QUARTZ

21, alpha, t-alpha-quartz, f-silice

SiO(2)

Hexagonal * P3(1)21 Z = 3

R =0.087 NR =153

3 .6 .9

Ref.Str.:

Ikuta D., Kawame N., Banno S., Hirajima T. et al. (2007)
* Amer. Mineral., 92, 57-63

R: Sample is on a thin section from Yangkou meta-igneous complex

in the middle part of the Sulu UHP terrain, eastern China.

See U(ij) in original. N.A.D.

Initial data from BDM-file

Lattice parameters (cub. angs.,degr.):

a =	4.923	alpha =	90.0
b =	4.923	beta =	90.0
c =	5.409	gamma =	120.0

Unit cell volume (cub. angs.) = 113.53

Molar volume (cub.cm/mol.) = 22.79

Co-ordinates, thermal parameters, occupation for atomic positions:

NoP	x/a	y/b	z/c	B(j)	atom / occupation
1	0.468	0.0	0.0	0.0	Si = 1.00
2	0.414	0.264	0.121	0.0	O = 1.00

Co-ordinates for all atomic positions :

No	NoP	x/a	y/b	z/c
1	1	0.468	0.0	0.0
2	2	0.414	0.264	0.121
3	1	0.0	0.468	0.6667
4	1	0.532	0.532	0.3333
5	2	0.736	0.15	0.7877
6	2	0.85	0.586	0.4543
7	2	0.264	0.414	0.5456
8	2	0.15	0.736	0.8789
9	2	0.586	0.85	0.2123

X-ray density (g/cm cub.) = 2.64

MU (1/cm) = 90.801 Mass attenuation coefficient (cm**2/g) = 34.452

Selected interatomic distances (cation-anion,anion-anion):

NoP	Atom	Rad.sph. (angs.)	C.N.	Distance (angs.)	NoP N.
1	Si	2.1	4		
				1.5918	2
				1.622	2
				1.5919	2
				1.6217	2
2	O	3.264	6		
				2.6398	2
				2.6398	2
				2.6288	2
				2.6042	2
				2.6155	2
				2.6154	2