275<br>±.005  |                  | 104° 42'<br>±15' |                  | r          | 177      |
| Ca <sub>2</sub> Mg <sub>5</sub> Si <sub>8</sub> O <sub>22</sub> F <sub>2</sub>                    | Fluor-Tremolite    | mon          | C2/m            | (12) tremolite    | 2  | 9.781<br>±.005  | 18.007<br>±.004 | 5.267<br>±.006  |                  | 104° 30'         |                  | 20         | 26       |
| Na <sub>2</sub> Mg <sub>3</sub> Fe <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub> | Mg-Riebecite       | mon          | I2/m            | (12) hornblende   | 2  | 10.04<br>±.01   | 18.02<br>±.01   | 5.28<br>±.01    |                  | 72° 00'<br>±30'  |                  | r          | 37       |
| Na <sub>2</sub> Mg <sub>3</sub> Al <sub>2</sub> Si <sub>8</sub> O <sub>22</sub> (OH) <sub>2</sub> | Glaucophane        | mon          |                 | hornblende        | 2  | 9.99<br>±.01    | 17.92<br>±.01   | 5.27<br>±.01    |                  | 71° 38'<br>±15'  |                  | r          | 38       |
| Be <sub>3</sub> Al <sub>2</sub> (Si <sub>6</sub> O <sub>18</sub> ) <sup>*</sup>                   | Beryl              | hex          | P6/mmc (192)    |                   | 2  | 9.215<br>±.005  |                 | 9.192<br>±.005  |                  |                  |                  | 25         | 154      |
| Mg <sub>2</sub> Al <sub>3</sub> (AlSi <sub>5</sub> O <sub>18</sub> )                              | Hi-Cordierite      | hex          | P6/mmc (192)    |                   | 2  | 9.7698<br>±.003 |                 | 9.3517<br>±.003 |                  |                  |                  | r          | 128      |

SILICATES continued

| Formula  | Name          | Cry.<br>Sys. | Space<br>Group  | Structure<br>Type | Z  | a <sub>o</sub>                          | b <sub>o</sub>             | c <sub>o</sub>             | α <sub>o</sub> or α <sub>r</sub> | β <sub>o</sub>    | γ <sub>o</sub>   | Temp<br>°C | Ref.          |
|--|---------------|--------------|-----------------|-------------------|----|---|----------------------------|----------------------------|----------------------------------|-------------------|------------------|------------|---------------|
| Mg <sub>2</sub> Al <sub>3</sub> (AlSi <sub>5</sub> O <sub>18</sub> )                               | Lo-Cordierite | orth         | Cccm (66)       |                   | 4  | 17.0621<br>±.005                        | 9.7208<br>±.003            | 9.3389<br>±.003            |                                  |                   |                  | r          | 128           |
| CaAl <sub>2</sub> Si <sub>2</sub> O <sub>8</sub> *   | Anorthite     | tri          | C $\bar{1}$ (2) | feldspar          | 4  | 8.1768<br>±.002                         | 12.8768<br>±.003           | 7.0845<br>±.002            | 93° 10.0'<br>±2'                 | 115° 50.8'<br>±2' | 91° 13.3'<br>±2' | r          | 25, 51        |
| NaAlSi <sub>3</sub> O <sub>8</sub> *   | Albite        | tri          | C $\bar{1}$ (2) | feldspar          | 4  | 8.1353<br>±.002                         | 12.7883<br>±.003           | 7.1542<br>±.002            | 94° 13.6'<br>±1'                 | 116° 31.1'<br>±1' | 87° 42.5'<br>±1' | r          | 25, 140<br>80 |
