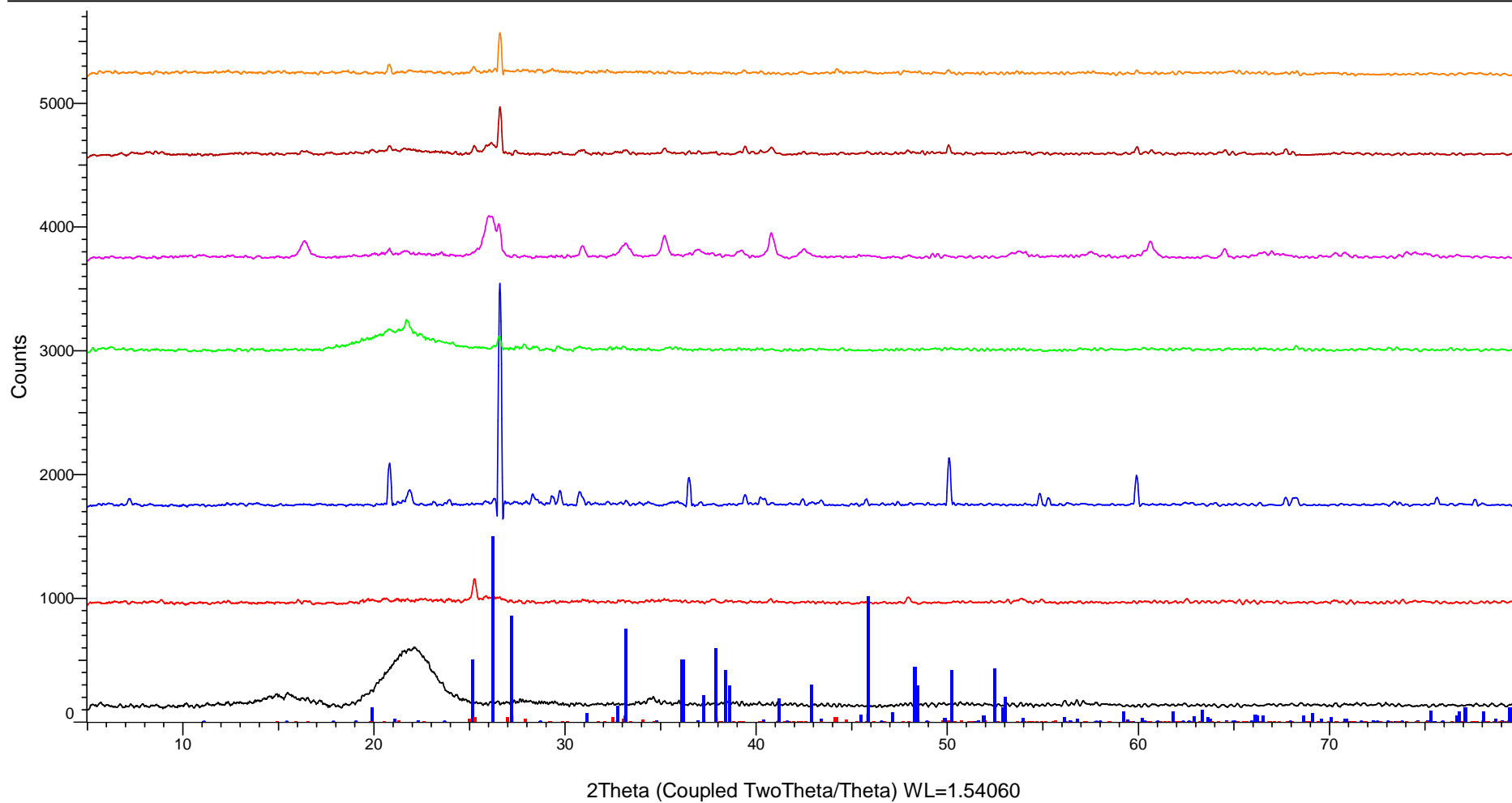


## Raw Rice Husk (Coupled TwoTheta/Theta)



Pattern: PDF 01-080-2147 (Tune Cell)    Radiation: 1.54060    Quality:  
User modified

<b>Formula</b> Si O2			<table><tr><th>d</th><th>2θ</th><th>I fix</th><th>h</th><th>k</th><th>l</th><th>d</th><th>2θ</th><th>I fix</th><th>h</th><th>k</th><th>l</th></tr><tr><td>4.4634<sub>1</sub></td><td>19.876</td><td>233</td><td>1</td><td>0</td><td>0</td><td>1.1384<sub>8</sub></td><td>85.158</td><td>13</td><td>1</td><td>3</td><td>2</td></tr><tr><td>3.5368<sub>2</sub></td><td>25.159</td><td>999</td><td>0</td><td>1</td><td>1</td><td>1.1223<sub>6</sub></td><td>86.679</td><td>13</td><td>0</td><td>1</td><td>5</td></tr><tr><td>2.5769<sub>5</sub></td><td>34.785</td><td>28</td><td>1</td><td>1</td><td>0</td><td>1.1158<sub>5</sub></td><td>87.312</td><td>9</td><td>4</td><td>0</td><td>0</td></tr><tr><td>2.4312<sub>3</sub></td><td>36.943</td><td>25</td><td>1</td><td>0</td><td>2</td><td>1.0994<sub>3</sub></td><td>88.956</td><td>13</td><td>2</td><td>1</td><td>4</td></tr><tr><td>2.3548<sub>4</sub></td><td>38.187</td><td>11</td><td>1</td><td>1</td><td>1</td><td>1.0957<sub>4</sub></td><td>89.335</td><td>4</td><td>0</td><td>4</td><td></td></tr><tr><td>2.2317<sub>0</sub></td><td>40.383</td><td>36</td><td>2</td><td>0</td><td>0</td><td>1.0720<sub>7</sub></td><td>91.864</td><td>10</td><td>2</td><td>2</td><td>3</td></tr><tr><td>2.0827<sub>5</sub></td><td>43.412</td><td>49</td><td>0</td><td>2</td><td>1</td><td>1.0574<sub>8</sub></td><td>93.509</td><td>3</td><td>1</td><td>1</td><td>5</td></tr><tr><td>1.9260<sub>3</sub></td><td>47.149</td><td>151</td><td>1</td><td>1</td><td>2</td><td>1.0424<sub>3</sub></td><td>95.284</td><td>2</td><td>1</td><td>3</td><td>3</td></tr><tr><td>1.7735<sub>7</sub></td><td>51.484</td><td>7</td><td>0</td><td>1</td><td>3</td><td>1.0413<sub>8</sub></td><td>95.411</td><td>2</td><td>0</td><td>4</td><td>2</td></tr><tr><td>1.7684<sub>1</sub></td><td>51.646</td><td>30</td><td>0</td><td>2</td><td>2</td><td>1.0382<sub>4</sub></td><td>95.792</td><td>4</td><td>0</td><td>3</td><td>4</td></tr><tr><td>1.6870<sub>1</sub></td><td>54.337</td><td>4</td><td>2</td><td>1</td><td>0</td><td>1.0290<sub>0</sub></td><td>96.937</td><td>2</td><td>0</td><td>2</td><td>5</td></tr><tr><td>1.6198<sub>4</sub></td><td>56.789</td><td>51</td><td>1</td><td>2</td><td>1</td><td>1.0239<sub>8</sub></td><td>97.574</td><td>4</td><td>3</td><td>2</td><td>0</td></tr><tr><td>1.5461<sub>6</sub></td><td>59.762</td><td>9</td><td>1</td><td>1</td><td>3</td><td>1.0083<sub>7</sub></td><td>99.619</td><td>7</td><td>2</td><td>3</td><td>1</td></tr><tr><td>1.4878<sub>0</sub></td><td>62.362</td><td>11</td><td>3</td><td>0</td><td>0</td><td>0.9740<sub>0</sub></td><td>104.53<sub>3</sub></td><td>2</td><td>4</td><td>1</td><td>0</td></tr><tr><td>1.4609<sub>9</sub></td><td>63.639</td><td>68</td><td>0</td><td>2</td><td>3</td><td>0.9663<sub>5</sub></td><td>105.71<sub>3</sub></td><td>9</td><td>0</td><td>0</td><td>6</td></tr><tr><td>1.4581<sub>0</sub></td><td>63.780</td><td>49</td><td>1</td><td>2</td><td>2</td><td>0.9663<sub>5</sub></td><td>105.71<sub>2</sub></td><td>9</td><td>0</td><td>4</td><td>3</td></tr><tr><td>1.4411<sub>1</sub></td><td>64.622</td><td>20</td><td>0</td><td>3</td><td>1</td><td>0.9655<sub>2</sub></td><td>105.84<sub>3</sub></td><td>9</td><td>3</td><td>2</td><td>2</td></tr><tr><td>1.3786<sub>5</sub></td><td>67.937</td><td>7</td><td>1</td><td>0</td><td>4</td><td>0.9630<sub>2</sub></td><td>106.23<sub>8</sub></td><td>2</td><td>2</td><td>2</td><td>4</td></tr><tr><td>1.3236<sub>7</sub></td><td>71.175</td><td>14</td><td>0</td><td>3</td><td>2</td><td>0.9605<sub>4</sub></td><td>106.63<sub>3</sub></td><td>10</td><td>1</td><td>4</td><td>1</td></tr><tr><td>1.2884<sub>8</sub></td><td>73.430</td><td>13</td><td>2</td><td>2</td><td>0</td><td>0.9556<sub>3</sub></td><td>107.42<sub>7</sub></td><td>7</td><td>1</td><td>2</td><td>5</td></tr><tr><td>1.2709<sub>4</sub></td><td>74.614</td><td>26</td><td>1</td><td>2</td><td>3</td><td>0.9444<sub>7</sub></td><td>109.29<sub>2</sub></td><td>3</td><td>1</td><td>0</td><td>6</td></tr><tr><td>1.2633<sub>7</sub></td><td>75.138</td><td>25</td><td>1</td><td>1</td><td>4</td><td>0.9413<sub>5</sub></td><td>109.82<sub>8</sub></td><td>5</td><td>3</td><td>1</td><td>4</td></tr><tr><td>1.2577<sub>9</sub></td><td>75.530</td><td>5</td><td>2</td><td>2</td><td>1</td><td>0.9232<sub>8</sub></td><td>113.08<sub>8</sub></td><td>5</td><td>1</td><td>4</td><td>2</td></tr><tr><td>1.2379<sub>3</sub></td><td>76.961</td><td>13</td><td>3</td><td>1</td><td>0</td><td>0.9146<sub>2</sub></td><td>114.74<sub>8</sub></td><td>3</td><td>0</td><td>3</td><td>5</td></tr><tr><td>1.2156<sub>1</sub></td><td>78.643</td><td>5</td><td>2</td><td>0</td><td>4</td><td>0.9048<sub>2</sub></td><td>116.71<sub>3</sub></td><td>2</td><td>1</td><td>1</td><td>6</td></tr><tr><td>1.2106<sub>4</sub></td><td>79.029</td><td>28</td><td>1</td><td>3</td><td>1</td><td>0.9048<sub>3</sub></td><td>116.71<sub>2</sub></td><td>2</td><td>2</td><td>3</td><td>3</td></tr><tr><td>1.1789<sub>4</sub></td><td>81.594</td><td>2</td><td>0</td><td>3</td><td>3</td><td>0.8926<sub>8</sub></td><td>119.28<sub>9</sub></td><td>2</td><td>5</td><td>0</td><td>0</td></tr><tr><td>1.1774<sub>2</sub></td><td>81.722</td><td>3</td><td>2</td><td>2</td><td>2</td><td>0.8867<sub>8</sub></td><td>120.60<sub>3</sub></td><td>5</td><td>0</td><td>2</td><td>6</td></tr></table>												