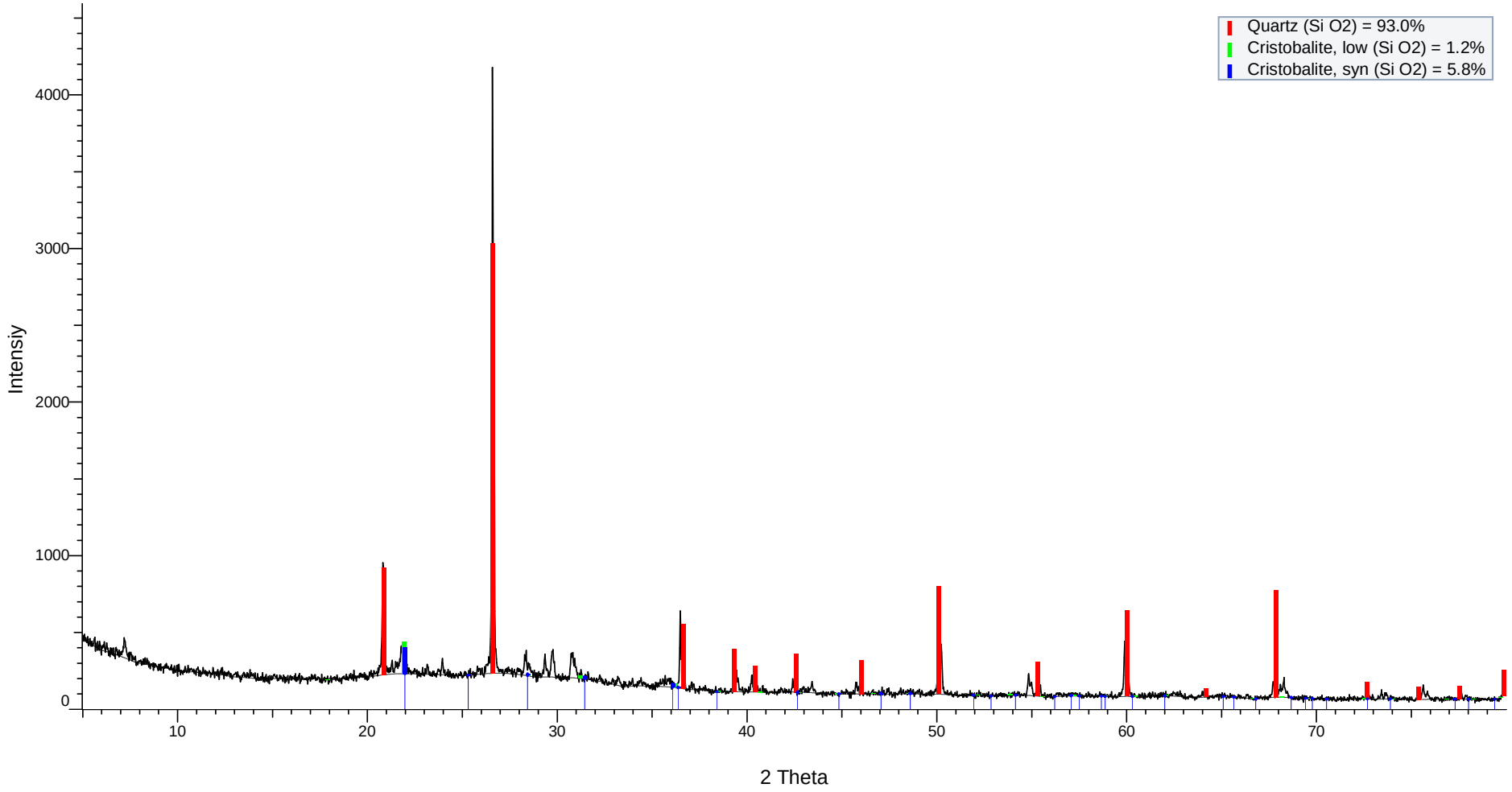
POFA (Coupled TwoTheta/Theta)



