Tilts and shifts in molecular perovskites

SUPPLEMENTARY INFORMATION

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Table S1 contains the data generated from the decompositions of a large number of molecular perovskites. For each entry, the chemical formula, space group, active distortion modes and a sensible set of primary order parameters are given. The number of possible order parameter generally increases as the symmetry decreases and in one case,[1] the number of possibilities exceeded the upper limit for what ISODISTORT[2] could provide. Another nontrivial example is the low-temperature phase of $[CH_3NH_3]Co(HCOO)_3$, where the of primary order parameters are R_5^-, M_2^+ and C, where C is either member of the set $\{\Gamma_{4,5}^+, R_{2,3}^-, X_{1,4}^-, M_5^+\}$. It should be remembered that an active mode may not be sufficiently strongly activated to be visible by inspection. For that reason, the (up to) three strongest distortion modes are highlighted in bold. Notation such as $M_{2,3}^+$ indicates that either M_2^+ or M_3^+ may be considered as a primary order parameter—this also applies to irreps separated by strokes, *e.g.* R_5^-/X_5^-. Distortion modes comprising propagation vector components other than 0 and $\frac{1}{2}$ are provided separately in Table S2.

Table S1: Structural details of the molecular perovskites considered here. Structures are at ambient conditions unless otherwise stated. Abbreviations are as follows: PPN = bis(triphenylphosphine)iminium, DAB = dabconium, TAz = triazolium, FA = formamidinium, MHy = methylhydrazinium, HIm = imidazolium, Ace = acetamidinium, Aze = azetidinium, Et = ethyl, Pr = propyl, *c*Pr = cyclopropyl, Bu = butyl, Bn = benzyl. M refers to several cations. $C^* \in \{\Gamma_4^+, \Gamma_5^+, R_2^-, R_3^-, X_1^-, X_4^-, M_5^+\}$.

s. g.	R_5^-	M_2^+	Γ_4^+	X_1^-	X_5^-	M_5^+	X_5^+	M_2^-	Γ_5^+	POPs	compound	condition	ref.
$P1$	**x**	x	**x**	x	x	x	**x**	x	x	-	$[(CH_3)_2NH_2]Fe(HCOO)_3$	7.9 GPa	1
$P1$	**x**		x						x	R_5^- Γ_4^-	$[MHy]Mn(HCOO)_3$	100 K	3
Cc	**x**		x						x	R_5^- Γ_4^-	$[(CH_3)_2NH_2]Mn(HCOO)_3$	100 K	4
$P2_1/c$	**x**	**x**	x	x	x	x			x	R_5^- M_2^+ C^*	$[CH_3NH_3]Co(HCOO)_3$	45 K	5
$P2_1/c$	**x**	**x**	x	x	x	x	**x**		x	R_5^- X_5^+	$[HIm]Mn(HCOO)_3$		6
$P2_1/c$	**x**		x				x	x	x	R_5^- X_5^+	$[Ace]Mn(HCOO)_3$	250 K	7
$P2_1/c$	**x**	**x**	x		x		**x**	x	x	R_5^- M_2^-/X_5^+	$[Aze]Mn(HCOO)_3$	180 K	8
$C2/c$	**x**		x						x	R_5^-	$[(CH_3)_2NH_2]Cu(HCOO)_3$		9
$C2/c$	**x**		x						**x**	R_5^-	$KM(HCOO)_3$		10,11
$C2/c$	**x**		x						**x**	R_5^-	$RbMn(HCOO)_3$		12
$C2/c$	**x**		x						x	R_5^-	$[FA]Mn(HCOO)_3$	110 K	13
$Pna2_1$	**x**	x			x		**x**		x	R_5^-/X_5^- X_5^+ $M_{2,3}^+$	$[C(NH_2)_3]Cu(HCOO)_3$		14
$Pna2_1$	**x**	**x**			x		**x**		x	R_5^-/X_5^- X_5^+ $M_{2,3}^+$	$[NH_2NH_3]Mn(HCOO)_3$	110 K	15
$Pna2_1$	**x**	**x**			x		**x**		x	R_5^-/X_5^- X_5^+ $M_{2,3}^+$	$[EtNH_3]M(HCOO)_3$		8,16
$Pna2_1$	x	**x**			**x**		**x**		x	R_5^-/X_5^- X_5^+ $M_{2,3}^+$	$[NH_4]Cd(HCOO)_3$		11
$Pnna$	**x**						**x**		x	R_5^- X_5^+	$[C(NH_2)_3]M(HCOO)_3$		14,17
$Pnma$	**x**	**x**			x				x	R_5^- M_2^+	$[CH_3NH_3]M(HCOO)_3$		8,18
$Pnma$	**x**	**x**			x				x	R_5^- M_2^+	$[NH_2NH_3]Mn(HCOO)_3$	400 K	15