d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l	4.4634 <sub>1</sub>	19.876	233	1	0	0	1.1384 <sub>8</sub>	85.158	13	1	3	2	3.5368 <sub>2</sub>	25.159	999	0	1	1	1.1223 <sub>6</sub>	86.679	13	0	1	5	2.5769 <sub>5</sub>	34.785	28	1	1	0	1.1158 <sub>5</sub>	87.312	9	4	0	0	2.4312 <sub>3</sub>	36.943	25	1	0	2	1.0994 <sub>3</sub>	88.956	13	2	1	4	2.3548 <sub>4</sub>	38.187	11	1	1	1	1.0957 <sub>4</sub>	89.335	4	0	4		2.2317 <sub>0</sub>	40.383	36	2	0	0	1.0720 <sub>7</sub>	91.864	10	2	2	3	2.0827 <sub>5</sub>	43.412	49	0	2	1	1.0574 <sub>8</sub>	93.509	3	1	1	5	1.9260 <sub>3</sub>	47.149	151	1	1	2	1.0424 <sub>3</sub>	95.284	2	1	3	3	1.7735 <sub>7</sub>	51.484	7	0	1	3	1.0413 <sub>8</sub>	95.411	2	0	4	2	1.7684 <sub>1</sub>	51.646	30	0	2	2	1.0382 <sub>4</sub>	95.792	4	0	3	4	1.6870 <sub>1</sub>	54.337	4	2	1	0	1.0290 <sub>0</sub>	96.937	2	0	2	5	1.6198 <sub>4</sub>	56.789	51	1	2	1	1.0239 <sub>8</sub>	97.574	4	3	2	0	1.5461 <sub>6</sub>	59.762	9	1	1	3	1.0083 <sub>7</sub>	99.619	7	2	3	1	1.4878 <sub>0</sub>	62.362	11	3	0	0	0.9740 <sub>0</sub>	104.53 <sub>3</sub>	2	4	1	0	1.4609 <sub>9</sub>	63.639	68	0	2	3	0.9663 <sub>5</sub>	105.71 <sub>3</sub>	9	0	0	6	1.4581 <sub>0</sub>	63.780	49	1	2	2	0.9663 <sub>5</sub>	105.71 <sub>2</sub>	9	0	4	3	1.4411 <sub>1</sub>	64.622	20	0	3	1	0.9655 <sub>2</sub>	105.84 <sub>3</sub>	9	3	2	2	1.3786 <sub>5</sub>	67.937	7	1	0	4	0.9630 <sub>2</sub>	106.23 <sub>8</sub>	2	2	2	4	1.3236 <sub>7</sub>	71.175	14	0	3	2	0.9605 <sub>4</sub>	106.63 <sub>3</sub>	10	1	4	1	1.2884 <sub>8</sub>	73.430	13	2	2	0	0.9556 <sub>3</sub>	107.42 <sub>7</sub>	7	1	2	5	1.2709 <sub>4</sub>	74.614	26	1	2	3	0.9444 <sub>7</sub>	109.29 <sub>2</sub>	3	1	0	6	1.2633 <sub>7</sub>	75.138	25	1	1	4	0.9413 <sub>5</sub>	109.82 <sub>8</sub>	5	3	1	4	1.2577 <sub>9</sub>	75.530	5	2	2	1	0.9232 <sub>8</sub>	113.08 <sub>8</sub>	5	1	4	2	1.2379 <sub>3</sub>	76.961	13	3	1	0	0.9146 <sub>2</sub>	114.74 <sub>8</sub>	3	0	3	5	1.2156 <sub>1</sub>	78.643	5	2	0	4	0.9048 <sub>2</sub>	116.71 <sub>3</sub>	2	1	1	6	1.2106 <sub>4</sub>	79.029	28	1	3	1	0.9048 <sub>3</sub>	116.71 <sub>2</sub>	2	2	3	3	1.1789 <sub>4</sub>	81.594	2	0	3	3	0.8926 <sub>8</sub>	119.28 <sub>9</sub>	2	5	0	0	1.1774 <sub>2</sub>	81.722	3	2	2	2	0.8867 <sub>8</sub>	120.60 <sub>3</sub>	5	0	2	6
d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l																																																																																																																																																																																																																																																																																																																																																															
4.4634 <sub>1</sub>	19.876	233	1	0	0	1.1384 <sub>8</sub>	85.158	13	1	3	2																																																																																																																																																																																																																																																																																																																																																															
3.5368 <sub>2</sub>	25.159	999	0	1	1	1.1223 <sub>6</sub>	86.679	13	0	1	5																																																																																																																																																																																																																																																																																																																																																															
2.5769 <sub>5</sub>	34.785	28	1	1	0	1.1158 <sub>5</sub>	87.312	9	4	0	0																																																																																																																																																																																																																																																																																																																																																															
2.4312 <sub>3</sub>	36.943	25	1	0	2	1.0994 <sub>3</sub>	88.956	13	2	1	4																																																																																																																																																																																																																																																																																																																																																															
2.3548 <sub>4</sub>	38.187	11	1	1	1	1.0957 <sub>4</sub>	89.335	4	0	4																																																																																																																																																																																																																																																																																																																																																																
