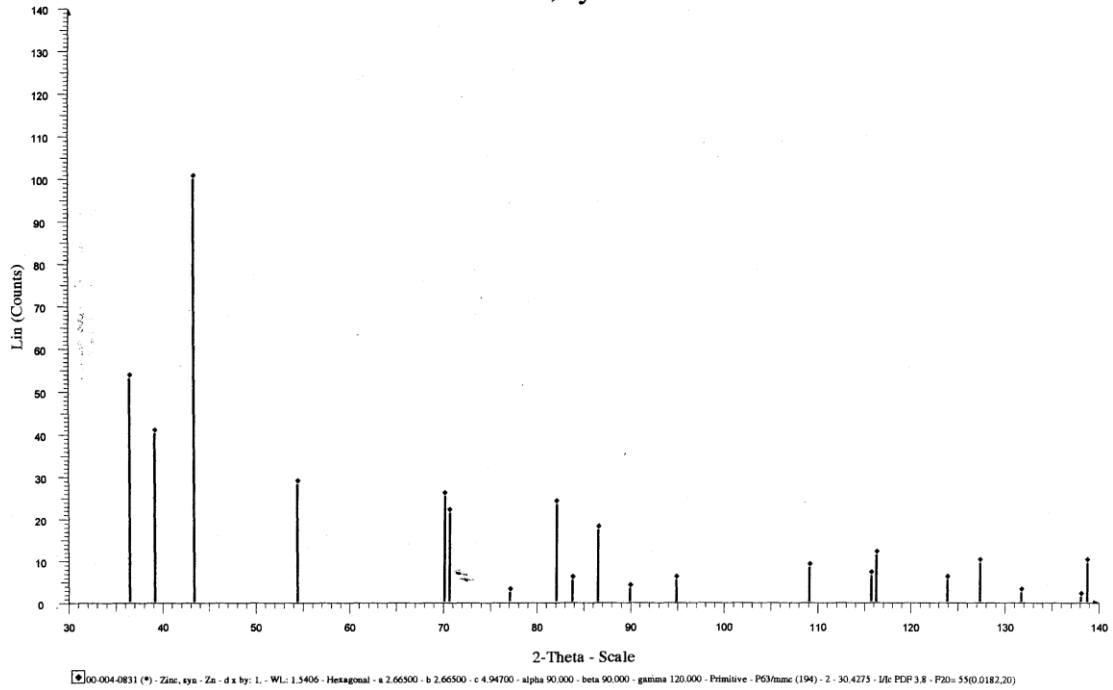


# Zinc, syn

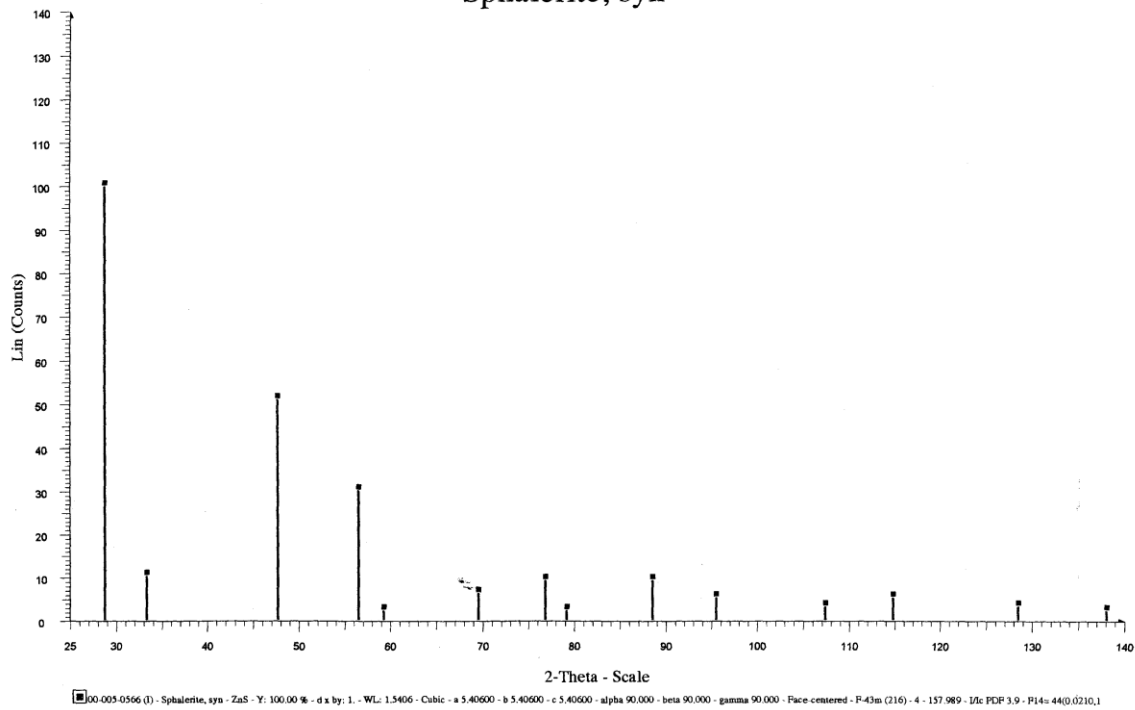


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| Pattern : 00-004-0831  |  | Radiation = 1.540560  |     | Quality : High |          |          |          |
|--|--|---|-----|----------------|----------|----------|----------|
| Zn   |  | <i>d</i> (Å)  |     | <i>i</i>       | <i>h</i> | <i>k</i> | <i>l</i> |
| Zinc   |  | 2.47300   | 53  | 0              | 0        | 0        | 2        |
| Zinc, syn  |  | 2.4800  | 40  | 1              | 0        | 0        | 0        |
|  |  | 2.09100   | 100 | 1              | 0        | 0        | 1        |
|  |  | 1.68700   | 28  | 1              | 0        | 0        | 2        |
|  |  | 1.34200   | 25  | 1              | 0        | 0        | 3        |
|  |  | 1.33200   | 21  | 1              | 1        | 0        | 0        |
|  |  | 1.23700   | 2   | 0              | 0        | 0        | 4        |
|  |  | 1.17290   | 23  | 1              | 1        | 1        | 2        |
|  |  | 1.15380   | 5   | 2              | 0        | 0        | 0        |
|  |  | 1.12380   | 17  | 2              | 0        | 0        | 1        |
|  |  | 1.09010   | 3   | 1              | 0        | 0        | 4        |
|  |  | 1.04560   | 5   | 2              | 0        | 0        | 2        |
|  |  | 0.94540   | 8   | 2              | 0        | 0        | 3        |
|  |  | 0.90930   | 6   | 1              | 0        | 0        | 5        |
|  |  | 0.90640   | 11  | 1              | 1        | 1        | 4        |
|  |  | 0.87220   | 5   | 2              | 1        | 0        | 0        |
|  |  | 0.85890   | 9   | 2              | 1        | 1        | 1        |
|  |  | 0.84370   | 2   | 2              | 0        | 0        | 4        |
|  |  | 0.82450   | 1   | 0              | 0        | 0        | 6        |
|  |  | 0.82250   | 9   | 2              | 1        | 1        | 2        |
| <b>Lattice :</b> Hexagonal<br><b>S.G. :</b> P63/mmc (194)<br><b>a =</b> 2.66500<br><b>c =</b> 4.94700<br><b>Z =</b> 2  |  | <b>Mol. weight =</b> 65.38<br><b>Volume [CD] =</b> 30.43<br><b>Dx =</b> 7.136<br><b>Dm =</b> 7.050<br><b>I/cor =</b> 3.80 |     |                |          |          |          |
| <b>Sample source or locality:</b> Sample from New Jersey Zinc Company, Sterling Hill, New Jersey, USA.<br><b>Temperature of data collection:</b> Pattern taken at 26 C.<br><b>Melting point:</b> 420°<br><b>Optical data:</b> B=2.58<br><b>Color:</b> Bluish white<br><b>Analysis:</b> Spectroscopic analysis shows faint traces of Pb, Cu, Mg, Si.<br><b>Data collection flag:</b> Ambient. |  |   |     |                |          |          |          |
| Swanson, Tatge., Natl. Bur. Stand. (U.S.), Circ. 539, volume I, page 16 (1953)<br>CAS Number: 7440-66-6  |  |   |     |                |          |          |          |
| <b>Radiation :</b> CuKα1<br><b>Lambda :</b> 1.54050<br><b>SS/FOM :</b> F20= 55(0.0182,20)  |  | <b>Filter :</b> Beta<br><b>d-sp :</b> Not given   |     |                |          |          |          |

# Sphalerite, syn



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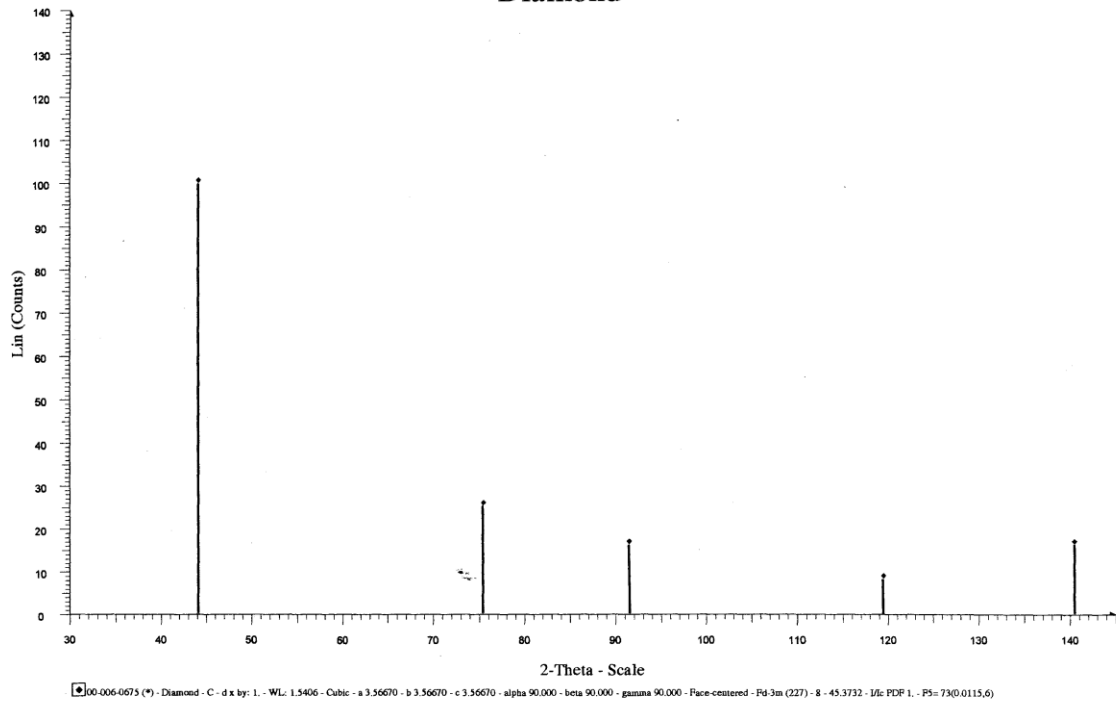
Pattern : 00-005-0586

Radiation = 1.540560

Quality : Indexed

| ZnS   |  | <i>d</i> (Å)                   | <i>i</i> | <i>h</i> | <i>k</i> | <i>l</i> |  |  |  |  |  |
|---|--|--------------------------------|----------|----------|----------|----------|--|--|--|--|--|
| Zinc Sulfide<br>Sphalerite, syn<br><b>Also called:</b> blende, zinc blende  |  | 3.12300                        | 100      | 1        | 1        | 1        |  |  |  |  |  |
|   |  | 2.70500                        | 10       | 2        | 0        | 0        |  |  |  |  |  |
|   |  | 1.91200                        | 51       | 2        | 2        | 0        |  |  |  |  |  |
|   |  | 1.63300                        | 30       | 3        | 1        | 1        |  |  |  |  |  |
|   |  | 1.56100                        | 2        | 2        | 2        | 2        |  |  |  |  |  |
|   |  | 1.35100                        | 6        | 4        | 0        | 0        |  |  |  |  |  |
|   |  | 1.24000                        | 9        | 3        | 3        | 1        |  |  |  |  |  |
|   |  | 1.20900                        | 2        | 4        | 2        | 0        |  |  |  |  |  |
|   |  | 1.10340                        | 9        | 4        | 2        | 2        |  |  |  |  |  |
|   |  | 1.04030                        | 5        | 5        | 1        | 1        |  |  |  |  |  |
|   |  | 0.95570                        | 3        | 4        | 4        | 0        |  |  |  |  |  |
|   |  | 0.91380                        | 5        | 5        | 3        | 1        |  |  |  |  |  |
|   |  | 0.85480                        | 3        | 6        | 2        | 0        |  |  |  |  |  |
|   |  | 0.82440                        | 2        | 5        | 3        | 3        |  |  |  |  |  |
| <b>Lattice :</b> Face-centered cubic  |  | <b>Mol. weight =</b> 97.44     |          |          |          |          |  |  |  |  |  |
| <b>S.G. :</b> F-43m (216)   |  | <b>Volume [CD] =</b> 157.99    |          |          |          |          |  |  |  |  |  |
| <b>a =</b> 5.40600  |  | <b>Dx =</b> 4.097              |          |          |          |          |  |  |  |  |  |
|   |  | <b>Dm =</b> 3.900              |          |          |          |          |  |  |  |  |  |
| <b>Z =</b> 4  |  | <b>V<sub>icor</sub> =</b> 3.90 |          |          |          |          |  |  |  |  |  |
| <p><b>Sample preparation:</b> Prepared at 940 C by RCA Laboratory.<br/> <b>Analysis:</b> Spectroscopic analysis: &lt;0.1% Cu; &lt;0.01% B, Fe, Mg, Si; &lt;0.001% Al, Ca.<br/> <b>Temperature of data collection:</b> Pattern taken at 26 C.<br/> <b>Additional pattern:</b> See 24-1137 for cadmium substitution.<br/> <b>General comments:</b> Opaque mineral optical data on specimen from Snailsbeach, Minsterly, Shropshire, England: RR<sub>2</sub>R<sub>m</sub>=16.7, Disp.=16, VHN<sub>100</sub>=218-227, Color values .303, .309, 16.6, Ref.: IMA Commission on Ore Microscopy QDF.<br/> <b>General comments:</b> Measured density and color from <i>Dana's System of Mineralogy, 7th Ed.</i>, 1211.<br/> <b>Color:</b> White, yellow white<br/> <b>Data collection flag:</b> Ambient.</p> |  |                                |          |          |          |          |  |  |  |  |  |
| Swanson, Fuyat., Natl. Bur. Stand. (U.S.), Circ. 539, volume II, page 16 (1953)   |  |                                |          |          |          |          |  |  |  |  |  |
| <b>Radiation :</b> CuKα1  |  | <b>Filter :</b> Beta           |          |          |          |          |  |  |  |  |  |
| <b>Lambda :</b> 1.54050   |  | <b>d-sp :</b> Not given        |          |          |          |          |  |  |  |  |  |
| <b>SS/FOM :</b> F14= 44(0.0210,15)  |  |                                |          |          |          |          |  |  |  |  |  |

# Diamond

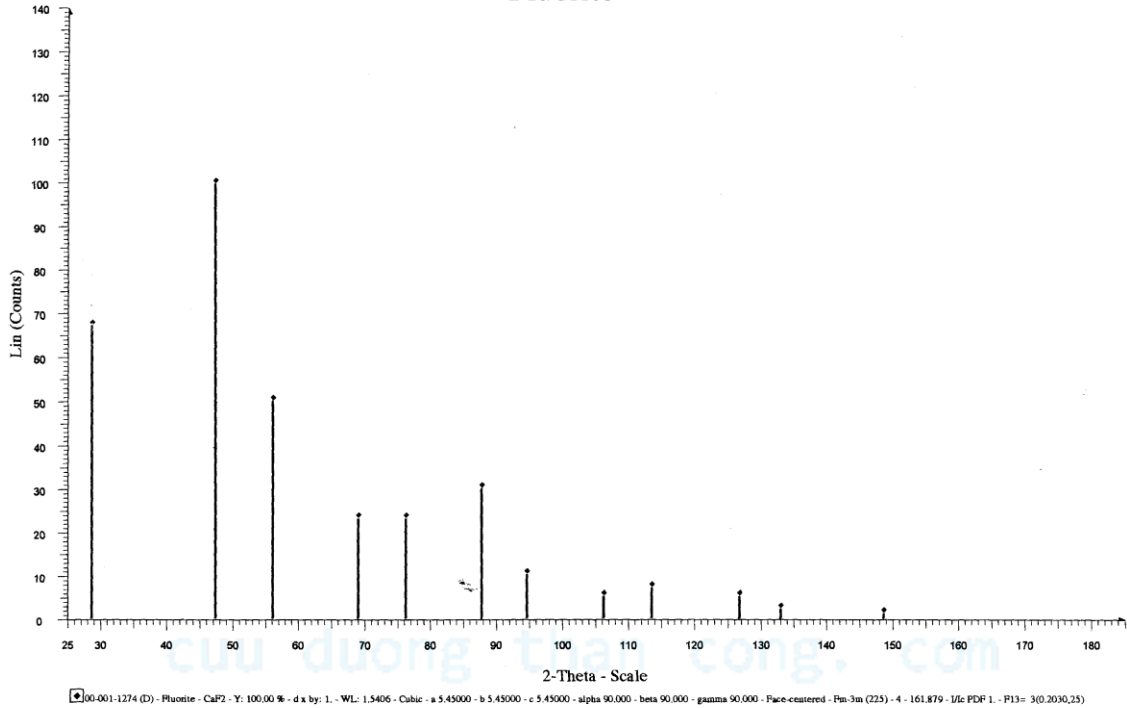


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|  |                     |  |   |  |  |  |
|--|---------------------|--|---|--|--|--|
| <b>Pattern :</b> 00-006-0675   |                     | <b>Radiation =</b> 1.540560  |   | <b>Quality :</b> High                            |  |  |
| <p>C</p> <p>Carbon<br/>Diamond<br/><b>Also called:</b> bort, carbonado</p>   |                     | <p><b>d (Å)</b></p> <p>2.06000<br/>1.26100<br/>1.07540<br/>0.89160<br/>0.81820</p> | <p><b>i</b></p> <p>100<br/>25<br/>16<br/>8<br/>16</p> | <p><b>h</b></p> <p>1<br/>2<br/>3<br/>4<br/>3</p> | <p><b>k</b></p> <p>1<br/>2<br/>1<br/>0<br/>3</p> | <p><b>l</b></p> <p>1<br/>0<br/>1<br/>0<br/>1</p> |
| <p><b>Lattice :</b> Face-centered cubic</p> <p><b>S.G. :</b> Fd-3m (227)</p>   |                     | <p><b>Mol. weight =</b> 12.01</p> <p><b>Volume [CD] =</b> 45.37</p>                |   |  |  |  |
| <p><b>a =</b> 3.56670</p>  |                     | <p><b>Dx =</b> 3.517</p> <p><b>Dm =</b> 3.511</p>                                  |   |  |  |  |
|  | <p><b>Z =</b> 8</p> |  |   |  |  |  |
| <p><b>Optical data:</b> B=2.4195<br/> <b>Color:</b> Colorless<br/> <b>Sample source or locality:</b> Specimen was an industrial abrasive powder.<br/> <b>Temperature of data collection:</b> Pattern taken at 26 C.<br/> <b>Additional pattern:</b> To replace 1-1249.<br/> <b>Additional pattern:</b> See ICSD 28857 (PDF 75-219); See ICSD 28858 (PDF 75-220); See ICSD 28859 (PDF 75-221); See ICSD 28860 (PDF 75-222); See ICSD 28861 (PDF 75-223); See ICSD 28862 (PDF 75-224); See ICSD 28863 (PDF 75-225); See ICSD 29066 (PDF 75-409); See ICSD 29151 (PDF 75-465); See ICSD 29324 (PDF 75-623); See ICSD 29325 (PDF 75-624); See ICSD 66464 (PDF 79-1467).<br/> <b>Data collection flag:</b> Ambient.</p> |                     |  |   |  |  |  |
| <p>Natl. Bur. Stand. (U.S.), Circ. 539, volume II, page 5 (1953)</p> <p>CAS Number: 7782-40-3</p>  |                     |  |   |  |  |  |
| <p><b>Radiation :</b> CuKα1</p> <p><b>Lambda :</b> 1.54050</p> <p><b>SS/FOM :</b> F5= 73(0.0115,6)</p>   |                     | <p><b>Filter :</b> Beta</p> <p><b>d-sp :</b> Not given</p>                         |   |  |  |  |

# Fluorite



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Pattern : 00-001-1274

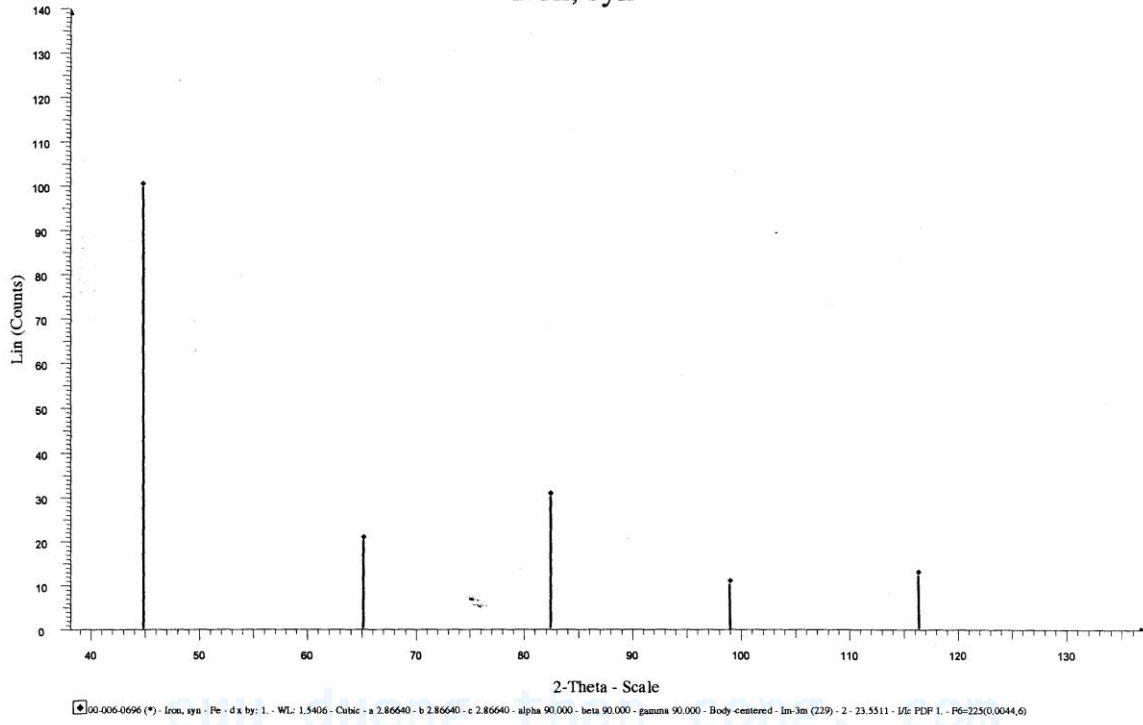
Radiation = 1.540560

Quality : Deleted

| CaF <sub>2</sub>  |  | <i>d</i> (Å)                | <i>l</i> | <i>h</i> | <i>k</i> | <i>l</i> |  |  |  |  |  |  |  |  |  |  |  |  |  |
|---|--|-----------------------------|----------|----------|----------|----------|--|--|--|--|--|--|--|--|--|--|--|--|--|
| Calcium Fluoride<br>Fluorite  |  | 3.16000                     | 67       | 1        | 1        | 1        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 1.93000                     | 100      | 2        | 2        | 0        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 1.85000                     | 50       | 3        | 1        | 1        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 1.37000                     | 23       | 4        | 0        | 0        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 1.26000                     | 23       | 3        | 3        | 1        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 1.12000                     | 30       | 4        | 2        | 2        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 1.05000                     | 10       | 5        | 1        | 1        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.97000                     | 5        | 4        | 4        | 0        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.93000                     | 7        | 5        | 3        | 1        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.87000                     | 5        | 6        | 2        | 0        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.84000                     | 2        |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.80000                     | 1        |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.77000                     | 2        |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.73000                     | 5        | 6        | 4        | 2        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.71000                     | 3        | 7        | 3        | 1        |  |  |  |  |  |  |  |  |  |  |  |  |  |
|   |  | 0.64000                     | 1        | 8        | 2        | 2        |  |  |  |  |  |  |  |  |  |  |  |  |  |
| <b>Lattice</b> : Face-centered cubic  |  | <b>Mol. weight</b> = 78.08  |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
| <b>S.G.</b> : Fm-3m (225)   |  | <b>Volume [CD]</b> = 161.88 |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
| <b>a</b> = 5.45000  |  | <b>Dx</b> = 3.204           |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
| <b>Z</b> = 4  |  | <b>Dm</b> = 3.180           |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
| <b>Deleted and rejected by:</b> Deleted by NBS card.<br><b>Color:</b> Colorless to varied<br><b>Melting point:</b> 1382<br><b>Optical data:</b> B=1.4339<br><b>Data collection flag:</b> Ambient. |  |                             |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Hanawalt. et al., Anal. Chem., volume 10, page 475 (1938)   |  |                             |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
| <b>Radiation</b> : MoK $\alpha$   |  | <b>Filter</b> : Beta        |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
| <b>Lambda</b> : 0.70900   |  | <b>d-sp</b> : Not given     |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |
| <b>SS/FOM</b> : F13= 3(0.2030,25)   |  |                             |          |          |          |          |  |  |  |  |  |  |  |  |  |  |  |  |  |



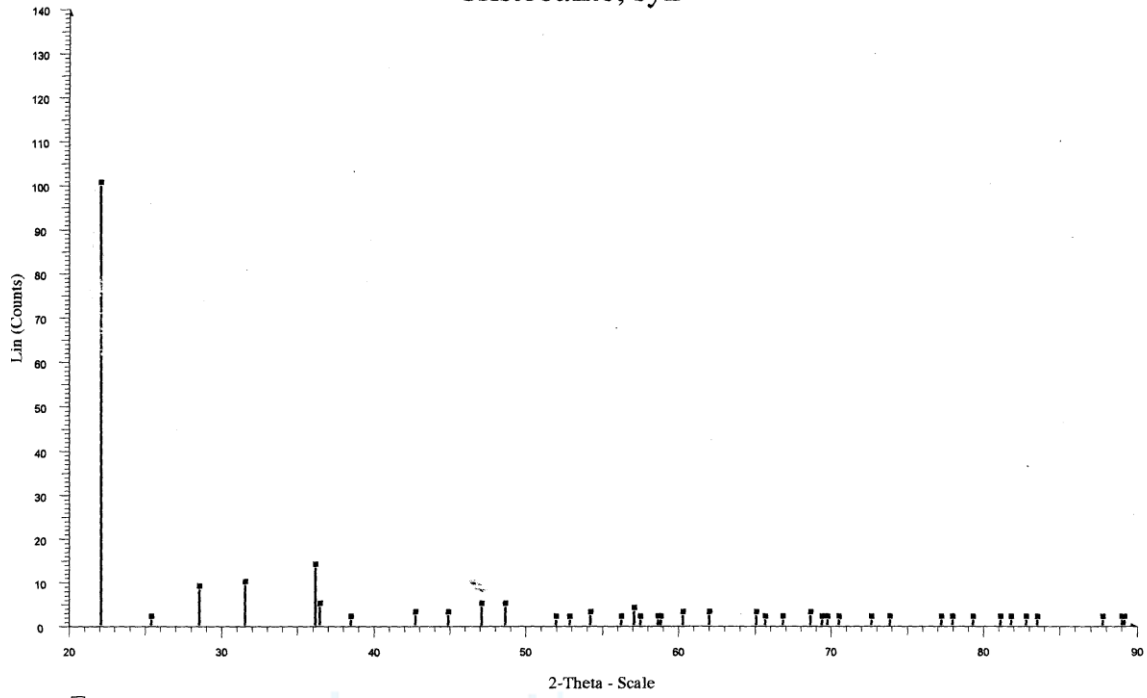
# Iron, syn



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| Pattern : 00-006-0696  |  | Radiation = 1.540560  |  | Quality : High                         |  |  |
|--|--|---|--|--|--|--|
| Fe<br><br>Iron<br>Iron, syn<br><b>Also called:</b> ferrite   |  | <b>d (Å)</b><br>2.02680<br>1.43320<br>1.17020<br>1.01340<br>0.90640<br>0.82750    | <b>i</b><br>100<br>20<br>30<br>10<br>12<br>6 | <b>h</b><br>1<br>2<br>2<br>2<br>3<br>2 | <b>k</b><br>1<br>0<br>1<br>2<br>1<br>2 | <b>l</b><br>0<br>0<br>1<br>0<br>0<br>2 |
| <b>Lattice :</b> Body-centered cubic<br><b>S.G. :</b> Im-3m (229)<br><b>a =</b> 2.86640<br><br><b>Z =</b> 2  |  | <b>Mol. weight =</b> 55.85<br><b>Volume [CD] =</b> 23.55<br><br><b>Dx =</b> 7.875 |  |  |  |  |
| <p><b>Color:</b> Gray, light gray metallic</p> <p><b>General comments:</b> Total impurities of sample &lt;0.0013% each metals and non-metals.</p> <p><b>Temperature of data collection:</b> Pattern taken at 25 C.</p> <p><b>Sample preparation:</b> The iron used was an exceptionally pure rolled sheet prepared at the NBS, Gaithersburg, Maryland, USA., [Moore, G., <i>J. Met.</i>, 6 1443 (1953)]. It was annealed in an H<sub>2</sub> atmosphere for 3 days at 1100 C and slowly cooled in a He atmosphere.</p> <p><b>General comments:</b> <math>\gamma</math>-Fe (fcc)=(1390 C) <math>\delta</math>-Fe (bcc).</p> <p><b>General comments:</b> Opaque mineral optical data on specimen from Meteorite: RR<sub>2</sub>R<sub>4</sub>=57.7, Disp=16, VHN=158 (mean at 100, 200, 300), Color values=.311, .316, 57.9, Ref.: IMA Commission on Ore Microscopy QDF.</p> <p><b>Additional pattern:</b> See ICSD 64795 (PDF 85-1410).</p> <p><b>Data collection flag:</b> Ambient.</p> |  |   |  |  |  |  |
| Swanson et al., Natl. Bur. Stand. (U.S.), Circ. 539, volume IV, page 3 (1955)<br>CAS Number: 7439-89-6   |  |   |  |  |  |  |
| <b>Radiation :</b> CuK $\alpha$ 1<br><b>Lambda :</b> 1.54050<br><b>SS/FOM :</b> F6=225(0.0044,6)   |  | <b>Filter :</b> Beta<br><b>d-sp :</b> Not given                                   |  |  |  |  |

