

Phenakite, Be₂SiO₄

Phenakite

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An exploratory examination of the electron density and electrostatic potential of phenakite

12.472 12.472 8.251 90 90 120 R-3

atom	x	y	z	Wyckoff
Si	0.19562	0.98402	0.74990	18f
Be1	0.1943	0.9841	0.4156	18f
Be2	0.1941	0.9822	0.0846	18f
O1	0.20975	0.12125	0.7503	18f
O2	0.33382	0.00040	0.74991	18f
O3	0.12223	0.91217	0.91497	18f
O4	0.12228	0.91342	0.58495	18f

(7 × 18f)

Raman Active Modes

WP	A _g	A _u	E _g ¹	E _u ¹	E _g ²	E _u ²
18f	3	·	3	·	3	·

Total number of modes:

$$21A_g + 21E_g^1 + 21E_g^2 = 63$$