

Orthoclase, KAlSi_3O_8

Orthoclase

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Characterization of lattice strain induced by neutron irradiation

8.59046 12.99323 7.18763 90 115.990 90 C2/m

atom	x	y	z	Wyckoff
K	0.2835	0	0.1364	4i
Si1	0.0104	0.1846	0.2241	8j
Si2	0.7093	0.11900	0.3411	8j
OA1	0	0.1481	0	4g
OA2	0.6316	0	0.2739	4i
OB	0.8311	0.1466	0.2320	8j
OC	0.0355	0.3120	0.2571	8j
OD	0.1838	0.1224	0.4099	8j

$$(5 \times 8j) + (2 \times 4i) + (1 \times 4g)$$

Raman Active Modes

WP	A_g	A_u	B_g	B_u
8j	3	·	3	·
4i	2	·	1	·
4g	1	·	2	·

Total number of modes:

$$20A_g + 19B_g = 39$$