Electronic Supplementary Material (ESI) for RSC Advances.

Structures, band gaps, and formation energies of highly stable phases of inorganic ABX_3 halides: A = Li, Na, K, Rb, Cs, Tl; B = Be, Mg, Ca, Ge, Sr, Sn, Pb; and X = F, Cl, Br & I

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Materials	Crystal	Space Group	No. of Atoms	a [Å]	b [Å]	c [Å]	α	β	γ	K Points	Density [g/cm^3]	E_g [eV]	Δf_E [eV/At]
CsBeBr3	Monoclinic	$P2_1/c$	20	11.105	7.770	9.338	85.011	89.999	89.994	2 3 3 0 0 0	3.146	5.817	-1.420
CsBeCl3	Triclinic	P1	40	11.320	10.883	11.206	87.949	82.553	87.499	2 2 2 0 0 0	2.389	6.644	-1.742
CsBeF3	Triclinic	P1	40	8.223	8.115	11.065	89.648	89.892	89.098	2 2 2 0 0 0	3.579	8.827	-3.205
CsCaBr3	Orthorhombic	Pnma	20	8.135	8.145	11.504	89.984	89.958	89.589	3 3 2 0 0 0	3.596	5.706	-2.029
CsCaCl3	Cubic	$Pm\bar{3}m$	5	5.463	5.463	5.463	90.000	90.000	90.000	4 4 4 0 0 0	2.844	6.684	-2.325
CsCaF3	Cubic	$Pm\bar{3}m$	5	4.574	4.574	4.574	90.000	90.000	90.000	4 4 4 0 0 0	3.991	8.994	-3.513
CsCaI3	Orthorhombic	Pnma	20	8.815	8.623	12.389	90.000	90.000	90.000	3 3 2 0 0 0	3.905	4.872	-1.645
CsGeBr3	Triclinic	P1	40	11.604	11.587	11.601	89.819	90.015	89.920	2 2 2 0 0 0	3.792	2.529	-1.164
CsGeCl3	Triclinic	P1	40	11.129	11.094	11.235	89.980	88.422	89.938	2 2 2 0 0 0	2.987	3.157	-1.391
CsGeF3	Triclinic	P1	40	9.853	10.107	10.184	83.655	89.259	89.839	2 2 2 0 0 0	3.448	5.596	-2.523
CsMgBr3	Cubic	$Pm\bar{3}m$	5	5.447	5.447	5.447	90.000	90.000	90.000	4 4 4 0 0 0	4.078	3.737	-1.666
CsMgCl3	Cubic	$Pm\bar{3}m$	5	5.131	5.131	5.131	90.000	90.000	90.000	4 4 4 0 0 0	3.240	5.317	-1.977

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CsMgF3	Cubic	$Pm\bar{3}m$	5	4.247	4.247	4.247	90.000	90.000	90.000	4 4 4 0 0 0	4.643	8.641	-3.232
CsMgI3	Monoclinic	Pm	40	11.865	11.818	11.778	89.866	89.697	90.155	2 2 2 0 0 0	4.327	2.212	-1.267
CsPbBr3	Orthorhombic	Pnma	20	8.525	8.299	11.866	89.994	89.999	89.998	3 3 2 0 0 0	4.588	1.797	-1.353
CsPbCl3	Orthorhombic	Pnma	40	11.368	11.379	11.378	88.990	90.000	90.000	2 2 2 0 0 0	4.030	2.148	-1.568
CsPbF3	Orthorhombic	Pnma	40	9.793	9.739	9.741	89.864	90.000	90.000	2 2 2 0 0 0	5.678	3.208	-2.560
CsPbI3	Orthorhombic	Pnma	20	8.712	9.099	12.646	90.005	90.002	89.997	3 3 2 0 0 0	4.776	1.329	-1.062
CsSnCl3	Triclinic	P1	40	11.400	11.440	11.458	89.479	89.801	89.912	2 2 2 0 0 0	3.182	2.660	-1.490
CsSnF3	Triclinic	P1	20	10.005	7.259	6.789	90.595	95.175	90.257	2 3 3 0 0 0	4.157	4.813	-2.553