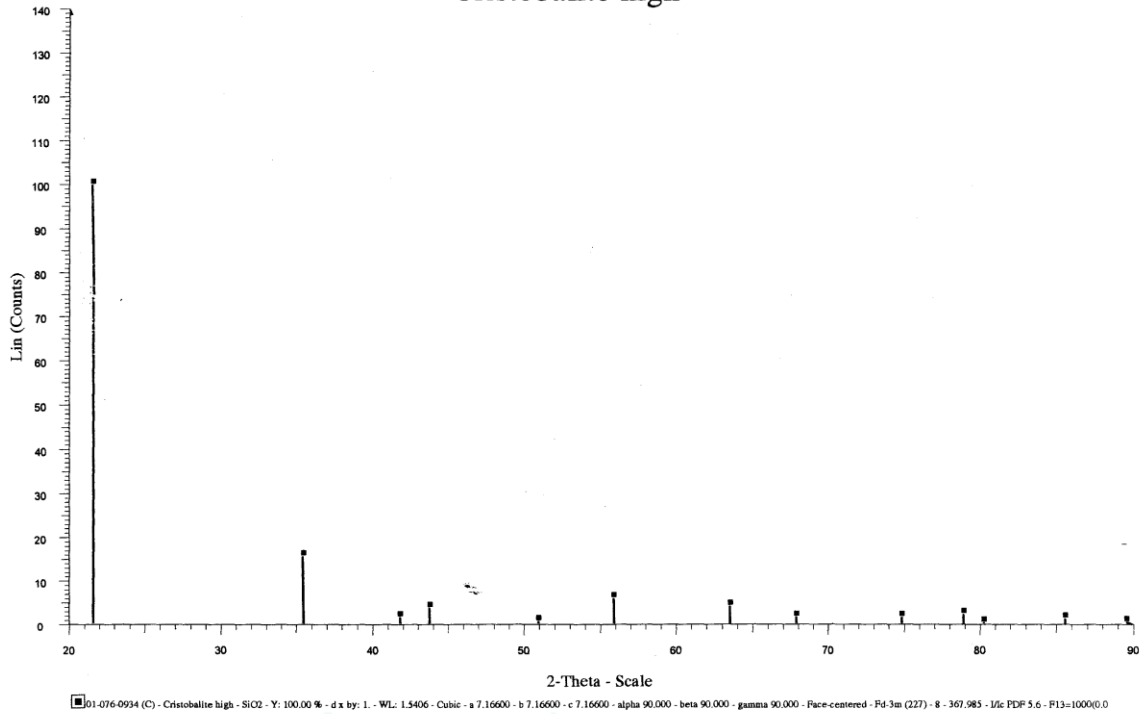
# Cristobalite, syn



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| Pattern : 00-039-1425  |  | Radiation = 1.540560   |     | Quality : High |          |          |          |
|--|--|--|-----|----------------|----------|----------|----------|
| SiO <sub>2</sub>   |  | <i>d</i> (Å)   |     | <i>i</i>       | <i>h</i> | <i>k</i> | <i>l</i> |
| Silicon Oxide<br>Cristobalite, syn   |  | 4.03974  | 100 | 1              | 0        | 0        | 1        |
|  |  | 3.51470  | 1   | 1              | 1        | 0        | 0        |
|  |  | 3.13592  | 8   | 1              | 1        | 1        | 1        |
|  |  | 2.84116  | 9   | 1              | 0        | 0        | 2        |
|  |  | 2.48740  | 13  | 2              | 0        | 0        | 0        |
|  |  | 2.46750  | 4   | 1              | 1        | 1        | 2        |
|  |  | 2.34170  | 1   | 2              | 0        | 0        | 1        |
|  |  | 2.11791  | 2   | 2              | 1        | 1        | 1        |
|  |  | 2.01957  | 2   | 2              | 0        | 0        | 2        |
|  |  | 1.92935  | 4   | 1              | 1        | 1        | 3        |
|  |  | 1.87147  | 4   | 2              | 1        | 2        | 2        |
|  |  | 1.75907  | 1   | 2              | 2        | 0        | 0        |
|  |  | 1.73033  | 1   | 0              | 0        | 0        | 4        |
|  |  | 1.69221  | 2   | 2              | 0        | 0        | 3        |
|  |  | 1.63488  | 1   | 1              | 0        | 0        | 4        |
|  |  | 1.61217  | 3   | 3              | 0        | 0        | 1        |
|  |  | 1.60131  | 1   | 2              | 1        | 3        | 3        |
|  |  | 1.57207  | 1   | 3              | 1        | 0        | 0        |
|  |  | 1.56745  | 1   | 2              | 2        | 2        | 2        |
|  |  | 1.53356  | 2   | 3              | 1        | 1        | 1        |
|  |  | 1.49520  | 2   | 3              | 0        | 0        | 2        |
|  |  | 1.43165  | 2   | 3              | 1        | 2        | 2        |
|  |  | 1.42102  | 1   | 2              | 0        | 0        | 4        |
|  |  | 1.39908  | 1   | 2              | 2        | 3        | 3        |
|  |  | 1.36560  | 2   | 2              | 1        | 4        | 4        |
|  |  | 1.35277  | 1   | 3              | 2        | 1        | 1        |
|  |  | 1.34650  | 1   | 3              | 0        | 0        | 3        |
|  |  | 1.33398  | 1   | 1              | 0        | 0        | 5        |
|  |  | 1.29976  | 1   | 3              | 1        | 3        | 3        |
|  |  | 1.28133  | 1   | 3              | 2        | 2        | 2        |
|  |  | 1.23318  | 1   | 2              | 2        | 4        | 4        |
|  |  | 1.22375  | 1   | 4              | 0        | 0        | 1        |
|  |  | 1.20599  | 1   | 4              | 1        | 0        | 0        |
|  |  | 1.18427  | 1   | 3              | 2        | 3        | 3        |
|  |  | 1.17576  | 1   | 2              | 1        | 5        | 5        |
|  |  | 1.16384  | 1   | 3              | 1        | 4        | 4        |
|  |  | 1.15546  | 1   | 3              | 3        | 1        | 1        |
|  |  | 1.11050  | 1   | 3              | 3        | 2        | 2        |
|  |  | 1.09783  | 1   | 4              | 2        | 1        | 1        |
|  |  | 1.09628  | 1   | 1              | 1        | 1        | 6        |
| <b>Lattice :</b> Tetragonal<br><b>S.G. :</b> P41212 (92)<br><b>a =</b> 4.97320<br><b>c =</b> 6.92360<br><b>Z =</b> 4   |  | <b>Mol. weight =</b> 60.08<br><b>Volume [CD] =</b> 171.24<br><b>Dx =</b> 2.331                           |     |                |          |          |          |
| <p><b>Sample preparation:</b> Cristobalite was prepared by the Trans Tech Company using Berkeley 5 micron MIN-U-SIL(R). A two kilogram sample was heated at 1600 C for eight hours. The sample was then air quenched, treated with 6N HCl and then jet-milled. The +325 mesh fraction was then removed by sieving.<br/> <b>Color:</b> Colorless<br/> <b>Structure:</b> The structure was determined by Peacor (1).<br/> <b>Temperature of data collection:</b> The temperature was ~25 C.<br/> <b>Polymorphism:</b> There are a number of other forms of Si O<sub>2</sub>.<br/> <b>Additional pattern:</b> To replace 11-695 and validated by calculated pattern.<br/> <b>Additional pattern:</b> See ICSD 75484 (PDF 82-1404); See ICSD 75490 (PDF 82-1410). See ICSD 30269 (PDF 75-923); See ICSD 34927 (PDF 76-935); See ICSD 34928 (PDF 76-936); See ICSD 34929 (PDF 76-937); See ICSD 47219 (PDF 77-1315); See ICSD 47220 (PDF 77-1316); See ICSD 47221 (PDF 77-1317);<br/> <b>Data collection flag:</b> Ambient.</p> |  |  |     |                |          |          |          |
| Wong-Ng, W., McMurdie, H., Paretzkin, B., Hubbard, C., Dragoo, A., NBS, Gaithersburg, MD, USA., ICDD Grant-in-Aid (1988)   |  |  |     |                |          |          |          |
| <b>Radiation :</b> CuKα1<br><b>Lambda :</b> 1.54060<br><b>SS/FOM :</b> F30= 84(0.0100,36)  |  | <b>Filter :</b> Monochromator crystal<br><b>d-sp :</b> Diffractometer<br><b>Internal standard :</b> W FP |     |                |          |          |          |

# Cristobalite high



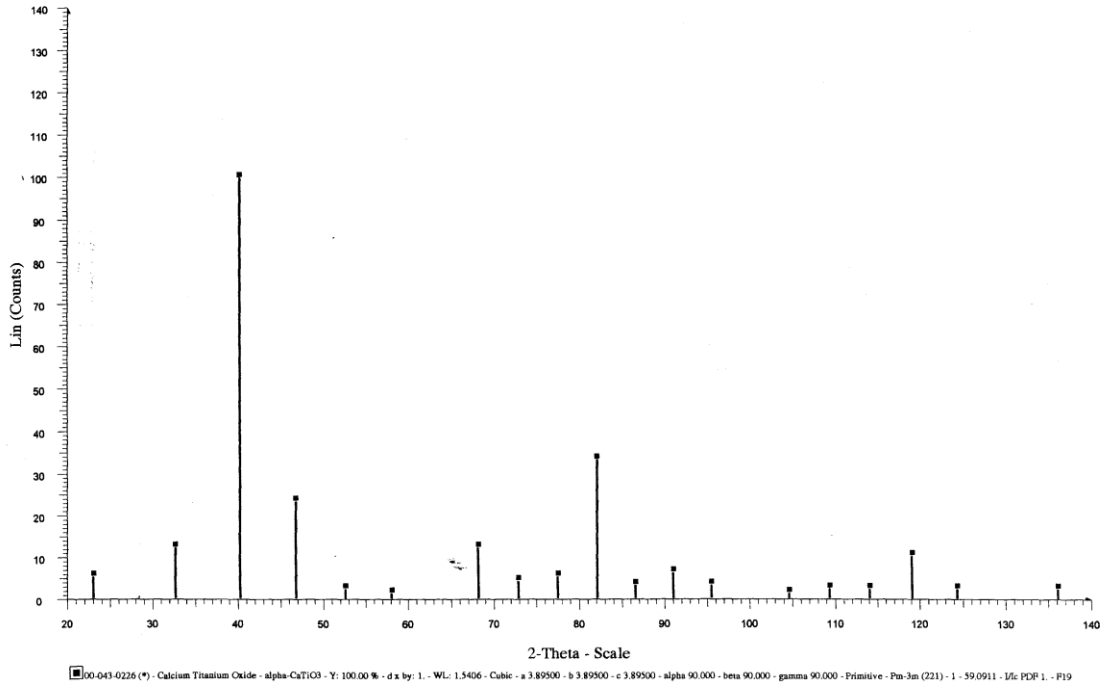
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| SiO <sub>2</sub>  |          | <table border="1"> <thead> <tr> <th><i>d</i> (Å)</th> <th><i>h</i></th> <th><i>k</i></th> <th><i>l</i></th> <th><i>h</i></th> <th><i>k</i></th> <th><i>l</i></th> </tr> </thead> <tbody> <tr><td>4.13729</td><td>999</td><td>1</td><td>1</td><td>1</td><td></td><td></td></tr> <tr><td>2.53356</td><td>154</td><td>2</td><td>2</td><td>2</td><td></td><td></td></tr> <tr><td>2.16063</td><td>13</td><td>3</td><td>1</td><td>1</td><td></td><td></td></tr> <tr><td>2.06865</td><td>34</td><td>2</td><td>2</td><td>2</td><td></td><td></td></tr> <tr><td>1.79150</td><td>3</td><td>4</td><td>0</td><td>0</td><td></td><td></td></tr> <tr><td>1.64399</td><td>57</td><td>3</td><td>3</td><td>1</td><td></td><td></td></tr> <tr><td>1.46275</td><td>39</td><td>4</td><td>2</td><td>2</td><td></td><td></td></tr> <tr><td>1.37910</td><td>13</td><td>5</td><td>1</td><td>1</td><td></td><td></td></tr> <tr><td>1.26678</td><td>13</td><td>4</td><td>4</td><td>0</td><td></td><td></td></tr> <tr><td>1.21127</td><td>20</td><td>5</td><td>3</td><td>1</td><td></td><td></td></tr> <tr><td>1.19433</td><td>1</td><td>4</td><td>4</td><td>2</td><td></td><td></td></tr> <tr><td>1.13304</td><td>10</td><td>6</td><td>2</td><td>0</td><td></td><td></td></tr> <tr><td>1.09280</td><td>2</td><td>5</td><td>3</td><td>3</td><td></td><td></td></tr> </tbody> </table> |          |          |          |          | <i>d</i> (Å) | <i>h</i> | <i>k</i> | <i>l</i> | <i>h</i> | <i>k</i> | <i>l</i> | 4.13729 | 999 | 1 | 1 | 1 |  |  | 2.53356 | 154 | 2 | 2 | 2 |  |  | 2.16063 | 13 | 3 | 1 | 1 |  |  | 2.06865 | 34 | 2 | 2 | 2 |  |  | 1.79150 | 3 | 4 | 0 | 0 |  |  | 1.64399 | 57 | 3 | 3 | 1 |  |  | 1.46275 | 39 | 4 | 2 | 2 |  |  | 1.37910 | 13 | 5 | 1 | 1 |  |  | 1.26678 | 13 | 4 | 4 | 0 |  |  | 1.21127 | 20 | 5 | 3 | 1 |  |  | 1.19433 | 1 | 4 | 4 | 2 |  |  | 1.13304 | 10 | 6 | 2 | 0 |  |  | 1.09280 | 2 | 5 | 3 | 3 |  |  |
|---|----------|--|----------|----------|----------|----------|--------------|----------|----------|----------|----------|----------|----------|---------|-----|---|---|---|--|--|---------|-----|---|---|---|--|--|---------|----|---|---|---|--|--|---------|----|---|---|---|--|--|---------|---|---|---|---|--|--|---------|----|---|---|---|--|--|---------|----|---|---|---|--|--|---------|----|---|---|---|--|--|---------|----|---|---|---|--|--|---------|----|---|---|---|--|--|---------|---|---|---|---|--|--|---------|----|---|---|---|--|--|---------|---|---|---|---|--|--|
| <i>d</i> (Å)  | <i>h</i> | <i>k</i>   | <i>l</i> | <i>h</i> | <i>k</i> | <i>l</i> |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 4.13729   | 999      | 1  | 1        | 1        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 2.53356   | 154      | 2  | 2        | 2        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 2.16063   | 13       | 3  | 1        | 1        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 2.06865   | 34       | 2  | 2        | 2        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.79150   | 3        | 4  | 0        | 0        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.64399   | 57       | 3  | 3        | 1        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.46275   | 39       | 4  | 2        | 2        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.37910   | 13       | 5  | 1        | 1        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.26678   | 13       | 4  | 4        | 0        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.21127   | 20       | 5  | 3        | 1        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.19433   | 1        | 4  | 4        | 2        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.13304   | 10       | 6  | 2        | 0        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| 1.09280   | 2        | 5  | 3        | 3        |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| <b>Lattice</b> : Face-centered cubic<br><b>S.G.</b> : Fd-3m (227)   |          | <b>Mol. weight</b> = 60.08<br><b>Volume [CD]</b> = 367.99  |          |          |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| <b>a</b> = 7.16600<br><br><b>Z</b> = 8  |          | <b>Dx</b> = 2.169<br><br><b>V<sub>cor</sub></b> = 5.60   |          |          |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| <b>ICSD collection code:</b> 034926<br><b>Temperature factor:</b> ATF<br><b>Remarks from ICSD/CSD:</b> REM TEM 583.<br><b>Sample source or locality:</b> Specimen from Ellora Caves, India.<br><b>Additional pattern:</b> See PDF 76-0931.<br><b>Data collection flag:</b> Non ambient temperature. |          |  |          |          |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| Peacor, D.R., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallichem., volume 138, page 274 (1973)<br>Calculated from ICSD using POWD-12++ (1997)   |          |  |          |          |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |
| <b>Radiation</b> : CuKα1<br><b>Lambda</b> : 1.54060<br><b>SS/FOM</b> : F13=1000(0.0002,13)  |          | <b>Filter</b> : Not specified<br><b>d-sp</b> : Calculated spacings   |          |          |          |          |              |          |          |          |          |          |          |         |     |   |   |   |  |  |         |     |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |         |    |   |   |   |  |  |         |   |   |   |   |  |  |

(7)

# Calcium Titanium Oxide



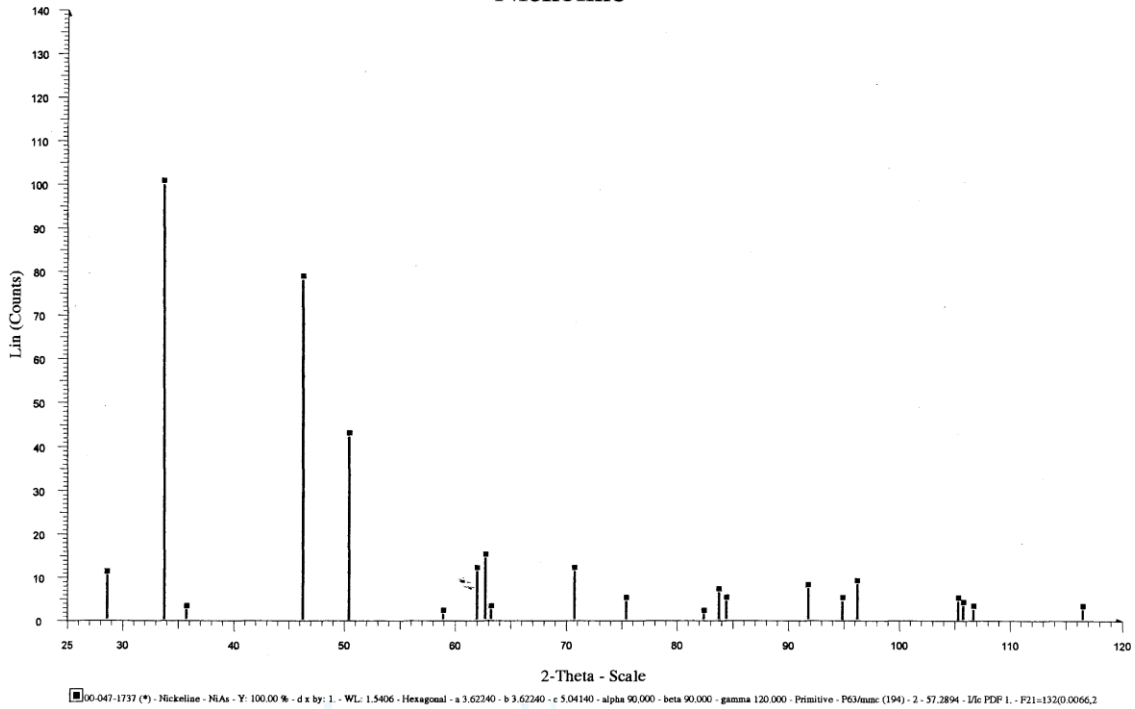
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| Pattern : 00-043-0226  |  | Radiation = 1.540560  |   | Quality : High  |  |   |
|--|--|---|---|---|--|---|
| $\alpha$ -CaTiO <sub>3</sub><br><br>Calcium Titanium Oxide   |  | <b>d (Å)</b><br>3.89500<br>2.75400<br>2.24900<br>1.94800<br>1.74200<br>1.59020<br>1.37720<br>1.29840<br>1.23180<br>1.17440<br>1.12440<br>1.08030<br>1.04100<br>0.97380<br>0.94470<br>0.91810<br>0.89360<br>0.87100<br>0.83050 | <b>i</b><br>5<br>12<br>100<br>23<br>2<br>1<br>12<br>4<br>5<br>33<br>3<br>6<br>3<br>1<br>2<br>2<br>2<br>10<br>2<br>2 | <b>h</b><br>1<br>1<br>1<br>2<br>2<br>1<br>3<br>3<br>3<br>3<br>2<br>0<br>1<br>4<br>3<br>3<br>3<br>4<br>3 | <b>k</b><br>0<br>1<br>1<br>0<br>1<br>1<br>2<br>0<br>1<br>1<br>2<br>2<br>0<br>2<br>3<br>3<br>3<br>3<br>2<br>3 | <b>l</b><br>0<br>0<br>1<br>0<br>0<br>2<br>0<br>0<br>1<br>1<br>3<br>3<br>2<br>0<br>1<br>0<br>1<br>0<br>2 |
| <b>Lattice :</b> Cubic<br><b>S.G. :</b> Pm-3m (221)<br><b>a =</b> 3.89500<br><br><b>Z =</b> 1  |  | <b>Mol. weight =</b> 135.98<br><b>Volume [CD] =</b> 59.09<br><b>Dx =</b> 3.821  |   |   |  |   |
| <p><b>Melting point:</b> 3150 K<br/> <b>Color:</b> Colorless<br/> <b>Sample source or locality:</b> Calcium titanate 99.5% purchased from Alfa Produkte, Karlsruhe, Germany, Lot No. 031280911, washed in acetic acid.<br/> <b>General comments:</b> Sample investigated at 1600 K in platinum can using a mirror furnace, intensities and d-values evaluated by Rietveld method, observed intensities are given.<br/> <b>General comments:</b> High temperature form.<br/> <b>Temperature of data collection:</b> Pattern taken at 1600 K.<br/> <b>Data collection flag:</b> Non ambient temperature.</p> |  |   |   |   |  |   |
| Fuess, H., Fachbereich Materialwissenschaft, Technische Hochschule Darmstadt, Germany., Private Communication (1991)   |  |   |   |   |  |   |
| <b>Radiation :</b> Neut<br><b>Lambda :</b> 1.59400<br><b>SS/FOM :</b> F19=134(0.0071,20)   |  | <b>Filter :</b> Monochromator crystal<br><b>d-sp :</b> Diffractometer<br><b>External standard :</b> Si  |   |   |  |   |



# Nickeline

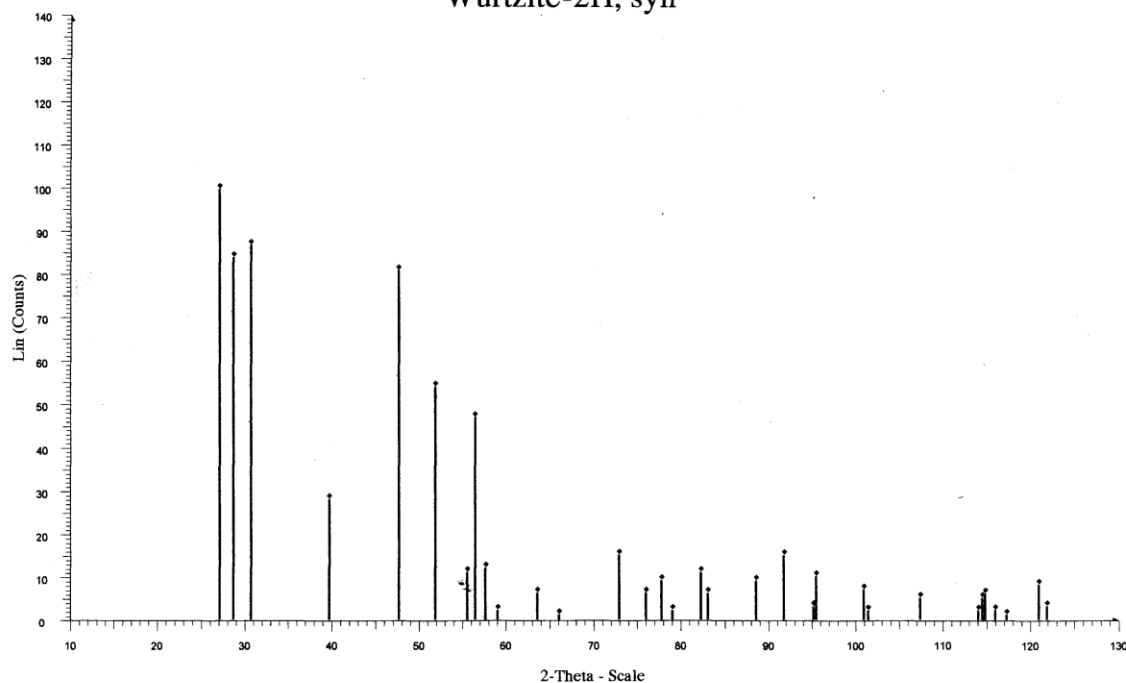


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| Pattern : 00-047-1737   |              | Radiation = 1.540560                  |  | Quality : High |          |          |          |
|---|--------------|---------------------------------------|--|----------------|----------|----------|----------|
| NiAs  |              | <b>d (Å)</b>                          |  | <b>i</b>       | <b>h</b> | <b>k</b> | <b>l</b> |
|   |              | 3.13600                               |  | 10             | 1        | 0        | 0        |
|   |              | 2.66400                               |  | 100            | 1        | 0        | 1        |
|   |              | 2.52100                               |  | 2              | 0        | 0        | 2        |
| Nickel Arsenide   |              | 1.96520                               |  | 78             | 1        | 0        | 2        |
| Nickeline   |              | 1.81140                               |  | 42             | 1        | 1        | 0        |
|   |              | 1.56830                               |  | 1              | 2        | 0        | 0        |
|   |              | 1.49770                               |  | 11             | 2        | 0        | 1        |
|   |              | 1.48150                               |  | 14             | 1        | 0        | 3        |
|   |              | 1.47090                               |  | 2              | 1        | 1        | 2        |
|   |              | 1.33170                               |  | 11             | 2        | 0        | 2        |
|   |              | 1.26030                               |  | 4              | 0        | 0        | 4        |
|   |              | 1.16920                               |  | 1              | 1        | 0        | 4        |
|   |              | 1.15420                               |  | 6              | 2        | 1        | 1        |
|   |              | 1.14660                               |  | 4              | 2        | 0        | 3        |
|   |              | 1.07290                               |  | 7              | 2        | 1        | 2        |
|   |              | 1.04570                               |  | 4              | 3        | 0        | 0        |
|   |              | 1.03460                               |  | 8              | 1        | 1        | 4        |
|   |              | 0.96877                               |  | 4              | 2        | 1        | 3        |
|   |              | 0.96590                               |  | 3              | 3        | 0        | 2        |
|   |              | 0.95997                               |  | 2              | 1        | 0        | 5        |
|   |              | 0.90567                               |  | 2              | 2        | 2        | 0        |
| <b>Lattice</b> : Hexagonal  |              | <b>Mol. weight</b> = 133.62           |  |                |          |          |          |
| <b>S.G.</b> : P63/mmc (194)   |              | <b>Volume [CD]</b> = 57.29            |  |                |          |          |          |
| <b>a</b> = 3.62240  |              | <b>Dx</b> = 7.746                     |  |                |          |          |          |
| <b>c</b> = 5.04140  | <b>Z</b> = 2 | <b>Dm</b> = 7.780                     |  |                |          |          |          |
| <p><b>Color</b>: Reddish orange metallic</p> <p><b>Sample source or locality</b>: Specimen from Cobalt, Ontario, Canada.</p> <p><b>Analysis</b>: X-ray emission analysis under SEM: major Ni and As and trace Co.</p> <p><b>General comments</b>: Average relative standard deviation in intensity of the 10 strongest reflections for three specimen mounts = 12.9%.</p> <p><b>General comments</b>: Validated with a calculated pattern.</p> <p><b>General comments</b>: Several unknown trace impurity reflections present.</p> <p><b>Data collection flag</b>: Ambient.</p> |              |                                       |  |                |          |          |          |
| <p>Martin, K., McCarthy, G., Bayliss, P., North Dakota State Univ., Fargo, ND, USA., ICDD Grant-in-Aid (1993)</p>   |              |                                       |  |                |          |          |          |
| <b>Radiation</b> : CuKα1  |              | <b>Filter</b> : Monochromator crystal |  |                |          |          |          |
| <b>Lambda</b> : 1.54056   |              | <b>d-sp</b> : Diffractometer          |  |                |          |          |          |
| <b>SS/FOM</b> : F21=132(0.0066,24)  |              | <b>Internal standard</b> : Si         |  |                |          |          |          |

# Wurtzite-2H, syn

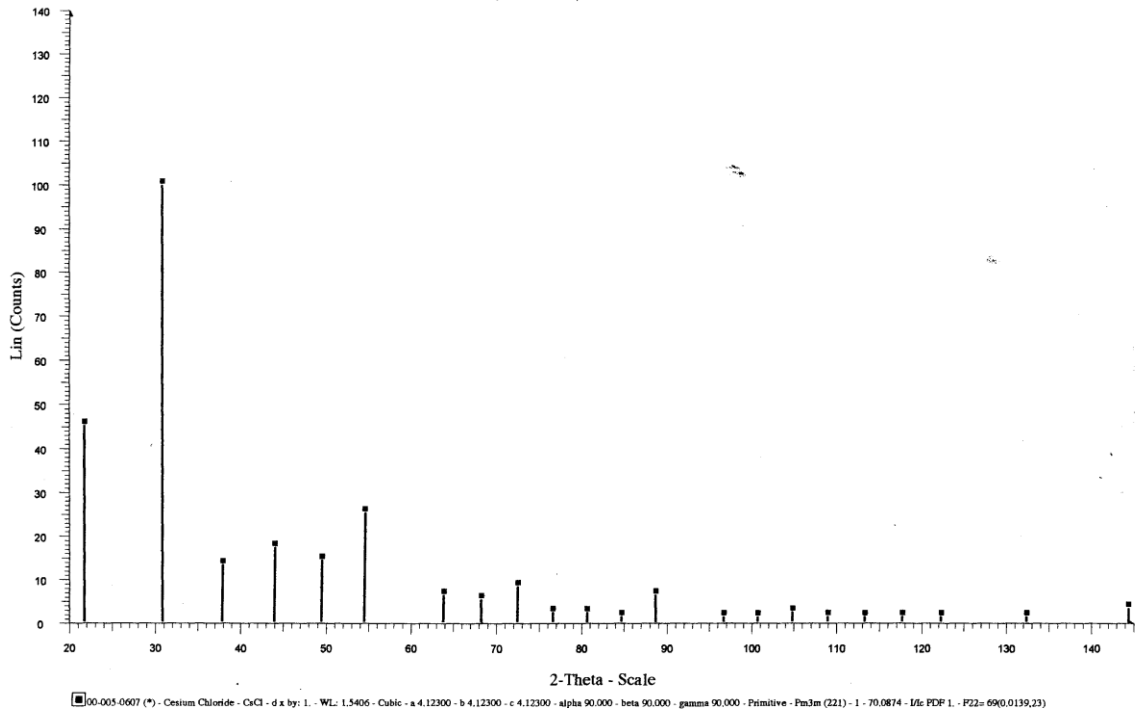


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# Cesium Chloride

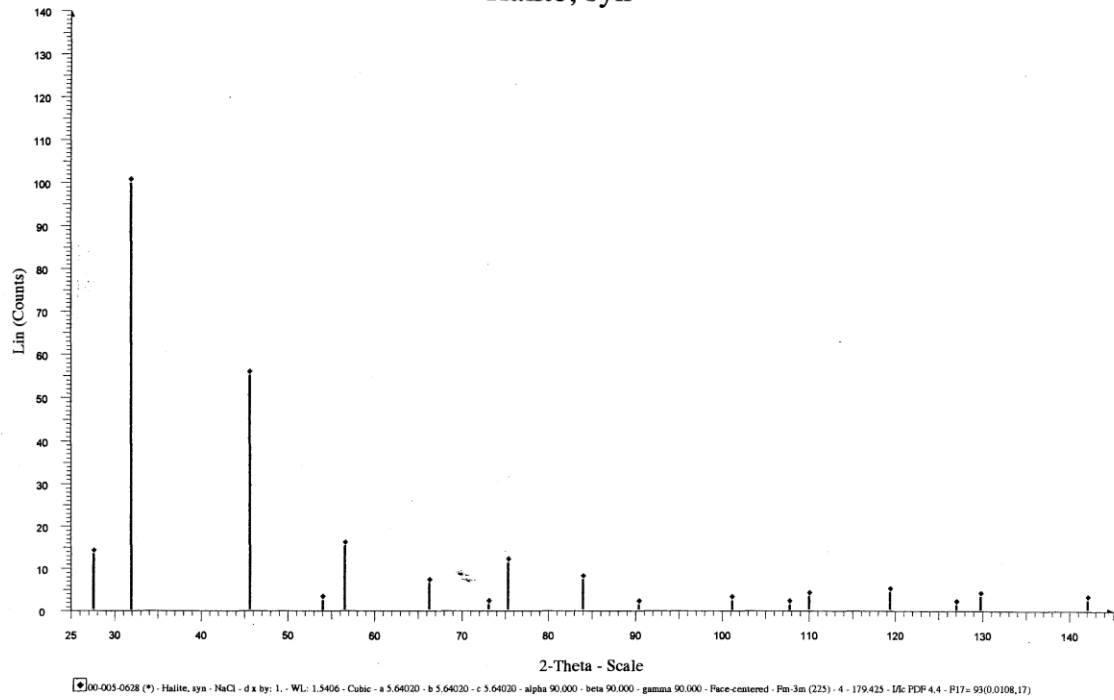


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|   |  |  |     |                |          |          |          |
|---|--|--|-----|----------------|----------|----------|----------|
| Pattern : 00-005-0607   |  | Radiation = 1.540560   |     | Quality : High |          |          |          |
| CsCl  |  | <i>d</i> (Å)   |     | <i>l</i>       | <i>h</i> | <i>k</i> | <i>l</i> |
| Cesium Chloride   |  | 4.12000  | 45  | 1              | 0        | 0        | 0        |
|   |  | 2.91700  | 100 | 1              | 1        | 1        | 0        |
|   |  | 2.38000  | 13  | 1              | 1        | 1        | 1        |
|   |  | 2.06200  | 17  | 2              | 0        | 0        | 0        |
|   |  | 1.84400  | 14  | 2              | 1        | 1        | 0        |
|   |  | 1.68300  | 25  | 2              | 1        | 1        | 1        |
|   |  | 1.45700  | 6   | 2              | 2        | 0        | 0        |
|   |  | 1.37400  | 5   | 3              | 0        | 0        | 0        |
|   |  | 1.30400  | 8   | 3              | 1        | 1        | 0        |
|   |  | 1.24300  | 2   | 3              | 1        | 1        | 1        |
|   |  | 1.19000  | 2   | 2              | 2        | 2        | 2        |
|   |  | 1.14340  | 1   | 3              | 2        | 0        | 0        |
|   |  | 1.10190  | 6   | 3              | 2        | 1        | 1        |
|   |  | 1.03090  | 1   | 4              | 0        | 0        | 0        |
|   |  | 0.99970  | 1   | 4              | 1        | 0        | 0        |
|   |  | 0.97190  | 2   | 3              | 3        | 0        | 0        |
|   |  | 0.94590  | 1   | 3              | 3        | 1        | 1        |
|   |  | 0.92190  | 1   | 4              | 2        | 0        | 0        |
|   |  | 0.89970  | 1   | 4              | 2        | 1        | 1        |
|   |  | 0.87910  | 1   | 3              | 3        | 2        | 2        |
|   |  | 0.84150  | 1   | 4              | 2        | 2        | 2        |
|   |  | 0.80860  | 3   | 5              | 1        | 0        | 0        |
| <b>Lattice :</b> Cubic<br><b>S.G. :</b> Pm3m (221)<br><b>a =</b> 4.12300<br><b>Z =</b> 1  |  | <b>Mol. weight =</b> 168.36<br><b>Volume [CD] =</b> 70.09<br><b>Dx =</b> 3.989 |     |                |          |          |          |
| <b>Color:</b> Colorless<br><b>Optical data:</b> B=1.639<br><b>Sample preparation:</b> Sample prepared at NBS. It was recrystallized three times from dilute hydrochloric acid and heated at 500 C liberating chlorine iodide.<br><b>Analysis:</b> Spectroscopic analysis: <0.01% Ca, K, Na; <0.001% Al, Ba, Cu, Fe, Mg, Si.<br><b>Temperature of data collection:</b> X-ray pattern at 25 C.<br><b>General comments:</b> Merck Index, 8th Ed., p. 225.<br><b>Data collection flag:</b> Ambient. |  |  |     |                |          |          |          |
| Swanson, Fuyat., Natl. Bur. Stand. (U.S.), Circ. 539, volume 2, page 44 (1953)<br>CAS Number: 7647-17-8   |  |  |     |                |          |          |          |
| <b>Radiation :</b> CuKα1<br><b>Lambda :</b> 1.54050<br><b>SS/FOM :</b> F22= 69(0.0139,23)   |  | <b>Filter :</b> Beta<br><b>d-sp :</b> Not given                                |     |                |          |          |          |

