Electronic Supplementary Material (ESI) for RSC Advances.

Lead-Free Europium and Ytterbium Perovskites

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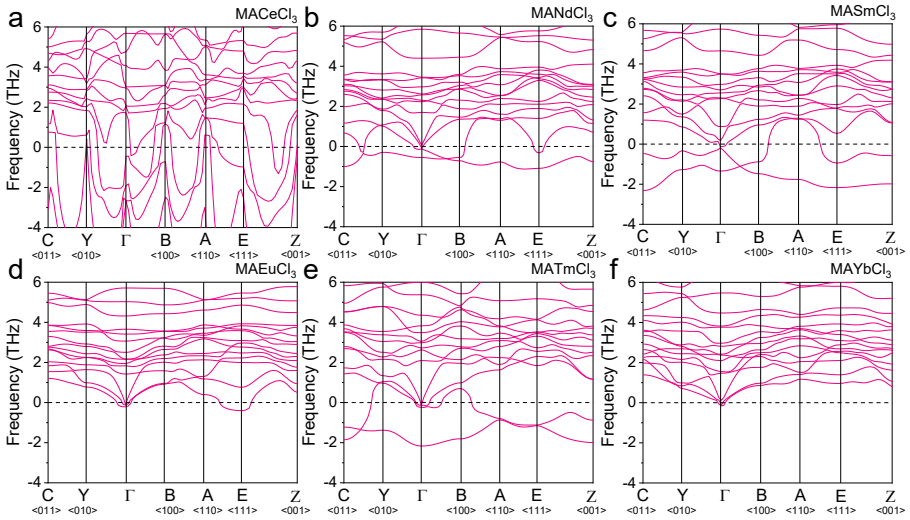

Figure S1. The phonon dispersion diagrams of lanthanide cations in MA-based chloride perovskite.

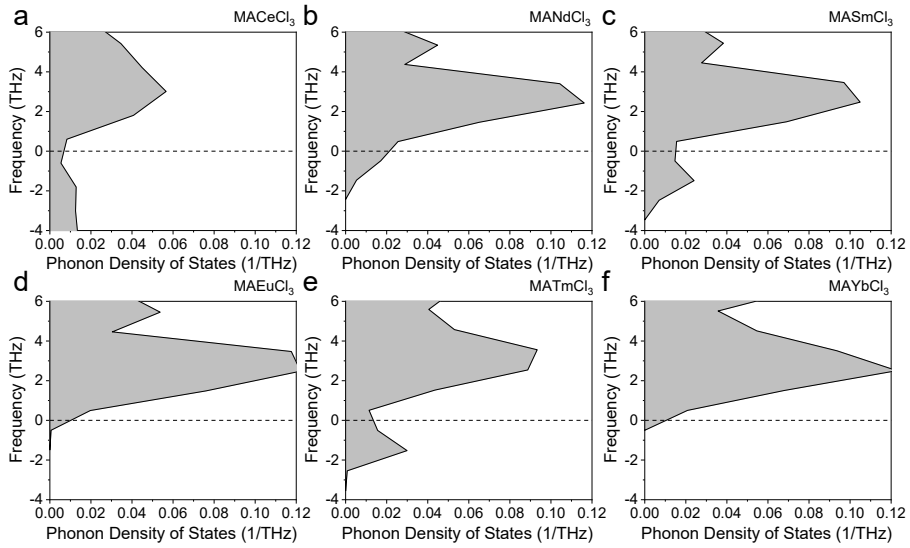

Figure S2. The phonon density of state of lanthanide cations in MA-based chloride perovskite.

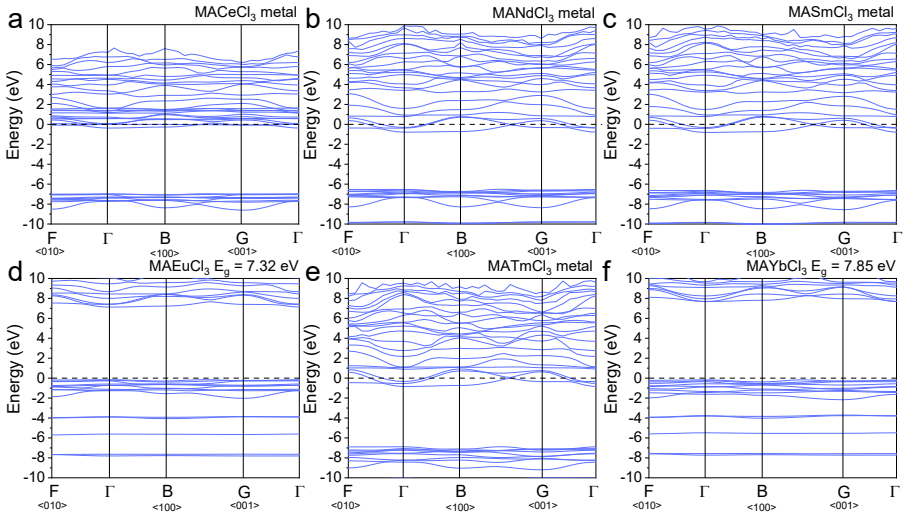

Figure S3. The band structure, without spin-polarized setting, of lanthanide cations in MA-based chloride perovskite.