CsSnI3	Orthorhombic	$Pmc2_1$	20	8.626	9.068	12.573	89.442	89.971	89.999	3 3 2 0 0 0	4.271	1.292	-0.989
CsSrBr3	Orthorhombic	Pnma	40	11.873	11.955	11.934	89.197	89.903	89.812	2 2 2 0 0 0	3.609	5.694	-2.067
CsSrF3	Triclinic	$P\bar{1}$	40	9.670	9.579	9.581	89.985	89.914	90.013	2 2 2 0 0 0	4.154	8.338	-3.462
CsSrI3	Orthorhombic	Pnma	20	9.173	8.870	12.718	90.000	89.988	89.996	3 3 2 0 0 0	3.859	4.828	-1.699
KBeCl3	Triclinic	P1	40	12.051	10.047	10.118	87.029	87.576	89.473	2 2 2 0 0 0	1.675	6.518	-1.719
KBeF3	Monoclinic	$P2_1/m$	40	10.274	7.737	8.597	91.025	90.009	89.940	2 2 2 0 0 0	2.043	8.752	-3.219
KCaBr3	Orthorhombic	Pnma	20	7.710	8.077	11.111	90.005	89.981	89.979	3 3 2 0 0 0	3.061	5.784	-2.000
KCaCl3	Orthorhombic	Pnma	20	7.326	7.646	10.547	90.000	90.000	90.000	3 3 2 0 0 0	2.086	6.882	-2.300
KCaF3	Orthorhombic	Pnma	20	6.303	6.197	8.822	89.998	90.001	89.975	3 3 2 0 0 0	2.625	8.781	-3.522
KCaI3	Orthorhombic	Pnma	20	8.239	8.734	11.955	89.974	90.065	90.006	3 3 2 0 0 0	3.551	4.805	-1.612
KGeBr3	Triclinic	P1	40	11.313	11.174	11.317	89.812	85.863	90.365	2 2 2 0 0 0	3.264	3.126	-1.125
KGeCl3	Triclinic	P1	40	10.845	10.923	10.700	89.357	89.592	86.777	2 2 2 0 0 0	2.286	3.905	-1.358
KGeF3	Triclinic	P1	40	9.279	9.338	9.624	85.561	87.704	91.238	2 2 2 0 0 0	2.692	5.523	-2.523
KMgBr3	Orthorhombic	Pnma	20	7.583	7.425	10.596	90.002	89.999	89.986	3 3 2 0 0 0	3.375	4.548	-1.641
KMgCl3	Orthorhombic	Pnma	20	7.090	7.021	10.012	89.997	90.001	90.001	3 3 2 0 0 0	2.262	5.929	-1.964
KMgF3	Cubic	$Pm\bar{3}m$	5	4.049	4.049	4.049	90.000	90.000	90.000	4 4 4 0 0 0	3.013	9.233	-3.359
KPbCl3	Triclinic	$P\bar{1}$	40	10.910	11.005	10.990	86.825	90.000	90.000	2 2 2 0 0 0	3.550	2.675	-1.545
KPbF3	Trigonal	Cc	40	9.412	9.408	9.414	89.802	89.850	89.843	2 2 2 0 0 0	4.834	4.532	-2.572
KPbI3	Orthorhombic	Pnma	20	8.365	8.954	12.174	90.168	90.008	89.988	3 3 2 0 0 0	4.567	1.667	-1.026
KSnCl3	Triclinic	P1	40	11.037	10.912	11.056	89.924	86.075	89.928	2 2 2 0 0 0	2.636	3.217	-1.463
KSnF3	Triclinic	P1	40	8.883	10.417	9.570	88.592	89.907	88.926	2 2 2 0 0 0	3.222	4.503	-2.558
KSrBr3	Cubic	$Pm\bar{3}m$	5	5.982	5.982	5.982	90.000	90.000	90.000	4 4 4 0 0 0	2.842	4.881	-1.951
KSrCl3	Orthorhombic	Pnma	20	7.569	7.959	10.912	90.013	90.032	89.908	3 3 2 0 0 0	2.355	6.611	-2.323

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KSrF3	Orthorhombic	Pnma	40	9.202	9.244	9.242	88.293	90.000	90.000	2 2 2 0 0 0	3.104	8.317	-3.468