# Halite, syn



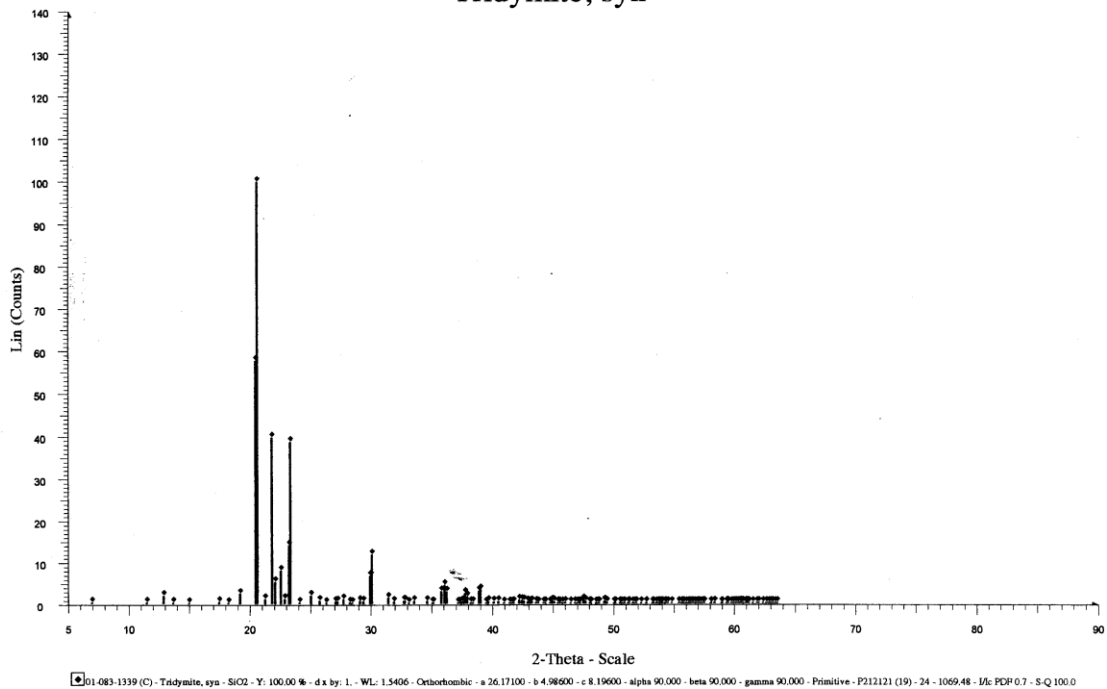
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| Pattern : 00-005-0628   |  | Radiation = 1.540560        |     | Quality : High |          |          |          |
|---|--|-----------------------------|-----|----------------|----------|----------|----------|
| NaCl  |  | <b>d (Å)</b>                |     | <b>i</b>       | <b>h</b> | <b>k</b> | <b>l</b> |
| Sodium Chloride<br>Halite, syn  |  | 3.26000                     | 13  | 1              | 1        | 1        | 1        |
|   |  | 2.92100                     | 100 | 2              | 0        | 0        | 0        |
|   |  | 1.99400                     | 55  | 2              | 2        | 2        | 0        |
|   |  | 1.70100                     | 2   | 3              | 1        | 1        | 1        |
|   |  | 1.62800                     | 15  | 2              | 2        | 2        | 2        |
|   |  | 1.41000                     | 6   | 4              | 0        | 0        | 0        |
|   |  | 1.29400                     | 1   | 3              | 3        | 1        | 1        |
|   |  | 1.26100                     | 11  | 4              | 2        | 0        | 0        |
|   |  | 1.15150                     | 7   | 4              | 2        | 2        | 2        |
|   |  | 1.08550                     | 1   | 5              | 1        | 1        | 1        |
|   |  | 0.99690                     | 2   | 4              | 4        | 0        | 0        |
|   |  | 0.95330                     | 1   | 5              | 3        | 1        | 1        |
|   |  | 0.94010                     | 3   | 6              | 0        | 0        | 0        |
|   |  | 0.89170                     | 4   | 6              | 2        | 0        | 0        |
|   |  | 0.86010                     | 1   | 5              | 3        | 3        | 3        |
|   |  | 0.85030                     | 3   | 6              | 2        | 2        | 2        |
|   |  | 0.81410                     | 2   | 4              | 4        | 4        | 4        |
| <b>Lattice</b> : Face-centered cubic  |  | <b>Mol. weight</b> = 58.44  |     |                |          |          |          |
| <b>S.G.</b> : Fm-3m (225)   |  | <b>Volume [CD]</b> = 179.43 |     |                |          |          |          |
| <b>a</b> = 5.64020  |  | <b>Dx</b> = 2.163           |     |                |          |          |          |
|   |  | <b>Dm</b> = 2.168           |     |                |          |          |          |
| <b>Z</b> = 4  |  | <b>I/cor</b> = 4.40         |     |                |          |          |          |
| <p><b>General comments:</b> An ACS reagent grade sample recrystallized twice from hydrochloric acid.<br/> <b>Temperature of data collection:</b> Pattern taken at 26 C.<br/> <b>Optical data:</b> B=1.542<br/> <b>Color:</b> Colorless<br/> <b>Melting point:</b> 804°<br/> <b>Additional pattern:</b> See ICSD 18189 (PDF 72-1668).<br/> <b>Data collection flag:</b> Ambient.</p> |  |                             |     |                |          |          |          |
| <p>Swanson, Fuyat., Natl. Bur. Stand. (U.S.), Circ. 539, volume II, page 41 (1953)<br/> CAS Number: 7647-14-5</p>   |  |                             |     |                |          |          |          |
| <b>Radiation</b> : CuKα1  |  | <b>Filter</b> : Beta        |     |                |          |          |          |
| <b>Lambda</b> : 1.54050   |  | <b>d-sp</b> : Not given     |     |                |          |          |          |
| <b>SS/FOM</b> : F17= 93(0.0108,17)  |  |                             |     |                |          |          |          |



# Tridymite, syn

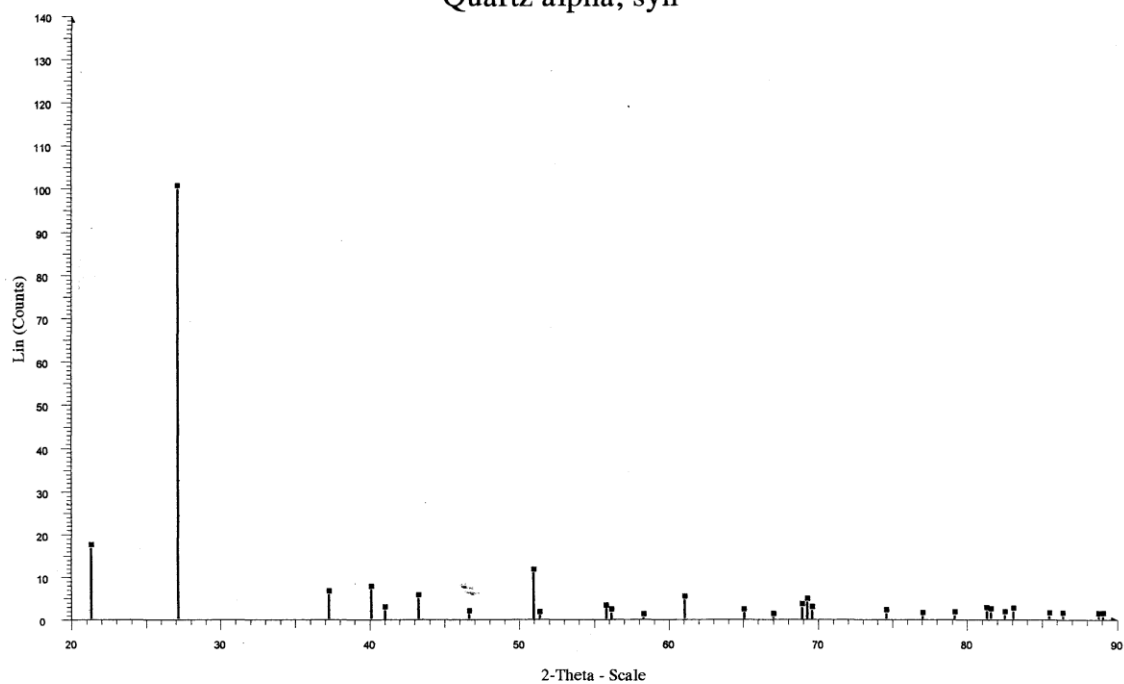


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| Pattern : 01-083-1339   |  | Radiation = 1.540560  |  | Quality : Calculated |  |    |  |   |  |   |  |
|---|--|-----------------------|--|----------------------|--|----|--|---|--|---|--|
| SiO <sub>2</sub>  |  | d (Å)                 |  | i                    |  | h  |  | k |  | l |  |
| Silicon Oxide   |  | 13.08550              |  | 2                    |  | 2  |  | 0 |  | 0 |  |
| Tridymite, syn  |  | 7.82142               |  | 2                    |  | 1  |  | 0 |  | 1 |  |
|   |  | 6.94600               |  | 18                   |  | 2  |  | 0 |  | 1 |  |
|   |  | 6.54275               |  | 2                    |  | 4  |  | 0 |  | 0 |  |
|   |  | 5.97328               |  | 1                    |  | 3  |  | 0 |  | 1 |  |
|   |  | 5.11330               |  | 3                    |  | 4  |  | 0 |  | 1 |  |
|   |  | 4.89790               |  | 1                    |  | 1  |  | 1 |  | 0 |  |
|   |  | 4.65823               |  | 23                   |  | 2  |  | 1 |  | 0 |  |
|   |  | 4.36183               |  | 575                  |  | 6  |  | 0 |  | 0 |  |
|   |  | 4.32884               |  | 999                  |  | 3  |  | 1 |  | 0 |  |
|   |  | 4.20437               |  | 10                   |  | 1  |  | 1 |  | 1 |  |
|   |  | 4.09800               |  | 395                  |  | 0  |  | 0 |  | 2 |  |
|   |  | 4.05049               |  | 51                   |  | 2  |  | 1 |  | 1 |  |
|   |  | *4.05049              |  | 51                   |  | 1  |  | 0 |  | 2 |  |
|   |  | 3.96572               |  | 78                   |  | 4  |  | 1 |  | 0 |  |
|   |  | 3.91071               |  | 10                   |  | 2  |  | 0 |  | 2 |  |
|   |  | 3.85050               |  | 138                  |  | 6  |  | 0 |  | 1 |  |
|   |  | 3.82775               |  | 385                  |  | 3  |  | 1 |  | 1 |  |
|   |  | 3.70913               |  | 2                    |  | 3  |  | 0 |  | 2 |  |
|   |  | 3.56979               |  | 18                   |  | 4  |  | 1 |  | 1 |  |
|   |  | 3.47300               |  | 6                    |  | 4  |  | 0 |  | 2 |  |
|   |  | 3.40152               |  | 1                    |  | 7  |  | 0 |  | 1 |  |
|   |  | 3.30387               |  | 3                    |  | 5  |  | 1 |  | 1 |  |
|   |  | 3.28291               |  | 4                    |  | 6  |  | 1 |  | 0 |  |
|   |  | 3.22670               |  | 9                    |  | 5  |  | 0 |  | 2 |  |
|   |  | 3.18590               |  | 2                    |  | 0  |  | 1 |  | 2 |  |
|   |  | 3.14298               |  | 1                    |  | 1  |  | 1 |  | 2 |  |
|   |  | 3.07712               |  | 5                    |  | 2  |  | 1 |  | 2 |  |
|   |  | 3.04753               |  | 4                    |  | 6  |  | 1 |  | 1 |  |
|   |  | 2.98884               |  | 65                   |  | 7  |  | 1 |  | 0 |  |
|   |  | *2.98884              |  | 65                   |  | 6  |  | 0 |  | 2 |  |
|   |  | 2.97598               |  | 116                  |  | 3  |  | 1 |  | 2 |  |
|   |  | 2.84980               |  | 13                   |  | 4  |  | 1 |  | 2 |  |
|   |  | 2.80991               |  | 3                    |  | 7  |  | 1 |  | 1 |  |
|   |  | 2.73520               |  | 6                    |  | 9  |  | 0 |  | 1 |  |
|   |  | *2.73520              |  | 6                    |  | 8  |  | 1 |  | 0 |  |
|   |  | 2.70882               |  | 1                    |  | 5  |  | 1 |  | 2 |  |
|   |  | 2.67434               |  | 5                    |  | 2  |  | 0 |  | 3 |  |
|   |  | 2.59453               |  | 5                    |  | 8  |  | 1 |  | 1 |  |
|   |  | 2.56215               |  | 2                    |  | 6  |  | 1 |  | 2 |  |
|   |  | 2.55685               |  | 2                    |  | 8  |  | 0 |  | 2 |  |
|   |  | 2.51191               |  | 28                   |  | 9  |  | 1 |  | 0 |  |
|   |  | 2.49300               |  | 43                   |  | 10 |  | 0 |  | 1 |  |
|   |  | *2.49300              |  | 43                   |  | 0  |  | 2 |  | 0 |  |
|   |  | 2.48177               |  | 27                   |  | 1  |  | 2 |  | 0 |  |
|   |  | 2.42194               |  | 1                    |  | 5  |  | 0 |  | 3 |  |
|   |  | 2.41805               |  | 1                    |  | 7  |  | 1 |  | 2 |  |
|   |  | 2.40185               |  | 3                    |  | 9  |  | 1 |  | 1 |  |
|   |  | 2.39704               |  | 4                    |  | 3  |  | 2 |  | 0 |  |
|   |  | *2.39704              |  | 4                    |  | 0  |  | 1 |  | 3 |  |
|   |  | 2.38510               |  | 24                   |  | 1  |  | 1 |  | 3 |  |
|   |  | *2.38510              |  | 24                   |  | 0  |  | 2 |  | 1 |  |
|   |  | 2.37526               |  | 15                   |  | 1  |  | 2 |  | 1 |  |
|   |  | 2.35673               |  | 2                    |  | 2  |  | 1 |  | 3 |  |
|   |  | 2.34845               |  | 2                    |  | 2  |  | 2 |  | 1 |  |
|   |  | 2.31728               |  | 29                   |  | 10 |  | 1 |  | 0 |  |
|   |  | *2.31728              |  | 29                   |  | 8  |  | 0 |  | 3 |  |
|   |  | 2.31036               |  | 32                   |  | 3  |  | 1 |  | 3 |  |
|   |  | 2.28488               |  | 1                    |  | 11 |  | 0 |  | 1 |  |
|   |  | 2.27500               |  | 4                    |  | 8  |  | 1 |  | 2 |  |
|   |  | 2.25074               |  | 3                    |  | 5  |  | 2 |  | 0 |  |
|   |  | *2.25074              |  | 3                    |  | 4  |  | 1 |  | 3 |  |
|   |  | 2.22987               |  | 4                    |  | 10 |  | 1 |  | 1 |  |
|   |  | 2.20588               |  | 1                    |  | 7  |  | 0 |  | 3 |  |
|   |  | *2.20588              |  | 1                    |  | 10 |  | 0 |  | 2 |  |
|   |  | 2.18092               |  | 1                    |  | 12 |  | 0 |  | 0 |  |
|   |  | *2.18092              |  | 1                    |  | 5  |  | 1 |  | 3 |  |
|   |  | 2.17039               |  | 1                    |  | 5  |  | 2 |  | 1 |  |
|   |  | 2.16442               |  | 2                    |  | 6  |  | 2 |  | 0 |  |
|   |  | 2.14180               |  | 8                    |  | 9  |  | 1 |  | 2 |  |
|   |  | 2.12985               |  | 7                    |  | 0  |  | 2 |  | 2 |  |
|   |  | 2.12283               |  | 6                    |  | 1  |  | 2 |  | 2 |  |
|   |  | 2.10758               |  | 3                    |  | 12 |  | 0 |  | 1 |  |
|   |  | 2.09996               |  | 2                    |  | 2  |  | 2 |  | 2 |  |
|   |  | *2.09996              |  | 2                    |  | 6  |  | 1 |  | 3 |  |
|   |  | 2.09288               |  | 3                    |  | 6  |  | 2 |  | 1 |  |
|   |  | 2.07417               |  | 2                    |  | 11 |  | 1 |  | 1 |  |
|   |  | *2.07417              |  | 2                    |  | 7  |  | 2 |  | 0 |  |
|   |  | 2.06907               |  | 1                    |  | 3  |  | 2 |  | 2 |  |
|   |  | 2.04900               |  | 1                    |  | 0  |  | 0 |  | 4 |  |
|   |  | 2.04275               |  | 1                    |  | 1  |  | 0 |  | 4 |  |
|   |  | 1.51915               |  | 1                    |  | 1  |  | 0 |  | 2 |  |
| Lattice : Orthorhombic  |  | Mol. weight = 60.08   |  |                      |  |    |  |   |  |   |  |
| S.G. : P212121 (19)   |  | Volume [CD] = 1069.48 |  |                      |  |    |  |   |  |   |  |
| a = 26.17100  |  | Dx = 2.239            |  |                      |  |    |  |   |  |   |  |
| b = 4.98600   |  | Dm = 2.200            |  |                      |  |    |  |   |  |   |  |
| c = 8.19600   |  |                       |  |                      |  |    |  |   |  |   |  |
| a/b = 5.24890   |  | Z = 24                |  | I/cor = 0.66         |  |    |  |   |  |   |  |
| c/b = 1.64380   |  |                       |  |                      |  |    |  |   |  |   |  |
| ICSD collection code: 100199  |  |                       |  |                      |  |    |  |   |  |   |  |
| Temperature factor: ATF   |  |                       |  |                      |  |    |  |   |  |   |  |
| Temperature of data collection: REM TEM 428.  |  |                       |  |                      |  |    |  |   |  |   |  |
| Remarks from ICSD/CSD: REM B Probably wrong: Distances Si3 - O12.                                     |  |                       |  |                      |  |    |  |   |  |   |  |
| Sample preparation: Prepared from fired silica brick.   |  |                       |  |                      |  |    |  |   |  |   |  |
| Remarks from ICSD/CSD: Origin shifted by 0.0.25 to fit correct origin.                                |  |                       |  |                      |  |    |  |   |  |   |  |
| Remarks from ICSD/CSD: Monoclinic cell at RT: 25.86, 4.99, 18.504, 117.66.                            |  |                       |  |                      |  |    |  |   |  |   |  |
| Remarks from ICSD/CSD: Cell at 493 K: 8.75, 5.03, 8.211.  |  |                       |  |                      |  |    |  |   |  |   |  |
| Polymorphism: Transforms at about 378 K.  |  |                       |  |                      |  |    |  |   |  |   |  |
| Test from ICSD: Calc. density unusual but tolerable.  |  |                       |  |                      |  |    |  |   |  |   |  |
| Data collection flag: Non ambient temperature.  |  |                       |  |                      |  |    |  |   |  |   |  |
| Kihara, K., Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem., volume 146, page 185 (1977) |  |                       |  |                      |  |    |  |   |  |   |  |
| Calculated from ICSD using POWD-12++  |  |                       |  |                      |  |    |  |   |  |   |  |

# Quartz alpha, syn



01-078-1259 (C) - Quartz alpha, syn - SiO<sub>2</sub> - Y: 100.00 % - d x by: 1 - Wt.: 1.5406 - Hexagonal - a 4.83180 - b 4.83180 - c 5.33370 - alpha 90.000 - beta 90.000 - gamma 120.000 - Primitive - P3121 (152) - 3 - 107.859 - U/c PDP 3.4 - P29=10000.

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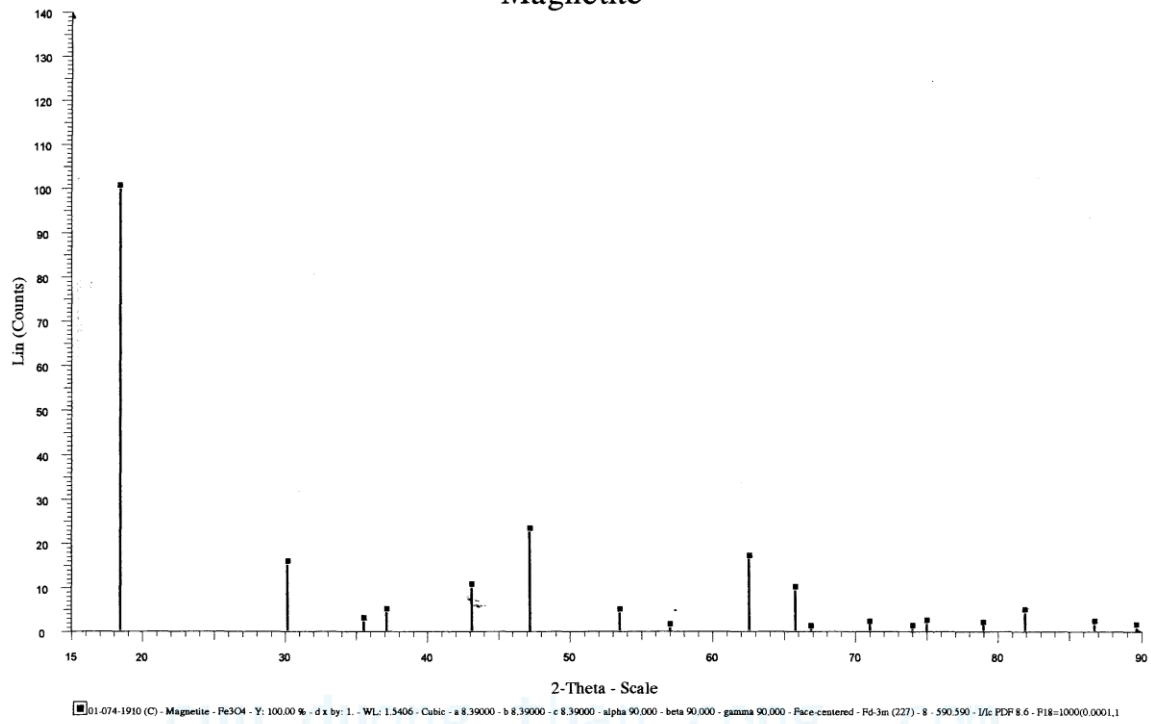
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| SiO <sub>2</sub>   |              | <table border="1"> <thead> <tr> <th><i>d</i> (Å)</th> <th><i>i</i></th> <th><i>h</i></th> <th><i>k</i></th> <th><i>l</i></th> </tr> </thead> <tbody> <tr><td>4.18446</td><td>165</td><td>1</td><td>0</td><td>0</td></tr> <tr><td>3.29221</td><td>999</td><td>0</td><td>1</td><td>1</td></tr> <tr><td>2.41590</td><td>53</td><td>1</td><td>1</td><td>0</td></tr> <tr><td>2.24894</td><td>65</td><td>1</td><td>0</td><td>2</td></tr> <tr><td>2.20068</td><td>18</td><td>1</td><td>1</td><td>1</td></tr> <tr><td>2.09223</td><td>45</td><td>2</td><td>0</td><td>0</td></tr> <tr><td>1.94774</td><td>8</td><td>0</td><td>2</td><td>1</td></tr> <tr><td>1.79046</td><td>106</td><td>1</td><td>1</td><td>2</td></tr> <tr><td>1.77790</td><td>6</td><td>0</td><td>0</td><td>3</td></tr> <tr><td>1.64610</td><td>21</td><td>2</td><td>0</td><td>2</td></tr> <tr><td>1.63633</td><td>12</td><td>0</td><td>1</td><td>3</td></tr> <tr><td>1.58158</td><td>1</td><td>2</td><td>1</td><td>0</td></tr> <tr><td>1.51632</td><td>42</td><td>1</td><td>2</td><td>1</td></tr> <tr><td>1.43194</td><td>12</td><td>1</td><td>1</td><td>3</td></tr> <tr><td>1.39482</td><td>1</td><td>3</td><td>0</td><td>0</td></tr> <tr><td>1.36034</td><td>25</td><td>2</td><td>1</td><td>2</td></tr> <tr><td>1.35481</td><td>37</td><td>2</td><td>0</td><td>3</td></tr> <tr><td>1.34944</td><td>18</td><td>3</td><td>0</td><td>1</td></tr> <tr><td>1.27048</td><td>10</td><td>1</td><td>0</td><td>4</td></tr> <tr><td>1.23598</td><td>4</td><td>0</td><td>3</td><td>2</td></tr> <tr><td>1.20795</td><td>6</td><td>2</td><td>2</td><td>0</td></tr> <tr><td>1.18168</td><td>15</td><td>2</td><td>1</td><td>3</td></tr> <tr><td>1.17811</td><td>13</td><td>2</td><td>2</td><td>1</td></tr> <tr><td>1.16741</td><td>7</td><td>1</td><td>1</td><td>4</td></tr> <tr><td>1.16056</td><td>15</td><td>3</td><td>1</td><td>0</td></tr> <tr><td>1.13403</td><td>4</td><td>3</td><td>1</td><td>1</td></tr> <tr><td>1.12447</td><td>3</td><td>2</td><td>0</td><td>4</td></tr> <tr><td>1.10034</td><td>3</td><td>2</td><td>2</td><td>2</td></tr> <tr><td>1.09740</td><td>3</td><td>3</td><td>0</td><td>3</td></tr> </tbody> </table> |          |          |  | <i>d</i> (Å) | <i>i</i> | <i>h</i> | <i>k</i> | <i>l</i> | 4.18446 | 165 | 1 | 0 | 0 | 3.29221 | 999 | 0 | 1 | 1 | 2.41590 | 53 | 1 | 1 | 0 | 2.24894 | 65 | 1 | 0 | 2 | 2.20068 | 18 | 1 | 1 | 1 | 2.09223 | 45 | 2 | 0 | 0 | 1.94774 | 8 | 0 | 2 | 1 | 1.79046 | 106 | 1 | 1 | 2 | 1.77790 | 6 | 0 | 0 | 3 | 1.64610 | 21 | 2 | 0 | 2 | 1.63633 | 12 | 0 | 1 | 3 | 1.58158 | 1 | 2 | 1 | 0 | 1.51632 | 42 | 1 | 2 | 1 | 1.43194 | 12 | 1 | 1 | 3 | 1.39482 | 1 | 3 | 0 | 0 | 1.36034 | 25 | 2 | 1 | 2 | 1.35481 | 37 | 2 | 0 | 3 | 1.34944 | 18 | 3 | 0 | 1 | 1.27048 | 10 | 1 | 0 | 4 | 1.23598 | 4 | 0 | 3 | 2 | 1.20795 | 6 | 2 | 2 | 0 | 1.18168 | 15 | 2 | 1 | 3 | 1.17811 | 13 | 2 | 2 | 1 | 1.16741 | 7 | 1 | 1 | 4 | 1.16056 | 15 | 3 | 1 | 0 | 1.13403 | 4 | 3 | 1 | 1 | 1.12447 | 3 | 2 | 0 | 4 | 1.10034 | 3 | 2 | 2 | 2 | 1.09740 | 3 | 3 | 0 | 3 |
|--|--------------|---|----------|----------|--|--------------|----------|----------|----------|----------|---------|-----|---|---|---|---------|-----|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|---|---|---|---|---------|-----|---|---|---|---------|---|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|---|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|---|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|---|---|---|---|---------|---|---|---|---|---------|----|---|---|---|---------|----|---|---|---|---------|---|---|---|---|---------|----|---|---|---|---------|---|---|---|---|---------|---|---|---|---|---------|---|---|---|---|---------|---|---|---|---|
| <i>d</i> (Å)   | <i>i</i>     | <i>h</i>  | <i>k</i> | <i>l</i> |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 4.18446  | 165          | 1   | 0        | 0        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 3.29221  | 999          | 0   | 1        | 1        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 2.41590  | 53           | 1   | 1        | 0        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 2.24894  | 65           | 1   | 0        | 2        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 2.20068  | 18           | 1   | 1        | 1        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 2.09223  | 45           | 2   | 0        | 0        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.94774  | 8            | 0   | 2        | 1        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.79046  | 106          | 1   | 1        | 2        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.77790  | 6            | 0   | 0        | 3        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.64610  | 21           | 2   | 0        | 2        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.63633  | 12           | 0   | 1        | 3        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.58158  | 1            | 2   | 1        | 0        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.51632  | 42           | 1   | 2        | 1        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.43194  | 12           | 1   | 1        | 3        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.39482  | 1            | 3   | 0        | 0        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.36034  | 25           | 2   | 1        | 2        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.35481  | 37           | 2   | 0        | 3        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.34944  | 18           | 3   | 0        | 1        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.27048  | 10           | 1   | 0        | 4        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.23598  | 4            | 0   | 3        | 2        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.20795  | 6            | 2   | 2        | 0        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.18168  | 15           | 2   | 1        | 3        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.17811  | 13           | 2   | 2        | 1        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.16741  | 7            | 1   | 1        | 4        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.16056  | 15           | 3   | 1        | 0        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.13403  | 4            | 3   | 1        | 1        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.12447  | 3            | 2   | 0        | 4        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.10034  | 3            | 2   | 2        | 2        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| 1.09740  | 3            | 3   | 0        | 3        |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| Silicon Oxide<br>Quartz α, syn   |              |   |          |          |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| <b>Lattice</b> : Hexagonal<br><b>S.G.</b> : P3121 (152)  |              | <b>Mol. weight</b> = 60.08<br><b>Volume [CD]</b> = 107.84   |          |          |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| <b>a</b> = 4.83180<br><br><b>c</b> = 5.33370   | <b>Z</b> = 3 | <b>Dx</b> = 2.776<br><br><b>l/lcor</b> = 3.42   |          |          |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| <b>ICSD collection code:</b> 062411<br><b>Temperature factor:</b> ATF<br><b>Remarks from ICSD/CSD:</b> REM TEM 488.<br><b>Remarks from ICSD/CSD:</b> REM PRE 23kbar.<br><b>Data collection flag:</b> Non ambient temperature and pressure. |              |   |          |          |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |
| Ogata, K., Takeuchi, Y., Kudoh, Y., Z. Kristallogr., volume 179, page 403 (1987)<br>Calculated from ICSD using POWD-12++ (1997)  |              |   |          |          |  |              |          |          |          |          |         |     |   |   |   |         |     |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |     |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |    |   |   |   |         |    |   |   |   |         |   |   |   |   |         |    |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |         |   |   |   |   |

