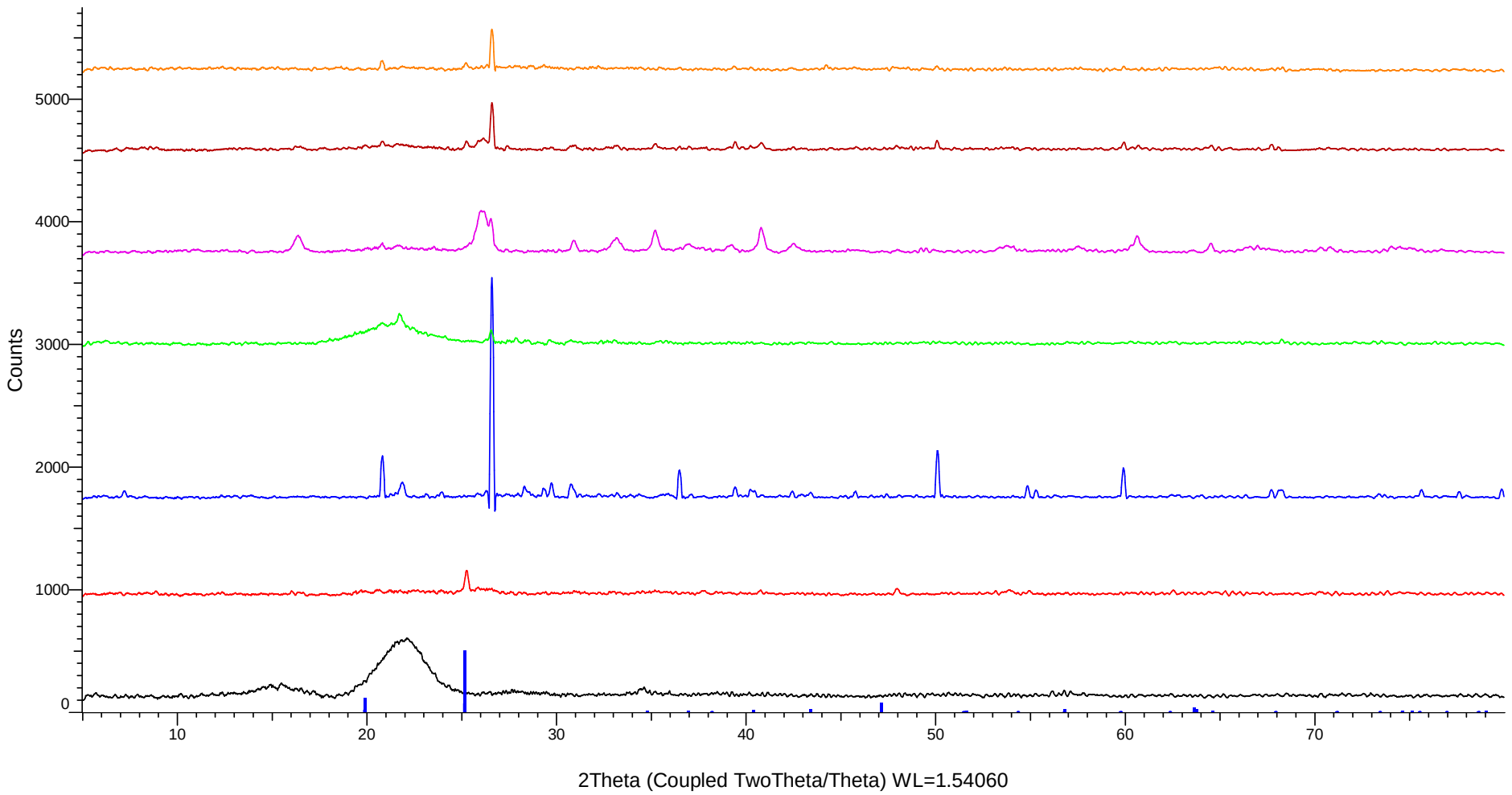
Raw Rice Husk (Coupled TwoTheta/Theta)



