

Jadeite, NaAlSi₂O₆

Jadeite

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The crystal structures of pyroxenes along the jadeite - hedenbergite and jadeite - aegirine joins

9.4278 8.5651 5.2262 90 107.624 90 C2/c

atom	x	y	z	Wyckoff
NaM2	0	0.3002	0.25	4e
AlM1	0	0.90604	0.25	4e
SiT	0.29072	0.09342	0.22822	8f
O1	0.1092	0.0760	0.1284	8f
O2	0.3610	0.2634	0.2935	8f
O3	0.3536	0.0071	0.0067	8f

$$(4 \times 8f) + (2 \times 4e)$$

Raman Active Modes

WP	A _g	A _u	B _g	B _u
8f	3	·	3	·
4e	1	·	2	·

Total number of modes:

$$14A_g + 16B_g = 30$$