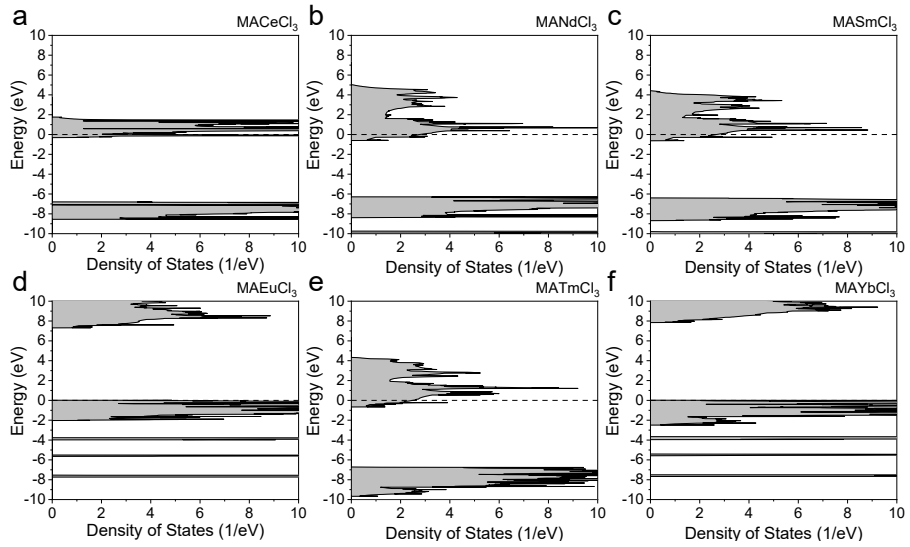

Figure S4. Without a spin-polarized setting, the electron density of the f state of lanthanide cations in MA-based chloride perovskite.

