

Calcite

IR and Raman Modes for R -3 c (167) [h axes]

Point group $D_{3d}(-3m)$

selection rules

Raman-active $\alpha_{xx} = \alpha_{yy} \neq \alpha_{zz}$
non-zero components

IR-active $\mu_z \neq 0$
 $\mu_x, \mu_y \neq 0$ + acoustic

$\alpha_{xx} = -\alpha_{yy} \neq \alpha_{xy}$
 $\alpha_{xz} \neq \alpha_{yz}$

rotation (inactive)

characters

normal modes

symmetry operations

number of operation of each class

Character Table

$D_{3d}(-3m)$	1	3	2	-1	-3	m_d	functions
Mult.	1	2	3	1	2	3	.
A_{1g}	1	1	1	1	1	1	x^2+y^2, z^2
A_{1u}	1	1	1	-1	-1	-1	.
A_{2g}	1	1	-1	1	1	-1	J_z
A_{2u}	1	1	-1	-1	-1	1	z
E_u	2	-1	0	-2	1	0	(x,y)
E_g	2	-1	0	2	-1	0	$(x^2-y^2, xy), (J_x, J_y)$ (xz, yz)

[List of irreducible representations in matrix form]

Mechanical Representation

WP	A_{1g}	A_{1u}	A_{2g}	A_{2u}	E_u	E_g	Modes
18e	1	1	2	2	3	3	Show
6b	.	1	.	1	2	.	Show
6a	.	.	1	1	1	1	Show

Show] option to obtain the symmetry adapted mo

Ca: (6b) : $A_{1u} + A_{2u} + 2E_u \rightarrow$ acoustic: $A_{2u} + E_u$ (the heaviest atom)

C : (6a) : $A_{2g} + A_{2u} + E_g + E_u$

O : (18a) : $A_{1g} + A_{1u} + 2A_{2g} + 2A_{2u} + 3E_g + 3E_u$

Total: $10A + 10E = 30 \Leftrightarrow 3N = 30$ ($N = 6:3 + 6:3 + 18:3 = 10$)

$\Gamma_{opt} = A_{1g}(R) + 2A_{1u}(ina) + 3A_{2g}(ina) + 3A_{2u}(IR) + 4E_g(R) + 5E_u(IR)$

\Rightarrow 5 Raman peaks and 8 IR peaks are expected