

Andalusite, Al₂OSiO₄

Andalusite

Burt J B, Ross N L, Angel R J, Koch M

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Equations of state and structures of andalusite to 9.8 GPa and sillimanite to 8.5 GPa

7.7930 7.89734 5.55583 90 90 90 Pnmm

atom	x	y	z	Wyckoff
Al1	0	0	0.2418	4e
Al2	0.3703	0.13879	0.5	4g
Si	0.2465	0.25237	0	4g
OA	0.4224	0.3638	0.5	4g
OB	0.4254	0.3619	0	4g
OC	0.1017	0.4012	0	4g
OD	0.2292	0.1341	0.2388	8h

$$(1 \times 8h) + (5 \times 4g) + (1 \times 4e)$$

Raman Active Modes

WP	A _g	A _u	B _{1g}	B _{1u}	B _{2g}	B _{2u}	B _{3g}	B _{3u}
8h	3	.	3	.	3	.	3	.
4g	2	.	2	.	1	.	1	.
4e	1	.	1	.	2	.	2	.

Total number of modes:

$$14A_g + 14B_{1g} + 10B_{2g} + 10B_{3g} = 48$$