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# Magnetite



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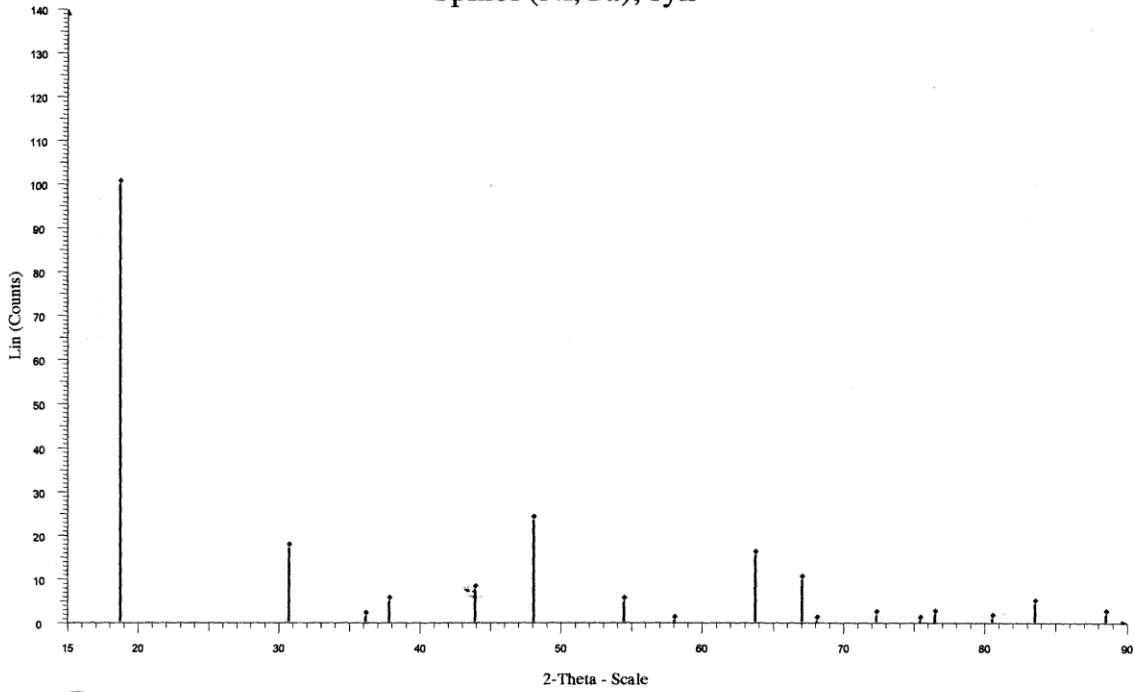
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| Fe <sub>3</sub> O <sub>4</sub>  |  | <i>d</i> (Å)                  | <i>l</i> | <i>h</i> | <i>k</i> | <i>l</i> |  |  |  |  |  |
|---|--|-------------------------------|----------|----------|----------|----------|--|--|--|--|--|
| Iron Oxide<br>Magnetite   |  | 4.84397                       | 999      | 1        | 1        | 1        |  |  |  |  |  |
|   |  | 2.96631                       | 147      | 2        | 2        | 0        |  |  |  |  |  |
|   |  | 2.52968                       | 19       | 3        | 1        | 1        |  |  |  |  |  |
|   |  | 2.42198                       | 39       | 2        | 2        | 2        |  |  |  |  |  |
|   |  | 2.09750                       | 96       | 4        | 0        | 0        |  |  |  |  |  |
|   |  | 1.92480                       | 223      | 3        | 3        | 1        |  |  |  |  |  |
|   |  | 1.71260                       | 38       | 4        | 2        | 2        |  |  |  |  |  |
|   |  | 1.61466                       | 4        | 5        | 1        | 1        |  |  |  |  |  |
|   |  | 1.48316                       | 161      | 4        | 4        | 0        |  |  |  |  |  |
|   |  | 1.41817                       | 89       | 5        | 3        | 1        |  |  |  |  |  |
|   |  | 1.39833                       | 1        | 4        | 4        | 2        |  |  |  |  |  |
|   |  | 1.32658                       | 11       | 6        | 2        | 0        |  |  |  |  |  |
|   |  | 1.27946                       | 1        | 5        | 3        | 3        |  |  |  |  |  |
|   |  | 1.26484                       | 14       | 6        | 2        | 2        |  |  |  |  |  |
|   |  | 1.21099                       | 9        | 4        | 4        | 4        |  |  |  |  |  |
|   |  | 1.17483                       | 37       | 7        | 1        | 1        |  |  |  |  |  |
|   |  | 1.12116                       | 12       | 6        | 4        | 2        |  |  |  |  |  |
|   |  | 1.09229                       | 3        | 7        | 3        | 1        |  |  |  |  |  |
| <b>Lattice</b> : Face-centered cubic  |  | <b>Mol. weight</b> = 231.54   |          |          |          |          |  |  |  |  |  |
| <b>S.G.</b> : Fd-3m (227)   |  | <b>Volume [CD]</b> = 590.59   |          |          |          |          |  |  |  |  |  |
| <b>a</b> = 8.39000  |  | <b>Dx</b> = 5.208             |          |          |          |          |  |  |  |  |  |
| <b>Z</b> = 8  |  | <b>V<sub>cor</sub></b> = 8.56 |          |          |          |          |  |  |  |  |  |
| <p><b>ICSD collection code:</b> 027899<br/> <b>Remarks from ICSD/CSD:</b> REM TEM below transition point of 120 K.<br/> <b>Remarks from ICSD/CSD:</b> REM B Author proposes an ordered distribution within the oct<br/> <b>Remarks from ICSD/CSD:</b> REM interstices..<br/> <b>Test from ICSD:</b> No R value given.<br/> <b>Test from ICSD:</b> At least one TF missing.<br/> <b>Additional pattern:</b> See entry 27898.<br/> <b>Additional pattern:</b> See PDF 74-1919 and PDF 74-1909.<br/> <b>Data collection flag:</b> Non ambient temperature.</p> |  |                               |          |          |          |          |  |  |  |  |  |
| <p>de Boer, F., van Santen, J.H., Verwey, E.J.W., J. Chem. Phys., volume 18, page 1032 (1950)<br/>           Calculated from ICSD using POWD-12++ (1997)</p>  |  |                               |          |          |          |          |  |  |  |  |  |

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# Spinel (Ni,Ga), syn



01-074-1913 (C) - Spinel (Ni,Ga), syn - NiFe2O4 - Y: 100.00 % - d x by: 1 - WL: 1.5406 - Cubic - a 8.25800 - b 8.25800 - c 8.25800 - alpha 90.000 - beta 90.000 - gamma 90.000 - Face-centered - Pd-3m (227) - h - 563.151 - I/Ic PDF 9.9 - P17=10

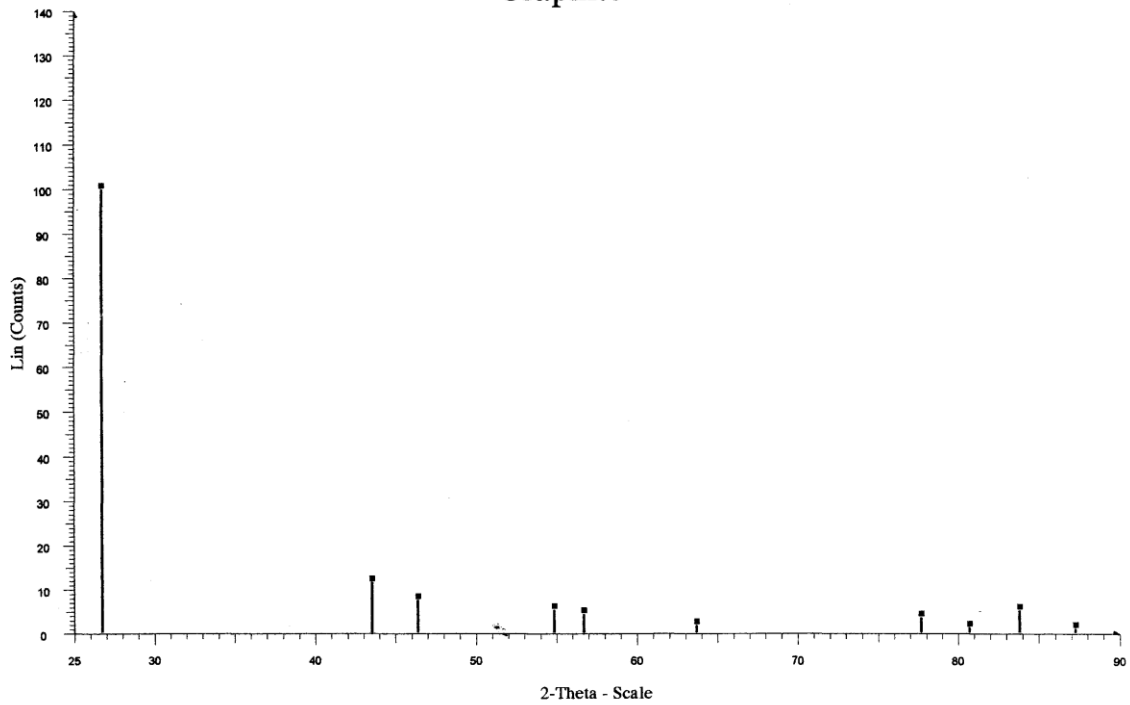
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| Pattern : 01-074-1913  |  | Radiation = 1.540560  |  | Quality : Calculated   |  |  |  |  |  |  |  |
|--|--|---|--|--|--|--|--|--|--|--|--|
| <p>NiFe<sub>2</sub>O<sub>4</sub></p> <p>Nickel Iron Oxide<br/>Spinel (Ni,Ga), syn</p>  |  | <p><b>d (Å)</b></p> <p>4.76776 999<br/>2.91964 158<br/>2.48988 11<br/>2.38388 45<br/>2.06450 71<br/>1.89452 232<br/>1.68566 45<br/>1.58925 2<br/>1.45982 152<br/>1.39586 94<br/>1.37633 1<br/>1.30570 14<br/>1.25933 1<br/>1.24494 15<br/>1.19194 6<br/>1.15635 40<br/>1.10352 15</p> |  | <p><b>i</b></p> <p>1<br/>2<br/>3<br/>2<br/>4<br/>3<br/>4<br/>5<br/>4<br/>5<br/>4<br/>6<br/>5<br/>6<br/>4<br/>7<br/>6</p> |  | <p><b>h</b></p> <p>1<br/>2<br/>1<br/>2<br/>0<br/>3<br/>2<br/>1<br/>4<br/>3<br/>4<br/>2<br/>3<br/>2<br/>4<br/>1<br/>4</p> |  | <p><b>k</b></p> <p>1<br/>2<br/>1<br/>2<br/>0<br/>3<br/>2<br/>1<br/>4<br/>3<br/>4<br/>0<br/>3<br/>2<br/>4<br/>1<br/>4</p> |  | <p><b>l</b></p> <p>1<br/>0<br/>1<br/>2<br/>0<br/>1<br/>2<br/>1<br/>0<br/>1<br/>2<br/>0<br/>3<br/>2<br/>4<br/>1<br/>2</p> |  |
| <p><b>Lattice</b> : Face-centered cubic</p> <p><b>S.G.</b> : Fd-3m (227)</p> <p><b>a</b> = 8.25800</p>   |  | <p><b>Mol. weight</b> = 234.39</p> <p><b>Volume [CD]</b> = 563.15</p> <p><b>Dx</b> = 5.529</p>  |  | <p><b>Z</b> = 8</p> <p><b>I/cor</b> = 9.92</p>   |  |  |  |  |  |  |  |
| <p><b>ICSD collection code:</b> 027903<br/> <b>Remarks from ICSD/CSD:</b> REM <math>\frac{1}{2}</math> MAG.<br/> <b>Test from ICSD:</b> No R value given.<br/> <b>Test from ICSD:</b> At least one TF missing.<br/> <b>Sample preparation:</b> Prepared from oxides at 1673 K for 1-2 hours.<br/> <b>Additional pattern:</b> See PDF 10-114.<br/> <b>Test from ICSD:</b> Calc. density unusual but tolerable.<br/> <b>Data collection flag:</b> Ambient.</p> |  |   |  |  |  |  |  |  |  |  |  |
| <p>Greenwald, S., Pickart, S.J., Grannis, F.H., J. Chem. Phys., volume 22, page 1597 (1954)<br/>           Calculated from ICSD using POWD-12++</p>  |  |   |  |  |  |  |  |  |  |  |  |
| <p><b>Radiation</b> : CuK<math>\alpha</math>1</p> <p><b>Lambda</b> : 1.54060</p> <p><b>SS/FOM</b> : F17=1000(0.0001,17)</p>  |  | <p><b>Filter</b> : Not specified</p> <p><b>d-sp</b> : Calculated spacings</p>   |  |  |  |  |  |  |  |  |  |



# Graphite



01-075-2078 (C) - Graphite - C - Wt.: 1.5406 - Rhombo.R.axes - Primitive - a 3.63500 - b 3.63500 - c 3.63500 - alpha 39.490 - beta 39.490 - gamma 39.490 - R-3m (166) - 2 - 17.4850 - I/c PDP 2.3 - F(0)=1000(0.0001,10)

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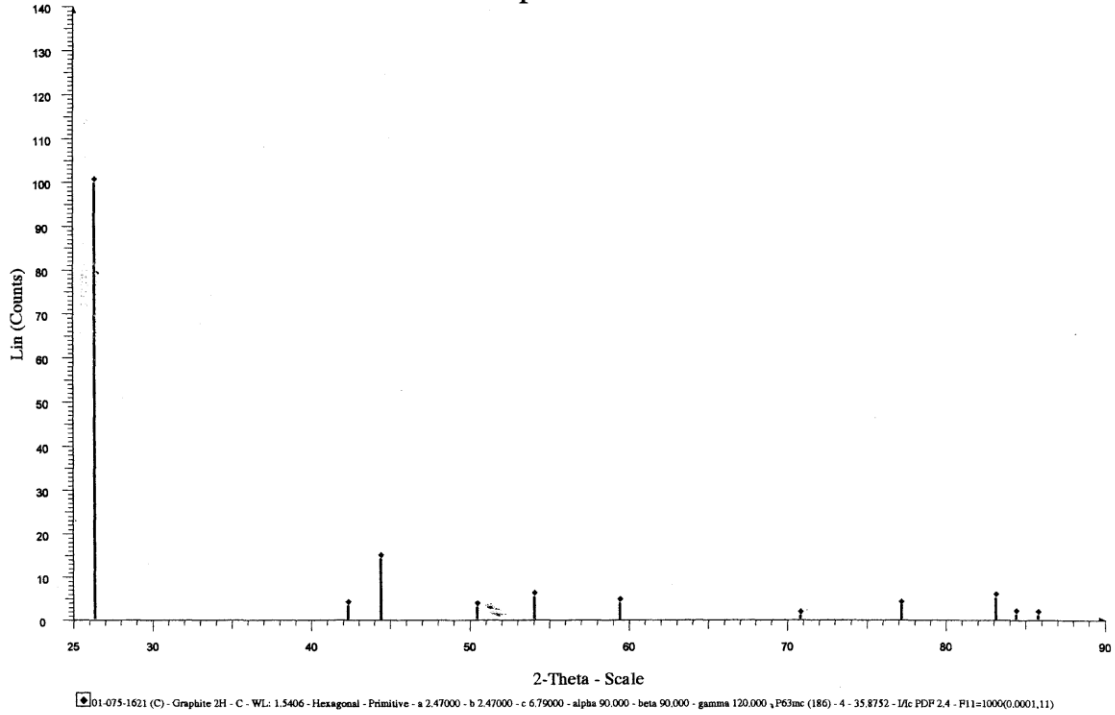
Pattern : 01-075-2078

Radiation = 1.540560

Quality : Calculated

| C  |  | <i>d</i> (Å)   | <i>l</i> | <i>h</i> | <i>k</i> | <i>l</i> |  |  |  |  |  |  |  |
|--|--|--|----------|----------|----------|----------|--|--|--|--|--|--|--|
| Graphite   |  | 3.34701  | 999      | 1        | 1        | 1        |  |  |  |  |  |  |  |
|  |  | 2.08083  | 113      | 0        | 1        | 0        |  |  |  |  |  |  |  |
|  |  | 1.95849  | 72       | 1        | 1        | 0        |  |  |  |  |  |  |  |
|  |  | 1.67351  | 50       | 2        | 2        | 2        |  |  |  |  |  |  |  |
|  |  | 1.62279  | 40       | 1        | 1        | 2        |  |  |  |  |  |  |  |
|  |  | 1.46021  | 14       | 2        | 2        | 1        |  |  |  |  |  |  |  |
|  |  | 1.22803  | 32       | -1       | 1        | 0        |  |  |  |  |  |  |  |
|  |  | 1.18926  | 10       | 2        | 3        | 2        |  |  |  |  |  |  |  |
|  |  | 1.15288  | 49       | 1        | 2        | 0        |  |  |  |  |  |  |  |
|  |  | 1.11567  | 7        | 3        | 3        | 3        |  |  |  |  |  |  |  |
| <b>Lattice</b> : Rhombohedral<br><b>S.G.</b> : R-3m (166)  |  | <b>Mol. weight</b> = 12.01<br><b>Volume [CD]</b> = 52.45               |          |          |          |          |  |  |  |  |  |  |  |
| <b>a</b> = 3.63500 <b>alpha</b> = 39.49<br><br><b>Z</b> = 2  |  | <b>Dx</b> = 2.281<br><br><b>I/cor</b> = 2.32                           |          |          |          |          |  |  |  |  |  |  |  |
| <b>ICSD collection code:</b> 031829<br><b>Remarks from ICSD/CSD:</b> PICT. $f^f$<br><b>Test from ICSD:</b> No R value given.<br><b>Test from ICSD:</b> At least one TF missing.<br><b>Data collection flag:</b> Ambient. |  |  |          |          |          |          |  |  |  |  |  |  |  |
| Lipson, H., Stokes, A.R., Proc. R. Soc. London, Ser. A, volume 181, page 101 (1942)<br>Calculated from ICSD using POWD-12++ (1997)   |  |  |          |          |          |          |  |  |  |  |  |  |  |
| <b>Radiation</b> : CuK $\alpha$ 1<br><br><b>Lambda</b> : 1.54060<br><br><b>SS/FOM</b> : F10=1000(0.0001,10)  |  | <b>Filter</b> : Not specified<br><br><b>d-sp</b> : Calculated spacings |          |          |          |          |  |  |  |  |  |  |  |

# Graphite 2H



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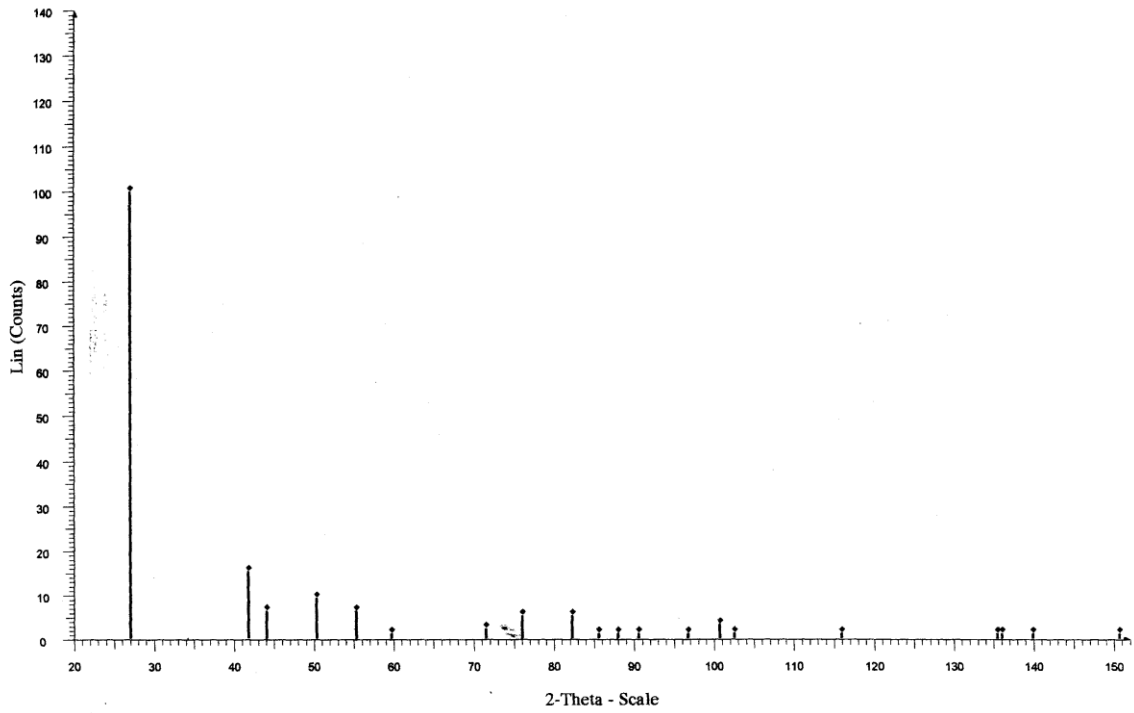
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|  |              |                             |          |                             |          |          |
|--|--------------|-----------------------------|----------|-----------------------------|----------|----------|
| <b>Pattern</b> : 01-075-1621   |              | <b>Radiation</b> = 1.540560 |          | <b>Quality</b> : Calculated |          |          |
| <b>C</b><br><br>Carbon<br>Graphite 2H  |              | <b>d (Å)</b>                | <b>l</b> | <b>h</b>                    | <b>k</b> | <b>i</b> |
|  |              | 3.39500                     | 999      | 0                           | 0        | 2        |
|  |              | 2.13908                     | 29       | 1                           | 0        | 0        |
|  |              | 2.04023                     | 138      | 1                           | 0        | 1        |
|  |              | 1.80980                     | 26       | 1                           | 0        | 2        |
|  |              | 1.69750                     | 50       | 0                           | 0        | 4        |
|  |              | 1.55463                     | 36       | 1                           | 0        | 3        |
|  |              | 1.32969                     | 6        | 1                           | 0        | 4        |
|  |              | 1.23500                     | 31       | 1                           | 1        | 0        |
|  |              | 1.18060                     | 48       | 1                           | 1        | 2        |
|  |              | 1.14648                     | 9        | 1                           | 0        | 5        |
|  |              | 1.13167                     | 7        | 0                           | 0        | 6        |
| <b>Lattice</b> : Hexagonal   |              | <b>Mol. weight</b> = 12.01  |          |                             |          |          |
| <b>S.G.</b> : P63mc (186)  |              | <b>Volume [CD]</b> = 35.88  |          |                             |          |          |
| <b>a</b> = 2.47000   |              | <b>Dx</b> = 2.224           |          |                             |          |          |
| <b>c</b> = 6.79000   | <b>Z</b> = 4 | <b>I/cor</b> = 2.37         |          |                             |          |          |
| <b>ICSD collection code</b> : 031170<br><b>Test from ICSD</b> : No R value given.<br><b>Test from ICSD</b> : At least one TF missing.<br><b>Sample source or locality</b> : Specimen from Kropfmuhl, Bavaria, Germany.<br><b>Test from ICSD</b> : Calc. density unusual but tolerable.<br><b>Data collection flag</b> : Ambient. |              |                             |          |                             |          |          |
| Hassel, O., Z. Phys., volume 25, page 317 (1924)<br>Calculated from ICSD using POWD-12++ (1997)  |              |                             |          |                             |          |          |

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# Boron Nitride



00-034-0421 (j) - Boron Nitride - BN - WL: 1.5406 - Hexagonal - Primitive - a 2.50441 - b 2.50441 - c 6.65620 - alpha 90.000 - beta 90.000 - gamma 120.000 - P63/mmc (194) - 2 - 36.1550 - I/c PDF 1 - P20= 720.0112,25)

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Pattern : 00-034-0421

Radiation = 1.540560

Quality : Indexed

BN

Boron Nitride

| d (Å)   | h   | k | l |
|---------|-----|---|---|
| 3.32813 | 100 | 0 | 0 |
| 2.16930 | 15  | 1 | 0 |
| 2.06190 | 6   | 1 | 0 |
| 1.81758 | 9   | 1 | 0 |
| 1.66362 | 6   | 0 | 0 |
| 1.55090 | 1   | 1 | 0 |
| 1.31985 | 2   | 1 | 0 |
| 1.25210 | 5   | 1 | 1 |
| 1.17205 | 5   | 1 | 1 |
| 1.13457 | 1   | 1 | 0 |
| 1.10946 | 1   | 0 | 0 |
| 1.08432 | 1   | 2 | 0 |
| 1.03115 | 1   | 2 | 0 |
| 1.00052 | 3   | 1 | 1 |
| 0.98770 | 1   | 1 | 0 |
| 0.90861 | 1   | 2 | 0 |
| 0.83185 | 1   | 0 | 0 |
| 0.83036 | 1   | 1 | 1 |
| 0.81973 | 1   | 2 | 1 |
| 0.79598 | 1   | 2 | 1 |

Lattice : Hexagonal

Mol. weight = 24.82

S.G. : P63/mmc (194)

Volume [CD] = 36.15

a = 2.50441

Dx = 2.280

c = 6.65620

Z = 2

Sample source or locality: The sample was obtained from the Carborundum Company, Niagara Falls, New York, USA.

Structure: The structure was done by Pease (1952).

Polymorphism: A high pressure wurtzite type form was described by Soma et al. (1974) and another high pressure zinc blende type structure was described by Coleburn and Forbes (1968).

Color: Colorless

Additional pattern: To replace 9-12.

Data collection flag: Ambient.

Coleburn, N. et al., J. Chem. Phys., volume 48, page 555 (1968)  
Natl. Bur. Stand. (U.S.) Monogr. 25, volume 20, page 22 (1983)

CAS Number: 10294-33-4

Radiation : CuKα1

Filter : Monochromator crystal

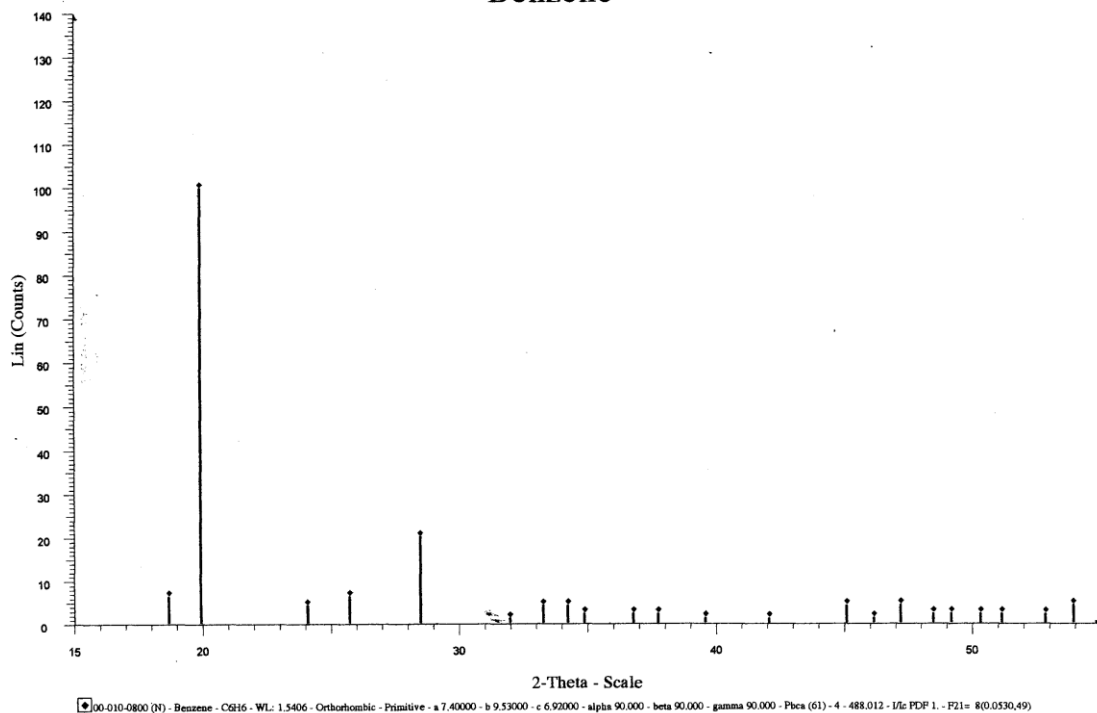
Lambda : 1.54060

d-sp : Diffractometer

SS/FOM : F20= 72(0.0112,25)

Internal standard : Si

# Benzene



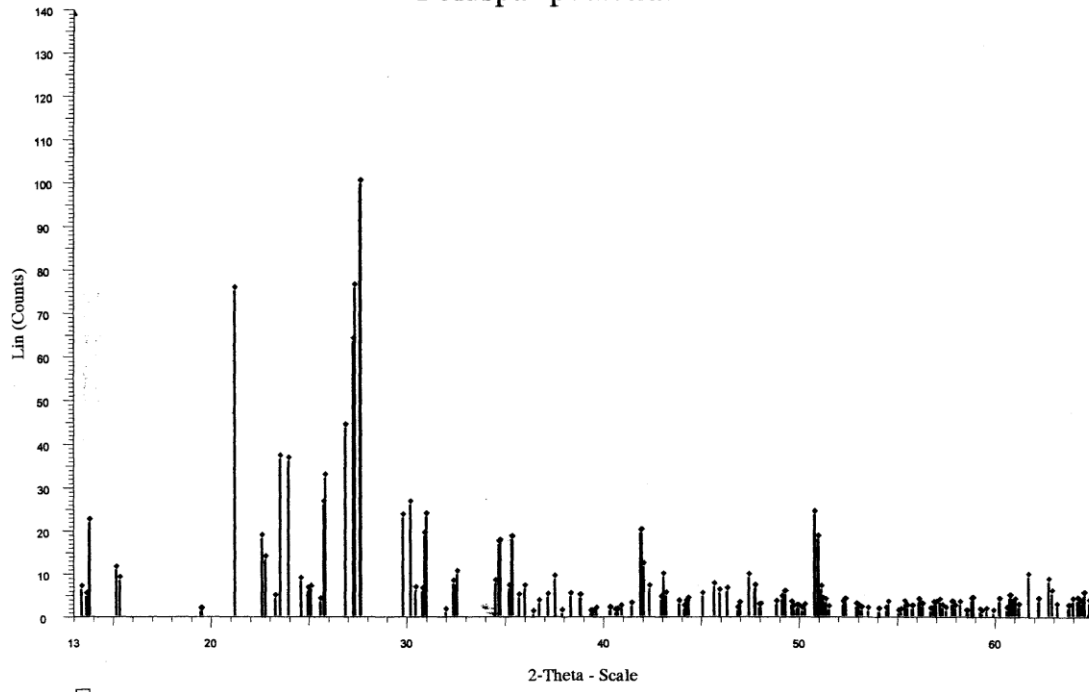
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| Pattern : 00-010-0800   |  | Radiation = 1.540560   |          | Quality : Not indexed |          |          |
|---|--|--|----------|-----------------------|----------|----------|
| C <sub>6</sub> H <sub>6</sub>   |  | <b>d (Å)</b>   | <b>l</b> | <b>h</b>              | <b>k</b> | <b>l</b> |
| Benzene   |  | 4.76000  | 6        | 0                     | 2        | 0        |
|   |  | 4.47000  | 100      | 1                     | 1        | 1        |
|   |  | 3.70000  | 4        | 2                     | 0        | 0        |
|   |  | 3.47000  | 6        | 1                     | 2        | 1        |
|   |  | 3.12000  | 20       | 1                     | 0        | 2        |
|   |  | 2.80300  | 1        | 0                     | 2        | 2        |
|   |  | 2.69400  | 4        | 2                     | 2        | 1        |
|   |  | 2.61700  | 4        | 1                     | 2        | 2        |
|   |  | 2.57100  | 2        |                       |          |          |
|   |  | 2.44500  | 2        | 2                     | 1        | 2        |
|   |  | 2.38800  | 2        | 0                     | 4        | 0        |
|   |  | 2.26200  | 1        | 2                     | 3        | 1        |
|   |  | 2.14900  | 1        | 1                     | 1        | 3        |
|   |  | 2.00900  | 4        | 3                     | 0        | 2        |
|   |  | 1.96600  | 1        | 3                     | 1        | 2        |
|   |  | 1.92200  | 4        | 2                     | 4        | 1        |
|   |  | 1.88200  | 2        | 3                     | 3        | 1        |
|   |  | 1.85400  | 2        | 3                     | 2        | 2        |
|   |  | 1.81200  | 2        | 2                     | 2        | 3        |
|   |  | 1.78400  | 2        | 1                     | 5        | 1        |
|   |  | 1.73100  | 2        | 0                     | 0        | 4        |
|   |  | 1.70000  | 4        | 3                     | 3        | 2        |
| <b>Lattice :</b> Orthorhombic<br><b>S.G. :</b> Pbc <sub>a</sub> (61)<br><b>a =</b> 7.40000<br><b>b =</b> 9.53000<br><b>c =</b> 6.92000<br><b>a/b =</b> 0.77650 <b>Z =</b> 4<br><b>c/b =</b> 0.72613 |  | <b>Mol. weight =</b> 78.11<br><b>Volume [CD] =</b> 488.01<br><b>Dx =</b> 1.063 |          |                       |          |          |
| <b>Temperature of data collection:</b> Pattern taken at -25 C.<br><b>Data collection flag:</b> Non ambient temperature.   |  |  |          |                       |          |          |
| Posner, A., Thesis, Polytechnic Institute of Brooklyn, Brooklyn, New York, USA., Private Communication (1949)<br>CAS Number: 71-43-2  |  |  |          |                       |          |          |
| <b>Radiation :</b> CuKα<br><b>Lambda :</b> 1.54180<br><b>SS/FOM :</b> F21= 8(0.0530,49)   |  | <b>Filter :</b> Beta<br><b>d-sp :</b> Other                                    |          |                       |          |          |