s. g.	R_5^-	M_2^+	Γ_4^+	X_1^-	X_5^-	M_5^+	X_5^+	M_2^-	Γ_5^+	POPs	compound	condition	ref.
$Pnma$	**x**	**x**			x				x	R_5^- M_2^+	$[Aze]Mn(HCOO)_3$		8
$Pnma$	**x**	**x**			x				x	R_5^- M_2^+	$[N(CH_3)_4]Mn(HCOO)_3$		19**?**
$Imma$	**x**								x	R_5^-	$[EtNH_3]Mg(HCOO)_3$	430 K	16
$Imma$	**x**								x	R_5^-	$[Ace]Mn(HCOO)_3$	330 K	7
$P\bar{4}2_1m$		**x**								M_2^+ Γ_5^-	$[HIm]Mn(HCOO)_3$	453 K	6
$R\bar{3}$	**x**		x						x	R_5^- $\Gamma_4^+/R_2^-/R_4^-$	$[EtNH_3]Mg(HCOO)_3$	378 K	16
$R3c$	**x**								x	R_5^- Γ_4^-	$[MHy]Mn(HCOO)_3$	230 K	3
$R\bar{3}c$	**x**								x	R_5^-	$[(CH_3)_2NH_2]M(HCOO)_3$		20
$R\bar{3}c$	**x**								x	R_5^-	$[C(NH_2)_3]Mn(HCOO)_3$	1.61 GPa	21
$R\bar{3}c$	**x**								x	R_5^-	$[C(NH_2)_3]Cd(HCOO)_3$		22
$R\bar{3}c$	**x**								x	R_5^-	$[FA]Mn(HCOO)_3$	355 K	13
$R\bar{3}c$	**x**								x	R_5^-	$[MHy]Mn(HCOO)_3$	330 K	3
$Im\bar{3}$		**x**								M_2^+	$[NH_4]Mn(HCOO)_3$		19
$P\bar{1}$	x	**x**	x	x	x	x			x	Λ_1 M_2^+	$[DAB]Mn(H_2POO)_3$	120 K	23
$P\bar{1}$	**x**		x						x	Λ_3	$[C(NH_2)_3]Mn(H_2POO)_3$		23
$C2/m$	**x**		x						x	R_5^-	$[C(NH_2)_3]Mn(H_2POO)_3$		23
$P2_1/c$	**x**		x				**x**	**x**	x	R_5^- M_2^-/X_5^+	$[TAz]Mn(H_2POO)_3$		23
$P2_1/c$	**x**		**x**				x	x	**x**	R_5^- M_2^-/X_5^+	$[FA]Mn(H_2POO)_3$	115 K	23
$P2_1/c$		**x**	x			x	x		x	S_3 B_1	$[(CH_3)_2NH_2]Mn(H_2POO)_3$		24
$P2_1/c$	x		x				**x**		x	X_5^+ S_2	$[HIm]Mn(H_2POO)_3$		23
$P2_1/c$	**x**	**x**	x		x	**x**			x	R_5^- M_2^+	$V(H_2POO)_3$		25
$P2_1/c$		**x**	x			**x**	**x**		x	X_5^+	$M(H_2POO)_3$		25
$C2/c$	**x**		x						x	R_5^-	$Al(H_2POO)_3$		25

