

Forsterite, Mg₂SiO₄

Forsterite

Kirfel A, Lippmann T, Blaha P, Schwarz K, Cox D F, Rosso K M, Gibbs G V

Physics and Chemistry of Minerals 32 (2005) 301-313

Electron density distribution and bond critical point properties for forsterite, Mg₂ SiO₄, determined with synchrotron single crystal X-ray diffraction data

4.752 10.192 5.978 90 90 90 Pbnm

atom	x	y	z	Wyckoff
Mg1	0	0	0	4a
Mg2	0.50846	0.77742	0.25	4c
Si	0.07353	0.59403	0.25	4c
O1	0.73408	0.59155	0.25	4c
O2	0.22160	0.44704	0.25	4c
O3	0.22253	0.66316	0.46697	8d

$$(1 \times 8d) + (4 \times 4c) + (1 \times 4a)$$

Raman Active Modes

WP	A _g	A _u	B _{1g}	B _{1u}	B _{2g}	B _{2u}	B _{3g}	B _{3u}
8d	3	·	3	·	3	·	3	·
4c	2	·	1	·	2	·	1	·
4a	·	·	·	·	·	·	·	·

Total number of modes:

$$11A_g + 7B_{1g} + 11B_{2g} + 7B_{3g} = 36$$