| NaAlSi <sub>3</sub> O <sub>8</sub>   | Hi-Albite     | tri          |                 | feldspar          | 4  | 8.171<br>±.005                          | 12.872<br>±.005            | 7.108<br>±.005             | 93° 28'<br>±10'                  | 116° 23'<br>±10'  | 90° 14'<br>±10'  | r          | 140, 80       |
| KAlSi <sub>3</sub> O <sub>8</sub> *  | Microcline    | tri          | C $\bar{1}$ (2) | feldspar          | 4  | 8.577<br>±.01                           | 12.967<br>±.01             | 7.223<br>±.01              | 90° 39'<br>±5'                   | 115° 56'<br>±5'   | 87° 42'<br>±5'   | r          | 80            |
| KAlSi <sub>3</sub> O <sub>8</sub>  | Sanidine      | mon          | C2/m (12)       | feldspar          | 4  | 8.617<br>±.005                          | 13.030<br>±.005            | 7.176<br>±.005             |                                  | 116° 4.6'<br>±10' |                  | r          | 31            |
| CaTiSiO <sub>5</sub> *   | Sphene        | mon          | A2/a (15)       |                   | 4  | 7.07 <sub>4</sub><br>±.010              | 8.71 <sub>8</sub><br>±.010 | 6.56 <sub>3</sub><br>±.010 |                                  | 113° 57'<br>±15'  |                  | r          | 32            |
| Zn <sub>4</sub> (OH) <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> ·H <sub>2</sub> O*                | Hemimorphite  | orth         | Imm2 (35)       | hemimorphite      | 2  | 8.370<br>±.005                          | 10.719<br>±.005            | 5.120<br>±.005             |                                  |                   |                  | 25         | 147           |
| (AlF) <sub>2</sub> SiO <sub>4</sub> *  | Topaz         | orth         | Pmnb (62)       |                   | 4  | 8.394<br>±.005                          | 8.792<br>±.007             | 4.649<br>±.003             |                                  |                   |                  |            | 156           |
| NaMg <sub>3</sub> Al <sub>6</sub> B <sub>3</sub> Si <sub>6</sub> O <sub>27</sub> (OH) <sub>4</sub> | Dravite       | hex-R        | R3m (160)       | tourmaline        | 3  | 15.93<br>±.01<br>a <sub>r</sub> = 9.50  |                            | 7.18<br>±.01               |                                  | 113° 53'          |                  | r          | 117           |
| CaMg <sub>4</sub> Al <sub>5</sub> B <sub>3</sub> Si <sub>6</sub> O <sub>27</sub> (OH) <sub>4</sub> | Uvite         | hex-R        | R3m (160)       | tourmaline        | 3  | 15.86<br>±.01<br>a <sub>r</sub> = 9.465 |                            | 7.19<br>±.01               |                                  | 114° 5'           |                  | r          | 117           |
| NaAlSi <sub>2</sub> O <sub>6</sub> ·H <sub>2</sub> O   | Analcite      | cub          | Ia3d (230)      | zeolite           | 16 | 13.733<br>±.005                         |                            |                            |                                  |                   |                  | r          | 123           |
| Na <sub>2</sub> Al <sub>2</sub> Si <sub>3</sub> O <sub>10</sub> ·2H <sub>2</sub> O                 | Natrolite     | orth         | Fdd2 (43)       |                   |    | 18.30<br>±.01                           | 18.63<br>±.01              | 6.60<br>±.01               |                                  |                   |                  | r          | 90            |