2.2317 <sub>0</sub>	40.383	36	2	0	0	1.0720 <sub>7</sub>	91.864	10	2	2	3																																																																																																																																																																																																																																																																																																																																																															
2.0827 <sub>5</sub>	43.412	49	0	2	1	1.0574 <sub>8</sub>	93.509	3	1	1	5																																																																																																																																																																																																																																																																																																																																																															
1.9260 <sub>3</sub>	47.149	151	1	1	2	1.0424 <sub>3</sub>	95.284	2	1	3	3																																																																																																																																																																																																																																																																																																																																																															
1.7735 <sub>7</sub>	51.484	7	0	1	3	1.0413 <sub>8</sub>	95.411	2	0	4	2																																																																																																																																																																																																																																																																																																																																																															
1.7684 <sub>1</sub>	51.646	30	0	2	2	1.0382 <sub>4</sub>	95.792	4	0	3	4																																																																																																																																																																																																																																																																																																																																																															
1.6870 <sub>1</sub>	54.337	4	2	1	0	1.0290 <sub>0</sub>	96.937	2	0	2	5																																																																																																																																																																																																																																																																																																																																																															
1.6198 <sub>4</sub>	56.789	51	1	2	1	1.0239 <sub>8</sub>	97.574	4	3	2	0																																																																																																																																																																																																																																																																																																																																																															
1.5461 <sub>6</sub>	59.762	9	1	1	3	1.0083 <sub>7</sub>	99.619	7	2	3	1																																																																																																																																																																																																																																																																																																																																																															
1.4878 <sub>0</sub>	62.362	11	3	0	0	0.9740 <sub>0</sub>	104.53 <sub>3</sub>	2	4	1	0																																																																																																																																																																																																																																																																																																																																																															
1.4609 <sub>9</sub>	63.639	68	0	2	3	0.9663 <sub>5</sub>	105.71 <sub>3</sub>	9	0	0	6																																																																																																																																																																																																																																																																																																																																																															
1.4581 <sub>0</sub>	63.780	49	1	2	2	0.9663 <sub>5</sub>	105.71 <sub>2</sub>	9	0	4	3																																																																																																																																																																																																																																																																																																																																																															
1.4411 <sub>1</sub>	64.622	20	0	3	1	0.9655 <sub>2</sub>	105.84 <sub>3</sub>	9	3	2	2																																																																																																																																																																																																																																																																																																																																																															
