

Supporting Information

Temperature-Dependent Raman Studies of FAPbBr₃ and MAPbBr₃ Perovskites: Effect of Phase Transitions on Molecular Dynamics and Lattice Distortion

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Table S1. Raman wavenumbers (in cm⁻¹) of MAPbBr₃ together with the proposed assignment.^a

300 K (<i>Pm</i> $\bar{3}$ <i>m</i>)	156 K (<i>I4/mcm</i>)	150 K (<i>P4/mmm</i> or <i>Imma</i>)	90 K (<i>Pnma</i>)	Assignment
1588w	1593w	1593w	1594m	$\delta_{as}(\text{NH}_3)$
1482m	1483m	1483m	1475s	$\delta_s(\text{NH}_3)$
1455sh	1458w	1459w	1463m + 1459sh	$\delta_{as}(\text{CH}_3)$
1430vw	1426w	1426w	1424w	$\delta_s(\text{CH}_3)$
1250vw	1256w	1257m	1262w	$\delta(\text{CN})$
971m	974m	976m	973s	$\nu(\text{CN})$
918w	919m	918m	917s	$\rho(\text{NH}_3)+\rho(\text{CH}_3)$
			551w	overtone
322m	322m	322m	363sh + 324m	MA-cage mode
138m	138m	139m	141m	T'(MA ⁺)+L(MA ⁺)+Pb-Br stretch
124m	126m	126m	127m	T'(MA ⁺)+L(MA ⁺)+Pb-Br stretch
111m	111m	112m	111m	T'(MA ⁺)+L(MA ⁺)+Pb-Br stretch
			98m	T'(MA ⁺)+L(MA ⁺)+Pb-Br stretch
			90m	T'(MA ⁺)+L(MA ⁺)+Pb-Br stretch
80m	81m	81m	81s	T'(MA ⁺)+L(MA ⁺)+Pb-Br stretch
			68vs	octahedra distortion (Pb-Br bend)
			63s	octahedra distortion (Pb-Br bend)
58s	58vs	58vs	54s	octahedra distortion (Pb-Br bend)
		47s	44s	octahedra twist (L(PbBr ₆))
		38s	35vs	octahedra twist (L(PbBr ₆))

^a key: vs, very strong; s, strong; m, medium; w, weak; vw, very weak; sh, shoulder; ν , stretching; δ , bending; ρ , rocking; L, librational mode; T', translational mode

Table S2. Raman wavenumbers (in cm⁻¹) of FAPbBr₃ together with the proposed assignment.^a

300 K	200 K	170 K	150 K	120 K	100 K	Assignment
1725vw	1724vw	1723vw	1722vw	1722vw	1721vw	$\delta(\text{NH}_2) + \nu_{\text{as}}(\text{CN})$
1653sh	1652sh	1652sh	1651sh	1649sh	1650sh	$\delta(\text{NH}_2)$
1625w	1624w	1623w	1623w	1622w	1622w	$\delta(\text{NH}_2)$
1562w	1560w	1559w	1558w	1558w	1558w	$\delta(\text{NH}_2)$
1530sh	1534sh	1535vw	1534vw	1533vw	1532vw	$\delta(\text{NH}_2)$
	1437w	1439w	1439w	1448w + 1428w	1444w + 1432w	$\delta(\text{CH})$
1395sh	1392m	1391m	1390m	1389m	1388m	$\delta(\text{CH})$
1369sh	1360w	1360w	1359w	1359w	1359w	$\rho(\text{NH}_2)$
1122m	1122m	1124m	1128w	1128w	1128w	$\rho(\text{NH}_2)$
1104w	1099w	1101m	1102m	1102m	1102m	$\nu(\text{CN}) + \rho(\text{NH}_2)$
861w	862w	865w	868w	870w	873w	overtone
719w	719w	759w + 721w	757w + 719w	758w + 719w	761w + 720w	$\omega(\text{NH}_2)$
602w	600w	598w	602w	602w	602m	$\tau(\text{NH}_2)$
521m	519m	519m	518s	518s	518s	$\delta(\text{NCN})$
307m	307m	307m	307m	307m	307m	FA-cage mode
109m	111m	111m	113m	115m	115m	T'(MA ⁺)+L(MA ⁺)+Pb-Br stretch
76w	72w	71w	69w	73w	74w	octahedra distortion (Pb-Br bend)
					64w	octahedra distortion (Pb-Br bend)
			48sh	53sh	52sh	octahedra distortion (Pb-Br bend)
				40sh	39sh	octahedra distortion (Pb-Br bend)
29vs	31vs	32vs	33vs	33vs	33vs	octahedra twist (L(PbBr ₆))

^a key: vs, very strong; s, strong; m, medium; w, weak; vw, very weak; sh, shoulder; ν , stretching; δ , bending; ρ , rocking; ω , wagging; τ , twist; L, librational mode; T', translational mode