## SILICATES continued

| Formula  | Name                      | Cry.<br>Sys. | Space<br>Group                                    | Structure<br>Type | Z   | a <sub>o</sub>              | b <sub>o</sub>              | c <sub>o</sub>              | α <sub>o</sub> | β <sub>o</sub>  | γ <sub>o</sub> | Temp<br>°C | Ref.     |
|--|---------------------------|--------------|---|-------------------|-----|-----------------------------|-----------------------------|-----------------------------|----------------|-----------------|----------------|------------|----------|
| NaAlSiO <sub>4</sub>   | Lo-Nepheline              | hex          | C6 <sub>3</sub> (178)                             |                   | 8   | 9.986<br>±.005              |                             | 8.330<br>±.004              |                |                 |                | r          | 33, 141  |
| NaAlSiO <sub>4</sub>   | Hi-Carnegeite             | cub          |   |                   | 4   | 7.325<br>±.007              |                             |                             |                |                 |                | 750        | 141      |
| KAlSiO <sub>4</sub> *  | Kaliophilite<br>natural   | hex          | P6 <sub>3</sub> 22 (182)                          |                   | 54  | 26.930<br>±.010             |                             | 8.522<br>±.004              |                |                 |                | r          | 141      |
| KAlSiO <sub>4</sub>  | Kaliophilite<br>synthetic | hex          | P6 <sub>3</sub> (173)<br>P6 <sub>3</sub> 22 (182) |                   | 2   | 5.180<br>±.002              |                             | 8.559<br>±.004              |                |                 |                | r          | 141      |
| KAlSiO <sub>4</sub>  | Kalsilite                 | hex          |   |                   | 2   | 5.159 <sub>7</sub><br>±.002 |                             | 8.7032<br>±.002             |                |                 |                | r          | 141      |
| -18- KAlSi <sub>2</sub> O <sub>6</sub> *   | Hi-Leucite                | cub          |   |                   |     | 13.43<br>±.01               |                             |                             |                |                 |                | 625        | 32       |
| LiAlSi <sub>2</sub> O <sub>6</sub>   | β-Spodumene               | tet          | P4 <sub>3</sub> 2 <sub>1</sub> 2 (96)             |                   |     | 7.5332<br>±.0008            |                             | 9.1540<br>±.0008            |                |                 |                | 25         | 138      |
| Ca <sub>2</sub> MgSi <sub>2</sub> O <sub>7</sub>                                     | Akermanite                | tet          |   |                   | 2   | 7.843 <sub>5</sub><br>±.003 |                             | 5.010<br>±.003              |                |                 |                | r          | 5        |
| Ca <sub>2</sub> Al <sub>2</sub> Si <sub>2</sub> O <sub>7</sub>                       | Gehlenite                 | tet          |   |                   | 2   | 7.690<br>±.003              |                             | 5.067 <sub>5</sub><br>±.003 |                |                 |                | r          | 5        |
| CaAl <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> (OH) <sub>2</sub> ·H <sub>2</sub> O | Lawsonite                 | orth         | Ccmm (63)   |                   | 4   | 8.787<br>±.005              | 5.836<br>±.005              | 13.123<br>±.008             |                |                 |                | r          | 112, 103 |
| 3Al <sub>2</sub> O <sub>3</sub> ·2SiO <sub>2</sub>                                   | 3·2 Mullite               | orth         |   |                   | 3   | 7.557<br>±.002              | 7.687 <sub>6</sub><br>±.002 | 2.884 <sub>2</sub><br>±.001 |                |                 |                | r          | 3        |
| 2Al <sub>2</sub> O <sub>3</sub> ·SiO <sub>2</sub>                                    | 2·1 Mullite               | orth         | Pbam (55)   |                   | 6/5 | 7.578 <sub>8</sub><br>±.001 | 7.690 <sub>9</sub><br>±.002 | 2.888 <sub>3</sub><br>±.001 |                |                 |                | r          | 3, 122   |
| Ca <sub>2</sub> Al <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub> (OH)                | Zoisite                   | orth         | Pnma (62)   |                   | 4   | 16.15<br>±.01               | 5.581<br>±.005              | 10.06<br>±.01               |                |                 |                | r          | 113      |
| Ca <sub>2</sub> Al <sub>3</sub> (SiO <sub>4</sub> ) <sub>3</sub> (OH)                | Clino zoisite             | mon          | P2 <sub>1</sub> /m (11)                           |                   | 2   | 8.887<br>±.007              | 5.581<br>±.005              | 10.14<br>±.01               |                | 115°56'<br>±20' |                | r          | 113      |

## REFERENCES

1. Abrahams and Calhoun, *Acta Cryst.* 6 , 105, 1953.
2. Adam and Rodgers, *Acta Cryst.* 12, 951, 1959.
3. Agrell and Smith, *J. Am. Ceram. Soc.* 43 69, 1960.
4. Allen, *Am. Min.* 37, 910, 1952.
5. Andrews, *Min. Mag.* 28, 374, 1948.
6. Aruja, *Min. Mag.* 31, 943, 1958.
7. Bannister, *Min. Mag.* 23, 195, 1932.
8. Berry and Thompson, *Mem. 85, Geol. Soc. Am.*, 281p., 1962.
9. Bethke, P. M., unpublished data.
10. Bethke and Barton, *U. S. Geol. Surv. Prof. Paper 424B*, 266, 1961.
11. Brophy, Scott, Snellgrove, *Am. Min.* 47, 112, 1962.
12. Brunauer, Kantro, and Weise, *Can. J. Chem.* 34, 729, 1956.
13. Buerger, *Am. Min.* 20, 36, 1935.
14. ———, *Zeit. Krist.* 97, 504, 1937.
15. ———, *Am. Min.* 23, 4, 1939.
16. ———, *Am. Min.* 27, 301, 1942.
17. ———, *Am. Min.* 32, 415, 1945.
18. ———, *Pro. Nat. Acad. Sci.* 42, 113, 1956.
19. Busing and Levey, *Acta Cryst.* 11, 798, 1958.
20. Bøhm and others, *Acta. Chem. Scand.* 9, 1510, 1955.
21. Caron and Donohue, *Acta Cryst.* 14, 548, 1961.
22. Chao, Evans, Skinner, and Milton, *Am. Min.* 46, 379, 1961.
23. Chao, Fahey, Littler, and Milton, *J. Geophys. Res.* 67, 419, 1962.
24. Christ, *Am. Min.* 41, 569, 1956.
25. Cole, Sorum and Taylor, *Acta Cryst.* 4, 20, 1951.
26. Comeforo and Kohn, *Am. Min.* 39, 537, 1954.
27. Cromer and Herrington, *J. Am. Chem. Soc.* 77, 4708, 1955.
28. deJong and Hoog, *Rec. Trav. Chim.* 46, 173, 1927.