1.3786 <sub>5</sub>	67.937	7	1	0	4	0.9630 <sub>2</sub>	106.23 <sub>8</sub>	2	2	2	4																																																																																																																																																																																																																																																																																																																																																															
1.3236 <sub>7</sub>	71.175	14	0	3	2	0.9605 <sub>4</sub>	106.63 <sub>3</sub>	10	1	4	1																																																																																																																																																																																																																																																																																																																																																															
1.2884 <sub>8</sub>	73.430	13	2	2	0	0.9556 <sub>3</sub>	107.42 <sub>7</sub>	7	1	2	5																																																																																																																																																																																																																																																																																																																																																															
1.2709 <sub>4</sub>	74.614	26	1	2	3	0.9444 <sub>7</sub>	109.29 <sub>2</sub>	3	1	0	6																																																																																																																																																																																																																																																																																																																																																															
1.2633 <sub>7</sub>	75.138	25	1	1	4	0.9413 <sub>5</sub>	109.82 <sub>8</sub>	5	3	1	4																																																																																																																																																																																																																																																																																																																																																															
1.2577 <sub>9</sub>	75.530	5	2	2	1	0.9232 <sub>8</sub>	113.08 <sub>8</sub>	5	1	4	2																																																																																																																																																																																																																																																																																																																																																															
1.2379 <sub>3</sub>	76.961	13	3	1	0	0.9146 <sub>2</sub>	114.74 <sub>8</sub>	3	0	3	5																																																																																																																																																																																																																																																																																																																																																															
1.2156 <sub>1</sub>	78.643	5	2	0	4	0.9048 <sub>2</sub>	116.71 <sub>3</sub>	2	1	1	6																																																																																																																																																																																																																																																																																																																																																															
1.2106 <sub>4</sub>	79.029	28	1	3	1	0.9048 <sub>3</sub>	116.71 <sub>2</sub>	2	2	3	3																																																																																																																																																																																																																																																																																																																																																															
1.1789 <sub>4</sub>	81.594	2	0	3	3	0.8926 <sub>8</sub>	119.28 <sub>9</sub>	2	5	0	0																																																																																																																																																																																																																																																																																																																																																															
1.1774 <sub>2</sub>	81.722	3	2	2	2	0.8867 <sub>8</sub>	120.60 <sub>3</sub>	5	0	2	6																																																																																																																																																																																																																																																																																																																																																															