Pattern: PDF 00-001-0649 Radiation: 1.54060 Quality: Blank

Formula	Si O2
Name	Silicon Oxide
Name (mineral)	Quartz
Name (common)	

Lattice:	Hexagonal
S.G.:	P3221 (154)

Mol. weight =	60.08
Volume [CD] =	112.28
Dx =	
Dm =	2.649
I/Icor =	-1.000

a =	4.90300	alpha =	
b =		beta =	
c =	5.39300	gamma =	
a/b =	1.00000	Z =	3
c/b =	1.09994		

Color: Colorless
Deleted Or Rejected By: Deleted by NBS 00-005-0490
Warning: Lines with abs(delta 2Theta)>0.2 DEG

Primary Reference
Publication: Anal. Chem.
Detail: volume 10, page 475 (1938)
Authors: Hanawalt, J., et al.

Radiation:	MoKα1	Filter:	F
Wavelength:	1.54060	d-spacing:	
SS/FOM:	6.4 (0.098,35)		

d	2θ	I fix	h	k	l
4.25000	20.885	26	1	0	0
3.35000	26.587	101	1	0	1
2.45000	36.650	16	1	1	0
2.29000	39.312	11	1	0	2
2.23000	40.416	7	1	1	1
2.12000	42.612	10	2	0	0
1.97000	46.035	9	2	0	1
1.82000	50.079	26	1	1	2
1.66000	55.296	9	1	0	3
1.54000	60.026	21	2	1	1
1.45000	64.179	3	1	1	3
1.38000	67.861	26	2	1	2
1.30000	72.675	5	1	0	4
1.26000	75.374	4	3	0	2
1.23000	77.549	4	2	2	0
1.20000	79.870	7	2	1	3
1.18000	81.506	9	1	1	4
1.16000	83.219	2	3	1	1
1.08000	90.998	5	3	1	2
1.05000	94.381	3	1	0	5
1.04000	95.578	2	4	0	1
1.02000	98.085	2	2	2	3

Pattern: PDF 01-071-3839 Radiation: 1.54060 Quality: Indexed

Formula	Si O2
Name	Silicon Oxide
Name (mineral)	Cristobalite, low
Name (common)	

Lattice:	Orthorhombic	Mol. weight =	60.08
S.G.:	P212121 (19)	Volume [CD] =	344.47
		Dx =	2.32
		Dm =	
		I/Icor =	5.650

a =	7.01000	alpha =	
b =	7.01000	beta =	
c =	7.01000	gamma =	
a/b =	1.00000	Z =	8
c/b =	1.00000		

ANX: AX2
Analysis: O2 Si1
Formula from original source: Si O2
ICSD Collection Code: 52371
Minor Warning: No R factors reported/abstracted. Magnitude of e.s.d. on cell dimension is >1000 ppm
Wyckoff Sequence: a6(P212121)
Unit Cell Data Source: Single Crystal

Structure
Publication: Amer. J. Sci.
Detail: volume 24, page 97 (1932)
Authors: Barth, T.F.W.
Primary Reference
Publication: Calculated from ICSD using POWD-12++

Radiation:	CuKα1	Filter:	Not specified
Wavelength:	1.54060	d-spacing:	
SS/FOM:	999.9 (0,30)		

