

Fluorapatite, $\text{Ca}_5(\text{PO}_4)_3\text{F}$

Fluorapatite

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Structural and vibrational behaviour of fluorapatite with pressure.

Part 1: in situ single-crystal X-ray diffraction investigation

9.375 9.375 6.887 90 90 120 $P6_3/m$

atom	x	y	z	Wyckoff
Ca1	2/3	1/3	0.0011	4f
Ca2	-0.00721	0.24154	0.25	6h
P	0.36853	0.39785	0.25	6h
O1	0.4844	0.3267	0.25	6h
O2	0.4666	0.5873	0.25	6h
O3	0.2572	0.3416	0.0705	12i
F	0	0	0.25	2a

$$(1 \times 12i) + (4 \times 6h) + (1 \times 4f) + (1 \times 2a)$$

Raman Active Modes

WP	A_g	A_u	B_g	B_u	E_{2g}^2	E_{2u}^2	E_{1g}^1	E_{1u}^1	E_{2g}^1	E_{2u}^1	E_{1g}^2	E_{1u}^2
12i	3	.	.	.	3	.	3	.	3	.	3	.
6h	2	.	.	.	2	.	1	.	2	.	1	.
4f	1	.	.	.	1	.	1	.	1	.	1	.
2a	1	.	.	.	1	.	.	.

Total number of modes:

$$12A_g + 13E_{2g}^2 + 8E_{1g}^1 + 13E_{2g}^1 + 8E_{1g}^2 = 54$$