<b>Lattice:</b> Hexagonal			<b>Mol. weight =</b> 60.08																																																																																																																																																																																																																																																																																																																																																																							
<b>S.G.:</b> P3221 (154)			<b>Volume [CD] =</b> 133.38																																																																																																																																																																																																																																																																																																																																																																							
			<b>Dx =</b> 2.24																																																																																																																																																																																																																																																																																																																																																																							
			<b>Dm =</b>																																																																																																																																																																																																																																																																																																																																																																							
			<b>I/Icor =</b> 2.880																																																																																																																																																																																																																																																																																																																																																																							
<b>a =</b> 5.15390		<b>alpha =</b> <b>beta =</b> <b>gamma</b> <b>=</b> <b>Z =</b> 3																																																																																																																																																																																																																																																																																																																																																																								
<b>b =</b>																																																																																																																																																																																																																																																																																																																																																																										
<b>c =</b> 5.79810																																																																																																																																																																																																																																																																																																																																																																										
<b>a/b</b> = 1.00000																																																																																																																																																																																																																																																																																																																																																																										
<b>c/b</b> = 1.12499																																																																																																																																																																																																																																																																																																																																																																										
<b>ANX:</b> AX2																																																																																																																																																																																																																																																																																																																																																																										
<b>Analysis:</b> O2 Si1																																																																																																																																																																																																																																																																																																																																																																										
Formula from original source: Si O2																																																																																																																																																																																																																																																																																																																																																																										