# Feldspar potassian



01-084-0710 (C) - Feldspar potassian - K<sub>2</sub>Si<sub>2</sub>O<sub>7</sub> - WL: 1.5406 - Triclinic - Base-centered - a 8.52900 - b 12.94500 - c 7.18900 - alpha 90.360 - beta 115.990 - gamma 88.800 - C-1 (0) - 4 - 713.294 - I/c PDF 0.6 - F30=161

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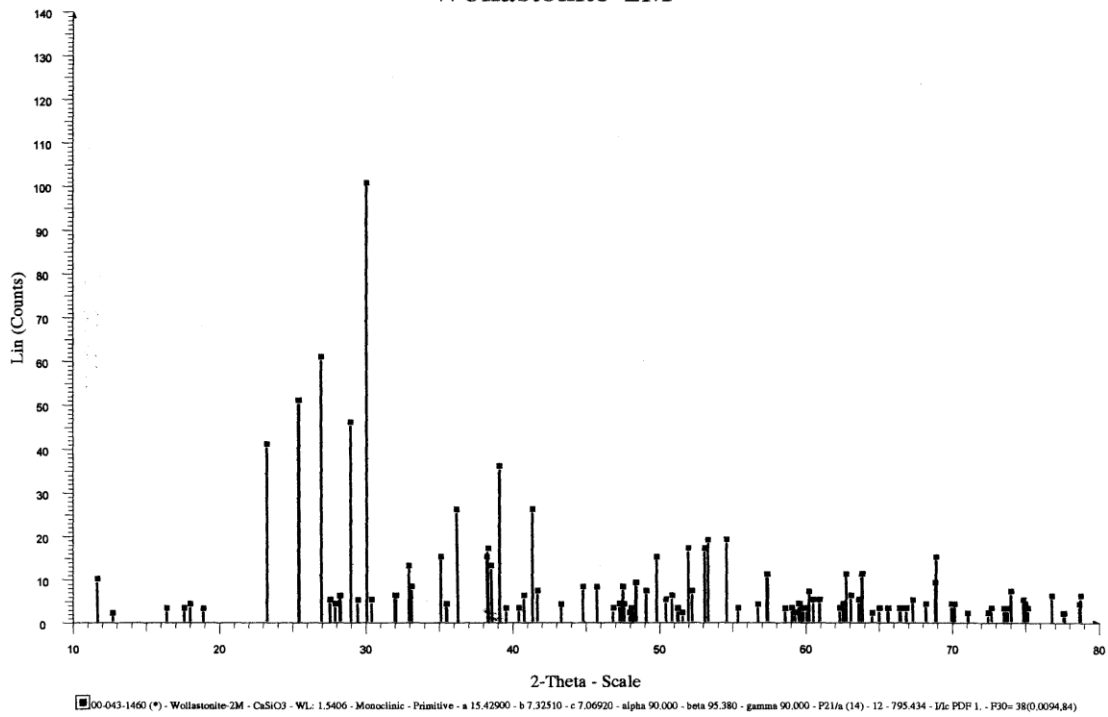
cuu duong than cong. com

| Pattern : 01-084-0710   |  | Radiation = 1.540560 |          |          |          |              | Quality : Calculated |          |          |    |   |   |
|---|--|----------------------|----------|----------|----------|--------------|----------------------|----------|----------|----|---|---|
| K <sub>5</sub> Na <sub>5</sub> AlSi <sub>3</sub> O <sub>8</sub> |  | <b>d (Å)</b>         | <b>h</b> | <b>k</b> | <b>l</b> | <b>d (Å)</b> | <b>h</b>             | <b>k</b> | <b>l</b> |    |   |   |
| Potassium Sodium Aluminum Silicate<br>Feldspar potassian        |  | 6.65436              | 80       | 1        | 1        | 0            | 1.64961              | 48       | 1        | -1 | 3 | 0 |
|   |  | 6.53730              | 43       | -1       | 1        | 0            | *1.64961             | 48       | 4        | 2  | 0 | 0 |
|   |  | 6.47105              | 215      | 0        | 2        | 0            | 1.83703              | 23       | 3        | 5  | 0 | 0 |
|   |  | *6.47105             | 215      | 0        | 0        | 1            | *1.83703             | 23       | -4       | -2 | 0 | 0 |
|   |  | 5.86265              | 105      | -1       | -1       | 1            | 1.83365              | 13       | -3       | 5  | 2 | 0 |
|   |  | 5.81467              | 80       | -1       | 1        | 1            | 1.82732              | 15       | -4       | 2  | 0 | 0 |
|   |  | 4.57966              | 8        | 0        | 2        | 1            | *1.82732             | 15       | 1        | -5 | 2 | 0 |
|   |  | *4.57966             | 8        | 0        | -2       | 1            | 1.81900              | 9        | -4       | 2  | 0 | 0 |
|   |  | 4.20164              | 750      | -2       | 0        | 1            | 1.81352              | 17       | -2       | -6 | 2 | 0 |
|   |  | 3.94828              | 178      | 1        | 1        | 1            | *1.79691             | 235      | -2       | 0  | 4 | 0 |
|   |  | 3.91876              | 129      | 1        | -1       | 1            | *1.79691             | 235      | 0        | 6  | 2 | 0 |
|   |  | 3.83245              | 37       | 2        | 0        | 0            | 1.79131              | 177      | 0        | -6 | 2 | 0 |
|   |  | 3.79242              | 363      | 1        | 3        | 0            | *1.79131             | 177      | 0        | -4 | 3 | 0 |
|   |  | 3.72737              | 358      | -1       | 3        | 0            | 1.76600              | 60       | -1       | -7 | 1 | 0 |
|   |  | 3.62703              | 80       | -1       | -3       | 1            | 1.78227              | 32       | -4       | -4 | 1 | 0 |
|   |  | 3.58056              | 55       | -1       | 3        | 1            | 1.77636              | 29       | -4       | -4 | 2 | 0 |
|   |  | 3.55676              | 59       | -2       | -2       | 1            | 1.77295              | 12       | -1       | 7  | 1 | 0 |
|   |  | 3.46207              | 30       | -2       | 2        | 1            | 1.75063              | 24       | -2       | 4  | 2 | 0 |
|   |  | 3.46807              | 257      | -1       | 1        | 2            | 1.74807              | 30       | 4        | 4  | 1 | 0 |
|   |  | 3.45753              | 319      | -1       | 1        | 2            | *1.74803             | 30       | -1       | -5 | 3 | 0 |
|   |  | 3.27116              | 435      | 2        | 2        | 0            | 1.73018              | 19       | 2        | -4 | 2 | 0 |
|   |  | 3.27233              | 633      | -2       | 0        | 2            | *1.73018             | 19       | -2       | 2  | 4 | 0 |
|   |  | 3.26665              | 757      | -2       | 0        | 2            | 1.72699              | 16       | -1       | -1 | 4 | 0 |
|   |  | 3.23067              | 999      | 0        | 4        | 0            | *1.72699             | 16       | -1       | -1 | 4 | 0 |
|   |  | *3.23067             | 999      | 0        | 0        | 2            | 1.72145              | 11       | 2        | 6  | 1 | 0 |
|   |  | 3.00231              | 228      | 1        | 3        | 1            | *1.72145             | 11       | 1        | 3  | 3 | 0 |
|   |  | 2.96369              | 257      | -1       | -3       | 1            | 1.71175              | 9        | 1        | -3 | 3 | 0 |
|   |  | 2.94042              | 57       | -2       | -2       | 2            | 1.69402              | 8        | 1        | 7  | 1 | 0 |
|   |  | 2.90733              | 54       | -2       | 2        | 2            | *1.69402             | 8        | -5       | -1 | 2 | 0 |
|   |  | 2.86986              | 184      | 0        | 4        | 1            | 1.68495              | 9        | -5       | 1  | 2 | 0 |
|   |  | 2.86986              | 184      | 0        | 2        | 2            | 1.68126              | 23       | -3       | -5 | 2 | 0 |
|   |  | 2.86940              | 229      | 0        | -4       | 1            | 1.66727              | 3        | 3        | 1  | 2 | 0 |
|   |  | *2.86940             | 229      | 0        | -2       | 2            | 1.66359              | 5        | 4        | 4  | 0 | 0 |
|   |  | 2.80144              | 5        | 0        | 0        | 1            | 1.65817              | 25       | 3        | 5  | 3 | 0 |
|   |  | 2.78928              | 72       | -1       | -3       | 2            | 1.65518              | 15       | -5       | -1 | 1 | 0 |
|   |  | 2.78106              | 65       | -3       | 1        | 1            | *1.65518             | 15       | -4       | -4 | 3 | 0 |
|   |  | 2.75324              | 94       | -1       | 3        | 2            | 1.64803              | 14       | -1       | -7 | 2 | 0 |
|   |  | 2.60183              | 73       | -3       | -1       | 2            | *1.64803             | 14       | -5       | 1  | 2 | 0 |
|   |  | 2.58879              | 164      | -2       | -4       | 1            | 1.63743              | 28       | -4       | 0  | 4 | 0 |
|   |  | *2.58879             | 164      | 2        | 2        | 1            | *1.63743             | 28       | 3        | 5  | 1 | 0 |
|   |  | 2.56319              | 168      | -3       | 1        | 2            | 1.63433              | 19       | -4       | 4  | 0 | 0 |
|   |  | 2.55147              | 60       | 1        | 1        | 2            | *1.63433             | 19       | -3       | -3 | 4 | 0 |
|   |  | 2.53966              | 178      | 1        | -1       | 2            | 1.62281              | 7        | -5       | -1 | 3 | 0 |
|   |  | *2.53966             | 178      | -2       | 4        | 1            | *1.62281             | 7        | -3       | 3  | 4 | 0 |
|   |  | 2.51626              | 39       | 3        | 1        | 0            | 1.61776              | 22       | 0        | 8  | 0 | 0 |
|   |  | 2.48701              | 60       | 2        | 4        | 0            | *1.61776             | 22       | -1       | -3 | 4 | 0 |
|   |  | *2.48701             | 60       | -3       | 1        | 0            | 1.61493              | 23       | -5       | 1  | 3 | 0 |
|   |  | 2.46754              | 2        | 1        | 5        | 0            | *1.61493             | 23       | -1       | 3  | 4 | 0 |
|   |  | 2.44798              | 26       | -2       | 4        | 0            | 1.60960              | 29       | 3        | -5 | 1 | 0 |
|   |  | 2.41913              | 41       | -1       | -5       | 1            | 1.60636              | 16       | 4        | 2  | 1 | 0 |
|   |  | 2.39492              | 85       | -1       | 5        | 1            | 1.60173              | 10       | 2        | 0  | 3 | 0 |
|   |  | *2.39492             | 85       | -3       | -3       | 1            | 1.59386              | 24       | -4       | -2 | 4 | 0 |
|   |  | 2.37366              | 4        | -2       | 0        | 3            | *1.59386             | 24       | 4        | -2 | 1 | 0 |
|   |  | *2.34801             | 43       | -3       | 3        | 1            | 1.58324              | 14       | -2       | 6  | 3 | 0 |
|   |  | 2.32106              | 39       | -1       | 1        | 3            | 1.58324              | 23       | -4       | 2  | 4 | 0 |
|   |  | *2.32106             | 39       | -2       | -4       | 2            | 1.57486              | 4        | -2       | -4 | 4 | 0 |
|   |  | 2.28994              | 2        | 0        | 4        | 2            | *1.57486             | 4        | -5       | 3  | 2 | 0 |
|   |  | *2.28994             | 2        | -2       | 4        | 2            | 1.56857              | 33       | 0        | 2  | 2 | 0 |
|   |  | 2.28256              | 1        | 0        | -4       | 2            | *1.56857             | 33       | 0        | -6 | 1 | 0 |
|   |  | 2.27424              | 9        | -3       | -3       | 2            | 1.56620              | 34       | -2       | 4  | 4 | 0 |
|   |  | 2.25740              | 10       | -3       | 3        | 2            | *1.56620             | 34       | 0        | -2 | 4 | 0 |
|   |  | *2.25740             | 10       | -2       | -2       | 3            | 1.55876              | 8        | 2        | 2  | 3 | 0 |
|   |  | 2.22219              | 4        | -2       | 2        | 3            | 1.55603              | 3        | -3       | -2 | 2 | 0 |
|   |  | 2.21812              | 5        | 3        | 3        | 0            | 1.55069              | 7        | 2        | -2 | 3 | 0 |
|   |  | *2.21812             | 5        | 1        | -3       | 2            | 1.54188              | 4        | -5       | -3 | 1 | 0 |
|   |  | 2.20596              | 15       | 1        | 5        | 1            | 1.53581              | 31       | -5       | -3 | 3 | 0 |
|   |  | 2.18040              | 20       | 1        | -5       | 1            | *1.53581             | 31       | -3       | 7  | 1 | 0 |
|   |  | *2.18040             | 20       | -3       | 3        | 0            | 1.52963              | 10       | 0        | 6  | 3 | 0 |
|   |  | 2.15702              | 192      | 0        | 6        | 0            | 1.52902              | 39       | -4       | -8 | 1 | 0 |
|   |  | *2.15702             | 192      | 0        | 0        | 3            | *1.52902             | 39       | 0        | -6 | 3 | 0 |
|   |  | 2.14945              | 113      | -3       | 1        | 3            | 1.52000              | 23       | -2       | -8 | 1 | 0 |
|   |  | 2.13506              | 80       | 2        | 4        | 1            | *1.52000             | 23       | -2       | -8 | 1 | 0 |
|   |  | 2.10580              | 35       | -1       | -5       | 2            | 1.52000              | 23       | -5       | 1  | 0 | 0 |
|   |  | *2.10580             | 35       | -4       | 0        | 1            |                      |          |          |    |   |   |

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# Wollastonite-2M

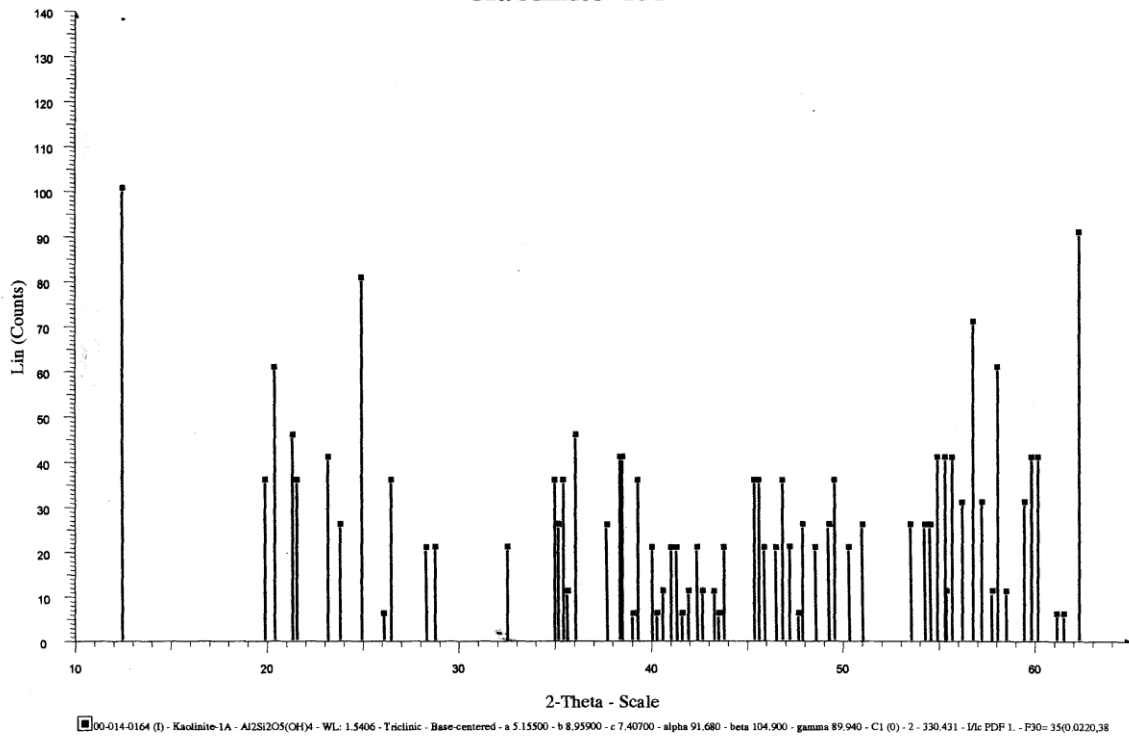


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| Pattern : 00-043-1460  |  | Radiation = 1.540560           |     |    |   |   | Quality : High |    |     |   |   |
|--|--|--------------------------------|-----|----|---|---|----------------|----|-----|---|---|
| CaSiO <sub>3</sub>   |  | d (Å)                          | i   | h  | k | l | d (Å)          | i  | h   | k | l |
| Calcium Silicate<br>Wollastonite-2M<br>Also called: parawollastonite |  | 7.68000                        | 9   | 2  | 0 | 0 | 1.60600        | 10 | 7   | 2 | 2 |
|  |  | 7.04000                        | 1   | 0  | 0 | 1 | *1.60600       | 10 | 5   | 2 | 3 |
|  |  | 5.45000                        | 2   | -2 | 0 | 1 | 1.57490        | 2  | 2   | 4 | 2 |
|  |  | 5.07500                        | 2   | 0  | 1 | 1 | *1.57490       | 2  | 3   | 3 | 3 |
|  |  | 4.96200                        | 3   | 2  | 0 | 1 | 1.56420        | 2  | 1   | 2 | 4 |
|  |  | 4.72500                        | 2   | 1  | 1 | 1 | 1.55920        | 1  | -8  | 0 | 3 |
|  |  | 3.84000                        | 40  | 4  | 0 | 0 | *1.55920       | 1  | -9  | 1 | 2 |
|  |  | 3.51900                        | 50  | 0  | 0 | 2 | 1.55180        | 3  | -3  | 2 | 4 |
|  |  | *3.51900                       | 50  | -4 | 0 | 1 | *1.55180       | 3  | -5  | 4 | 1 |
|  |  | 3.31900                        | 60  | -2 | 0 | 2 | 1.54640        | 2  | -9  | 2 | 0 |
|  |  | 3.24800                        | 4   | 0  | 2 | 1 | *1.54640       | 2  | 4   | 0 | 4 |
|  |  | *3.24800                       | 4   | 4  | 0 | 1 | 1.53910        | 2  | 6   | 3 | 2 |
|  |  | 3.20700                        | 3   | -1 | 2 | 1 | *1.53910       | 2  | -9  | 2 | 1 |
|  |  | 3.17000                        | 5   | 0  | 1 | 2 | 1.53610        | 6  | 10  | 0 | 0 |
|  |  | *3.17000                       | 5   | -4 | 1 | 1 | 1.52950        | 4  | -7  | 2 | 3 |
|  |  | 3.09100                        | 45  | 2  | 0 | 2 | *1.52950       | 4  | 3   | 4 | 2 |
|  |  | 3.04000                        | 4   | -2 | 2 | 1 | 1.51970        | 4  | -4  | 4 | 2 |
|  |  | 2.97800                        | 100 | -3 | 2 | 0 | *1.51970       | 4  | 5   | 4 | 1 |
|  |  | 2.94700                        | 4   | 2  | 2 | 1 | 1.48950        | 2  | -6  | 4 | 0 |
|  |  | 2.79900                        | 5   | -3 | 1 | 2 | 1.48420        | 3  | 9   | 2 | 1 |
|  |  | *2.79900                       | 5   | -3 | 2 | 1 | *1.48420       | 3  | 8   | 2 | 2 |
|  |  | 2.72500                        | 12  | -4 | 0 | 2 | 1.48020        | 10 | 3   | 2 | 4 |
|  |  | 2.71100                        | 7   | -5 | 1 | 1 | 1.47340        | 5  | -6  | 4 | 1 |
|  |  | 2.56000                        | 14  | 6  | 0 | 0 | *1.47340       | 5  | 4   | 4 | 2 |
|  |  | 2.53300                        | 3   | -4 | 2 | 1 | 1.46270        | 4  | -9  | 2 | 2 |
|  |  | *2.53300                       | 3   | -1 | 2 | 2 | *1.46270       | 4  | -5  | 4 | 2 |
|  |  | 2.48100                        | 25  | -6 | 0 | 1 | 1.45840        | 10 | -1  | 5 | 0 |
|  |  | *2.48100                       | 25  | 4  | 0 | 2 | *1.45840       | 10 | -6  | 3 | 3 |
|  |  | 2.35400                        | 14  | -5 | 2 | 0 | 1.44340        | 1  | 0   | 4 | 3 |
|  |  | 2.35000                        | 16  | -6 | 1 | 1 | *1.44340       | 1  | 10  | 1 | 1 |
|  |  | *2.35000                       | 16  | 4  | 1 | 2 | 1.43410        | 2  | 0   | 5 | 1 |
|  |  | 2.33700                        | 12  | -3 | 2 | 2 | *1.43410       | 2  | -2  | 4 | 3 |
|  |  | *2.33700                       | 12  | 6  | 0 | 1 | 1.42500        | 2  | -2  | 3 | 4 |
|  |  | 2.30600                        | 35  | -5 | 1 | 2 | *1.42500       | 2  | 8   | 0 | 3 |
|  |  | *2.30600                       | 35  | -2 | 0 | 3 | 1.40680        | 2  | 0   | 0 | 5 |
|  |  | 2.28200                        | 2   | -5 | 2 | 1 | *1.40680       | 2  | -7  | 4 | 0 |
|  |  | 2.23400                        | 2   | 0  | 1 | 3 | 1.39910        | 2  | -6  | 4 | 2 |
|  |  | 2.21500                        | 5   | 3  | 2 | 2 | *1.39910       | 2  | -9  | 3 | 0 |
|  |  | 2.18600                        | 25  | -4 | 2 | 2 | 1.39050        | 4  | 6   | 0 | 4 |
|  |  | *2.18600                       | 25  | 5  | 2 | 1 | 1.37410        | 3  | 3   | 5 | 1 |
|  |  | 2.16900                        | 6   | -6 | 0 | 2 | *1.37410       | 3  | 9   | 2 | 2 |
|  |  | 2.09100                        | 3   | -4 | 0 | 3 | 1.36310        | 8  | 7   | 4 | 1 |
|  |  | 2.02500                        | 7   | -5 | 2 | 2 | *1.36310       | 8  | 5   | 2 | 4 |
|  |  | 1.96380                        | 7   | 3  | 1 | 3 | 1.36200        | 14 | 2   | 0 | 5 |
|  |  | *1.96380                       | 7   | 6  | 0 | 2 | *1.36200       | 14 | 10  | 0 | 2 |
|  |  | 1.94010                        | 2   | 1  | 2 | 3 | 1.34410        | 3  | -10 | 0 | 3 |
|  |  | 1.92180                        | 3   | 4  | 0 | 3 | *1.34410       | 3  | 1   | 5 | 2 |
|  |  | *1.92180                       | 3   | 8  | 0 | 0 | 1.34030        | 3  | -7  | 2 | 4 |
|  |  | 1.91540                        | 7   | 2  | 3 | 2 | 1.32540        | 1  | 8   | 2 | 3 |
|  |  | *1.91540                       | 7   | 6  | 1 | 2 | *1.32540       | 1  | -8  | 4 | 0 |
|  |  | 1.91150                        | 3   | -5 | 3 | 0 | 1.30380        | 1  | -11 | 2 | 1 |
|  |  | 1.89820                        | 1   | -8 | 0 | 1 | 1.30020        | 2  | -10 | 3 | 0 |
|  |  | 1.89430                        | 2   | 5  | 2 | 2 | *1.30020       | 2  | 6   | 2 | 4 |
|  |  | 1.88890                        | 2   | -5 | 1 | 3 | 1.28640        | 2  | 8   | 4 | 1 |
|  |  | 1.88150                        | 8   | -7 | 2 | 0 | *1.28640       | 2  | -6  | 0 | 5 |
|  |  | *1.88150                       | 8   | -7 | 1 | 2 | 1.28330        | 2  | 4   | 0 | 5 |
|  |  | 1.85680                        | 6   | -8 | 1 | 0 | 1.28010        | 6  | 12  | 0 | 0 |
|  |  | *1.85680                       | 6   | -7 | 2 | 1 | *1.28010       | 6  | 7   | 4 | 2 |
|  |  | 1.83130                        | 14  | 0  | 4 | 0 | 1.26750        | 4  | -8  | 4 | 2 |
|  |  | 1.80980                        | 4   | 8  | 0 | 1 | *1.26750       | 4  | -9  | 1 | 4 |
|  |  | 1.79620                        | 5   | 3  | 2 | 3 | 1.26580        | 3  | -6  | 1 | 5 |
|  |  | 1.78220                        | 2   | 7  | 2 | 1 | *1.26580       | 3  | -2  | 4 | 4 |
|  |  | *1.78220                       | 2   | -2 | 4 | 0 | 1.26370        | 2  | 4   | 1 | 5 |
|  |  | 1.77230                        | 1   | 0  | 4 | 1 | *1.26370       | 2  | 11  | 2 | 1 |
|  |  | 1.75940                        | 16  | 0  | 0 | 4 | 1.24050        | 5  | 8   | 0 | 4 |
|  |  | 1.75120                        | 6   | -2 | 0 | 4 | *1.24050       | 5  | -7  | 3 | 4 |
|  |  | 1.72450                        | 16  | -5 | 2 | 3 | 1.22920        | 1  | -4  | 4 | 4 |
|  |  | 1.71800                        | 18  | 2  | 4 | 1 | *1.22920       | 1  | 8   | 3 | 3 |
|  |  | *1.71800                       | 18  | -1 | 1 | 4 | 1.21510        | 3  | 9   | 4 | 1 |
|  |  | 1.68110                        | 18  | 2  | 0 | 4 | *1.21510       | 3  | -10 | 0 | 4 |
|  |  | 1.65960                        | 2   | -4 | 0 | 4 | 1.21410        | 5  | -9  | 2 | 4 |
|  |  | 1.62280                        | 3   | -1 | 4 | 2 | *1.21410       | 5  | -6  | 5 | 2 |
| Radiation : CuKα1  |  | Filter : Monochromator crystal |     |    |   |   |                |    |     |   |   |
| Lambda : 1.54060   |  | d-sp : Diffractometer          |     |    |   |   |                |    |     |   |   |
| SE/COM : F30-3810 0004 841   |  | Internal standard : Si         |     |    |   |   |                |    |     |   |   |