d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l
4.95682	17.880	24	0	1	1	1.60820	57.238	36	1	3	3
4.95682	17.880	24	1	0	1	1.56748	58.869	22	0	4	2
4.04723	21.944	999	1	1	1	1.56748	58.869	22	4	0	2
3.50500	25.391	6	2	0	0	1.52971	60.472	31	4	2	1
3.50500	25.391	6	0	0	2	1.52971	60.472	31	2	4	1
3.13497	28.448	61	2	0	1	1.49454	62.050	33	2	3	3
3.13497	28.448	61	0	2	1	1.49454	62.050	33	3	3	2
2.86182	31.229	71	1	1	2	1.43091	65.140	7	2	2	4
2.86182	31.229	71	1	2	1	1.43091	65.140	7	2	4	2
2.47841	36.215	138	0	2	2	1.40200	66.656	10	0	4	3
2.47841	36.215	138	2	0	2	1.40200	66.656	10	4	0	3
2.33667	38.496	21	2	1	2	1.37477	68.155	42	1	3	4
2.33667	38.496	21	1	2	2	1.37477	68.155	42	3	1	4
2.21676	40.668	25	1	3	0	1.34908	69.637	15	1	5	1
2.21676	40.668	25	3	1	0	1.34908	69.637	15	5	1	1
2.11359	42.748	13	3	1	1	1.30172	72.563	22	2	4	3
2.11359	42.748	13	1	1	3	1.30172	72.563	22	4	2	3
2.02361	44.749	38	2	2	2	1.27985	74.008	11	1	5	2
1.94422	46.682	17	3	2	0	1.27985	74.008	11	5	1	2
1.94422	46.682	17	0	3	2	1.23920	76.868	7	4	0	4
1.87350	48.555	25	1	3	2	1.23920	76.868	7	0	4	4
1.87350	48.555	25	3	1	2	1.22028	78.285	20	4	4	1
1.75250	52.150	2	4	0	0	1.22028	78.285	20	2	2	5
1.75250	52.150	2	0	0	4	1.20221	79.694	17	5	3	0
1.70017	53.882	51	2	2	3	1.20221	79.694	17	3	5	0
1.70017	53.882	51	3	2	2	1.18491	81.097	17	5	1	3
1.65227	55.577	10	0	3	3	1.18491	81.097	17	1	3	5
1.65227	55.577	10	1	4	1	1.16833	82.496	11	0	6	0
1.60820	57.238	36	3	1	3	1.16833	82.496	11	4	2	4

d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l
1.15244	83.889	2	6	1	0	0.95394	107.703	8	3	3	6	0.82614	137.628	3	6	6	0
1.15244	83.889	2	0	1	6	0.95394	107.703	8	5	5	2	0.82046	139.724	2	8	0	3
1.13717	85.279	8	1	1	6	0.93675	110.633	5	4	6	2	0.82046	139.724	2	3	8	0
1.13717	85.279	8	3	5	2	0.93675	110.633	5	6	4	2	0.81490	141.914	8	3	1	8
1.10838	88.051	5	2	0	6	0.92850	112.120	3	4	4	5	0.81490	141.914	8	3	7	4
1.10838	88.051	5	0	2	6	0.92850	112.120	3	2	2	7	0.80945	144.217	7	5	5	5
1.09478	89.435	13	6	2	1	0.92046	113.621	3	7	3	0	0.80945	144.217	7	7	1	5
1.09478	89.435	13	0	4	5	0.92046	113.621	3	0	3	7	0.80410	146.656	5	6	2	6
1.08167	90.819	2	1	5	4	0.91262	115.141	9	1	7	3	0.80410	146.656	5	2	6	6
1.08167	90.819	2	1	4	5	0.91262	115.141	9	7	1	3	0.79886	149.264	5	8	2	3
1.06902	92.203	3	3	5	3	0.89754	118.238	3	4	6	3	0.79886	149.264	5	2	8	3
1.06902	92.203	3	3	3	5	0.89754	118.238	3	6	4	3						
1.05680	93.588	9	2	6	2	0.89027	119.821	5	1	5	6						
1.05680	93.588	9	6	2	2	0.89027	119.821	5	5	1	6						
1.04499	94.976	7	2	4	5	0.87625	123.065	3	0	0	8						
1.04499	94.976	7	4	2	5	0.87625	123.065	3	0	8	0						
1.03357	96.366	4	3	1	6	0.86948	124.732	3	4	0	7						
1.03357	96.366	4	1	3	6	0.86948	124.732	3	2	6	5						
1.01181	99.159	2	4	4	4	0.86287	126.433	2	1	8	1						
1.00143	100.564	2	6	2	3	0.86287	126.433	2	4	7	1						
1.00143	100.564	2	2	6	3	0.85641	128.173	3	3	7	3						
0.99136	101.975	5	3	5	4	0.85641	128.173	3	7	3	3						
0.99136	101.975	5	5	3	4	0.85009	129.955	5	8	0	2						
0.98160	103.394	13	1	1	7	0.85009	129.955	5	0	8	2						
0.98160	103.394	13	5	1	5	0.84390	131.785	6	8	2	1						
0.97211	104.820	9	6	0	4	0.84390	131.785	6	4	2	7						
0.97211	104.820	9	0	4	6	0.83785	133.669	3	3	6	5						
0.96290	106.257	6	2	0	7	0.83785	133.669	3	5	3	6						
0.96290	106.257	6	6	4	1	0.82614	137.628	3	2	2	8						