ICSD Collection Code: 70006																																																																																																																																																																																																																																																																																																																																																																										
Hypothetical Structure: Structure calculated theoretically																																																																																																																																																																																																																																																																																																																																																																										
Calculated Pattern Original Remarks: Stable up to 846 K, above P6222, above 1143 K tridymite is stable																																																																																																																																																																																																																																																																																																																																																																										
Minor Warning: No e.s.d reported/abstracted on the cell dimension																																																																																																																																																																																																																																																																																																																																																																										
Wyckoff Sequence: c a(P3221)																																																																																																																																																																																																																																																																																																																																																																										
Unit Cell Data Source: Single Crystal																																																																																																																																																																																																																																																																																																																																																																										
<b>Structure</b>																																																																																																																																																																																																																																																																																																																																																																										
Publication: Phys. Rev. B: Condens. Matter. Mater. Phys.																																																																																																																																																																																																																																																																																																																																																																										
Detail: volume 44, page 489 (1991)																																																																																																																																																																																																																																																																																																																																																																										
Authors: Chelikowsky, J.R., Troullier, N., Martins, J.L., King, Jr., H.E.																																																																																																																																																																																																																																																																																																																																																																										
Primary Reference																																																																																																																																																																																																																																																																																																																																																																										
Publication: Calculated from ICSD using POWD-12++																																																																																																																																																																																																																																																																																																																																																																										