# Kaolinite-1A

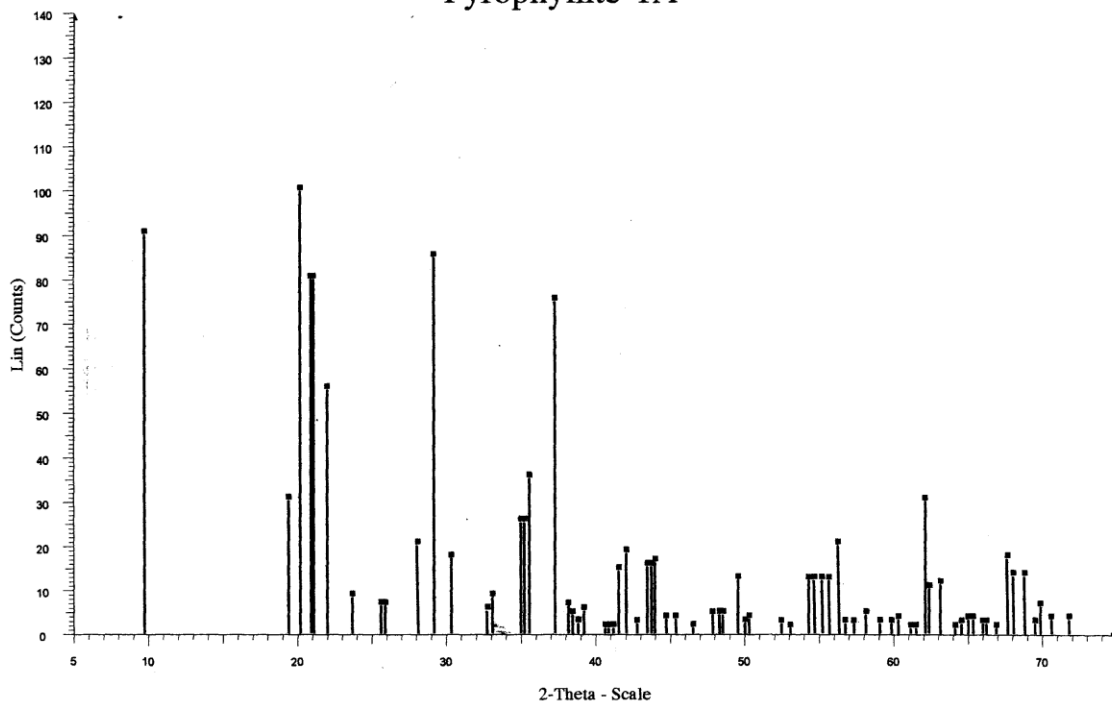


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| Pattern : 00-014-0164  |                      | Radiation = 1.540560                  |          | Quality : Indexed |          |          |
|--|----------------------|---------------------------------------|----------|-------------------|----------|----------|
| Al <sub>2</sub> Si <sub>2</sub> O <sub>5</sub> (OH) <sub>4</sub>   |                      | <b>d (Å)</b>                          | <b>l</b> | <b>h</b>          | <b>k</b> | <b>i</b> |
| Aluminum Silicate Hydroxide<br>Kaolinite-1A  |                      | 7.17000                               | 100      | 0                 | 0        | 1        |
|  |                      | 4.47800                               | 35       | 0                 | 2        | 0        |
|  |                      | 4.36600                               | 60       | -1                | 1        | 0        |
|  |                      | 4.18600                               | 45       | -1                | -1       | 1        |
|  |                      | 4.13900                               | 35       | -1                | 1        | 1        |
|  |                      | 3.84700                               | 40       | 0                 | -2       | 1        |
|  |                      | 3.74500                               | 25       | 0                 | 2        | 1        |
|  |                      | 3.57900                               | 80       | 0                 | 0        | 2        |
|  |                      | 3.42000                               | 5        | 1                 | -1       | 1        |
|  |                      | 3.37600                               | 35       | 1                 | 1        | 1        |
|  |                      | 3.15500                               | 20       | -1                | -1       | 2        |
|  |                      | 3.10700                               | 20       | -1                | 1        | 2        |
|  |                      | 2.75400                               | 20       | 0                 | 2        | 2        |
|  |                      | 2.56600                               | 35       | -2                | 0        | 1        |
|  |                      | 2.55300                               | 25       | 1                 | 3        | 0        |
|  |                      | 2.53500                               | 35       | -1                | -3       | 1        |
|  |                      | 2.51900                               | 10       | 1                 | -1       | 2        |
|  |                      | 2.49500                               | 45       | 2                 | 0        | 0        |
|  |                      | 2.38500                               | 25       | 0                 | 0        | 3        |
|  |                      | 2.34700                               | 40       | -2                | 0        | 2        |
|  |                      | 2.33800                               | 40       | 1                 | -3       | 1        |
|  |                      | 2.30500                               | 5        | -1                | 1        | 3        |
|  |                      | 2.29300                               | 35       | 1                 | 3        | 1        |
|  |                      | 2.26300                               | 20       | -1                | -3       | 2        |
|  |                      | 2.23700                               | 5        | 0                 | 4        | 0        |
|  |                      | 2.21800                               | 10       | -2                | 2        | 1        |
|  |                      | 2.19700                               | 20       | -1                | 3        | 2        |
|  |                      | 2.18600                               | 20       | 2                 | 0        | 1        |
|  |                      | 2.17300                               | 5        | 2                 | 2        | 0        |
|  |                      | 2.15100                               | 10       | 0                 | -4       | 1        |
|  |                      | 2.13300                               | 20       | 0                 | -2       | 3        |
|  |                      | 2.11600                               | 10       | 0                 | 4        | 1        |
|  |                      | 2.09300                               | 10       | -2                | -2       | 2        |
|  |                      | 2.08000                               | 5        | 0                 | 2        | 3        |
|  |                      | 2.06400                               | 20       | -2                | 2        | 2        |
|  |                      | 1.99700                               | 35       | -2                | 0        | 3        |
|  |                      | 1.98700                               | 35       | 1                 | -3       | 2        |
|  |                      | 1.97400                               | 20       | 2                 | -2       | 1        |
|  |                      | 1.95200                               | 20       | 2                 | 2        | 1        |
|  |                      | 1.93900                               | 35       | 1                 | 3        | 2        |
|  |                      | 1.92100                               | 20       | 0                 | -4       | 2        |
|  |                      | 1.90600                               | 5        | 1                 | 1        | 3        |
|  |                      | 1.89700                               | 25       | -1                | -3       | 3        |
|  |                      | 1.87000                               | 20       | 0                 | 4        | 2        |
|  |                      | 1.84500                               | 25       | -1                | 3        | 3        |
|  |                      | 1.83800                               | 35       | -2                | -2       | 3        |
|  |                      | 1.81000                               | 20       | -2                | 2        | 3        |
|  |                      | 1.78900                               | 25       | 0                 | 0        | 4        |
|  |                      | 1.71000                               | 25       | 2                 | -2       | 2        |
|  |                      | 1.68900                               | 25       | -1                | 5        | 0        |
|  |                      | 1.68100                               | 25       | -1                | -5       | 1        |
|  |                      | 1.66900                               | 40       | -2                | 4        | 0        |
|  |                      | 1.66000                               | 40       | 2                 | 4        | 0        |
|  |                      | 1.65600                               | 10       | 0                 | -4       | 3        |
|  |                      | 1.64900                               | 40       | -3                | 1        | 2        |
|  |                      | 1.63300                               | 30       | -3                | 1        | 0        |
|  |                      | 1.62000                               | 70       | 1                 | 3        | 3        |
|  |                      | 1.60700                               | 30       | 0                 | 4        | 3        |
|  |                      | 1.59400                               | 10       | -1                | -5       | 2        |
|  |                      | 1.58600                               | 60       | -1                | -3       | 4        |
|  |                      | 1.57200                               | 10       | 2                 | -4       | 1        |
|  |                      | 1.55300                               | 30       | -2                | 2        | 4        |
|  |                      | 1.54500                               | 40       | 1                 | -1       | 4        |
|  |                      | 1.53700                               | 40       | 2                 | 0        | 3        |
|  |                      | 1.51400                               | 5        | 3                 | -1       | 1        |
|  |                      | 1.50500                               | 5        | -2                | -4       | 3        |
|  |                      | 1.48900                               | 90       | -3                | -3       | 1        |
| <b>Lattice</b> : Anorthic (triclinic)  |                      | <b>Mol. weight</b> = 258.16           |          |                   |          |          |
| <b>S.G.</b> : C1 (0)   |                      | <b>Volume [CD]</b> = 165.22           |          |                   |          |          |
| <b>a</b> = 5.15500   | <b>alpha</b> = 91.68 | <b>Dx</b> = 2.595                     |          |                   |          |          |
| <b>b</b> = 8.95900   | <b>beta</b> = 104.90 | <b>Dm</b> = 2.645                     |          |                   |          |          |
| <b>c</b> = 7.40700   | <b>gamma</b> = 89.94 |                                       |          |                   |          |          |
| <b>a/b</b> = 0.57540   | <b>Z</b> = 2         |                                       |          |                   |          |          |
| <b>c/b</b> = 0.82677   |                      |                                       |          |                   |          |          |
| <b>Optical data</b> : A=1.559(6), B=1.564(5), Q=1.565(5), Sign=-, 2V=24-50°  |                      |                                       |          |                   |          |          |
| <b>Color</b> : White   |                      |                                       |          |                   |          |          |
| <b>Sample source or locality</b> : Specimen from Scalby, Yorkshire, England, UK.   |                      |                                       |          |                   |          |          |
| <b>General comments</b> : Validated by calculated pattern Borg and Smith, GSA Memoir, 122.   |                      |                                       |          |                   |          |          |
| <b>Additional pattern</b> : To replace 5-143 and 12-447.   |                      |                                       |          |                   |          |          |
| <b>Additional pattern</b> : See ICSD 20593 (PDF 72-2300); ICSD 27713 (PDF 74-1784); ICSD 27715 (PDF 74-1786); ICSD 68698 (PDF 80-886); ICSD 31135 (PDF 75-1593); ICSD 63192 (PDF 78-1996); ICSD 68697 (PDF 80-885); ICSD 66571 (PDF 79-1570); ICSD 63315 (PDF 78-2109); ICSD 80082 (PDF 83-971). |                      |                                       |          |                   |          |          |
| <b>Data collection flag</b> : Ambient.   |                      |                                       |          |                   |          |          |
| Goodyear, Duffin., Mineral. Mag., volume 32, page 902 (1961)   |                      |                                       |          |                   |          |          |
| <b>Radiation</b> : CuKα  |                      | <b>Filter</b> : Monochromator crystal |          |                   |          |          |
| <b>Lambda</b> : 1.54180  |                      | <b>d-sp</b> : Other                   |          |                   |          |          |
| <b>SS/FOM</b> : F30= 35(0.0220,38)   |                      |                                       |          |                   |          |          |

# Pyrophyllite-1A



00-025-0022 (1) - Pyrophyllite-1A - Al<sub>2</sub>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub> - WL: 1.5406 - Triclinic - Base-centered - a 5.16100 - b 8.95700 - c 9.35100 - alpha 91.030 - beta 100.370 - gamma 89.750 - C-1 (0) - 2 - 425.140 - I/c PDF 1 - F30= 27(0.02)

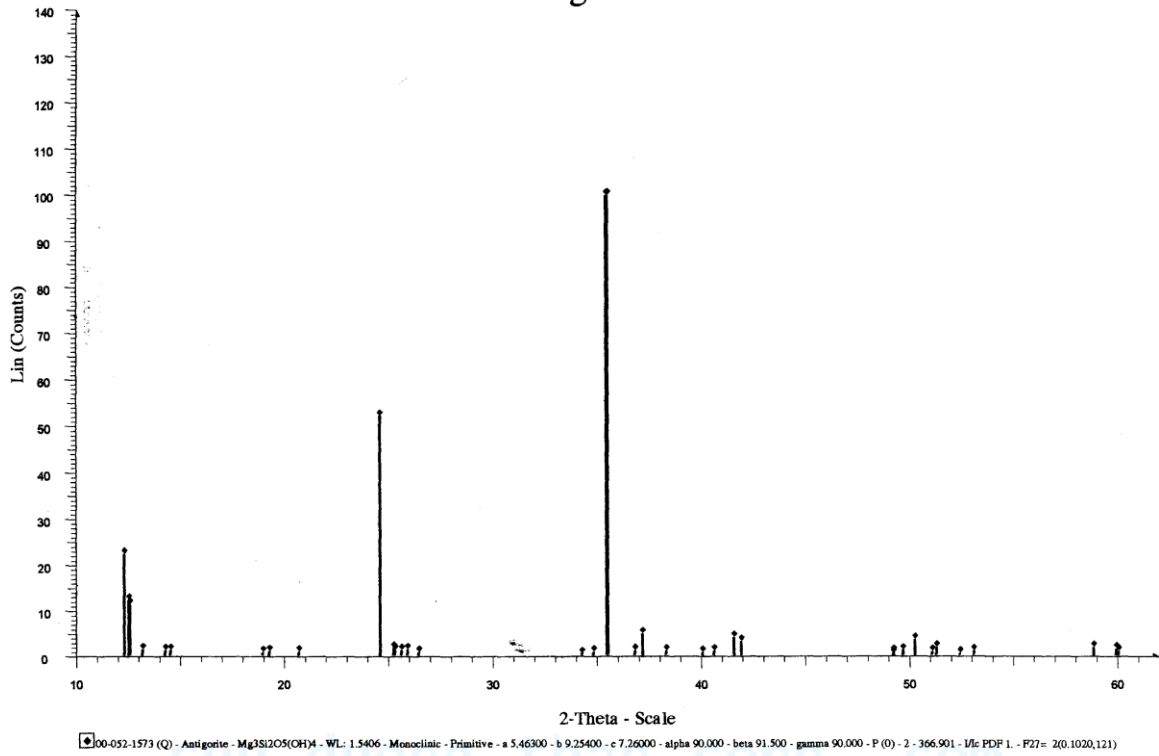
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| Pattern : 00-025-0022   |  | Radiation = 1.540560   |          | Quality : Indexed  |          |                   |  |
|---|--|--|----------|--|----------|-------------------|--|
| Al <sub>2</sub> Si <sub>4</sub> O <sub>10</sub> (OH) <sub>2</sub>   |  | <b>d (Å)</b>   | <b>l</b> | <b>h</b>   | <b>k</b> | <b>l</b>          |  |
| Aluminum Silicate Hydroxide<br>Pyrophyllite-1A  |  | 9.20000  | 90       | 0  | 0        | 1                 |  |
|   |  | 4.60000  | 30       | 0  | 0        | 2                 |  |
|   |  | 4.42000  | 100      | 1  | 1        | 0                 |  |
|   |  | 4.26000  | 80       | -1   | -1       | 1                 |  |
|   |  | 4.23000  | 80       | -1   | 1        | 1                 |  |
|   |  | 4.06000  | 55       | 0  | -2       | 1                 |  |
|   |  | 3.77000  | 8        | 1  | -1       | 1                 |  |
|   |  | 3.49000  | 6        | -1   | -1       | 2                 |  |
|   |  | 3.45000  | 6        | -1   | 1        | 2                 |  |
|   |  | 3.18000  | 20       | 0  | 2        | 2                 |  |
|   |  | 3.07000  | 85       | 0  | 0        | 3                 |  |
|   |  | 2.95300  | 17       | 1  | 1        | 2                 |  |
|   |  | 2.74100  | 5        | -1   | -1       | 3                 |  |
|   |  | 2.71000  | 8        | -1   | 1        | 3                 |  |
|   |  | 2.56900  | 25       | -2   | 0        | 1                 |  |
|   |  | 2.54700  | 25       | 0  | -2       | 3                 |  |
|   |  | 2.53200  | 35       | -1   | 3        | 1                 |  |
|   |  | 2.41600  | 75       | -2   | 0        | 2                 |  |
|   |  | 2.35900  | 6        | 1  | -1       | 3                 |  |
|   |  | 2.34100  | 4        | 2  | 0        | 1                 |  |
|   |  | 2.32200  | 2        | -1   | 3        | 2                 |  |
|   |  | 2.30000  | 5        | 0  | 0        | 4                 |  |
|   |  | 2.22200  | 1        | -2   | 2        | 1                 |  |
|   |  | 2.20900  | 1        | 2  | 2        | 0                 |  |
|   |  | 2.19500  | 1        | -1   | -1       | 4                 |  |
|   |  | 2.17200  | 14       | -1   | 1        | 4                 |  |
|   |  | 2.15200  | 18       | 1  | 3        | 2                 |  |
|   |  | 2.11600  | 2        | -2   | 2        | 2                 |  |
|   |  | 2.08300  | 15       | -1   | -3       | 3                 |  |
|   |  | 2.07000  | 15       | 2  | 0        | 2                 |  |
|   |  | 2.05400  | 16       | 0  | -2       | 4                 |  |
|   |  | 2.02600  | 3        | 0  | -4       | 2                 |  |
|   |  | 1.99800  | 3        | 0  | 4        | 2                 |  |
|   |  | 1.95200  | 1        | -2   | -2       | 3                 |  |
|   |  | 1.90000  | 4        | 1  | -3       | 3                 |  |
|   |  | 1.88300  | 4        | 2  | -2       | 2                 |  |
|   |  | 1.87500  | 4        | 1  | 3        | 3                 |  |
|   |  | 1.84100  | 12       | 0  | 0        | 5                 |  |
|   |  | 1.82300  | 2        | 0  | -4       | 3                 |  |
|   |  | 1.81200  | 3        | -1   | -3       | 4                 |  |
|   |  | 1.74400  | 2        | -2   | -2       | 4                 |  |
|   |  | 1.72200  | 1        | -2   | 2        | 4                 |  |
|   |  | 1.68900  | 12       | -1   | 5        | 0                 |  |
|   |  | 1.67700  | 12       | 2  | -2       | 3                 |  |
|   |  | 1.66100  | 12       | -3   | 1        | 0                 |  |
|   |  | 1.65000  | 12       | -2   | -4       | 2                 |  |
|   |  | 1.63300  | 20       | -2   | 4        | 2                 |  |
|   |  | 1.62100  | 2        | 2  | -4       | 1                 |  |
|   |  | 1.60700  | 2        | 1  | 1        | 5                 |  |
|   |  | 1.58500  | 4        | -3   | -1       | 3                 |  |
|   |  | 1.56500  | 2        | 1  | -5       | 2                 |  |
|   |  | 1.54400  | 2        | -2   | -2       | 5                 |  |
|   |  | 1.53200  | 3        | 0  | 0        | 6                 |  |
|   |  | 1.51400  | 1        | 2  | 4        | 2                 |  |
|   |  | 1.50500  | 1        | -1   | 5        | 3                 |  |
|   |  | 1.49300  | 30       | -3   | -3       | 1                 |  |
|   |  | 1.48700  | 10       | -3   | 3        | 1                 |  |
|   |  | 1.47200  | 11       | -3   | 3        | 0                 |  |
|   |  | 1.45100  | 1        | -2   | -4       | 4                 |  |
|   |  | 1.44300  | 2        | 0  | 2        | 6                 |  |
|   |  | 1.43300  | 3        | 0  | -4       | 5                 |  |
|   |  | 1.42500  | 3        | 1  | 3        | 5                 |  |
|   |  | 1.41400  | 2        | 1  | 5        | 4                 |  |
| <b>Sample source or locality:</b> Specimen from Coromandel region, New Zealand.<br><b>General comments:</b> Calibrated with Si powder (a=5.43062 at 21 C).<br><b>Analysis:</b> No analysis given.<br><b>Additional pattern:</b> To replace 3-574 and 24-11.<br><b>Color:</b> White<br><b>Optical data:</b> Sign=, 2V=-60°<br><b>Additional pattern:</b> See ICSD 25-22 (PDF 75-856).<br><b>Data collection flag:</b> Ambient. |  | <b>Mol. weight = 360.31</b>  |          | <b>Volume [CD] = 212.57</b>  |          | <b>Dx = 2.815</b> |  |
| <b>Lattice :</b> Anorthic (triclinic)<br><b>S.G. :</b> C-1 (0)  |  | <b>a = 5.16100</b><br><b>b = 8.95700</b><br><b>c = 9.35100</b><br><b>a/b = 0.57620</b><br><b>c/b = 1.04399</b> |          | <b>alpha = 91.03</b><br><b>beta = 100.37</b><br><b>gamma = 89.75</b><br><b>Z = 2</b> |          |                   |  |
| Wardle, Brindley., Am. Mineral., volume 57, page 732 (1972)   |  |  |          |  |          |                   |  |



# Antigorite



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Pattern : 00-052-1573

Radiation = 1.540560

Quality : Questionable

$Mg_3Si_2O_5(OH)_4$

Magnesium Silicate Hydroxide  
Antigorite

Lattice : Monoclinic

S.G. : P (0)

a = 5.46300

b = 9.25400

c = 7.26000

a/b = 0.59034

c/b = 0.78453

beta = 91.50

Z = 2

Mol. weight = 277.11

Volume [CD] = 366.90

Dx = 2.508

Color: Light green

Sample source or locality: Specimen from Jin-gatou, Sasaguri-cho, Japan.

General comments: Incommensurate structure.

Analysis: Analysis (wt.%): Si 4.193, Cr 0.021, Fe<sup>+3</sup> 0.102, Fe<sup>+2</sup> 0.390, Mg 5.503, Ni 0.021.

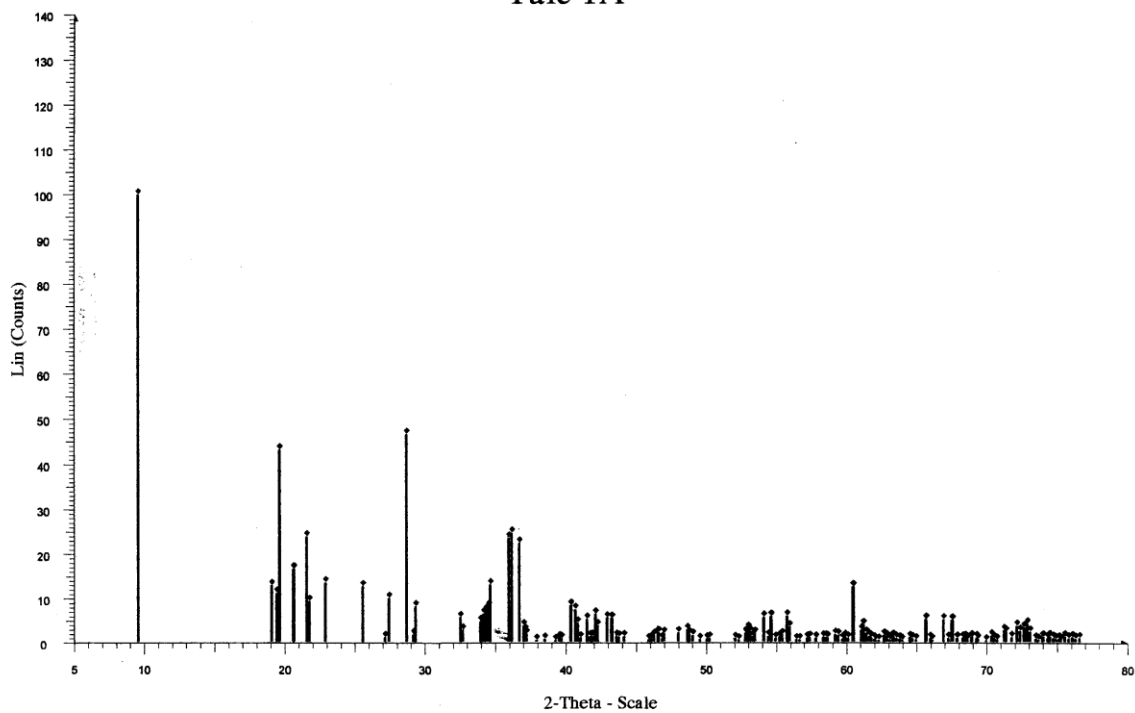
Data collection flag: Ambient.

| d (Å)   | i   | h  | k | l  |
|---------|-----|----|---|----|
| 7.27000 | 220 | 0  | 0 | 1  |
| 7.14000 | 120 |    |   |    |
| 7.10000 | 110 |    |   |    |
| 6.77000 | 11  |    |   |    |
| 6.25000 | 9   |    |   |    |
| 6.14000 | 9   |    |   |    |
| 4.88500 | 4   | 1  | 1 | 0  |
| 4.61800 | 7   | 0  | 2 | 0  |
| 4.21400 | 6   | 1  | 0 | 1  |
| 3.61100 | 520 | 0  | 0 | 2  |
| 3.57400 | 10  | 1  | 2 | 0  |
| 3.53800 | 14  |    |   |    |
| 3.48500 | 9   |    |   |    |
| 3.44800 | 11  |    |   |    |
| 3.39100 | 5   | 0  | 1 | 2  |
| 2.61000 | 3   | 2  | 1 | 0  |
| 2.58200 | 5   | -2 | 0 | 1  |
| 2.53200 | 999 | 2  | 0 | 1  |
| 2.53200 | 999 | 1  | 3 | -1 |
| 2.44700 | 8   | 2  | 1 | 1  |
| 2.41690 | 46  | 0  | 0 | 3  |
| 2.37570 | 7   | -2 | 2 | 0  |
| 2.26370 | 5   | -2 | 2 | 1  |
| 2.21830 | 7   | 2  | 2 | 1  |
| 2.17290 | 38  | 1  | 3 | -2 |
| 2.15600 | 29  | 2  | 0 | 2  |
| 1.86040 | 3   | 0  | 5 | 0  |
| 1.85040 | 7   |    |   |    |
| 1.83680 | 10  | -2 | 0 | 3  |
| 1.81390 | 33  | 0  | 0 | 4  |
| 1.78740 | 6   | 2  | 0 | 3  |
| 1.77860 | 15  | 0  | 1 | 4  |
| 1.74610 | 3   | -3 | 1 | 1  |
| 1.72740 | 8   | 3  | 1 | 1  |
| 1.56870 | 17  | 3  | 3 | 0  |
| 1.54200 | 12  | 0  | 6 | 0  |
| 1.53830 | 7   | 3  | 3 | -1 |

Uehara, S., Shirozu, H., Mineral. J., volume 12, page 299 (1985)

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# Talc 1A

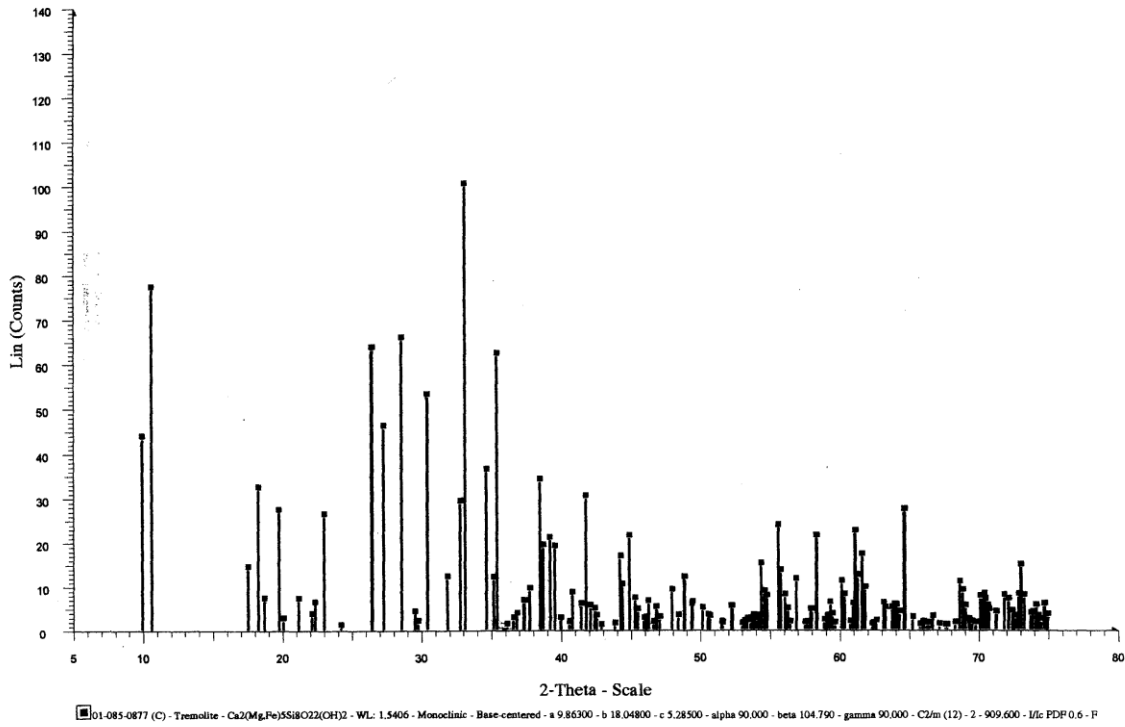


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cuu duong than cong. com

| Pattern : 01-073-0147  |  | Radiation = 1.540560              |          |          |          |          | Quality : Calculated |          |          |          |          |
|--|--|-----------------------------------|----------|----------|----------|----------|----------------------|----------|----------|----------|----------|
| Mg <sub>3</sub> (Si <sub>2</sub> O <sub>5</sub> ) <sub>2</sub> (OH) <sub>2</sub> |  | <b>d (Å)</b>                      | <b>i</b> | <b>h</b> | <b>k</b> | <b>l</b> | <b>d (Å)</b>         | <b>i</b> | <b>h</b> | <b>k</b> | <b>l</b> |
| Magnesium Silicate Hydroxide<br>Talc 1A  |  | 9.35425                           | 999      | 0        | 0        | 1        | *1.58281             | 6        | 1        | 5        | 2        |
|  |  | 4.87713                           | 126      | 0        | 0        | 2        | 1.57970              | 9        | -1       | 3        | 5        |
|  |  | 4.58926                           | 106      | 0        | 2        | 0        | 1.57465              | 9        | -2       | 4        | 3        |
|  |  | 4.07942                           | 426      | -1       | 1        | 0        | 1.57200              | 7        | 2        | -4       | 2        |
|  |  | *4.53942                          | 426      | 1        | -1       | 0        | 1.56504              | 15       | 0        | 0        | 6        |
|  |  | 4.32794                           | 183      | -1       | -1       | 1        | *1.55384             | 13       | -1       | -5       | 3        |
|  |  | *4.32794                          | 183      | 1        | 1        | 1        | *1.55384             | 13       | -2       | -2       | 5        |
|  |  | 4.13678                           | 236      | 0        | -2       | 1        | 1.54843              | 4        | -2       | 2        | 5        |
|  |  | 4.10368                           | 90       | 0        | 2        | 1        | 1.54250              | 10       | -1       | 5        | 3        |
|  |  | 3.89605                           | 132      | 1        | -1       | 1        | *1.54250             | 10       | -1       | -1       | 6        |
|  |  | 3.49484                           | 123      | -1       | 1        | 2        | 1.53720              | 8        | 0        | 6        | 0        |
|  |  | 3.28247                           | 8        | 0        | -2       | 2        | *1.52975             | 123      | 0        | 6        | 0        |
|  |  | 3.25222                           | 97       | 0        | 2        | 2        | *1.52975             | 123      | -3       | -3       | 1        |
|  |  | 3.11806                           | 464      | 0        | 0        | 3        | 1.51586              | 25       | -3       | 3        | 0        |
|  |  | 3.08786                           | 14       | 1        | -1       | 2        | 1.51314              | 37       | 3        | 3        | 0        |
|  |  | 3.05185                           | 78       | 1        | 1        | 2        | *1.51314             | 37       | 0        | -6       | 1        |
|  |  | 2.75581                           | 53       | -1       | -1       | 3        | 1.50726              | 18       | 0        | 6        | 0        |
|  |  | 2.74288                           | 25       | -1       | 1        | 3        | 1.50235              | 11       | -3       | 2        | 2        |
|  |  | 2.63831                           | 44       | -1       | 3        | 0        | 1.50021              | 8        | -3       | 3        | 2        |
|  |  | *2.63831                          | 44       | 1        | 3        | 0        | 1.49540              | 4        | -3       | -1       | 4        |
|  |  | 2.62570                           | 62       | -2       | 0        | 1        | 1.49312              | 2        | -3       | 1        | 4        |
|  |  | 2.61456                           | 89       | 2        | 0        | 0        | 1.48873              | 2        | 1        | -5       | 3        |
|  |  | 2.59694                           | 78       | -1       | -3       | 1        | 1.47950              | 13       | 0        | 0        | 6        |
|  |  | 2.59111                           | 128      | 0        | -2       | 3        | *1.47930             | 11       | 0        | -4       | 5        |
|  |  | 2.59111                           | 128      | -1       | 3        | 1        | 1.47577              | 10       | 1        | 5        | 3        |
|  |  | 2.49849                           | 233      | 1        | -3       | 1        | 1.47164              | 3        | 0        | 2        | 6        |
|  |  | 2.48549                           | 245      | 1        | 3        | 1        | 1.46713              | 11       | 1        | 3        | 5        |
|  |  | 2.44948                           | 222      | -2       | 0        | 2        | *1.46713             | 11       | -2       | -4       | 4        |
|  |  | 2.42893                           | 35       | 1        | -1       | 3        | 1.46193              | 6        | 3        | 3        | 1        |
|  |  | 2.42264                           | 24       | 2        | 0        | 1        | 1.45636              | 4        | 0        | -4       | 5        |
|  |  | 2.41780                           | 18       | 1        | 1        | 3        | *1.45636             | 4        | -2       | 4        | 4        |
|  |  | 2.37285                           | 2        | -1       | 3        | 2        | 1.45321              | 2        | 2        | -4       | 3        |
|  |  | 2.33656                           | 4        | 0        | 0        | 4        | 1.44284              | 8        | 0        | 4        | 5        |
|  |  | 2.29483                           | 1        | 0        | 4        | 0        | *1.44284             | 8        | 2        | 4        | 3        |
|  |  | 2.27978                           | 7        | -2       | -2       | 1        | 1.44062              | 6        | -2       | 0        | 6        |
|  |  | *2.27978                          | 7        | -2       | 2        | 1        | 1.43863              | 5        | -3       | 3        | 3        |
|  |  | 2.27380                           | 5        | -2       | 2        | 0        | *1.43863             | 5        | -1       | -5       | 6        |
|  |  | 2.26871                           | 5        | 2        | 2        | 0        | 1.42087              | 50       | 2        | 0        | 5        |
|  |  | 2.23550                           | 81       | 1        | -3       | 2        | *1.42087             | 50       | 1        | -1       | 6        |
|  |  | *2.23550                          | 81       | 0        | -4       | 1        | 1.41436              | 6        | 3        | -1       | 3        |
|  |  | 2.21899                           | 72       | 1        | 3        | 2        | 1.41162              | 3        | 3        | 1        | 3        |
|  |  | 2.20808                           | 41       | -1       | -1       | 4        | 1.39642              | 49       | -1       | -3       | 6        |
|  |  | 2.19889                           | 7        | -1       | 1        | 4        | 1.39012              | 8        | -1       | -3       | 2        |
|  |  | 2.17828                           | 50       | -2       | 0        | 3        | *1.38586             | 48       | 3        | 3        | 2        |
|  |  | 2.16587                           | 10       | -2       | 2        | 2        | 1.37892              | 6        | 0        | -6       | 3        |
|  |  | 2.15784                           | 11       | -2       | 2        | 2        | *1.37892             | 6        | -2       | -2       | 6        |
|  |  | 2.14505                           | 61       | 2        | -2       | 1        | 1.37144              | 7        | -2       | 2        | 6        |
|  |  | *2.14505                          | 61       | 2        | 0        | 2        | *1.37144             | 7        | -3       | 1        | 5        |
|  |  | 2.13842                           | 35       | 2        | 2        | 1        | 1.36789              | 9        | 0        | 6        | 3        |
|  |  | 2.10636                           | 52       | -1       | -3       | 3        | 1.36548              | 4        | 1        | -5       | 4        |
|  |  | 2.08913                           | 51       | 0        | -2       | 4        | 1.35985              | 10       | 2        | -2       | 5        |
|  |  | 2.08913                           | 51       | -1       | 3        | 3        | *1.35985             | 10       | -3       | -3       | 4        |
|  |  | 2.07513                           | 11       | 0        | 2        | 4        | 1.35472              | 8        | -3       | 3        | 4        |
|  |  | 2.06838                           | 9        | 0        | -4       | 2        | *1.35472             | 8        | 2        | 2        | 5        |
|  |  | 2.05184                           | 10       | 0        | 4        | 2        | 1.35249              | 4        | 1        | 5        | 4        |
|  |  | 1.97790                           | 3        | 1        | -1       | 4        | 1.34286              | 1        | -2       | -4       | 5        |
|  |  | 1.97004                           | 4        | -2       | -2       | 3        | 1.33632              | 12       | 0        | 0        | 7        |
|  |  | 1.97004                           | 4        | 1        | 1        | 4        | 1.33330              | 7        | -1       | -1       | 7        |
|  |  | 1.96232                           | 12       | -2       | 2        | 3        | *1.33330             | 7        | -2       | 4        | 5        |
|  |  | 1.95044                           | 19       | 1        | -3       | 3        | 1.33009              | 3        | 2        | -4       | 4        |
|  |  | *1.95044                          | 19       | 2        | -2       | 2        | *1.33009             | 3        | -1       | 1        | 7        |
|  |  | 1.93853                           | 4        | 2        | 2        | 2        | 1.32158              | 25       | -2       | 6        | 0        |
|  |  | 1.93294                           | 17       | 1        | 3        | 3        | *1.32158             | 25       | -2       | 6        | 1        |
|  |  | 1.89500                           | 19       | -2       | 0        | 4        | 1.31916              | 21       | 2        | 4        | 4        |
|  |  | 1.87085                           | 28       | 0        | 0        | 5        | *1.31916             | 21       | 2        | 6        | 0        |
|  |  | 1.86818                           | 18       | 2        | 0        | 3        | 1.31285              | 9        | -4       | 0        | 2        |
|  |  | 1.85715                           | 12       | 0        | -4       | 3        | 1.30728              | 35       | 4        | 0        | 0        |
|  |  | 1.83924                           | 3        | 0        | 4        | 3        | 1.30376              | 23       | 1        | -3       | 6        |
|  |  | 1.82154                           | 4        | -1       | -1       | 5        | *1.29947             | 31       | -2       | -6       | 4        |
|  |  | 1.81495                           | 6        | -1       | 3        | 4        | 1.29847              | 31       | 3        | -3       | 3        |
|  |  | *1.81495                          | 6        | -1       | 1        | 5        | 1.29556              | 40       | 0        | -4       | 6        |
|  |  | 1.75771                           | 5        | -2       | -2       | 4        | *1.29556             | 40       | -2       | 6        | 2        |
|  |  | 1.74742                           | 2        | -2       | 2        | 4        | 1.29235              | 21       | 3        | -1       | 4        |
|  |  | 1.73321                           | 18       | -1       | 5        | 0        | *1.29235             | 21       | 3        | 3        | 3        |
|  |  | *1.73321                          | 18       | -3       | -1       | 1        | 1.28618              | 5        | 0        | -2       | 7        |
|  |  | 1.72717                           | 28       | -2       | 4        | 1        | *1.28618             | 5        | 0        | -6       | 4        |
|  |  | *1.72717                          | 28       | 0        | 2        | 5        | 1.28351              | 3        | 0        | 4        | 6        |
|  |  | 1.72417                           | 21       | 2        | 2        | 3        | *1.27828             | 10       | 0        | 2        | 7        |
|  |  | *1.72417                          | 21       | 2        | 4        | 0        | 1.27828              | 10       | -4       | 0        | 3        |
|  |  | 1.71708                           | 10       | -1       | 5        | 1        | *1.27427             | 7        | 0        | 6        | 4        |
|  |  | 1.71309                           | 17       | -3       | 1        | 0        | 1.27246              | 11       | -2       | 0        | 7        |
|  |  | *1.71309                          | 17       | 3        | 1        | 0        | *1.27246             | 11       | -4       | -2       | 1        |
|  |  | 1.69397                           | 54       | 1        | -3       | 4        | 1.26805              | 7        | 4        | 0        | 1        |
|  |  | *1.69397                          | 54       | -3       | 1        | 2        | *1.26805             | 7        | -1       | -7       | 1        |
|  |  | 1.68322                           | 11       | 1        | 5        | 1        | 1.26533              | 4        | -1       | 7        | 1        |
|  |  | 1.67910                           | 56       | 1        | 3        | 4        | *1.26533             | 4        | -3       | 5        | 0        |
|  |  | *1.67910                          | 56       | -2       | -4       | 2        | 1.26289              | 5        | 3        | 5        | 0        |
|  |  | 1.66978                           | 5        | 2        | -4       | 1        | *1.26289             | 5        | -4       | 2        | 2        |
|  |  | 1.66218                           | 9        | 2        | 4        | 1        | 1.26044              | 3        | -3       | 3        | 5        |
|  |  | 1.65648                           | 14       | -1       | -5       | 2        | 1.25619              | 11       | 4        | 2        | 0        |
|  |  | *1.65648                          | 14       | 1        | -1       | 5        | *1.25619             | 11       | 2        | 0        | 6        |
|  |  | 1.64697                           | 57       | -2       | 0        | 5        | 1.25267              | 6        | -3       | -1       | 6        |
|  |  | *1.64697                          | 57       | 0        | -4       | 4        | 1.24925              | 9        | 2        | -6       | 2        |
|  |  | 1.64190                           | 32       | 3        | -1       | 1        | *1.24925             | 9        | -2       | 6        | 3        |
|  |  | 1.62961                           | 3        | 0        | 4        | 4        | 1.24577              | 5        | 1        | -5       | 5        |
|  |  | 1.62263                           | 3        | 2        | 0        | 4        | 1.24174              | 7        | 2        | -7       | 2        |
|  |  | 1.60868                           | 6        | -3       | -1       | 3        | *1.24174             | 7        | -1       |          |          |
|  |  | *1.60868                          | 6        | -3       | 1        | 3        |                      |          |          |          |          |
|  |  | 1.60354                           | 8        | 1        | -5       | 2        |                      |          |          |          |          |
|  |  | 1.59281                           | 6        | -1       | -3       | 5        |                      |          |          |          |          |
| <b>Radiation :</b> CuKα1   |  | <b>Filter :</b> Not specified     |          |          |          |          |                      |          |          |          |          |
| <b>Lambda :</b> 1.54060  |  | <b>d-sp :</b> Calculated spacings |          |          |          |          |                      |          |          |          |          |
| <b>SS/FOM :</b> F30=166(0.0048,38)   |  |                                   |          |          |          |          |                      |          |          |          |          |