s. g.	R_5^-	M_2^+	Γ_4^+	X_1^-	X_5^-	M_5^+	X_5^+	M_2^-	Γ_5^+	POPs	compound	condition	ref.
$C2/c$	**x**		x						**x**	R_5^-	$[FA]Mn(H_2POO)_3$		23
$R\bar{3}$	**x**		x						**x**	Λ_1 R_5^-	$[DAB]Mn(H_2POO)_3$		23
$P2_1/c$	**x**		x				**x**	x	x	Λ_3	$[Bu_3NCH_3]Mn[N(CN)_2]_3$	295 K	26
$P2_1/c$	**x**		x				**x**	**x**	x	R_5^- M_2^-/X_5^+	$[Et_3PCH_2CHCH_2]Mn[N(CN)_2]_3$		27
$P2_1/c$	**x**		x				**x**	**x**	x	R_5^- M_2^-/X_5^+	$[SPh_3]Mn[N(CN)_2]_3$		28
$P2_1/c$	**x**		x				**x**	**x**	x	R_5^- M_2^-/X_5^+	$[Et_3P(CH_2)_2Cl]Mn[N(CN)_2]_3$		29
$P2_1/c$	**x**		x				**x**	**x**	x	R_5^- X_5^+	$[Et_3PCH_2OCH_3]Mn[N(CN)_2]_3$	173 K	27
$P2_1/c$	**x**		x				**x**	**x**	x	R_5^- X_5^+	$[Et_3PPr]Cd[N(CN)_2]_3$	223 K	30
$P2_1/c$	**x**	x	x		x		**x**	**x**	x	R_5^- M_2^-/X_5^+	$[NPr_4]Mn[N(CN)_2]_3$	3.3 GPa	31
$P2_1/c$	**x**	**x**	x		x		x	**x**	x	R_5^- M_2^-/X_5^+	$[NPr_4]Cd[N(CN)_2]_3$	100 K	32
$C2/c$	**x**		x						x	R_5^-	$[Et_3P(CH_2)_2F]Cd[N(CN)_2]_3$		33
$C2/c$	**x**		x						x	R_5^-	$[Et_3P(CH_2)_2F]Mn[N(CN)_2]_3$		29
$P2_12_12_1$	**x**	x			**x**		x	**x**	x	R_5^- X_5^- M_2^-	$[Et_3PPr]M[N(CN)_2]_3$		27,30
$P2_12_12_1$	**x**	x			**x**		x	**x**	x	R_5^- X_5^- M_2^-	$[Et_3PCH_2OCH_3]Mn[N(CN)_2]_3$		27
$P2_12_12_1$	**x**	x			**x**		x	**x**	x	R_5^- X_5^- M_2^-	$[Et_3P(CH_2)_2Cl]Cd[N(CN)_2]_3$		33
$Pnna$	**x**			x			x	x	x	Σ_3 R_5^- S_1	$[NPr_4]M[N(CN)_2]_3$		34,35
$Pbcn$	**x**	**x**			x		x	**x**		R_5^- M_2^-	$[NPr_4]Mn[N(CN)_2]_3$	0.5 GPa	31
$Pbcn$	**x**	x			**x**		x	**x**		R_5^- M_2^-	$[Et_3P(CH_2)_2Cl]Cd[N(CN)_2]_3$	333 K	33
$Pbcn$	**x**	x			x		x	**x**		R_5^- M_2^-	$[Et_3P(CH_2)_2F]Mn[N(CN)_2]_3$	347 K	29
$Pnma$	**x**	**x**			x				x	R_5^- M_2^+	$[Et_3NBn]Fe[N(CN)_2]_3$		36
$Pnma$	**x**	**x**			x				x	R_5^- M_2^+	$[Bu_3NBn]Co[N(CN)_2]_3$		36
$Pnma$	**x**	**x**			x				x	R_5^- M_2^+	$[Bu_3NCH_3]Mn[N(CN)_2]_3$	375 K	26
$Cmce$	**x**						**x**	**x**		R_5^- M_2^-/X_5^+	$[Et_3P(CH_2)_2F]Cd[N(CN)_2]_3$	373 K	33