<b>Radiation:</b> CuKα1			<b>Filter:</b> Not specified																																																																																																																																																																																																																																																																																																																																																																							
<b>Wavelength:</b> 1.54060			<b>d-spacing:</b>																																																																																																																																																																																																																																																																																																																																																																							
<b>SS/FOM:</b> 999.9 (0,31)																																																																																																																																																																																																																																																																																																																																																																										

d	2θ	l fix	h	k	l
0.8842 1	121.19 2	2	0	4	4
0.8822 9	121.63 5	3	0	5	1
0.8697 9	124.65 5	4	1	4	3
0.8619 4	126.67 9	3	2	2	5
0.8589 8	127.47 0	2	3	3	0
0.8531 5	129.08 1	5	0	5	2
0.8497 1	130.06 4	4	3	3	1
0.8463 1	131.06 4	7	3	1	5
0.8435 0	131.90 7	5	4	2	0
0.8385 2	133.45 5	2	1	2	6
0.8363 4	134.15 5	9	2	3	4
0.8347 2	134.68 6	2	2	4	1
0.8235 9	138.55 1	2	3	3	2
0.8144 0	142.11 9	4	0	1	7
0.8104 1	143.79 7	5	0	3	6
0.8104 1	143.79 6	5	5	0	3
0.8099 2	144.01 0	4	2	4	2
0.8084 4	144.66 1	5	1	4	4
0.8040 5	146.67 9	2	0	4	5
0.8016 5	147.84 6	3	5	1	0

Pattern: PDF 01-070-9854 (Tune Cell)    Radiation: 1.54060    Quality:  
User modified

<b>Formula</b> Ca ( C O3 )														
<b>Name</b> Calcium Carbonate														
<b>Name (mineral)</b> Aragonite														
<b>Name (common)</b>														
<b>Lattice:</b> Triclinic			<b>Mol. weight</b> = 100.09 <b>Volume [CD]</b> = 226.96 <b>Dx</b> = 2.93 <b>Dm</b> = <b>I/Icor</b> = 0.330											
<b>S.G.:</b> P-1 (2)														
<b>a</b> = 5.73940	<b>alpha</b> = 89.999													
<b>b</b> = 4.96160	<b>beta</b> = 90.012													
<b>c</b> = 7.97000	<b>gamma</b> = 89.996													
<b>a/b</b> = 1.15676		<b>Z</b> = 4												
<b>c/b</b> = 1.60634														
<b>ANX:</b> ABX3														
<b>Analysis:</b> C1 Ca1 O3														
<b>Formula from original source:</b> Ca (C O3)														
<b>ICSD Collection Code:</b> 280991														
<b>Note:</b> Structure determined on a twinned crystal														
<b>Sample Source or Locality:</b> Specimen from British Museum, UK														
<b>Wyckoff Sequence:</b> i10(P1-)														
<b>Unit Cell Data Source:</b> Single Crystal														
<b>Structure</b>														
<b>Publication:</b> Acta Crystallogr., Sec. B: Struct. Sci.														
<b>Detail:</b> volume 58, page 448 (2002)														
<b>Authors:</b> Bevan, D.J.M., Rossmanith, E., Mylrea, D.K., Ness, S.E., Taylor, M.R., Cuff, C.														
<b>Primary Reference</b>														
<b>Publication:</b> Calculated from ICSD using POWD-12++														
<b>Radiation:</b> CuKα1			<b>Filter:</b> Not specified <b>d-spacing:</b>											
<b>Wavelength:</b> 1.54060														
<b>SS/FOM:</b> 148.1 (0.0023,88)														

d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l
7.97000	11.093	2	0	0	1	2.34204	38.404	278	0	-1	3
5.73940	15.426	2	1	0	0	2.32895	38.629	194	-2	0	2
4.96160	17.863	2	0	1	0	2.32849	38.637	194	2	0	2
4.65698	19.042	3	1	0	1	2.18957	41.195	128	1	2	1
4.65791	19.038	3	-1	0	1	2.18945	41.198	128	1	-2	
4.21206	21.075	18	0	-1	1	2.16829	41.618	6	1	-1	3
4.21212	21.075	18	0	1	1	2.16836	41.617	6	1	1	3
3.98500	22.291	9	0	0	2	2.10603	42.909	200	0	-2	2
3.75361	23.684	2	1	1	0	2.10606	42.908	200	0	2	2
3.75336	23.686	2	-1	1	0	1.99250	45.486	40	0	0	4
3.39585	26.222	1000	-1	1	1	1.97702	45.863	676	1	-2	2
3.39568	26.223	1000	1	1	1	1.97712	45.860	676	1	2	2
3.27367	27.219	572	-1	0	2	1.94972	46.542	6	-2	0	3
3.27302	27.224	572	1	0	2	1.94931	46.553	6	2	0	3
3.10698	28.710	2	0	1	2	1.88242	48.310	298	-1	0	4
3.10693	28.710	2	0	-1	2	1.88218	48.317	298	1	0	4
2.86970	31.141	48	2	0	0	1.87668	48.467	194	-2	2	0
2.73204	32.753	86	1	-1	2	1.87681	48.464	194	2	2	0
2.73218	32.752	86	1	1	2	1.86038	48.920	5	-3	0	1
2.69983	33.155	502	2	0	1	1.86020	48.925	5	3	0	1
2.70019	33.151	502	-2	0	1	1.82678	49.880	22	-2	2	1
2.48080	36.179	338	0	2	0	1.82666	49.884	22	2	-2	1
2.48405	36.130	338	-2	1	0	1.81435	50.246	278	2	1	3
2.41110	37.263	144	-1	0	3	1.81427	50.248	278	2	-1	3
2.41072	37.269	144	1	0	3	1.75978	51.918	33	1	-1	4
2.37154	37.908	397	2	1	1	1.75983	51.916	33	1	1	4
2.37140	37.910	397	2	-1	1	1.74176	52.495	289	3	-1	1
2.34208	38.404	278	0	1	3	1.74191	52.491	289	-3	1	1

d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l
1.7288 <sub>4</sub>	52.918	77	1	-2	3	1.4883 <sub>3</sub>	62.338	2	3	2	1	1.3283 <sub>3</sub>	70.887	19	0	0	6	1.1936 <sub>2</sub>	80.383	4	3	-3	2
1.7289 <sub>2</sub>	52.916	77	1	2	3	1.4815 <sub>4</sub>	62.655	2	3	1	3	1.3293 <sub>8</sub>	70.823	19	3	-1	4	1.1888 <sub>5</sub>	80.772	53	3	1	5