## REFERENCES

29. Djurle, *Acta Chem. Scand.* 12, 1415, 1958.
30. ———, *Acta Chem. Scand.* 12, 1427, 1958.
31. Donnay and Donnay, *Am. J. Sci.* Bowen vol., 115, 1952.
32. Donnay and Nowacki, *Crystal Data*, Memoir 60, Geol. Soc. Am., 1954.
33. Donnay, Schairer, and Donnay, *Min. Mag.* 32, 93, 1959.
34. Duncanson and Stevenson, *Pro. Phys. Soc.* 72, 1001, 1958.
35. Earley, *Am. Min.* 34, 433, 1949.
36. ———, *Am. Min.* 35, 337, 1950.
37. Ernst, *Geochim. et. Cosmochim. Acta.* 19, 10, 1960.
38. Ernst, *Am. J. Sci.* 259, 735, 1961.
39. Fisher, *Am. Min.* 37, 95, 1952.
40. Fournier, R. O., private communication June 1960.
41. Francombe, *Brit. J. Appl. Phys.* 9, 415, 1958.
42. Frondel and Hurlburt, *J. Chem. Phys.* 23, 1215, 1955.
43. Frueh, *Geol. Soc. Am. Bull.* 67, 1697, 1956.
44. ———, *Am. Min.* 44, 693, 1959.
45. ———, *Zeit. Krist.* 112, 44, 1959.
46. Fuchs and Gebert, *Am. Min.* 43, 243, 1958.
47. Gaines, *Am. Min.* 42, 766, 1957.
48. Goldschmidt, *Norsk. Vidensk. Akad. Oslo I Maf. Nat. Klasse*, no. 8, 1927.
49. Goldsmith and Graf, *Geochim. et Cosmochim. Acta* 11, 310, 1957.
50. Goldsmith and Laves, *Geochim. et. Cosmochim. Acta* 5, 1, 1954.
51. ———, *Zeit. f. Krist.* 106, 213, 1955.
52. Goodyear and Duffin, *Min. Mag.* 32, 902, 1961.
53. Gordon, *Am. Min.* 36, 918, 1951.

## REFERENCES

54. Goryunova and Fedorova, Sov. Phys. Solid State, 1, 307, 1959.
55. Graf, Am. Min. 46, 1283, 1961.
56. Grønqvold, Haraldson and Vinovde, Acta Chem. Scand. 14, 1879, 1960.
57. Grønqvold, Haraldson and Vihovde, Acta Chem. Scand. 8, 1927, 1954.
58. Grønqvold and Jacobsen, Acta Chem. Scand. 10, 1440, 1956.
59. Grønqvold and Westrum, J. Am. Chem. Soc. 81, 1780, 1959.
60. ———, Inorg. Chem. 1, 36, 1962.
61. Gruner, Zeit. f. Krist. 88, 412, 1934.
62. Güntert and Faessler, Zeit. Krist. 107, 357, 1956.
63. Hall, U. S. Geol. Surv. Prof. Paper 424B, 271, 1961.
64. Heller, McGannon, and Weber, J. Appl. Phys. 21, 1283, 1950.
65. Hess, Am. J. Sci. Bowen vol., 173, 1952.
66. Hewitt, Econ. Geol. 43, 408, 1948.
67. Hiller, Neues Jahrb. Mineral. Monatsch, 265, 1951.
68. Hurlburt, Am. Min. 46, 549, 1961.
69. Ievins, Straumanis, and Karlsons, Zeit.f. Phys. Chem. 40B, 347, 1938.
70. Jan, Steinman, and Dinichert, J. Phys. Chem. Solids 12, 349, 1960.
71. Jay, Pro. Roy. Soc. A142, 237, 1933.
72. Jeffery and Heller, Acta Cryst. 6, 807, 1953.
73. Jurriaanse, Zeit. Krist. 90, 322, 1953.
74. Kay and Bailey, Acta Cryst. 10, 219, 1957.
75. Kohn and Hatch, Am. Min. 40, 10, 1955.
76. Kullerud, Unpublished data.
77. Kullerud and Yund, J. Petrology 3, 126, 1962.
78. Kuno and Hess, Am. J. Sci. 251, 741, 1953.
79. LaPlaca and Post, Acta Cryst. 13, 503, 1960.