s. g.	R_5^-	M_2^+	Γ_4^+	X_1^-	X_5^-	M_5^+	X_5^+	M_2^-	Γ_5^+	POPs	compound	condition	ref.
$Cmce$					**x**			**x**		X_5^- M_2^-	$[Et_3PPr]Cd[N(CN)_2]_3$	427 K	30
$Ibam$		x						**x**		M_2^-	$[Et_3PPr]Cd[N(CN)_2]_3$	397 K	30
$Ibam$	**x**								x	R_5^- R_3^-/Γ_5^+	$[NPr_4]M[N(CN)_2]_3$	323 K	34
$P\bar{4}2_1c$	**x**	**x**			x		x	**x**		R_5^- M_2^-	$[NPr_4]M[N(CN)_2]_3$	200 K	32,34,35
$I4/mcm$	**x**									R_5^-	$[NPr_4]M[N(CN)_2]_3$	368 K	32,34
$P\bar{1}$			**x**						x	Γ_4^+	$[(CH_3)_2NH_2]Cd(N_3)_3$	150 K	37
$P2_1$		x	x			**x**		**x**	**x**	M_2^+ M_5^+ M_2^-	$[(CH_3)_2NH_2]Mn(N_3)_3$	173 K	38
Cc			x	x	x		**x**		**x**	X_5^+ Γ_4^-	$[Et_2(CH_3)NH]Mn(N_3)_3$		39
$P2_1/m$			**x**		**x**				x	X_5^-	$[N(CH_3)_4]M(N_3)_3$		38,40,41
$P2_1/c$			x	**x**	**x**			x	**x**	Γ_5^+ X_5^- M_2^-	$[(CH_3)_3NH]M(N_3)_3$	173 K	38,42
$P2_1/c$			x					**x**	x	Σ_2 M_2^-	$[CH_3NH_3]Mn(N_3)_3$	173 K	38
$P2_1/c$	**x**		x				x	**x**	x	R_5^- M_2^-/X_5^+	$[CH_3NH_3]Mn(N_3)_3$	320 K	38
$C2/c$			x	**x**	**x**				**x**	Γ_5^+ X_5^-/X_1^-	$[(CH_3)_3NH]M(N_3)_3$		38,42
$C2/c$	**x**		**x**						x	R_5^-	$[N(CH_3)_4]Cd(N_3)_3$	220 K	41
$Pbca$	**x**						x		x	Σ_3 R_5^-	$[c\mathrm{PrNH_3}]Mn(N_3)_3$		43
$Cmce$	x						**x**	**x**		X_5^+ M_2^-	$[(CH_3)_2NH_2]Mn(N_3)_3$	323 K	38
$P4/nmm$								**x**		M_2^-	$[N(CH_3)_4]Ca(N_3)_3$		44
$R\bar{3}$			**x**						x	Γ_4^+	$[(CH_3)_2NH_2]Cd(N_3)_3$	273 K	37
$R\bar{3}m$									**x**	Γ_5^+	$[(CH_3)_3NH]Mn(N_3)_3$	360 K	38
$Pm\bar{3}m$											$[N(CH_3)_4]M(N_3)_3$	333 K	38,40,41
$C2/c$	**x**		x						x	R_5^-	$[PPN]Mn[Au(CN)_2]_3$		45
$R\bar{3}c$	**x**								x	R_5^-	$[PPN]Ni[Au(CN)_2]_3$		46

s. g.	R_5^-	M_2^+	Γ_4^+	X_1^-	X_5^-	M_5^+	X_5^+	M_2^-	Γ_5^+	POPs	compound	condition	ref.
$Pa\bar{3}$					x	**x**				X_5^-	$[PPN]Cd[Ag(CN)_2]_3$		45

Table S2: Compounds exhibiting distortion modes with unusual periodicities.

compound	$\langle\frac{1}{4}, \frac{1}{4}, 0\rangle$	$\langle\frac{1}{4}, \frac{1}{4}, \frac{1}{4}\rangle$	$\langle\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\rangle$	$\langle\frac{1}{4}, \frac{1}{2}, \frac{1}{4}\rangle$	$\langle\frac{1}{6}, \frac{1}{2}, \frac{1}{3}\rangle$	ref.
[DAB]Mn(H_2POO)$_3$, 120 K		Λ_1 Λ_2 Λ_3				23
[$C(NH_2)_3$]Mn(H_2POO)$_3$		Λ_1 Λ_2 Λ_3				23
[$(CH_3)_2NH_2$]Mn(H_2POO)$_3$	Σ_1 Σ_2		S_3 S_4	A_2	B_1	24
[HIm]Mn(H_2POO)$_3$	Σ_3 Σ_4		S_1 S_2			23
[DAB]Mn(H_2POO)$_3$		Λ_1 Λ_2				23
[CH_3NH_3]Mn(N_3)$_3$, 173 K	Σ_2 Σ_4					38
[cPrNH$_3$]Mn(N_3)$_3$, 173 K	Σ_3	S_2				43
[Bu_3NCH_3]Mn[$N(CN)_2$]$_3$		Λ_2 Λ_3				26
[NPr_4]M[$N(CN)_2$]$_3$	Σ_3 Σ_4		S_1 S_2			35

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