KSrI3	Orthorhombic	Pnma	40	12.322	12.352	12.330	86.050	89.774	90.278	2 2 2 0 0 0	3.592	4.716	-1.663
LiBeBr3	Triclinic	P1	40	13.835	9.496	10.908	74.900	84.702	93.421	2 2 2 0 0 0	2.370	5.553	-1.274
LiBeCl3	Triclinic	P1	40	9.922	12.136	8.957	81.235	81.088	78.381	2 2 2 0 0 0	1.507	6.933	-1.626
LiBeF3	Monoclinic	Pm	40	8.607	5.331	9.199	90.027	88.995	90.032	2 2 2 0 0 0	2.297	9.987	-3.222
LiCaBr3	Trigonal	R3	40	7.901	7.095	10.502	83.809	83.835	83.835	2 2 2 0 0 0	3.235	5.928	-1.898
LiCaCl3	Trigonal	R3	40	13.389	13.396	19.211	89.988	90.059	119.963	2 2 2 0 0 0	2.048	7.130	-2.218
LiCaF3	Orthorhombic	Pnma	20	5.257	5.788	7.470	90.002	90.010	89.940	3 3 2 0 0 0	3.040	10.035	-3.583
LiCaI3	Triclinic	P1	40	11.570	11.462	11.598	84.590	84.592	86.102	2 2 2 0 0 0	3.695	4.824	-1.480
LiGeBr3	Triclinic	P1	40	11.451	11.247	11.499	89.422	75.128	94.853	2 2 2 0 0 0	2.864	3.761	-1.003
LiGeCl3	Triclinic	P1	40	11.344	10.823	10.697	89.001	85.424	88.856	2 2 2 0 0 0	1.881	4.917	-1.255
LiGeF3	Triclinic	P1	40	9.098	9.702	8.158	86.975	84.933	87.829	2 2 2 0 0 0	2.522	5.334	-2.528
LiMgBr3	Trigonal	R3c	40	10.008	9.977	9.950	85.645	85.639	85.603	2 2 2 0 0 0	3.624	4.915	-1.558
LiMgCl3	Trigonal	R3c	10	6.367	5.519	5.831	62.420	62.403	59.969	3 3 3 0 0 0	2.239	6.538	-1.897
LiMgF3	Trigonal	R3c	10	5.085	4.409	4.632	62.287	62.284	59.978	3 3 3 0 0 0	2.834	9.781	-3.388
LiPbBr3	Triclinic	P1	40	10.968	11.074	11.110	81.250	82.403	85.491	2 2 2 0 0 0	4.468	2.821	-1.209
LiPbF3	Triclinic	P1	40	9.656	8.052	8.200	73.818	77.155	76.169	2 2 2 0 0 0	5.651	5.044	-2.622
LiPbI3	Triclinic	P1	40	11.870	11.868	11.700	83.533	84.576	85.291	2 2 2 0 0 0	4.795	2.137	-0.894
LiSnF3	Triclinic	P1	40	10.585	7.856	8.927	84.638	82.595	69.471	2 2 2 0 0 0	3.291	4.788	-2.589
LiSrF3	Triclinic	P1	40	8.683	8.043	8.246	75.400	77.831	75.443	2 2 2 0 0 0	3.497	8.484	-3.547
NaBeBr3	Triclinic	P1	40	9.344	13.218	10.498	113.014	88.819	96.862	2 2 2 0 0 0	2.781	5.553	-1.302
NaBeCl3	Triclinic	P1	40	8.840	10.854	11.267	68.254	84.929	85.771	2 2 2 0 0 0	1.700	6.560	-1.643
NaBeF3	Triclinic	P1	40	7.521	9.660	7.475	90.369	77.803	102.629	2 2 2 0 0 0	2.192	8.866	-3.187
NaCaBr3	Triclinic	P1	40	10.900	10.935	10.899	85.815	86.056	85.867	2 2 2 0 0 0	3.096	5.515	-1.914
NaCaCl3	Trigonal	R3	40	7.582	7.073	10.322	86.025	86.023	86.024	2 2 2 0 0 0	2.033	6.679	-2.222
NaCaF3	Trigonal	R3c	10	5.831	5.073	5.164	61.807	61.862	60.104	3 3 3 0 0 0	2.613	8.708	-3.498
