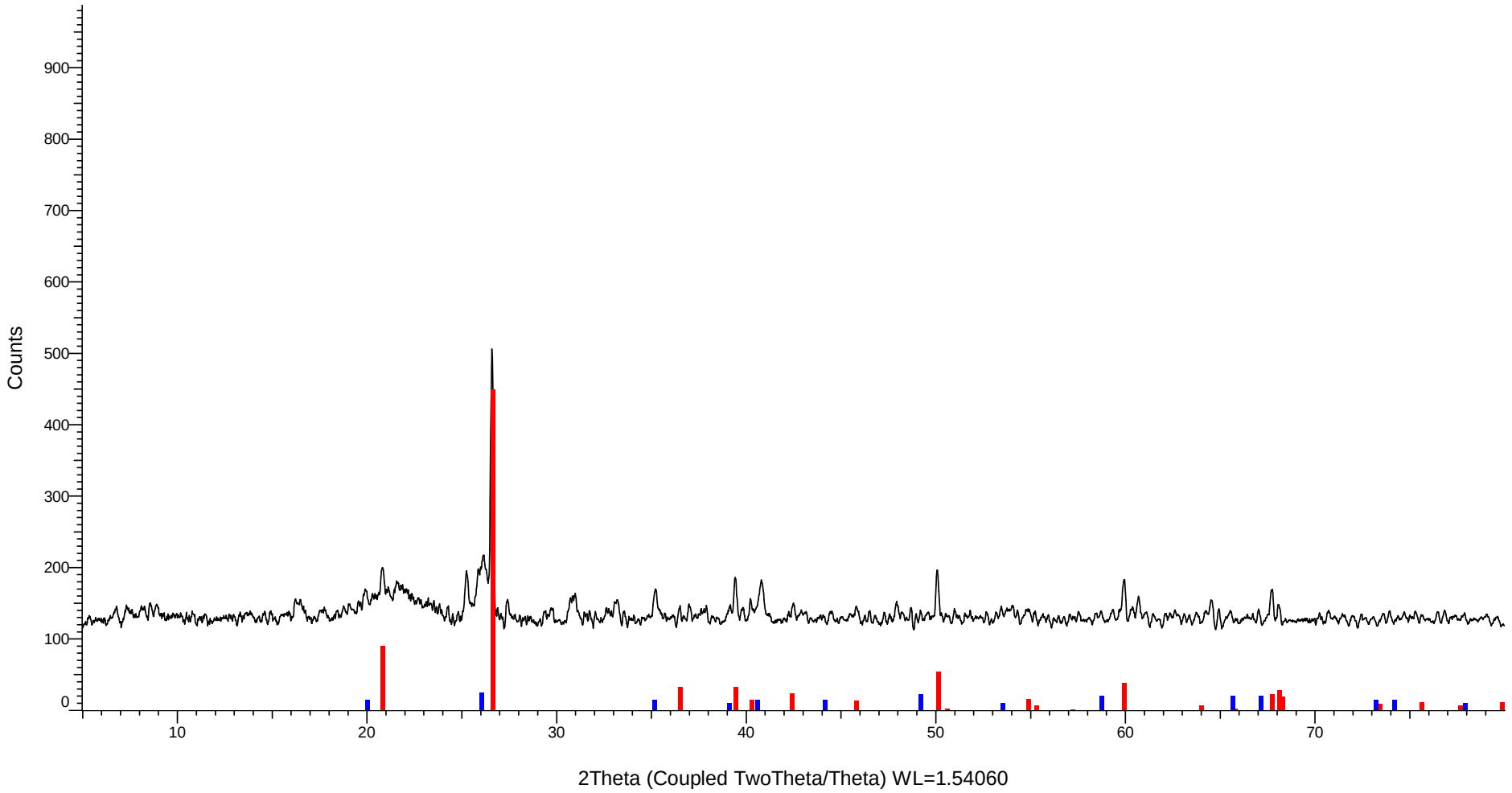
OPT5 Before (Coupled TwoTheta/Theta)



Pattern: PDF 00-007-0346 Radiation: 1.54060 Quality: Low precision

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

Lattice:	Hexagonal
S.G.:	P6222 (180)

Mol. weight =	60.08
Volume [CD] =	121.44
Dx =	
Dm =	
I/Icor =	-1.000

a =	5.11000	alpha =	
b =		beta =	
c =	5.37000	gamma =	
a/b =	1.00000	Z =	3
c/b =	1.05088		

Deleted Or Rejected By: Deleted: JVS during 6-10 revision
Sample Preparation: Fired to 1000 C, the sample develops β-quartz which is retained down to room temperature
Sample Source or Locality: Sample of montmorillonite from Otay, California, USA
Warning: One or more of the three strongest lines are unindexed

Primary Reference
Publication: Am. Mineral.
Detail: volume 36, page 182 (1951)
Authors: Bradley, Grim.