# REFERENCES

80. Laves, J. Geol. 60, 549, 1952.
81. Lepp, Am. Min. 41, 347, 1956.
82. Liebau, Hilmer and Lindeman, Acta Cryst. 12, 182, 1959.
83. Lundquist, Ark. Kem. Min. Geol. 17B, n.12, 1943.
84. ———, Ark. Kem. Min. Geol. 24A, n.21, 1947.
85. ———, Ark. Kem. Min. Geol. 24A, n.22, 1947.
86. ———, Ark. Kem. Min. Geol. 24A, n.23, 1947.
87. Lundquist and Westgren, Zeit. anorg. Chem. 239, 85, 1938.
88. McConnell, Min. Mag. 32, 534, 1960.
89. McConnell, Science 136, 241, 1962.
90. Meier, Zeit.f. Krist. 113, 430, 1960.
91. Midgley, Acta, Cryst. 5, 307, 1952.
92. Morimoto, Min. J. (Japan) 2, 1, 1956.
93. ———, Ann. Rept. Dir. Geophys. Lab. 58, 193, 1959.
94. Morimoto and Clark, Am. Min. 46, 1448, 1961.
95. Morimoto and Kullerud, Am. Min. 46, 1270, 1961.
96. Mosberg and others, U. S. Geol. Surv. Prof. Paper 424C, 347, 1961.
97. Mrose, Chao, Fahey, and Milton, Am. Min. 46, 420, 1961.
98. Murdoch and Berry, Am. Min. 39, 475, 1954.
99. Nelson and Riley, Pro. Phys. Soc. 57, 477, 1945.
100. Newman, Min. Mag. 32, 683, 1961.
101. Oftedal, Zeit. Phys. Chem. 135, 291, 1928.
102. O'Daniel and Tscheischwili, Zeit.f. Krist. 104, 124, 1942.
103. Pabst, Zeits, Krist. 115, 307, 1961. (Min. Abstracts 15, 337, 1962.)
104. Palache, Berman, and Frondel, Dana's System of Mineralogy 7th Ed. 2 volumes, John Wiley, New York 1944, 1951.
105. Parker, Am. Min. 47, 127, 1962.
106. Peacock, Am. J. Sci. XXX, 495, 1935.
107. ———, Univ. Toronto Stud. Geol. Ser. 42, 101, 1939.

# REFERENCES

108. ———, Trans. Roy. Soc. Can. IV 36, 107, 1942.
109. ———, Am. Min. 27, 229, 1942.
110. Peacock and McAndrew, Am. Min. 35, 425, 1950.
111. Oswald, Z. Krist. 116, 210, 1961.
112. Pistorious, Am. Min. 46, 982, 1961.
113. ———, J. Geol. 69, 604, 1961.
114. Posner, Perloff, and Diorio, Acta Cryst. 11, 308, 1958.
115. Primak, Kaufman and Ward, J. Am. Chem. Soc. 70, 2043, 1948.
116. Rahlfs, Zeit. Phys. Chem. B31, 157, 1936.
117. Robbins, Ann. Rept. Dir. Geophys. Lab. 58, 137, 1959.
118. Roseboom, Am. Min. 47, 310, 1962.
119. ———, unpublished data
120. Ross and Edwards, Acta Cryst. 12, 258, 1959.
121. Ruben and Others, J. Am. Chem. Soc. 83, 821, 1961.
122. Sadanga, Tokonami and Takeuchi, Acta Cryst. 15, 65, 1962.
123. Saha, Am. Min. 44, 300, 1959.
124. Sahama and Hytonen, Am. Min. 43, 862, 1958.
125. Sakata, Jap. J. Geol. Geog. 28, 161, 1957.
126. Salkovitz, J. Metals 8, 176, 1956.
127. Sasaki, Min. J. (Japan) 2, 375, 1959.
128. Schreyer, J. Pet. 2, XXX, 1961.
129. Shropshire, Keat, and Vaughan, Zeit.f. Krist, 112, 409, 1959.
130. Skinner, Am. Min. 41, 428, 1956.
131. ———, Am. Min. 42, 39, 1957.
132. ———, Am. Min. 46, 1399, 1961.
133. ———, unpublished data.
134. Skinner, Appelman, and Clark, Am. J. Sci. 259, 651, 1961.