NaCaI3	Trigonal	R3c	40	8.628	8.013	11.715	85.767	85.767	85.767	2 2 2 0 0 0	3.639	4.665	-1.523
NaGeBr3	Triclinic	P1	40	11.042	10.875	10.990	85.882	86.207	84.695	2 2 2 0 0 0	3.376	3.662	-1.036
NaGeCl3	Triclinic	P1	40	10.583	10.678	10.401	85.118	88.218	91.062	2 2 2 0 0 0	2.283	4.548	-1.273
NaGeF3	Triclinic	P1	40	8.378	8.454	10.479	87.244	86.591	85.552	2 2 2 0 0 0	2.734	5.119	-2.478
NaGeI3	Triclinic	P1	40	11.579	11.728	11.746	87.038	86.041	85.866	2 2 2 0 0 0	3.967	2.685	-0.737

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NaMgBr3	Orthorhombic	Pnma	20	7.024	7.412	10.298	90.035	89.959	90.044	3 3 2 0 0 0	3.556	4.732	-1.567
NaMgCl3	Orthorhombic	Pnma	20	6.616	6.958	9.655	90.001	90.018	90.030	3 3 2 0 0 0	2.296	6.276	-1.897
NaMgF3	Orthorhombic	Pnma	20	5.568	5.424	7.764	90.000	90.002	90.001	3 3 2 0 0 0	2.954	9.010	-3.328
NaPbBr3	Trigonal	R3c	10	3.833	6.623	6.874	62.061	62.207	60.234	6 3 3 0 0 0	4.480	2.874	-1.251
NaPbCl3	Trigonal	R3c	10	6.816	3.647	6.015	56.383	56.391	56.339	3 6 4 0 0 0	3.735	3.460	-1.484
NaPbF3	Trigonal	R3c	10	5.350	3.203	5.076	60.636	60.124	60.642	3 6 3 0 0 0	5.548	5.374	-2.570
NaSnBr3	Orthorhombic	$Pna2_1$	20	7.453	8.191	10.925	89.938	89.983	90.039	3 3 2 0 0 0	3.799	3.324	-1.163
NaSnCl3	Triclinic	P1	40	10.958	10.710	10.787	83.769	84.465	83.408	2 2 2 0 0 0	2.603	3.742	-1.373
NaSnF3	Monoclinic	Cc	40	6.482	6.416	8.617	87.897	87.893	90.574	2 2 2 0 0 0	3.683	4.548	-2.532
NaSrBr3	Monoclinic	Cc	40	11.222	11.185	11.174	86.144	86.145	86.113	2 2 2 0 0 0	3.318	5.561	-1.967
NaSrF3	Orthorhombic	Pnma	20	5.803	6.264	8.451	89.934	90.039	90.009	3 3 2 0 0 0	3.624	8.608	-3.459
RbBeCl3	Triclinic	P1	40	9.430	9.579	12.791	89.881	88.521	90.143	2 2 2 0 0 0	2.309	6.248	-1.733
RbBeF3	Monoclinic	$P2_1/c$	40	10.809	7.822	7.774	92.196	90.000	90.000	2 2 2 0 0 0	3.062	8.800	-3.209
RbCaBr3	Orthorhombic	Pnma	20	8.131	7.898	11.299	90.000	90.000	90.000	3 3 2 0 0 0	3.344	5.768	-2.006
RbCaCl3	Orthorhombic	Pnma	20	7.683	7.534	10.734	89.999	89.994	89.985	3 3 2 0 0 0	2.479	6.762	-2.303
RbCaF3	Orthorhombic	Pnma	40	9.000	9.005	8.998	89.865	89.956	90.045	2 2 2 0 0 0	3.325	8.600	-3.511
RbCaI3	Orthorhombic	Pnma	20	8.416	8.795	12.142	89.998	89.998	89.999	3 3 2 0 0 0	3.742	4.821	-1.621
RbGeBr3	Triclinic	P1	40	11.477	11.434	11.491	88.846	86.492	90.461	2 2 2 0 0 0	3.505	3.033	-1.137
RbGeCl3	Triclinic	P1	40	10.930	11.143	11.128	86.208	89.986	89.838	2 2 2 0 0 0	2.592	3.875	-1.367
RbGeF3	Triclinic	P1	40	9.658	9.467	9.934	88.054	86.668	90.940	2 2 2 0 0 0	3.149	5.500	-2.514