# Tremolite



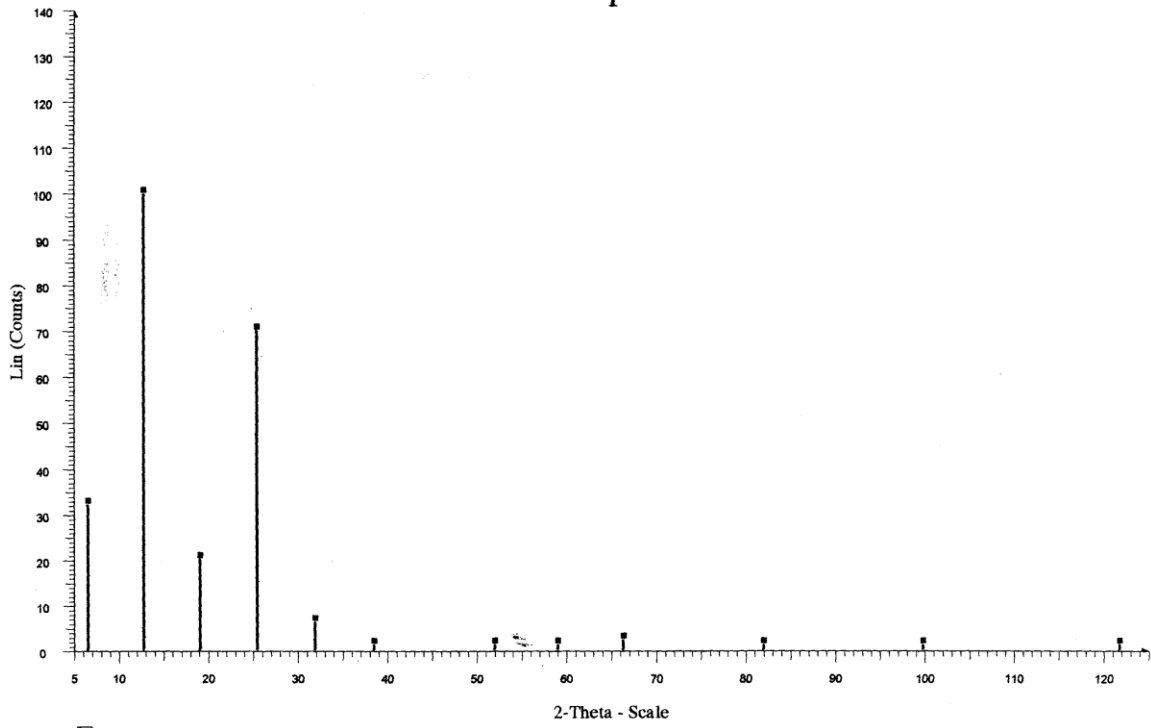
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| Pattern : 01-085-0877  |               | Radiation = 1.540560 |          |          |          |          | Quality : Calculated |          |          |          |          |
|--|---------------|----------------------|----------|----------|----------|----------|----------------------|----------|----------|----------|----------|
| Ca <sub>2</sub> (Mg,Fe) <sub>5</sub> Si <sub>6</sub> O <sub>22</sub> (OH) <sub>2</sub> |               | <i>d</i> (Å)         | <i>i</i> | <i>h</i> | <i>k</i> | <i>l</i> | <i>d</i> (Å)         | <i>i</i> | <i>h</i> | <i>k</i> | <i>l</i> |
| Magnesium Calcium Silicate Hydroxide<br>Tremolite                                      |               | 9.02400              | 429      | 0        | 2        | 0        | 1.56765              | 7        | 3        | 5        | 2        |
| Lattice : Base-centered monoclinic   |               | 8.43156              | 785      | 1        | 1        | 0        | *1.56785             | 7        | -1       | 9        | 2        |
| S.G. : C2/m (12)   |               | 5.08812              | 134      | 1        | 3        | 0        | 1.56471              | 6        | 5        | 3        | 1        |
| Mol. weight = 812.37   |               | 4.88226              | 314      | -1       | 1        | 0        | *1.56471             | 6        | 0        | 4        | 3        |
| Volume [CD] = 909.60   |               | 4.76811              | 62       | 2        | 0        | 0        | 1.56857              | 36       | -4       | 0        | 3        |
| Dx = 2.966   |               | 4.51200              | 284      | 0        | 4        | 0        | *1.56837             | 36       | 6        | 0        | 0        |
| Dm = 2.900   |               | 4.44651              | 16       | 0        | 2        | 1        | 1.57817              | 205      | -5       | 5        | 2        |
| I/cor = 0.64   |               | 4.21578              | 81       | 2        | 2        | 0        | *1.57817             | 205      | -1       | 5        | 3        |
| a = 9.86300  | beta = 104.79 | 4.03802              | 26       | -2       | 0        | 1        | 1.56528              | 12       | -4       | 2        | 3        |
| b = 18.04800   |               | 3.98911              | 53       | 1        | 1        | 1        | *1.56528             | 12       | 6        | 2        | 0        |
| c = 5.28500  | Z = 2         | 3.87638              | 254      | -1       | 3        | 1        | 1.56128              | 21       | 2        | 10       | 1        |
| a/b = 0.54649  |               | 3.86583              | 1        | -2       | 2        | 1        | *1.56128             | 21       | -1       | 11       | 1        |
| c/b = 0.29283  |               | 3.38251              | 628      | 1        | 3        | 1        | 1.56636              | 22       | -5       | 7        | 1        |
|  |               | 3.27727              | 452      | 2        | 4        | 0        | 1.55615              | 53       | 4        | 0        | 2        |
|  |               | 3.13055              | 650      | 3        | 1        | 1        | 1.55279              | 29       | 1        | 3        | 3        |
|  |               | 3.03025              | 33       | -3       | 1        | 1        | 1.54789              | 5        | 3        | 9        | 1        |
|  |               | 3.00896              | 10       | -2       | 4        | 1        | 1.53695              | 101      | -6       | 0        | 2        |
|  |               | *3.00896             | 10       | 0        | 6        | 0        | 1.53332              | 70       | 5        | 7        | 0        |
|  |               | 2.94222              | 523      | 2        | 2        | 1        | *1.53332             | 70       | -3       | 5        | 3        |
|  |               | *2.94222             | 523      | -1       | 5        | 1        | 1.52278              | 6        | 1        | 11       | 1        |
|  |               | 2.81053              | 113      | 3        | 3        | 0        | *1.51827             | 50       | 1        | 9        | 2        |
|  |               | 2.73728              | 283      | -3       | 3        | 1        | 1.51389              | 216      | -8       | 2        | 2        |
|  |               | 2.70644              | 999      | 1        | 5        | 1        | *1.51389             | 216      | -2       | 6        | 3        |
|  |               | 2.59222              | 355      | 0        | 6        | 1        | 1.51105              | 115      | -3       | 9        | 2        |
|  |               | 2.55495              | 110      | 0        | 0        | 2        | 1.50400              | 163      | 0        | 12       | 0        |
|  |               | 2.53781              | 615      | -2       | 0        | 2        | *1.50400             | 163      | 5        | 5        | 1        |
|  |               | 2.48892              | 3        | 1        | 7        | 0        | 1.49908              | 87       | -4       | 4        | 3        |
|  |               | 2.45632              | 17       | 0        | 2        | 2        | *1.49908             | 87       | 8        | 4        | 0        |
|  |               | 2.44304              | 27       | -2       | 2        | 2        | 1.48818              | 3        | 2        | 0        | 3        |
|  |               | 2.41227              | 57       | -2       | 6        | 1        | 1.48637              | 4        | 4        | 8        | 1        |
|  |               | *2.41227             | 57       | -4       | 0        | 1        | 1.48217              | 10       | 0        | 6        | 3        |
|  |               | 2.36557              | 85       | 3        | 5        | 0        | 1.47111              | 51       | 4        | 4        | 2        |
|  |               | *2.36557             | 85       | 4        | 0        | 0        | *1.47111             | 51       | -2       | 10       | 2        |
|  |               | 2.34026              | 333      | -3       | 5        | 0        | 1.46835              | 41       | 2        | 2        | 3        |
|  |               | 2.32741              | 184      | -4       | 2        | 1        | *1.46835             | 41       | 1        | 5        | 3        |
|  |               | 2.29871              | 201      | -1       | 7        | 1        | 1.45797              | 41       | 3        | 11       | 0        |
|  |               | 2.28001              | 181      | -3       | 1        | 2        | 1.45486              | 48       | -8       | 4        | 2        |
|  |               | 2.25689              | 18       | 3        | 3        | 1        | *1.45486             | 48       | -5       | 7        | 2        |
|  |               | *2.25689             | 18       | 0        | 8        | 0        | 1.45145              | 46       | -1       | 7        | 3        |
|  |               | 2.22525              | 6        | 0        | 4        | 2        | 1.44744              | 31       | -3       | 11       | 1        |
|  |               | 2.21194              | 78       | -2       | 4        | 2        | *1.44064             | 264      | -6       | 8        | 0        |
|  |               | 2.18113              | 49       | 1        | 7        | 1        | 1.42849              | 19       | -5       | 3        | 3        |
|  |               | 2.16291              | 295      | 2        | 6        | 1        | 1.42649              | 19       | 2        | 6        | 0        |
|  |               | 2.14707              | 45       | -3       | 3        | 2        | 1.41843              | 2        | -6       | 0        | 1        |
|  |               | 2.13208              | 36       | -1       | 5        | 2        | 1.41452              | 6        | -3       | 7        | 3        |
|  |               | 2.12522              | 22       | -4       | 4        | 1        | *1.41452             | 6        | 2        | 4        | 3        |
|  |               | 2.10790              | 2        | 4        | 4        | 0        | 1.40941              | 5        | -2       | 12       | 1        |
|  |               | 2.06381              | 4        | 0        | 6        | 1        | 1.40662              | 5        | -4       | 6        | 3        |
|  |               | 2.04514              | 159      | 2        | 0        | 2        | *1.40662             | 5        | 6        | 6        | 0        |
|  |               | 2.03926              | 95       | 2        | 8        | 0        | 1.40123              | 20       | 6        | 2        | 1        |
|  |               | 2.01848              | 206      | -4       | 0        | 2        | *1.40123             | 20       | -6       | 9        | 1        |
|  |               | *2.01848             | 206      | 3        | 5        | 1        | 1.39208              | 3        | 5        | 7        | 1        |
|  |               | 2.00241              | 62       | 3        | 7        | 0        | 1.38371              | 1        | -2       | 8        | 3        |
|  |               | 1.99456              | 36       | 2        | 2        | 2        | *1.38214             | 1        | 4        | 6        | 2        |
|  |               | 1.97541              | 16       | 4        | 0        | 1        | 1.38214              | 1        | 5        | 9        | 0        |
|  |               | *1.97541             | 16       | -3       | 7        | 1        | 1.37179              | 6        | -7       | 3        | 1        |
|  |               | 1.97030              | 19       | -4       | 2        | 2        | 1.36567              | 100      | 5        | 1        | 2        |
|  |               | *1.97030             | 19       | -2       | 8        | 1        | 1.36180              | 81       | -5       | 5        | 3        |
|  |               | 1.96241              | 56       | 1        | 9        | 0        | 1.35845              | 45       | 0        | 8        | 3        |
|  |               | 1.94686              | 8        | 0        | 6        | 2        | 1.35845              | 45       | 7        | 1        | 0        |
|  |               | *1.94686             | 8        | -5       | 1        | 1        | 1.35417              | 14       | 2        | 12       | 1        |
|  |               | 1.93875              | 43       | -2       | 6        | 2        | 1.35322              | 10       | 2        | 10       | 2        |
|  |               | *1.93875             | 43       | -3       | 5        | 2        | *1.35322             | 10       | 6        | 4        | 1        |
|  |               | 1.93012              | 19       | 4        | 2        | 1        | 1.35037              | 9        | -7       | 1        | 2        |
|  |               | 1.89698              | 82       | 5        | 1        | 0        | 1.34557              | 6        | -6       | 0        | 3        |
|  |               | 1.88028              | 23       | -4       | 6        | 1        | 1.34036              | 67       | 1        | 11       | 2        |
|  |               | 1.86505              | 111      | -1       | 9        | 1        | *1.34036             | 67       | -1       | 13       | 1        |
|  |               | *1.86505             | 111      | 2        | 4        | 2        | 1.33539              | 73       | 5        | 3        | 2        |
|  |               | 1.84533              | 49       | -1       | 7        | 2        | *1.33539             | 73       | -3       | 11       | 2        |
|  |               | 1.84292              | 53       | -4       | 4        | 2        | 1.33366              | 60       | 2        | 6        | 3        |
|  |               | 1.81807              | 40       | 5        | 3        | 0        | 1.33128              | 45       | 3        | 9        | 2        |
|  |               | 1.80480              | 24       | 0        | 10       | 0        | *1.33128             | 45       | -6       | 2        | 3        |
|  |               | 1.80058              | 21       | 1        | 9        | 1        | 1.32970              | 36       | 3        | 3        | 3        |
|  |               | 1.77308              | 8        | 3        | 1        | 2        | 1.32222              | 31       | -5       | 9        | 2        |
|  |               | 1.77018              | 5        | 3        | 7        | 1        | *1.32222             | 31       | -7       | 3        | 2        |
|  |               | 1.75036              | 44       | -5       | 1        | 2        | 1.31247              | 70       | -7       | 5        | 1        |
|  |               | *1.75036             | 44       | -1       | 1        | 3        | 1.30753              | 61       | -1       | 1        | 4        |
|  |               | 1.72628              | 4        | 1        | 7        | 2        | *1.30753             | 61       | -2       | 2        | 4        |
|  |               | *1.72628             | 4        | 1        | 7        | 2        | 1.30291              | 33       | -3       | 1        | 4        |

Hawthorne, F.C., Grundy, H.D., Can. Mineral., volume 14, page 334 (1976)  
 Calculated from ICSD using POWD-12++

# Chlorite-serpentine



00-052-1044 (1) - Chlorite-serpentine -  $(Mg,Al)_6(Si,Al)_4O_{10}(OH)_8$  - WL: 1.5406 - Hexagonal - Primitive - a 5.34000 - b 5.34000 - c 14.10900 - alpha 90.000 - beta 90.000 - gamma 120.000 - P (0) - 1 - 348.425 - I/c PDF 1 - P12

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Pattern : 00-052-1044

Radiation = 1.540560

Quality : Indexed



Magnesium Aluminum Silicate Hydroxide  
Chlorite-serpentine

| $d$ (Å)  | $l$ | $h$ | $k$ | $l$ |
|----------|-----|-----|-----|-----|
| 14.15000 | 32  | 0   | 0   | 1   |
| 7.04000  | 100 | 0   | 0   | 2   |
| 4.70000  | 20  | 0   | 0   | 3   |
| 3.52500  | 70  | 0   | 0   | 4   |
| 2.82500  | 6   | 0   | 0   | 5   |
| 2.35300  | 1   | 0   | 0   | 6   |
| 1.76300  | 1   | 0   | 0   | 8   |
| 1.56800  | 1   | 0   | 0   | 9   |
| 1.41200  | 2   | 0   | 0   | 10  |
| 1.17700  | 1   | 0   | 0   | 12  |
| 1.00830  | 1   | 0   | 0   | 14  |
| 0.88180  | 1   | 0   | 0   |     |

Lattice : Hexagonal

Mol. weight = 554.22

S.G. : P (0)

Volume [CD] = 348.43

a = 5.34000

Dx = 2.641

c = 14.10900

Z = 1

Sample source or locality: Specimen from Tuscaloosa Formation,  
Louisiana, USA.

General comments: Only 00l reflections are recorded.

Data collection flag: Ambient.

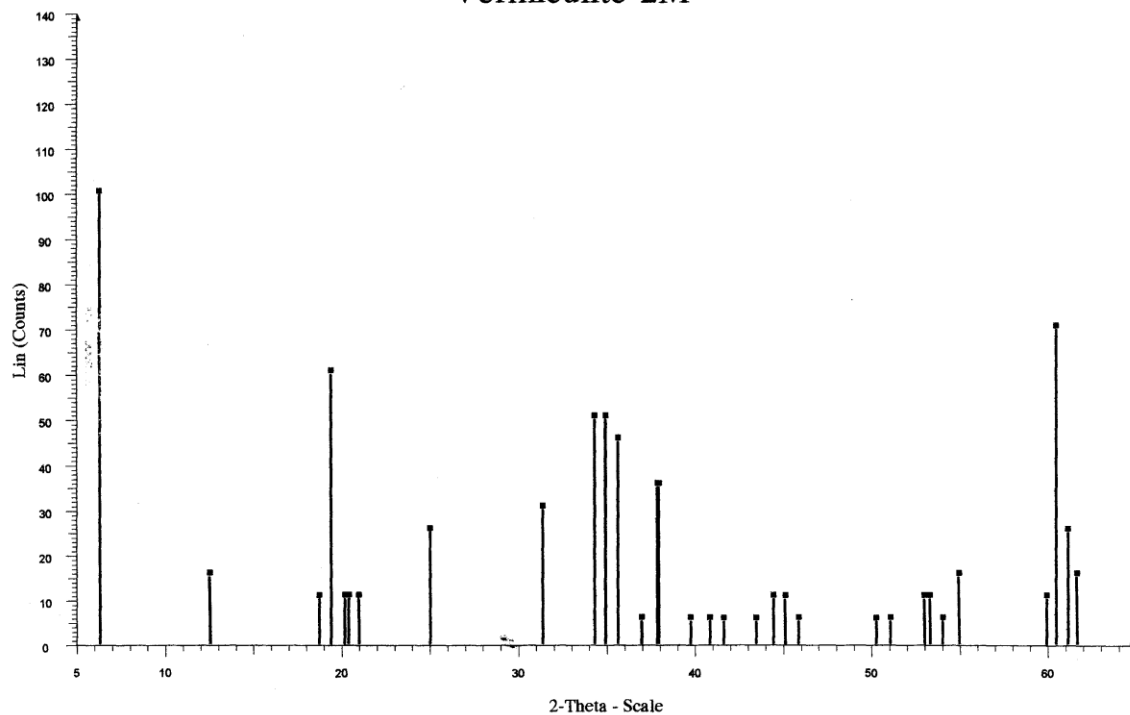
Reynolds, Jr., R., DiStefano, M., Lahann, R., Clays Clay Miner., volume 40,  
page 262 (1992)

cuu duong than cong, com

cuu duong than cong, com



# Vermiculite-2M



00-016-0613 (1) - Vermiculite-2M - Mg<sub>x</sub>(Mg,Fe)<sub>3</sub>(Si,Al)<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>·4H<sub>2</sub>O - WL: 1.5406 - Monoclinic - Base-centered - a 5.24000 - b 9.17000 - c 28.60000 - alpha 90.000 - beta 94.600 - gamma 90.000 - C2/c (15) - 4 - 1369.83 - 1

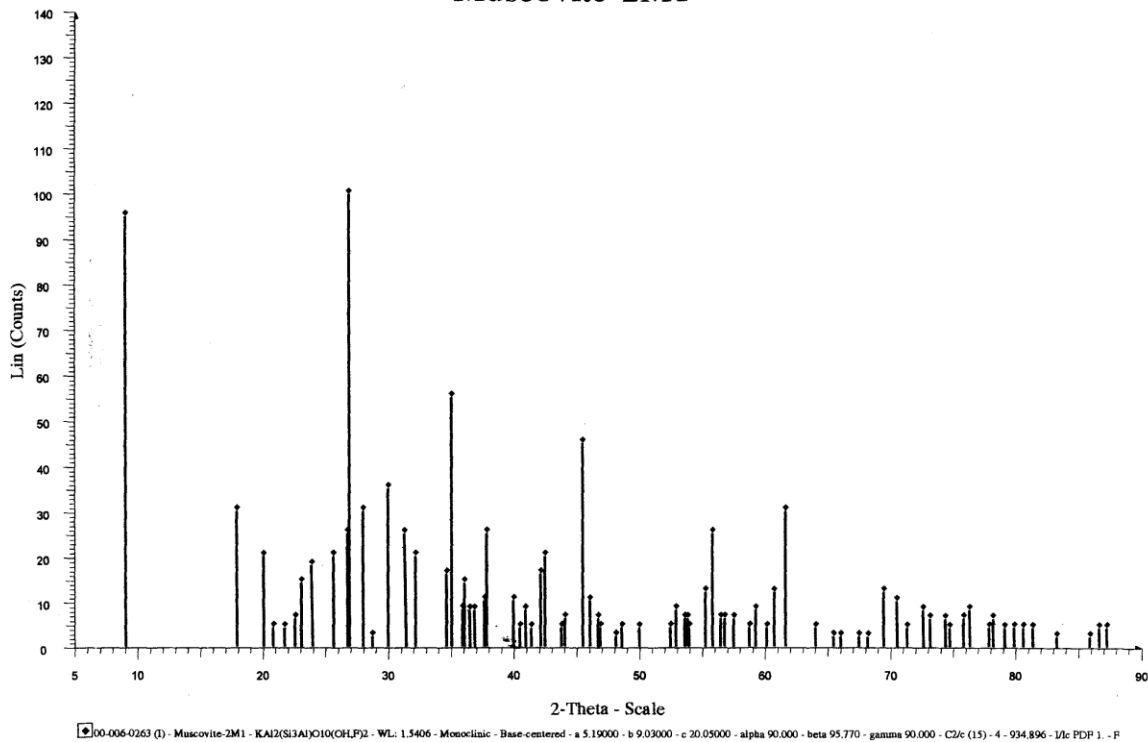
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| Pattern : 00-016-0613   |  | Radiation = 1.540560  |  | Quality : Indexed   |  |   |
|---|--|---|--|---|--|---|
| <p><b>Mg<sub>x</sub>(Mg,Fe)<sub>3</sub>(Si,Al)<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>·4H<sub>2</sub>O</b></p> <p>Magnesium Iron Aluminum Silicate Hydroxide Hydrate<br/>Vermiculite-2M</p>   |  | <p><b>d (Å)</b></p> <p>14.20000<br/>7.14000<br/>4.76000<br/>4.57000<br/>4.41000<br/>4.35000<br/>4.25000<br/>3.58000<br/>2.85000<br/>2.61500<br/>2.57000<br/>2.52500<br/>2.43000<br/>2.38000<br/>2.36500<br/>2.26500<br/>2.20000<br/>2.17000<br/>2.08000<br/>2.04000<br/>2.01000<br/>1.97500<br/>1.82000<br/>1.79000<br/>1.72500<br/>1.71500<br/>1.69500<br/>1.66500<br/>1.54300<br/>1.52800<br/>1.51400<br/>1.50200</p> | <p><b>i</b></p> <p>100<br/>15<br/>10<br/>60<br/>10<br/>10<br/>10<br/>25<br/>30<br/>50<br/>50<br/>45<br/>5<br/>35<br/>35<br/>5<br/>5<br/>5<br/>5<br/>10<br/>10<br/>10<br/>5<br/>5<br/>5<br/>10<br/>10<br/>5<br/>10<br/>15<br/>10<br/>70<br/>25<br/>15</p> | <p><b>h</b></p> <p>0<br/>0<br/>0<br/>0<br/>-1<br/>0<br/>1<br/>0<br/>0<br/>-1<br/>-1<br/>-2<br/>-1<br/>0<br/>-2<br/>-2<br/>-2<br/>-1<br/>1<br/>0<br/>-2<br/>-1<br/>1<br/>2<br/>2<br/>-2<br/>-3<br/>-2<br/>-1<br/>1<br/>1<br/>1<br/>0<br/>1<br/>0<br/>1<br/>1</p> | <p><b>k</b></p> <p>0<br/>0<br/>0<br/>2<br/>1<br/>2<br/>1<br/>0<br/>0<br/>3<br/>3<br/>0<br/>3<br/>0<br/>0<br/>2<br/>2<br/>1<br/>3<br/>0<br/>0<br/>-1<br/>-1<br/>1<br/>2<br/>2<br/>4<br/>1<br/>1<br/>4<br/>5<br/>5<br/>5<br/>6<br/>3<br/>6<br/>5</p> | <p><b>l</b></p> <p>2<br/>4<br/>6<br/>0<br/>2<br/>2<br/>2<br/>8<br/>10<br/>2<br/>3<br/>4<br/>5<br/>12<br/>6<br/>2<br/>4<br/>12<br/>8<br/>14<br/>10<br/>10<br/>10<br/>11<br/>9<br/>1<br/>1<br/>4<br/>5<br/>8<br/>0<br/>15<br/>9</p> |
| <p><b>Lattice</b> : Base-centered monoclinic</p> <p><b>S.G.</b> : C2/c (15)</p> <p><b>a</b> = 5.24000<br/><b>b</b> = 9.17000<br/><b>c</b> = 28.60000<br/><b>a/b</b> = 0.57143<br/><b>c/b</b> = 3.11887</p>  |  | <p><b>Volume [CD]</b> = 1369.83</p> <p><b>beta</b> = 94.60</p> <p><b>Dm</b> = 2.260</p> <p><b>Z</b> = 4</p>   |  |   |  |   |
| <p><b>Optical data</b>: A=1.525, B=1.545, <math>n_x = 1.545</math>, Sign=, 2V=0°<br/><b>Color</b>: Brown, green<br/><b>Sample source or locality</b>: Specimen from Ajmer-Marwar, India (Indian Museum 8247).<br/><b>Analysis</b>: Analysis (wt.%): Si O<sub>2</sub> 34.92, Al<sub>2</sub> O<sub>3</sub> 13.97, Fe<sub>2</sub> O<sub>3</sub> 6.25, FeO 0.52, MgO 20.37, CaO 2.15, Na<sub>2</sub> O 0.32, H<sub>2</sub> O 21.00.<br/><b>Additional pattern</b>: To replace 10-418 and validated by calculated pattern 34-166.<br/><b>Additional pattern</b>: See ICSD 37442 (PDF 77-22).<br/><b>Data collection flag</b>: Ambient.</p> |  |   |  |   |  |   |
| <p>Mukherjee., Clay Miner. Bull., volume 5, page 194 (1963)</p> <p>CAS Number: 1318-00-9</p>  |  |   |  |   |  |   |