## REFERENCES

135. Skinner and Barton, *Am. Min.* 45, 612, 1960.
136. Skinner, Barton, and Kullerud, *Econ. Geol.* 54, 1040, 1959.
137. Skinner and Bethke, *Am. Min.* 46, 1382, 1961.
138. Skinner and Evans, *Am. J. Sci.* 258A, 312, 1960.
139. Smith, *Ann. Rept. Dir. Geophys. Lab.* 52, 61, 1953.
140. ———, *Min. Mag.* 31, 47, 1956.
141. Smith and Tuttle, *Am. J. Sci.* 255, 282, 1957.
142. Stemple and Brindley, *J. Am. Ceram. Soc.* 43, 34, 1960.
143. Straumanis, *J. Appl. Phys.* 20, 726, 1949.
144. Straumanis, Ejima, and James, *Acta Cryst.* 13, 1022 1960.
145. Structure Reports, 184, 1951.
146. Swanson and Tatge, *U. S. Nat. Bur. Stds. Circular 539*, v. 1, Washington, D. C., 1953.
147. Swanson and Fuyat, *U. S. Nat. Bur. Stds. Circular 539*, v.2, Washington, D. C., 1953.
148. Swanson, Fuyant, and Ugrinie, *U. S. Nat. Bur. Stds. Circular 539*, v.3, Washington, D. C., 1954.
149. ———, *U. S. Nat. Bur. Stds Circular 539*, v.4, Washington, D. C., 1955.
150. Swanson, Gilfrich, and Ugrinic, *U. S. Nat. Bur. Stds. Circular 539*, v.5, Washington, D. C., 1955.
151. Swanson, Gilfrich, and Cook, *U. S. Nat. Bur. Stds. Circular 539*, v.6, Washington, D. C., 1956.
152. ———, *U. S. Nat. Bur. Stds. Circular 539*, v.7, Washington, D. C. 1957.
153. Swanson and others, *U. S. Nat. Bur. Stds Circular 539*, v.8, Washington, D. C., 1959.
154. ———, *U. S. Nat. Bur. Stds. Circular 539*, v.9, Washington, D. C. 1960.
155. ———, *U. S. Nat. Bur. Stds. Circular 539*, v.10, Washington, D.C. 1960.
156. ———, *U. S. Nat. Bur. Stds. Monogr. 25*, sec. 1, Washington, D. C. 1962.
157. Taylor and Underwood, *Acta Cryst.* 13, 361, 1960.

## REFERENCES

158. Tengner, Zeit. anorg. Chem. 239, 126, 1938.
159. Thomassen, Zeit. Phys. Chem. 4, Abt. B, 277, 1929.
160. Tolliday, Nature 182, 1012, 1958.
161. Tombs and Rooksby, Acta Cryst. 4, 474, 1951.
162. Toulmin, Priestley, 3d, in press.
163. Turnock, A. C., private communication, February 1961.
164. Ulrich and Zachariasen, Zeit. Krist. 62, 260, 1925.
165. Van Hook and Keith, Am. Min. 43, 69, 1958.
166. Waldbaum, D. R., private communication, August 1961.
167. Wasserstein, Am. Min. 36, 102, 1951.
168. Wiese and Muldower, Phy. and Chem. Solids 15, 13, 1960.
169. Willis and Rooksby, Pro. Phys. Soc. 65B, 950, 1952.
170. ———, Acta Cryst. 6, 827, 1953.
171. Wolfe, Am. Min. 40, 249, 1955.
172. Wones, D. R., private communication, February 1961.
173. Yoder and Eugster, Geochim. et. Cosmochim. Acta 6, 157, 1954.
174. ———, Geochim. et. Cosmochim. Acta 8, 225, 1955.
175. Yoder and Sahama, Am. Min. 42, 475, 1957.
176. Yund, Ann. Rept. Dir. Geophys. Lab. Wash. 56, 148, 1959.
177. Zussman, Acta Cryst. 12, 309, 1959.
178. Cooper, Bond and Abrahams, Acta Cryst. 14, 1008, 1961.
179. Cooper, Acta Cryst. 15, 578, 1962.
180. Skinner and Appleman, Abstract, Geol. Soc. America, Houston, Texas meeting, 1962.
181. Ito, Morimoto and Sadanaga, Acta Cryst. 5, 775, 1952.
182. Frondel, Dana's System of Mineralogy, 7th ed., vol. 111, Silica Minerals, John Wiley, New York, 1962.
183. Parrish, Acta Cryst. 13, 838, 1960.