

Zoisite, $\text{Ca}_2\text{Al}_3(\text{Si}_2\text{O}_7)(\text{SiO}_4)\text{O}(\text{OH})$

Zoisite

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The pressure behavior of clinozoisite and zoisite: An X-ray diffraction study

16.212 5.555 10.034 90 90 90 Pnma

atom	x	y	z	Wyckoff
Ca1	0.3668	0.25	0.4373	4c
Ca2	0.4518	0.25	0.1150	4c
Si1	0.0813	0.25	0.1055	4c
Si2	0.4105	0.75	0.2824	4c
Si3	0.1600	0.25	0.4357	4c
Al1	0.2497	0.9970	0.1897	8d
Al2	0.1055	0.75	0.3004	4c
O1	0.1307	-0.0006	0.1453	8d
O2	0.1011	0.0137	0.4309	8d
O3	0.3587	0.9897	0.2450	8d
O4	0.2193	0.75	0.3004	4c
O5	0.2275	0.25	0.3119	4c
O6	0.2718	0.75	0.0600	4c
O7	0.9916	0.25	0.1639	4c
O8	0.9960	0.75	0.2952	4c
O9	0.4211	0.75	0.4431	4c
O10	0.2682	0.25	0.0754	4c
H	0.263	0.25	0.976	4c

$(4 \times 8d) + (14 \times 4c)$

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	-

Total number of modes:

$$40A_g + 26B_{1g} + 40B_{2g} + 26B_{3g} = 132$$