RbMgBr3	Tetragonal	I4/mcm	40	10.929	10.677	10.682	89.993	89.963	90.075	2 2 2 0 0 0	3.725	4.047	-1.643
RbMgCl3	Cubic	$Pm\bar{3}m$	5	5.061	5.061	5.061	90.000	90.000	90.000	4 4 4 0 0 0	2.768	5.512	-1.968
RbMgF3	Cubic	$Pm\bar{3}m$	5	4.126	4.126	4.126	90.000	90.000	90.000	4 4 4 0 0 0	3.942	9.213	-3.312
RbPbBr3	Orthorhombic	Pnma	20	8.038	8.492	11.642	89.993	89.979	90.005	3 3 2 0 0 0	4.450	2.050	-1.331
RbPbCl3	Orthorhombic	Pnma	20	7.727	8.094	11.110	90.000	89.985	90.039	3 3 2 0 0 0	3.814	2.458	-1.550
RbPbF3	Orthorhombic	Pnma	20	6.841	6.688	9.526	90.003	90.007	89.991	3 3 2 0 0 0	5.329	3.681	-2.557
RbPbI3	Orthorhombic	Pnma	20	8.539	9.049	12.372	90.004	89.931	90.005	3 3 2 0 0 0	4.679	1.534	-1.037
RbSnCl3	Triclinic	P1	40	11.141	11.283	11.236	86.891	89.684	89.850	2 2 2 0 0 0	2.921	2.973	-1.469
RbSnF3	Triclinic	P1	40	9.793	9.073	10.732	89.071	88.494	88.927	2 2 2 0 0 0	3.639	4.437	-2.545
RbSrBr3	Orthorhombic	Pnma	20	8.101	8.504	11.650	89.997	90.009	90.009	3 3 2 0 0 0	3.416	5.634	-2.045
RbSrCl3	Orthorhombic	Pnma	20	7.718	8.066	11.102	89.980	90.070	90.109	3 3 2 0 0 0	2.686	6.609	-2.327

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RbSrF3	Orthorhombic	Pnma	20	6.725	6.608	9.405	89.989	90.010	90.055	3 3 2 0 0 0	3.656	8.222	-3.456
RbSrI3	Orthorhombic	Pnma	40	12.490	12.561	12.548	86.762	89.982	90.046	2 2 2 0 0 0	3.737	4.745	-1.674
TlBeF3	Monoclinic	$P2_1/c$	40	7.793	7.823	10.647	84.246	89.888	89.946	2 2 2 0 0 0	5.542	5.379	-2.841
TlCaF3	Cubic	$Pm\bar{3}m$	5	4.529	4.513	4.515	89.987	89.640	90.100	4 4 4 0 0 0	5.424	5.445	-3.150
TlCaI3	Orthorhombic	Pnma	20	8.154	8.735	11.890	89.894	89.972	89.997	3 3 2 0 0 0	4.903	3.895	-1.325
TlGeBr3	Triclinic	P1	40	11.231	11.289	11.324	85.888	89.395	90.891	2 2 2 0 0 0	4.781	3.373	-0.811
TlGeF3	Triclinic	P1	40	9.369	9.696	9.646	89.270	89.678	93.608	2 2 2 0 0 0	5.067	4.396	-2.144
TlGeI3	Triclinic	P1	40	11.815	11.813	11.821	89.740	89.681	94.131	2 2 2 0 0 0	5.295	2.440	-0.543
TlMgCl3	Orthorhombic	Ama2	20	7.104	7.102	10.089	90.012	90.009	89.515	3 3 2 0 0 0	4.372	5.186	-1.621
TlMgF3	Cubic	$Pm\bar{3}m$	5	4.145	4.145	4.145	90.000	90.000	90.000	4 4 4 0 0 0	6.661	5.106	-2.942
TlPbF3	Trigonal	R3c	10	5.631	3.437	5.565	62.829	62.798	62.633	3 6 3 0 0 0	7.234	4.324	-2.209
TlSnF3	Triclinic	P1	40	10.369	9.440	9.131	89.626	83.452	89.735	2 2 2 0 0 0	5.652	4.036	-2.195
TlSrF3	Monoclinic	Cc	10	5.760	3.389	5.450	60.364	60.013	60.346	3 6 3 0 0 0	5.488	5.657	-3.110