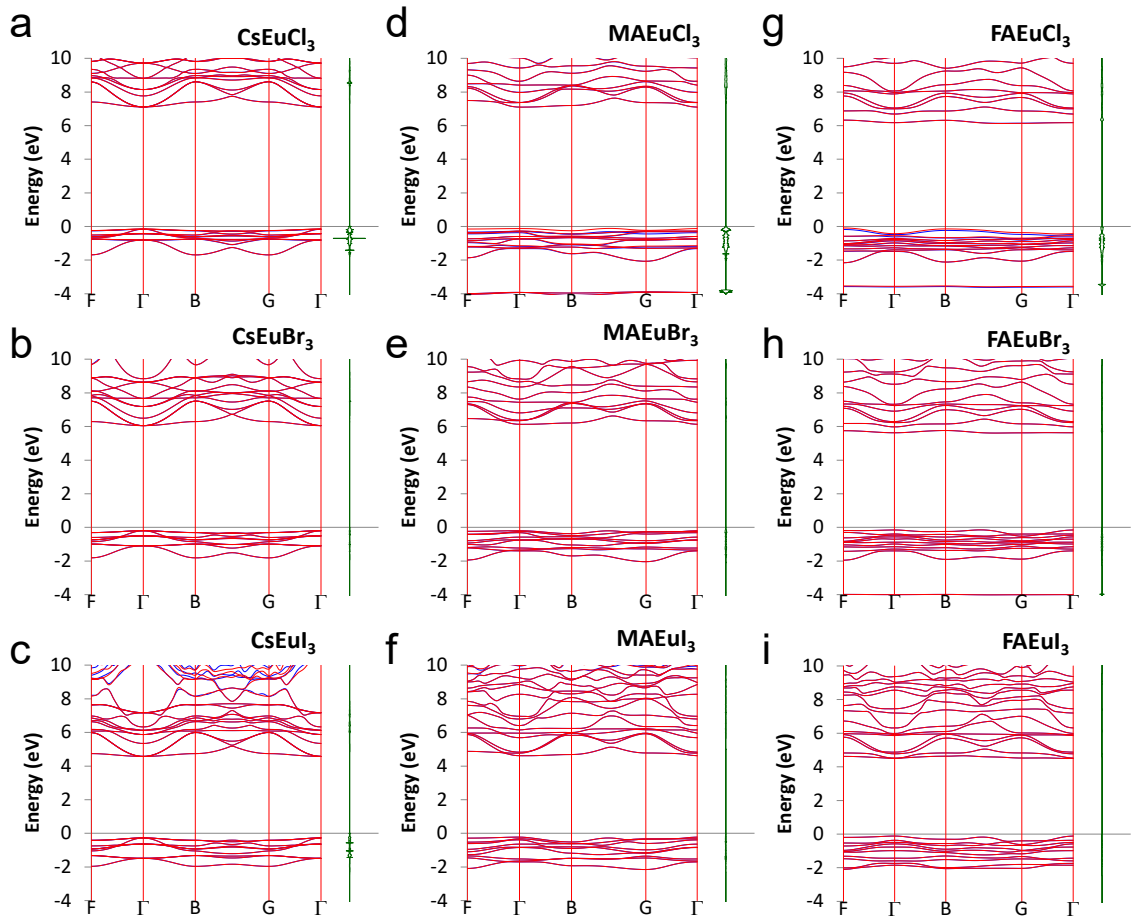

Figure S5. The electronic structure, spin-polarized setting, of the Eu^{2+}-based perovskites. (Blue line: spin down, Red line: spin down)

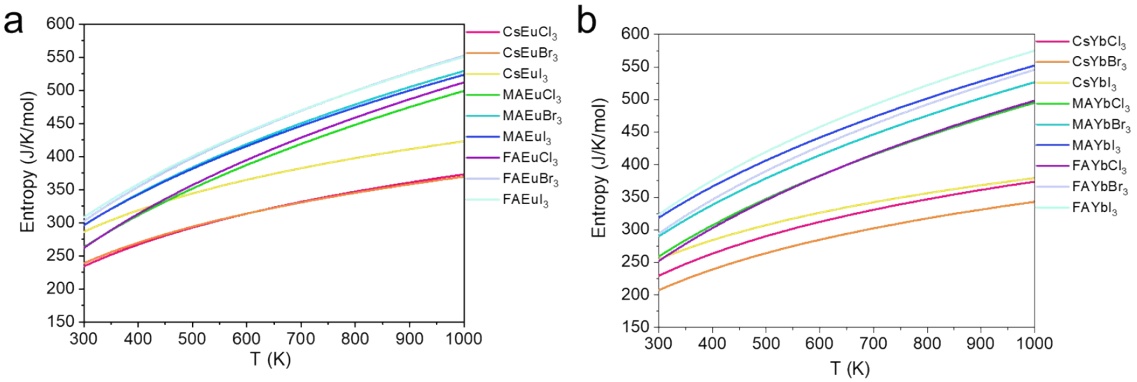

Figure S6. The entropy calculation of (a) Eu^{2+} and (b) Yb^{2+} cations in perovskite.

Table S1. The electrical conductivity and carrier mobility of $CsEuCl_3$, $CsEuBr_3$, and $CsEuI_3$.

T (K)	$CsEuCl_3$		$CsEuBr_3$		$CsEuI_3$	
	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)
300	0	0	0	0	-6.99×10^{-34}	0
400	0	0	-3.79×10^{-34}	0	2.26×10^{-9}	1.45
500	0	0	2.70×10^{-10}	1.11	9.55×10^{-7}	1.34
600	6.10×10^{-34}	0	6.14×10^{-8}	1.02	5.56×10^{-5}	1.24
700	9.77×10^{-31}	0	3.03×10^{-6}	0.96	1.04×10^{-3}	1.17
800	3.66×10^{-9}	0.77	5.75×10^{-5}	0.91	9.48×10^{-3}	1.10
900	1.07×10^{-7}	0.74	5.73×10^{-4}	0.86	5.36×10^{-2}	1.04
1000	1.61×10^{-6}	0.71	3.64×10^{-3}	0.82	0.22	0.99

Table S2. The electrical conductivity and carrier mobility of $MAEuCl_3$, $MAEuBr_3$, and $MAEuI_3$.

T (K)	$MAEuCl_3$		$MAEuBr_3$		$MAEuI_3$	
	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)
300	0	0	0	0	-1.25×10^{-33}	0
400	0	0	-5.14×10^{-35}	0	2.16×10^{-9}	1.26
500	0	0	1.41×10^{-10}	0.72	8.37×10^{-7}	1.14
600	-4.96×10^{-33}	0	3.32×10^{-8}	0.66	4.60×10^{-6}	1.05
700	-6.55×10^{-31}	0	1.67×10^{-6}	0.62	8.24×10^{-4}	0.98
800	2.37×10^{-9}	0.38	3.19×10^{-5}	0.58	7.29×10^{-3}	0.93
900	6.74×10^{-8}	0.36	3.19×10^{-4}	0.55	0.04	0.88
1000	9.85×10^{-7}	0.34	2.03×10^{-3}	0.52	0.16	0.84

Table S3. The electrical conductivity and carrier mobility of $FAEuCl_3$, $FAEuBr_3$, and $FAEuI_3$.