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

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

Lattice:	Hexagonal	Mol. weight =	60.08
S.G.:	P3221 (154)	Volume [CD] =	133.38
		Dx =	2.24
		Dm =	
		I/Icor =	2.880

a =	5.15390	alpha =	
b =		beta =	
c =	5.79810	gamma =	
a/b =	1.00000	Z =	3
c/b =	1.12499		

ANX: AX2
Analysis: 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

Structure
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++

Radiation:	CuKα1	Filter:	Not specified
Wavelength:	1.54060	d-spacing:	
SS/FOM:	999.9 (0,31)		

d	2θ	I fix	h	k	l	d	2θ	I fix	h	k	l
4.46341	19.876	233	1	0	0	1.13848	85.158	13	1	3	2
3.53682	25.159	999	0	1	1	1.12236	86.679	13	0	1	5
2.57695	34.785	28	1	1	0	1.11585	87.312	9	4	0	0
2.43123	36.943	25	1	0	2	1.09943	88.956	13	2	1	4
2.35484	38.187	11	1	1	1	1.09574	89.335	4	0	4	1
2.23170	40.383	36	2	0	0	1.07207	91.864	10	2	2	3
2.08275	43.412	49	0	2	1	1.05748	93.509	3	1	1	5
1.92603	47.149	151	1	1	2	1.04243	95.284	2	1	3	3
1.77357	51.484	7	0	1	3	1.04138	95.411	2	0	4	2
1.76841	51.646	30	0	2	2	1.03824	95.792	4	0	3	4
1.68701	54.337	4	2	1	0	1.02900	96.937	2	0	2	5
1.61984	56.789	51	1	2	1	1.02398	97.574	4	3	2	0
1.54616	59.762	9	1	1	3	1.00837	99.619	7	2	3	1
1.48780	62.362	11	3	0	0	0.97400	104.533	2	4	1	0
1.46099	63.639	68	0	2	3	0.96635	105.713	9	0	0	6
1.45810	63.780	49	1	2	2	0.96635	105.712	9	0	4	3
1.44111	64.622	20	0	3	1	0.96552	105.843	9	3	2	2
1.37865	67.937	7	1	0	4	0.96302	106.238	2	2	2	4
1.32367	71.175	14	0	3	2	0.96054	106.633	10	1	4	1
1.28848	73.430	13	2	2	0	0.95563	107.427	7	1	2	5
1.27094	74.614	26	1	2	3	0.94447	109.292	3	1	0	6
1.26337	75.138	25	1	1	4	0.94135	109.828	5	3	1	4
1.25779	75.530	5	2	2	1	0.92328	113.088	5	1	4	2
1.23793	76.961	13	3	1	0	0.91462	114.748	3	0	3	5
1.21561	78.643	5	2	0	4	0.90482	116.713	2	1	1	6
1.21064	79.029	28	1	3	1	0.90483	116.712	2	2	3	3
1.17894	81.594	2	0	3	3	0.89268	119.289	2	5	0	0
1.17742	81.722	3	2	2	2	0.88678	120.603	5	0	2	6

d	2θ	I fix	h	k	l
0.88421	121.192	2	0	4	4
0.88229	121.635	3	0	5	1
0.86979	124.655	4	1	4	3
0.86194	126.679	3	2	2	5
0.85898	127.470	2	3	3	0
0.85315	129.081	5	0	5	2
0.84971	130.064	4	3	3	1
0.84631	131.064	7	3	1	5
0.84350	131.907	5	4	2	0
0.83852	133.455	2	1	2	6
0.83634	134.155	9	2	3	4
0.83472	134.686	2	2	4	1
0.82359	138.551	2	3	3	2
0.81440	142.119	4	0	1	7
0.81041	143.797	5	0	3	6
0.81041	143.796	5	5	0	3
0.80992	144.010	4	2	4	2
0.80844	144.661	5	1	4	4
0.80405	146.679	2	0	4	5
0.80165	147.846	3	5	1	0