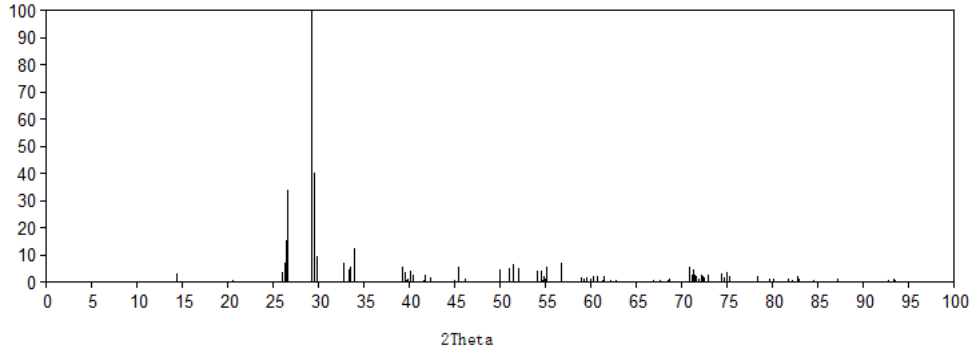
PDF Card No.: 04-015-7165 Quality:I

Sub-File Name:	Inorganic, Mineral, Alloy&Metal, Pharmaceutical, LPF Pattern
Formula:	Si O2
Name:	coesite I/Ic (RIR)= 0.83
Crystal System:	Monoclinic Space Group: C2/c(15) Dmeas:
Cell Parameters:	a= 6.9520 b= 12.1986 c= 7.0942
	Alpha= 90.000 Beta= 120.820 Gamma= 90.000
	Volume= 516.661 Z= 16
Reference:	Angel R.J., Shaw C.S.J., Gibbs G.V. Phys. Chem. Miner. 30(2003)167-176.
Radiation:	CuKa1 Wavelength= 1.54060
2Theta range:	14.51 - 96.23
Database comments:	ANX: AX2. LPF Collection Code: 1220073. Pressure of Data Collection: 6.16 GPa. Calculated Pattern Original Remarks: LPF Editor Comment: unit for isotropic displacement parameters omitted, assumed to be EPSILON2. LPF Editor Comment: experimental procedure described in Phys. Earth Planet. Inter. (2001) 124, 71. Minor Warning: No e.s.d reported/abstracted on the cell dimension. Wyckoff Sequence: f5 e a. Unit Cell Data Source: Single Crystal.

Relative Intensity



No.	2Theta	d-Value	Intensity	h	k	l	No.	2Theta	d-Value	Intensity	h	k	l
1	14.51	6.099	3.5	0	2	0	21	40.47	2.227	3.2	-3	1	1
2	16.22	5.460	0.3	-1	1	1	22	41.60	2.169	1.3	-2	2	3
3	16.52	5.362	0.2	1	1	0	23	41.84	2.158	2.9	-2	4	2
4	20.59	4.310	1.1	0	2	1	24	42.33	2.133	1.9	2	4	0
5	26.14	3.406	4.1	-1	1	2	25	42.60	2.121	0.5	2	2	1
6	26.31	3.384	7.4	-1	3	1	26	44.53	2.033	0.1	0	6	0
7	26.50	3.361	16.0	1	3	0	27	44.97	2.014	1.1	-1	3	3
8	26.71	3.335	34.2	1	1	1	28	45.13	2.007	0.6	-1	5	2
9	29.26	3.050	100.0	0	0	2	29	45.42	1.995	6.1	1	5	1
10	29.56	3.019	40.6	-2	2	1	30	45.82	1.979	0.1	-3	3	1
11	29.91	2.985	9.8	2	0	0	31	46.18	1.964	1.7	3	1	0
12	32.84	2.725	7.3	0	4	1	32	47.13	1.927	0.1	0	2	3
13	33.39	2.681	5.0	2	2	0	33	49.30	1.847	0.3	-2	4	3
14	33.50	2.673	5.8	-1	3	2	34	50.08	1.820	4.9	-3	3	3
15	33.95	2.638	12.8	1	3	1	35	51.05	1.787	5.3	3	3	0

Supplementary File S4. Table S1. ICCD Reference data of coesite.