1.7248 <sub>2</sub>	53.051	133	-3	0	2	1.4817 <sub>6</sub>	62.645	2	-3	1	3	1.3161 <sub>0</sub>	71.647	2	-3	2	3	1.1888 <sub>2</sub>	80.775	53	3	-1	5
1.7245 <sub>4</sub>	53.061	133	3	0	2	1.4760 <sub>9</sub>	62.913	30	1	-3	2	1.3159 <sub>0</sub>	71.660	2	3	-2	3	1.1858 <sub>9</sub>	81.016	6	-4	-2	2
1.6977 <sub>3</sub>	53.966	23	2	-2	2	1.4761 <sub>5</sub>	62.910	30	1	3	2	1.3058 <sub>3</sub>	72.299	8	1	2	5	1.1857 <sub>0</sub>	81.032	6	4	-2	2
1.6979 <sub>2</sub>	53.959	23	-2	2	2	1.4670 <sub>9</sub>	63.343	65	1	-1	5	1.3057 <sub>9</sub>	72.301	8	1	-2	5	1.1710 <sub>4</sub>	82.263	86	0	2	6
1.6365 <sub>1</sub>	56.159	26	2	0	4	1.4672 <sub>5</sub>	63.336	65	-1	-1	5	1.3025 <sub>9</sub>	72.507	5	4	1	2	1.1710 <sub>2</sub>	82.265	86	0	-2	6
1.6368 <sub>3</sub>	56.147	26	-2	0	4	1.4348 <sub>5</sub>	64.939	4	4	0	0	1.3025 <sub>4</sub>	72.510	5	4	-1	2	1.1632 <sub>4</sub>	82.936	7	2	-3	4
1.6289 <sub>1</sub>	56.444	10	3	-1	2	1.4328 <sub>9</sub>	65.039	6	-2	3	0	1.2941 <sub>9</sub>	73.054	2	-1	0	6	1.1642 <sub>5</sub>	82.849	7	4	0	4
1.6289 <sub>8</sub>	56.442	10	3	1	2	1.4329 <sub>7</sub>	65.035	6	2	3	0	1.2940 <sub>7</sub>	73.062	2	1	0	6	1.1598 <sub>8</sub>	83.230	29	1	-4	2
1.6193 <sub>6</sub>	56.807	18	0	-3	1	1.4159 <sub>7</sub>	65.914	5	3	-2	2	1.2831 <sub>4</sub>	73.786	2	0	-1	6	1.1599 <sub>2</sub>	83.226	29	1	4	2
1.6193 <sub>7</sub>	56.807	18	0	3	1	1.4160 <sub>6</sub>	65.909	5	3	2	2	1.2831 <sub>5</sub>	73.786	2	0	1	6	1.1474 <sub>3</sub>	84.339	2	-1	2	6
1.5940 <sub>0</sub>	57.796	2	0	0	5	1.4121 <sub>0</sub>	66.118	39	4	0	1	1.2611 <sub>6</sub>	75.293	62	2	3	3	1.1473 <sub>3</sub>	84.348	2	1	-2	6
1.5891 <sub>7</sub>	57.988	2	-1	3	0	1.4122 <sub>0</sub>	66.112	39	-4	0	1	1.2610 <sub>8</sub>	75.298	62	2	-3	3	1.1385 <sub>6</sub>	85.150	8	-2	4	0
1.5892 <sub>3</sub>	57.986	2	1	3	0	1.4102 <sub>5</sub>	66.216	33	2	-3	1	1.2521 <sub>9</sub>	75.928	2	1	1	6	1.1385 <sub>7</sub>	85.149	8	0	0	7
1.5584 <sub>7</sub>	59.243	59	1	-3	1	1.4103 <sub>0</sub>	66.213	33	-2	3	1	1.2521 <sub>7</sub>	75.929	2	1	-1	6	1.1361 <sub>9</sub>	85.370	3	-5	0	1
1.5585 <sub>6</sub>	59.239	59	-1	-3	1	1.4040 <sub>2</sub>	66.547	34	0	-3	3	1.2420 <sub>2</sub>	76.661	33	-4	2	0	1.1361 <sub>2</sub>	85.376	3	5	0	1
1.5534 <sub>6</sub>	59.453	12	0	-2	4	1.4040 <sub>4</sub>	66.546	34	0	3	3	1.2421 <sub>0</sub>	76.656	33	4	2	0	1.1334 <sub>8</sub>	85.623	3	4	1	4
1.5534 <sub>9</sub>	59.452	12	0	2	4	1.3783 <sub>4</sub>	67.954	3	-4	1	0	1.2404 <sub>0</sub>	76.780	56	0	4	0	1.1334 <sub>4</sub>	85.627	3	4	-1	4
1.5357 <sub>8</sub>	60.208	21	1	0	5	1.3784 <sub>0</sub>	67.951	3	4	1	0	1.2359 <sub>5</sub>	77.107	81	3	-3	1	1.1318 <sub>2</sub>	85.779	5	3	-3	3
1.5359 <sub>5</sub>	60.200	21	-1	0	5	1.3660 <sub>2</sub>	68.652	32	2	-2	4	1.2360 <sub>4</sub>	77.100	81	3	3	1	1.1318 <sub>9</sub>	85.772	5	3	3	3
1.5327 <sub>0</sub>	60.341	5	2	-2	3	1.3660 <sub>9</sub>	68.648	32	2	2	4	1.2233 <sub>7</sub>	78.049	59	4	-1	3	1.1271 <sub>0</sub>	86.225	16	2	-4	1
1.5327 <sub>9</sub>	60.337	5	2	2	3	1.3581 <sub>4</sub>	69.107	47	4	-1	1	1.2234 <sub>2</sub>	78.046	59	4	1	3	1.1271 <sub>3</sub>	86.222	16	-2	4	1
1.5176 <sub>0</sub>	61.005	2	0	-1	5	1.3581 <sub>9</sub>	69.104	47	4	1	1	1.2148 <sub>2</sub>	78.705	16	2	-2	5	1.1254 <sub>6</sub>	86.382	36	-1	3	5
1.5176 <sub>1</sub>	61.005	2	0	1	5	1.3501 <sub>0</sub>	69.577	19	-4	0	2	1.2150 <sub>0</sub>	78.691	16	-2	2	5	1.1253 <sub>8</sub>	86.390	36	1	-3	5
1.4994 <sub>3</sub>	61.825	57	1	-2	4	1.3499 <sub>2</sub>	69.588	19	4	0	2	1.2058 <sub>4</sub>	79.406	81	3	-2	4	1.1168 <sub>5</sub>	87.214	2	-1	0	7
1.4994 <sub>9</sub>	61.822	57	1	2	4	1.3416 <sub>8</sub>	70.078	26	-2	-1	5	1.2053 <sub>6</sub>	79.444	81	2	0	6	1.1167 <sub>6</sub>	87.222	2	1	0	7
1.4882 <sub>2</sub>	62.342	2	3	-2	1	1.3414 <sub>3</sub>	70.092	26	2	-1	5	1.1937 <sub>0</sub>	80.377	4	3	3	2	1.1097 <sub>3</sub>	87.916	5	0	1	7

d	2θ	l fix	h	k	l	d	2θ	l fix	h	k	l
1.1097 <sub>2</sub>	87.917	5	0	-1	7	1.0425 <sub>0</sub>	95.275	12	4	-1	5
1.1075 <sub>4</sub>	88.135	23	-5	-1	1	1.0356 <sub>9</sub>	96.104	39	1	-4	4
1.1074 <sub>4</sub>	88.145	23	5	-1	1	1.0349 <sub>5</sub>	96.195	39	2	-1	7
1.1029 <sub>4</sub>	88.598	14	1	-4	3						
1.1029 <sub>7</sub>	88.596	14	5	0	2						
1.0980 <sub>6</sub>	89.097	2	3	2	5						
1.0980 <sub>1</sub>	89.102	2	3	-2	5						
1.0947 <sub>3</sub>	89.441	15	2	-4	2						
1.0948 <sub>2</sub>	89.430	15	-2	-4	2						
1.0895 <sub>0</sub>	89.986	13	1	-1	7						
1.0895 <sub>9</sub>	89.977	13	-1	1	7						
1.0843 <sub>0</sub>	90.537	13	-2	2	6						
1.0841 <sub>4</sub>	90.554	13	2	-2	6						
1.0766 <sub>7</sub>	91.360	2	5	-1	2						
1.0767 <sub>0</sub>	91.356	2	5	1	2						
1.0738 <sub>7</sub>	91.666	10	4	-3	1						
1.0739 <sub>2</sub>	91.661	10	-4	3	1						
1.0656 <sub>9</sub>	92.575	14	-2	3	5						
1.0655 <sub>6</sub>	92.590	14	2	-3	5						
1.0595 <sub>5</sub>	93.272	2	3	3	4						
1.0594 <sub>8</sub>	93.280	2	3	-3	4						
1.0582 <sub>4</sub>	93.422	3	2	0	7						
1.0583 <sub>9</sub>	93.405	3	-2	0	7						
1.0530 <sub>1</sub>	94.028	14	0	-4	4						
1.0539 <sub>3</sub>	93.922	14	4	-2	4						
1.0465 <sub>7</sub>	94.787	2	-2	-4	3						
1.0464 <sub>7</sub>	94.800	2	2	-4	3						
1.0427 <sub>3</sub>	95.247	12	-4	-1	5						