Pattern: PDF 00-039-1425 Radiation: 1.54060 Quality: Star (*)

Formula	Si O2
Name	Silicon Oxide
Name (mineral)	Cristobalite, syn
Name (common)	

Lattice:	Tetragonal	Mol. weight =	60.08
S.G.:	P41212 (92)	Volume [CD] =	171.24
		Dx =	
		Dm =	
		I/Icor =	-1.000

a =	4.97320	alpha =	
b =		beta =	
c =	6.92360	gamma =	
a/b =	1.00000	Z =	4
c/b =	1.39218		

Additional Patterns: See PDF 01-082-1404, 01-082-1410, 01-075-0923, 01-076-0935, 01-076-0936, 01-076-0937, 01-077-1315, 01-077-1316 and 01-077-1317. To replace 00-011-0695 and validated by calculated pattern
Color: Colorless
Polymorphism/Phase Transition: There are a number of other forms of "Si O2"
Sample Preparation: 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
Structures: The structure was determined by Peacor (1)
Temperature of Data Collection: Pattern taken ~298 K
Unit Cell Data Source: Powder Diffraction

Structure
Publication: Z. Kristallogr., Kristallgeom., Kristallphys., Kristallchem.
Detail: volume 138, page 274 (1973)
Authors: 1. Peacor, D.
Primary Reference
Publication: ICDD Grant-in-Aid
Authors: Wong-Ng, W., McMurdie, H., Paretzkin, B., Hubbard, C., Dragoo, A., NBS, Gaithersburg, MD, USA.

Radiation:	CuKα1	Filter:	M
Wavelength:	1.54060	d-spacing:	
SS/FOM:	83.3 (0.01,36)		

d	2θ	I fix	h	k	l
4.03974	21.985	101	1	0	1
3.51470	25.320	2	1	1	0
3.13592	28.439	9	1	1	1
2.84116	31.462	10	1	0	2
2.48740	36.080	13	2	0	0
2.46750	36.381	5	1	1	2
2.34170	38.410	2	2	0	1
2.11791	42.656	3	2	1	1
2.01957	44.843	3	2	0	2
1.92935	47.063	5	1	1	3
1.87147	48.611	5	2	1	2
1.75907	51.940	2	2	2	0
1.73033	52.869	2	0	0	4
1.69221	54.156	3	2	0	3
1.63488	56.220	2	1	0	4
1.61217	57.084	4	3	0	1
1.60131	57.507	2	2	1	3
1.57207	58.680	2	3	1	0
1.56745	58.870	2	2	2	2
1.53356	60.304	3	3	1	1
1.49520	62.019	3	3	0	2
1.43165	65.102	3	3	1	2
1.42102	65.650	2	2	0	4
1.39908	66.813	2	2	2	3
1.36560	68.676	3	2	1	4
1.35277	69.420	2	3	2	1
1.34650	69.790	2	3	0	3
1.33398	70.542	2	1	0	5
1.29976	72.690	2	3	1	3
1.28133	73.908	2	3	2	2
1.23318	77.312	2	2	2	4
1.22375	78.020	2	4	0	1
1.20599	79.394	2	4	1	0
1.18427	81.150	2	3	2	3
1.17576	81.862	2	2	1	5
1.16384	82.884	2	3	1	4
1.15546	83.620	2	3	3	1
1.11050	87.840	2	3	3	2
1.09783	89.120	2	4	2	1
1.09628	89.280	2	1	1	6