

Symmetry Modes Summary for *Cmce* to *Pbca* phase transition.

Atoms	WP	Modes
Cl3	16g	GM1+(3) Y2+(3)
Cl1 Cl4 Cd1	8f	GM1+(2) Y2+(1)
Cl2	8e	GM1+(1) Y2+(2)

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	Cmce (64)	10	0.237(2)
(1,0,0)	Y2+	(a)	Pbca (61)	8	1.565(2)

Global distortion: 1.5833 Å

Symmetry Modes Summary for *Pbca* to *P2₁2₁2₁* phase transition

Atoms	WP	Modes
Cl1 Cl5 Cd1 Cl3 Cl4 Cl2	8c	GM1+(3) GM1-(3)
Cd2	4a	GM1-(3)

Note: The primary mode is written in bold letters

Summary of Amplitudes

K-vector	Irrep	Direction	Isotropy Subgroup	Dimension	Amplitude (Å)
(0,0,0)	GM1+	(a)	Pbca (61)	18	0.183(3)
(0,0,0)	GM1-	(a)	P2 ₁ 2 ₁ 2 ₁ (19)	21	1.008(3)

Global distortion: 1.0244 Å