Radiation:		Filter:	Not specified
Wavelength:	1.54060	d-spacing:	
SS/FOM:	5.8 (0.091,34)		

d	2θ	I fix	h	k	l
4.43000	20.027	61	1	0	0
3.42000	26.033	101	1	0	1
2.55000	35.165	61	1	1	0
2.30000	39.134	40	1	0	2
2.22000	40.606	61	2	0	0
2.05000	44.142	61	2	0	1
1.85000	49.212	91	1	1	2
1.71000	53.547	40	2	0	2
1.57000	58.765	80			
1.42100	65.651	80	2	1	2
1.39300	67.143	80	2	0	3
1.29200	73.198	61	3	0	2
1.27700	74.200	61	2	2	0
1.22500	77.926	40	3	1	0
1.19600	80.191	61	3	1	1
1.19000	80.678	40	1	1	4
1.11300	87.592	20	3	1	2
1.10500	88.390	20	4	0	0
1.04400	95.095	20	1	0	5

Pattern: PDF 01-079-1910 Radiation: 1.54060 Quality: Star (*)

Formula	Si O2
Name	Silicon Oxide
Name (mineral)	Quartz, syn
Name (common)	α-Si O2

Lattice:	Hexagonal	Mol. weight =	60.08
S.G.:	P3121 (152)	Volume [CD] =	113.05
		Dx =	2.65
		Dm =	
		I/Icor =	3.070

a =	4.91400	alpha =	
b =		beta =	
c =	5.40600	gamma =	
a/b =	1.00000	Z =	3
c/b =	1.10012		

ANX: AX2
Analysis: O2 Si1
Formula from original source: Si O2
ICSD Collection Code: 67121
Calculated Pattern Original Remarks: Isotropic temperature factors obtained from room pressure refinement. Refinement was constrained to have a twin fraction of .035+3. Stable up to 846 K, above P6222, above 1143 K tridymite is stable
Wyckoff Sequence: c a(P3121)
Unit Cell Data Source: Single Crystal

Structure
Publication: Solid State Commun.
Detail: volume 72, page 507 (1989)
Authors: Hazen, R.M., Finger, L.W., Hemley, R.J., Mao, H.K.
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
4.25565	20.857	200	1	0	0
3.34387	26.637	1000	0	1	1
2.45700	36.542	72	1	1	0
2.28166	39.462	72	0	1	2
2.23681	40.287	32	1	1	1
2.12782	42.448	53	2	0	0
1.97997	45.790	30	0	2	1
1.81812	50.134	120	1	1	2
1.80200	50.614	4	0	0	3
1.67193	54.868	36	0	2	2
1.65937	55.319	16	1	0	3
1.60848	57.227	2	2	1	0
1.54169	59.953	85	2	1	1
1.45309	64.026	16	1	1	3
1.41855	65.779	4	3	0	0
1.38226	67.735	51	2	1	2
1.37513	68.134	63	0	2	3
1.37210	68.306	41	0	3	1
1.28810	73.455	20	0	1	4
1.25608	75.651	25	0	3	2
1.22850	77.662	14	2	2	0
1.19998	79.871	26	1	2	3
1.19796	80.033	8	2	2	1
1.18418	81.157	22	1	1	4
1.18030	81.480	24	3	1	0
1.15314	83.826	16	1	3	1
1.14083	84.941	2	0	2	4
1.11841	87.062	1	2	2	2
1.11462	87.433	2	0	3	3
1.08168	90.817	23	1	3	2
1.06391	92.776	4	4	0	0
1.04791	94.628	13	1	0	5
1.04389	95.108	8	0	4	1
1.03473	96.223	13	1	2	4
1.01506	98.730	11	2	2	3
0.98962	102.225	8	1	1	5
0.98962	102.225	8	0	4	2
0.98736	102.551	6	3	1	3
0.97850	103.854	4	0	3	4
0.97631	104.182	7	3	2	0
0.96390	106.098	1	0	2	5
0.96077	106.596	13	3	2	1
0.92866	112.090	1	4	1	0
0.91825	114.044	6	2	3	2
0.91615	114.449	11	0	4	3
0.91525	114.624	13	1	4	1
0.90906	115.851	4	2	2	4
0.90100	117.506	1	0	0	6
0.89732	118.285	8	2	1	5
0.88901	120.103	8	1	3	4

0.88146	121.828	2	0	1	6
0.87827	122.581	6	4	1	2
0.85990	127.222	2	0	3	5
0.85842	127.623	1	3	2	3
0.84592	131.180	2	1	1	6
0.84077	132.748	1	0	5	1
0.83597	134.277	1	0	4	4
0.82968	136.381	11	2	0	6
0.82549	137.861	12	1	4	3
0.81900	140.284	4	3	3	0
0.81183	143.187	14	2	2	5
0.81183	143.187	14	0	5	2
0.80976	144.079	4	3	3	1
0.80424	146.590	8	4	2	0