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# Muscovite-2M1

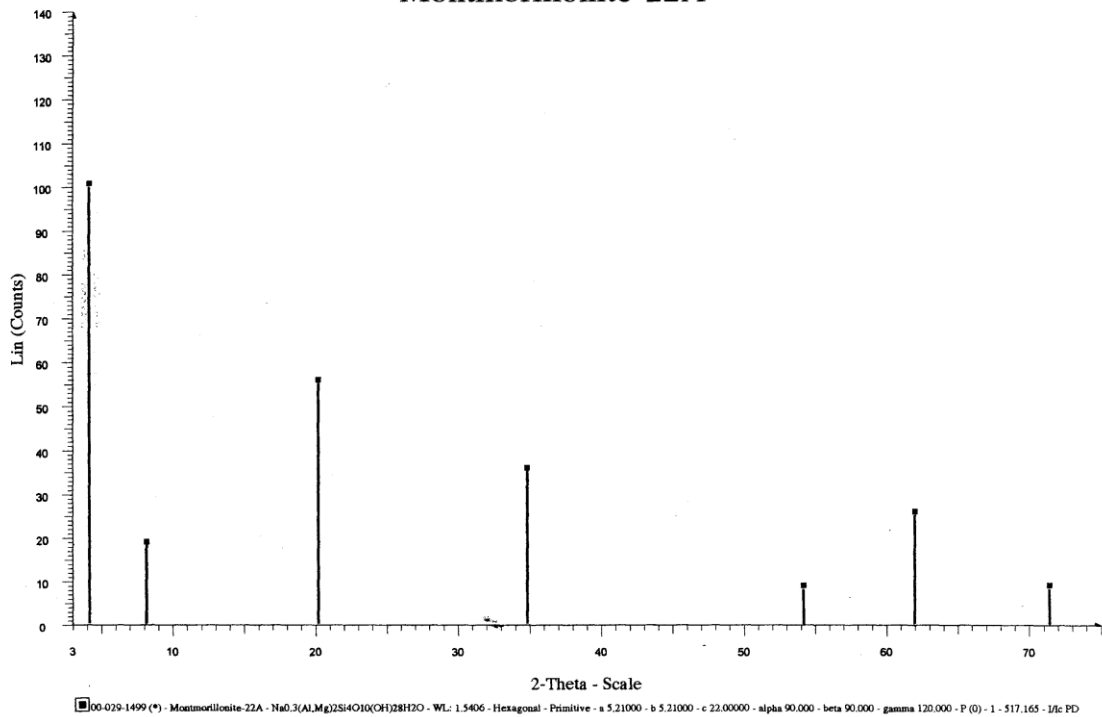


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cuu duong than cong. com

| Pattern : 00-006-0263   |  | Radiation = 1.540560  |          |          |          |          | Quality : Indexed |          |          |          |          |
|---|--|---|----------|----------|----------|----------|-------------------|----------|----------|----------|----------|
| $KAl_2(Si_3Al)O_{10}(OH,F)_2$<br><br>Potassium Aluminum Silicate Hydroxide<br>Muscovite-2M1   |  | <i>d</i> (Å)  | <i>l</i> | <i>h</i> | <i>k</i> | <i>l</i> | <i>d</i> (Å)      | <i>l</i> | <i>h</i> | <i>k</i> | <i>l</i> |
|   |  | 9.95000   | 95       | 0        | 0        | 2        | 1.18280           | 4        | -1       | 7        | 6        |
|   |  | 4.97000   | 30       | 0        | 0        | 4        | 1.15820           | 2        | 0        | 6        | 11       |
|   |  | 4.47000   | 20       | -1       | 1        | 1        | 1.13000           | 2        | 2        | 6        | 8        |
|   |  | 4.30000   | 4        | 1        | 1        | 1        | 1.12200           | 4        | 1        | 5        | 13       |
|   |  | 4.11000   | 4        | 0        | 2        | 2        | 1.11670           | 4        | 0        | 6        | 12       |
|   |  | 3.95000   | 6        | 1        | 1        | 2        |                   |          |          |          |          |
|   |  | 3.88000   | 14       | -1       | 1        | 3        |                   |          |          |          |          |
|   |  | 3.73000   | 18       | 0        | 2        | 3        |                   |          |          |          |          |
|   |  | 3.48000   | 20       | -1       | 1        | 4        |                   |          |          |          |          |
|   |  | 3.34000   | 25       | 0        | 2        | 4        |                   |          |          |          |          |
|   |  | 3.32000   | 100      | 0        | 0        | 6        |                   |          |          |          |          |
|   |  | 3.19000   | 30       | 1        | 1        | 4        |                   |          |          |          |          |
|   |  | 3.12000   | 2        | -1       | 1        | 5        |                   |          |          |          |          |
|   |  | 2.98700   | 35       | 0        | 2        | 5        |                   |          |          |          |          |
|   |  | 2.85900   | 25       | 1        | 1        | 5        |                   |          |          |          |          |
|   |  | 2.78900   | 20       | -1       | 1        | 6        |                   |          |          |          |          |
|   |  | 2.59600   | 16       | -1       | 3        | 1        |                   |          |          |          |          |
|   |  | 2.56600   | 55       | 1        | 1        | 6        |                   |          |          |          |          |
|   |  | 2.50500   | 8        | -1       | 1        | 7        |                   |          |          |          |          |
|   |  | 2.49100   | 14       | 0        | 0        | 8        |                   |          |          |          |          |
|   |  | 2.46500   | 8        | -1       | 3        | 3        |                   |          |          |          |          |
|   |  | 2.45000   | 8        | 2        | 0        | 2        |                   |          |          |          |          |
|   |  | 2.39800   | 10       | -2       | 0        | 4        |                   |          |          |          |          |
|   |  | 2.38400   | 25       | 1        | 3        | 3        |                   |          |          |          |          |
|   |  | 2.25400   | 10       | 0        | 4        | 0        |                   |          |          |          |          |
|   |  | 2.23600   | 4        | -1       | 3        | 5        |                   |          |          |          |          |
|   |  | 2.20800   | 8        | 2        | 2        | 1        |                   |          |          |          |          |
|   |  | 2.18900   | 4        | 0        | 2        | 8        |                   |          |          |          |          |
|   |  | 2.14900   | 16       | 2        | 2        | 2        |                   |          |          |          |          |
|   |  | 2.13200   | 20       | 1        | 3        | 5        |                   |          |          |          |          |
|   |  | 2.07000   | 4        | 2        | 2        | 3        |                   |          |          |          |          |
|   |  | 2.05300   | 6        | 0        | 4        | 4        |                   |          |          |          |          |
|   |  | 1.99300   | 45       | 0        | 0        | 10       |                   |          |          |          |          |
|   |  | 1.97200   | 10       | -1       | 3        | 7        |                   |          |          |          |          |
|   |  | 1.95100   | 6        | 2        | 0        | 6        |                   |          |          |          |          |
|   |  | 1.94100   | 4        | -2       | 2        | 6        |                   |          |          |          |          |
|   |  | 1.89400   | 2        | -2       | 0        | 8        |                   |          |          |          |          |
|   |  | 1.87100   | 4        | 1        | 3        | 7        |                   |          |          |          |          |
|   |  | 1.82200   | 4        | 0        | 2        | 10       |                   |          |          |          |          |
|   |  | 1.74600   | 4        | -2       | 2        | 8        |                   |          |          |          |          |
|   |  | 1.73100   | 8        | -1       | 3        | 9        |                   |          |          |          |          |
|   |  | 1.71000   | 6        | 2        | 0        | 8        |                   |          |          |          |          |
|   |  | 1.70400   | 6        | -1       | 5        | 1        |                   |          |          |          |          |
|   |  | 1.69900   | 4        | -3       | 1        | 1        |                   |          |          |          |          |
|   |  | 1.66200   | 12       | 0        | 0        | 12       |                   |          |          |          |          |
|   |  | 1.64600   | 25       | 1        | 3        | 9        |                   |          |          |          |          |
|   |  | 1.63100   | 6        | -1       | 5        | 4        |                   |          |          |          |          |
|   |  | 1.62000   | 6        | 2        | 4        | 3        |                   |          |          |          |          |
|   |  | 1.60300   | 6        | -2       | 4        | 5        |                   |          |          |          |          |
|   |  | 1.57300   | 4        | -3       | 1        | 6        |                   |          |          |          |          |
|   |  | 1.55900   | 8        | -2       | 2        | 10       |                   |          |          |          |          |
|   |  | 1.54100   | 4        | -1       | 5        | 6        |                   |          |          |          |          |
|   |  | 1.52400   | 12       | -1       | 3        | 11       |                   |          |          |          |          |
|   |  | 1.50400   | 30       | -2       | 4        | 7        |                   |          |          |          |          |
|   |  | 1.45300   | 4        | 0        | 2        | 13       |                   |          |          |          |          |
|   |  | 1.42400   | 2        | 0        | 0        | 14       |                   |          |          |          |          |
|   |  | 1.41400   | 2        | 0        | 4        | 11       |                   |          |          |          |          |
|   |  | 1.38800   | 2        | 1        | 5        | 8        |                   |          |          |          |          |
|   |  | 1.37500   | 2        | -3       | 3        | 7        |                   |          |          |          |          |
|   |  | 1.35200   | 12       | -1       | 3        | 13       |                   |          |          |          |          |
| <b>Lattice</b> : Base-centered monoclinic<br><b>S.G.</b> : C2/c (15)  |  | <b>Mol. weight</b> = 398.31<br><b>Volume [CD]</b> = 934.90<br><b>Dx</b> = 2.830 |          |          |          |          |                   |          |          |          |          |
| <b>a</b> = 5.19000<br><b>b</b> = 9.03000<br><b>c</b> = 20.05000<br><b>a/b</b> = 0.57475<br><b>c/b</b> = 2.22038   |  | <b>beta</b> = 95.77<br><b>Z</b> = 4   |          |          |          |          |                   |          |          |          |          |
| <b>Optical data</b> : A=1.50-1.56, Q=1.59-1.61, Sign=-, 2V=36-50°<br><b>General comments</b> : Space group by Jackson, West, Z. <i>Kristallogr.</i> , 76 211 (1930) and Hendricks, Jefferson, <i>Am. Mineral.</i> , 24 729 (1939).<br><b>General comments</b> : Other sources give refractive indexes for muscovites: $n_{\alpha}=1.55-1.57$ , $n_{\beta}=1.58-1.61$ , $n_{\gamma}=1.59-1.62$ .<br><b>General comments</b> : Locality not given.<br><b>Color</b> : Colorless<br><b>Additional pattern</b> : See ICSD 15868 (PDF 72-496); See ICSD 25803 (PDF 74-345); See ICSD 28553 (PDF 74-2428); See ICSD 30297 (PDF 75-948); See ICSD 34353 (PDF 76-637); See ICSD 34406 (PDF 76-668); See ICSD 34921 (PDF 76-929); See ICSD 60569 (PDF 77-2255); See ICSD 202260 (PDF 84-1302); See ICSD 202262 (PDF 84-1304); See ICSD 68547 (PDF 80-742); See ICSD 67629 (PDF 79-2363); See ICSD 74608 (PDF 82-576); See ICSD 79027 (PDF 82-2450); See ICSD 79029 (PDF 85-2147).<br><b>Data collection flag</b> : Ambient. |  |   |          |          |          |          |                   |          |          |          |          |
| Gillery, F., Penn State Univ., University Park, PA, USA., Private Communication   |  |   |          |          |          |          |                   |          |          |          |          |

# Montmorillonite-22A



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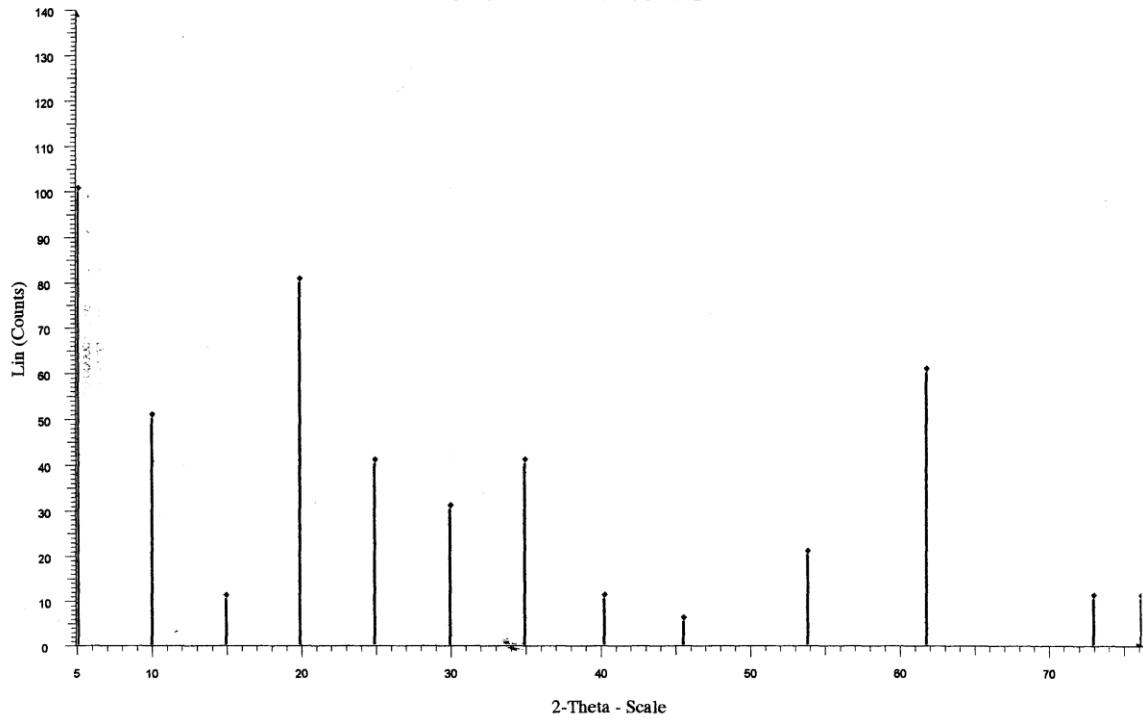
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|  |              |   |   |   |   |   |
|--|--------------|---|---|---|---|---|
| <b>Pattern</b> : 00-029-1499   |              | <b>Radiation</b> = 1.540560   |   | <b>Quality</b> : High                       |   |   |
| $\text{Na}_{0.3}(\text{Al,Mg})_2\text{Si}_4\text{O}_{10}(\text{OH})_2 \cdot 8\text{H}_2\text{O}$<br><br>Sodium Magnesium Aluminum Silicate Hydroxide Hydrate<br>Montmorillonite-22A  |              | <b>d (Å)</b><br>21.50000<br>10.60000<br>4.45000<br>2.58000<br>1.69000<br>1.49500<br>1.32500 | <b>l</b><br>100<br>18<br>55<br>35<br>8<br>25<br>8 | <b>h</b><br>0<br>0<br>1<br>1<br>0<br>2<br>3 | <b>k</b><br>0<br>0<br>0<br>0<br>0<br>0<br>0 | <b>i</b><br>1<br>2<br>1<br>7<br>13<br>11<br>8 |
| <b>Lattice</b> : Hexagonal<br><b>S.G.</b> : P (0)  |              | <b>Mol. weight</b> = 511.33<br><b>Volume [CD]</b> = 517.16<br><b>Dx</b> = 1.642             |   |   |   |   |
| <b>a</b> = 5.21000<br><br><b>c</b> = 22.00000  | <b>Z</b> = 1 |   |   |   |   |   |
| <p><b>Sample source or locality:</b> Specimen from Wyoming, USA.<br/> <b>Sample preparation:</b> Stored over water, four days, 100% relative humidity.<br/> <b>General comments:</b> Reflection at 3.15 (l=40) was deleted, because it was probably cristobalite.<br/> <b>Data collection flag:</b> Ambient.</p> |              |   |   |   |   |   |
| Brindley, G., Penn State Univ., University Park, PA, USA., ICDD Grant-in-Aid (1977)<br>CAS Number: 1318-93-0   |              |   |   |   |   |   |

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# Montmorillonite-18A



00-012-0219 (1) - Montmorillonite-18A - Na<sub>0.3</sub>(AlMg)<sub>2</sub>Si<sub>4</sub>O<sub>10</sub>(OH)<sub>2</sub>·2H<sub>2</sub>O - WL: 1.5406 - Hexagonal - Primitive - a 5.19500 - b 5.19500 - c 17.93000 - alpha 90.000 - beta 90.000 - gamma 120.000 - P (0) - 1 - 419.066 - I/I: PDF

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| Pattern : 00-012-0219   |  | Radiation = 1.540560  |          | Quality : Indexed |          |          |
|---|--|---|----------|-------------------|----------|----------|
| $\text{Na}_{0.3}(\text{AlMg})_2\text{Si}_4\text{O}_{10}\text{OH}_2 \cdot 6\text{H}_2\text{O}$<br><br>Sodium Magnesium Aluminum Silicate Hydroxide Hydrate<br>Montmorillonite-18A  |  | <i>d</i> (Å)  | <i>i</i> | <i>h</i>          | <i>k</i> | <i>l</i> |
|   |  | 17.60000  | 100      | 0                 | 0        | 1        |
|   |  | 9.00000   | 50       | 0                 | 0        | 2        |
|   |  | 5.99000   | 10       | 0                 | 0        | 3        |
|   |  | 4.49000   | 80       | 0                 | 0        | 4        |
|   |  | 3.58000   | 40       | 0                 | 0        | 5        |
|   |  | 2.99000   | 30       | 0                 | 0        | 6        |
|   |  | 2.57000   | 40       | 1                 | 1        | 1        |
|   |  | 2.24200   | 10       | 0                 | 0        | 8        |
|   |  | 1.98900   | 5        | 0                 | 0        | 9        |
|   |  | 1.69900   | 20       | 2                 | 1        | 0        |
|   |  | 1.50400   | 60       | 3                 | 0        | 0        |
|   |  | 1.29400   | 10       | 3                 | 0        | 7        |
|   |  | 1.25000   | 10       | 3                 | 1        | 0        |
| <b>Latitude :</b> Hexagonal<br><b>S.G. :</b> P (0)<br><b>a =</b> 5.19500<br><b>c =</b> 17.93000<br><b>Z =</b> 1   |  | <b>Mol. weight =</b> 507.91<br><b>Volume [CD] =</b> 419.07<br><b>Dx =</b> 2.013 |          |                   |          |          |
| <b>Optical data:</b> A=1.48-1.61, B=1.50-1.64, Q=1.50-1.64, Sign=, 2V=15(15)°<br><b>Color:</b> White, yellow, green<br><b>Sample source or locality:</b> Specimen from Chambers, Arizona, USA.<br><b>Sample preparation:</b> Glycol sodium saturated.<br><b>Additional pattern:</b> To replace 12-204.<br><b>Data collection flag:</b> Ambient. |  |   |          |                   |          |          |
| Earley et al., Am. Mineral., volume 38, page 707 (1953)<br>CAS Number: 1318-93-0  |  |   |          |                   |          |          |

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Pattern : 00-013-0135

Radiation = 1.540560

Quality : Not indexed



Calcium Magnesium Aluminum Silicate Hydroxide Hydrate  
Montmorillonite-15A

| d (Å)   | i   | h | k | l  |
|---------|-----|---|---|----|
| 15.0000 | 100 | 0 | 0 | 1  |
| 5.01000 | 60  | 0 | 0 | 3  |
| 4.50000 | 80  | 1 | 0 | 0  |
| 3.77000 | 20  | 0 | 0 | 4  |
| 3.50000 | 10  |   |   |    |
| 3.30000 | 10  | 1 | 0 | 3  |
| 3.02000 | 60  | 0 | 0 | 5  |
| 2.58000 | 40  | 1 | 1 | 0  |
| 2.50000 | 40  | 0 | 0 | 6  |
| 2.26000 | 10  | 2 | 0 | 0  |
| 2.15000 | 10  | 0 | 0 | 7  |
| 1.88000 | 10  | 0 | 0 | 8  |
| 1.70000 | 30  | 2 | 1 | 0  |
| 1.50000 | 50  | 0 | 0 | 10 |
| 1.49300 | 50  | 3 | 0 | 0  |
| 1.28500 | 20  | 2 | 2 | 1  |
| 1.24300 | 20  | 3 | 1 | 0  |

Lattice : Hexagonal

Mol. weight = 440.39

S.G. : P (0)

Volume [CD] = 347.55

a = 5.16900

Dx = 2.104

Dm = 2.300

c = 15.02000

Z = 1

Optical data: A=1.545(6), B=1.57(7), Q=1.57(7), Sign=-, 2V=0(15)°

Color: White, yellow, green

Sample source or locality: Specimen from Skyrvedalen, Hemsedal, Norway.

Analysis: Analysis (wt.%): Si O2 59.58, Al2 O3 22.96, Fe2 O3 0.47, MgO 3.67, CaO 3.38, Na2 O 0.06, loss 110-950° 9.61.

Footnote for d-spacings and Intensities: 1 15.0 expands to 18.0 with glycerol treatment.

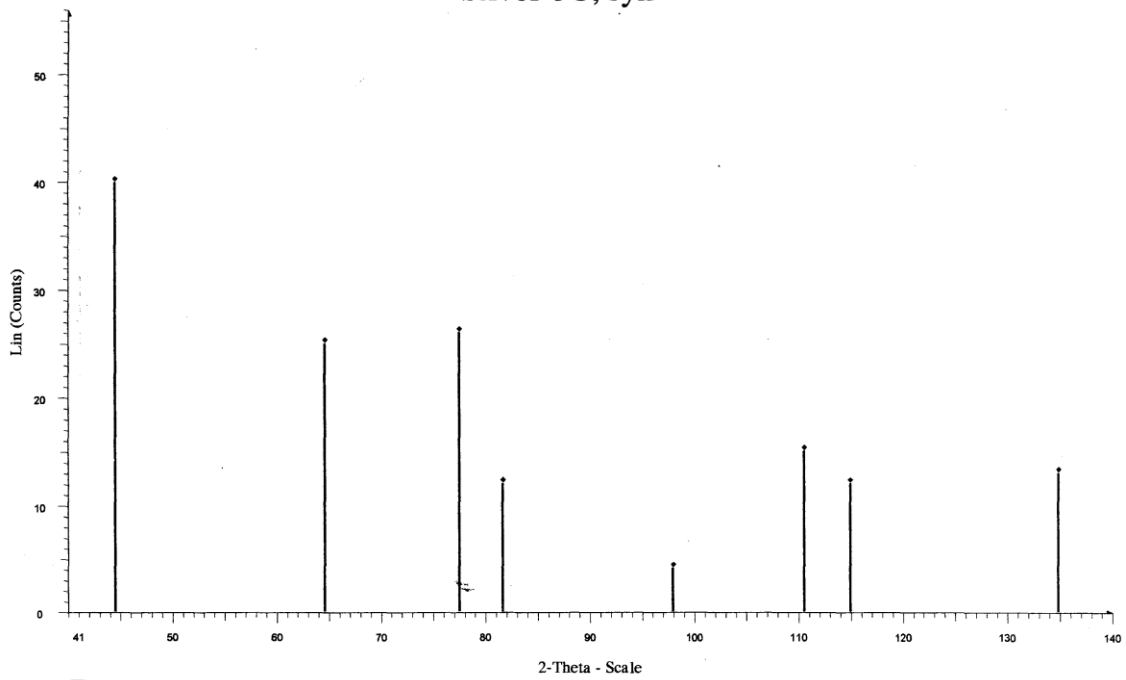
Data collection flag: Ambient.

Rosenquist., Nor. Geol. Tidsskr., volume 39, page 350 (1959)

CAS Number: 1318-93-0

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# Silver-3C, syn



00-004-0783 (1) - Silver-3C, syn - Ag - d x by: 1. - WL: 1.5406 - Cubic - a 4.08620 - b 4.08620 - c 4.08620 - alpha 90.000 - beta 90.000 - gamma 90.000 - Face-centered - Pm-3m (225) - 4 - 68.2274 - Ifc PDF 5.2 - P9= 65(0.0153,9)

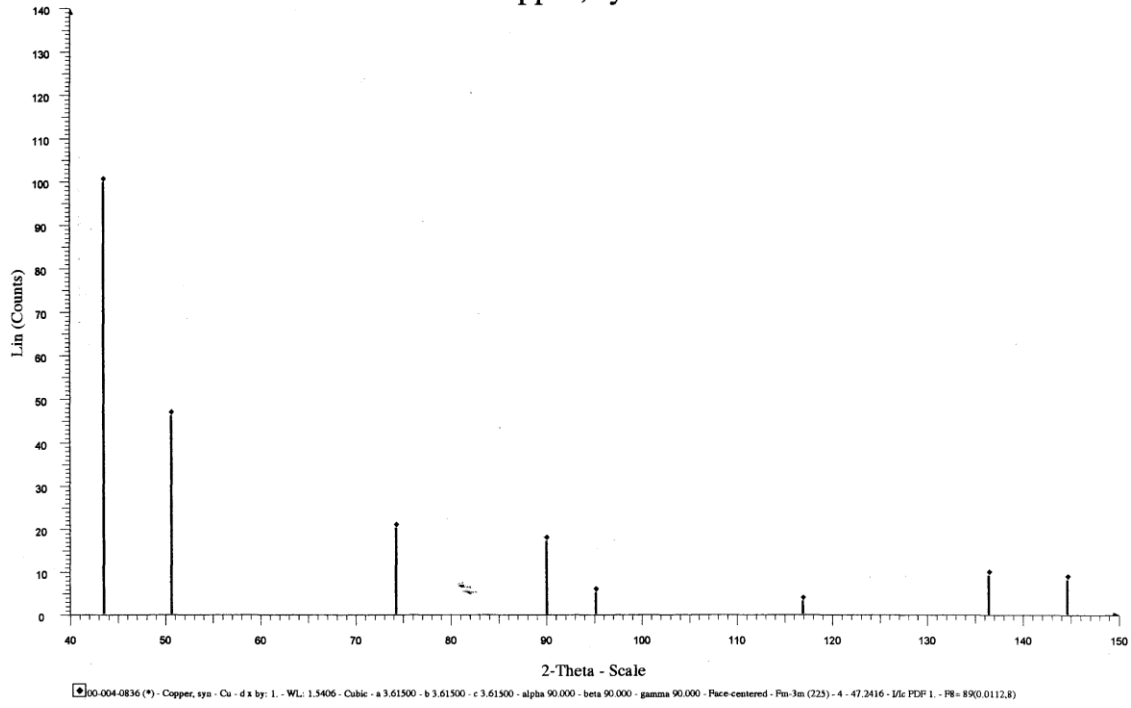
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| Pattern : 00-004-0783  |  | Radiation = 1.540560   |   | Quality : Indexed  |  |  |
|--|--|--|---|--|--|--|
| <p>Ag</p> <p>Silver</p> <p>Silver-3C, syn</p>  |  | <p><b>d (Å)</b></p> <p>2.35900</p> <p>2.04400</p> <p>1.44500</p> <p>1.23100</p> <p>1.17960</p> <p>1.02150</p> <p>0.93750</p> <p>0.91370</p> <p>0.83410</p> | <p><b>i</b></p> <p>100</p> <p>40</p> <p>25</p> <p>26</p> <p>12</p> <p>4</p> <p>15</p> <p>12</p> <p>13</p> | <p><b>h</b></p> <p>1</p> <p>2</p> <p>2</p> <p>3</p> <p>2</p> <p>4</p> <p>3</p> <p>4</p> <p>4</p> | <p><b>k</b></p> <p>1</p> <p>0</p> <p>2</p> <p>1</p> <p>2</p> <p>0</p> <p>3</p> <p>2</p> <p>2</p> | <p><b>l</b></p> <p>1</p> <p>0</p> <p>0</p> <p>1</p> <p>2</p> <p>0</p> <p>1</p> <p>0</p> <p>2</p> |
| <p><b>Lattice :</b> Face-centered cubic</p> <p><b>S.G. :</b> Fm-3m (225)</p> <p><b>a =</b> 4.08620</p> <p><b>Z =</b> 4</p>   |  | <p><b>Mol. weight =</b> 107.87</p> <p><b>Volume [CD] =</b> 68.23</p> <p><b>Dx =</b> 10.501</p> <p><b>Dm =</b> 10.500</p> <p><b>V/cor =</b> 5.20</p>        |   |  |  |  |
| <p><b>Color:</b> Light gray metallic</p> <p><b>Sample source or locality:</b> Sample obtained from Johnson Matthey Company, Ltd.</p> <p><b>General comments:</b> Purity &gt;99.999%.</p> <p><b>Analysis:</b> Spectrographic analysis indicated faint traces of Ca, Fe and Cu.</p> <p><b>Temperature of data collection:</b> Pattern taken at 27 C.</p> <p><b>Optical data:</b> B=0.181</p> <p><b>Melting point:</b> 960.6°</p> <p><b>General comments:</b> Opaque mineral optical data on specimen from Great Bear Lake, Canada: RR<sub>2</sub>R<sub>s</sub>=94.1, Disp.=16, VHN<sub>100</sub>=55-63, Color values 314, 321, 94.2, Ref.: IMA Commission on Ore Microscopy QDF.</p> <p><b>Additional pattern:</b> See ICSD 64706 (PDF 87-597).</p> <p><b>Data collection flag:</b> Ambient.</p> |  |  |   |  |  |  |
| <p>Swanson, Tatge., Natl. Bur. Stand. (U.S.), Circ. 539, volume 1, page 23 (1953)</p> <p>CAS Number: 7440-22-4</p>   |  |  |   |  |  |  |
| <p><b>Radiation :</b> CuKα1</p> <p><b>Lambda :</b> 1.54056</p> <p><b>SS/FOM :</b> F9= 65(0.0153,9)</p>   |  | <p><b>Filter :</b> Beta</p> <p><b>d-sp :</b> Not given</p>   |   |  |  |  |

# Copper, syn

(2)



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| Pattern : 00-004-0836  |  | Radiation = 1.540560                                     |          | Quality : High |          |          |
|--|--|--|----------|----------------|----------|----------|
| Cu   |  | <i>d</i> (Å)   | <i>i</i> | <i>h</i>       | <i>k</i> | <i>l</i> |
|  |  | 2.08800  | 100      | 1              | 1        | 1        |
|  |  | 1.80800  | 46       | 2              | 0        | 0        |
|  |  | 1.27800  | 20       | 2              | 2        | 0        |
| Copper   |  | 1.09000  | 17       | 3              | 1        | 1        |
| Copper, syn  |  | 1.04360  | 5        | 2              | 2        | 2        |
|  |  | 0.90380  | 3        | 4              | 0        | 0        |
|  |  | 0.82930  | 9        | 3              | 3        | 1        |
|  |  | 0.80830  | 8        | 4              | 2        | 0        |
| <b>Lattice</b> : Face-centered cubic<br><b>S.G.</b> : Fm-3m (225)  |  | <b>Mol. weight</b> = 63.55<br><b>Volume [CD]</b> = 47.24 |          |                |          |          |
| <b>a</b> = 3.61500<br><br><b>Z</b> = 4   |  | <b>Dx</b> = 8.935<br><b>Dm</b> = 8.950                   |          |                |          |          |
| <b>Melting point:</b> 1083°<br><b>Sample preparation:</b> It had been heated in an H <sub>2</sub> atmosphere at 300 C.<br><b>Sample source or locality:</b> Sample from metallurgical laboratory of NBS, Gaithersburg, Maryland, USA.<br><b>General comments:</b> Impurities from 0.001-0.01%, Ag, Al, Bi, Fe, Si, Zn.<br><b>Reflectance:</b> Opaque mineral optical data on specimen from unspecified locality, R <sub>3</sub> R% = 60.65, Disp. = Std.<br><b>Vickers hardness number:</b> VHN <sub>100</sub> = 96-104.<br><b>General comments:</b> Measured density and color from Dana's System of Mineralogy, 7th Ed., 199.<br><b>Color:</b> Red<br><b>Additional pattern:</b> See ICSD 64699 (PDF 85-1326).<br><b>Temperature of data collection:</b> Pattern taken at 26 C.<br><b>Data collection flag:</b> Ambient. |  |  |          |                |          |          |
| Swanson, Tatge., Natl. Bur. Stand. (U.S.), Circ. 539, volume I, page 15 (1953)<br>CAS Number: 7440-50-8  |  |  |          |                |          |          |

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