T (K)	$FAEuCl_3$		$FAEuBr_3$		$FAEuI_3$	
	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)
300	0	0	0	0	-9.64×10^{-36}	0
400	0	0	-3.22×10^{-33}	0	4.20×10^{-10}	1.24
500	-4.17×10^{-35}	0	5.23×10^{-10}	0.43	2.12×10^{-7}	1.00
600	-1.39×10^{-30}	0	9.47×10^{-8}	0.36	1.42×10^{-5}	0.86
700	8.69×10^{-9}	0.35	3.98×10^{-6}	0.31	2.98×10^{-4}	0.78
800	3.30×10^{-7}	0.32	6.65×10^{-5}	0.27	2.99×10^{-3}	0.72
900	5.60×10^{-6}	0.30	6.01×10^{-4}	0.24	0.02	0.68
1000	5.38×10^{-5}	0.27	3.53×10^{-3}	0.22	0.08	0.64

Table S4. The electrical conductivity and carrier mobility of $CsYbCl_3$, $CsYbBr_3$, and $CsYbI_3$.

T (K)	$CsYbCl_3$		$CsYbBr_3$		$CsYbI_3$	
	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)
300	0	0	0	0	0	0
400	0	0	0	0	0	0
500	0	0	0	0	-2.08×10^{-32}	0
600	0	0	-1.44×10^{-31}	0	6.99×10^{-10}	1.35
700	0	0	1.52×10^{-9}	1.88	6.57×10^{-8}	1.26
800	0	0	8.12×10^{-8}	1.82	2.02×10^{-6}	1.19
900	-4.08×10^{-32}	0	1.82×10^{-6}	1.76	2.93×10^{-5}	1.12
1000	-2.17×10^{-30}	0	2.21×10^{-5}	1.70	2.52×10^{-4}	1.06
1100	2.37×10^{-9}	0.61	1.72×10^{-4}	1.66	1.48×10^{-3}	1.00

Table S5. The electrical conductivity and carrier mobility of $MAYbCl_3$, $MAYbBr_3$, and $MAYbI_3$.

T (K)	$MAYbCl_3$		$MAYbBr_3$		$MAYbI_3$	
	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)
300	0	0	0	0	0	0
400	0	0	0	0	0	0
500	0	0	0	0	-2.43×10^{-32}	0
600	0	0	0	0	6.64×10^{-10}	1.16
700	0	0	-3.53×10^{-33}	0	5.75×10^{-8}	1.07
800	0	0	-8.18×10^{-31}	0	1.67×10^{-6}	0.99
900	-1.39×10^{-32}	0	1.84×10^{-9}	0.55	2.33×10^{-5}	0.93
1000	-8.18×10^{-31}	0	3.94×10^{-8}	0.52	1.95×10^{-4}	0.87
1100	9.21×10^{-10}	0.32	4.88×10^{-7}	0.50	1.12×10^{-3}	0.83

Table S6. The electrical conductivity and carrier mobility of $FAYbCl_3$, $FAYbBr_3$, and $FAYbI_3$.

T (K)	$FAYbCl_3$		$FAYbBr_3$		$FAYbI_3$	
	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)	Electrical conductivity ($ohm^{-1}\,m^{-1}$)	Carrier mobility ($cm^2V^{-1}s^{-1}$)
300	0	0	0	0	0	0
400	0	0	0	0	0	0
500	0	0	0	0	-6.25×10^{-32}	0
600	0	0	-1.50×10^{-32}	0	1.40×10^{-9}	0.92
700	-3.88×10^{-32}	0	2.00×10^{-10}	0.36	1.10×10^{-7}	0.82
800	2.34×10^{-10}	0.30	1.17×10^{-8}	0.31	2.99×10^{-6}	0.75
900	9.09×10^{-9}	0.27	2.81×10^{-7}	0.27	3.95×10^{-5}	0.69
1000	1.70×10^{-7}	0.24	3.59×10^{-6}	0.23	3.15×10^{-4}	0.65
1100	1.86×10^{-6}	0.22	2.90×10^{-5}	0.21	1.74×10^{-3}	0.62

Crystal information

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Title CH_6NCeCl_3 ($MACeCl_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.59058	5.60133	5.71131	90.0000	89.1600	90.0000

Unit-cell volume = 178.828635 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.35093	0.51930	0.64410	1.000	1.000	1a	1
2 H	H_2	0.35093	0.82054	0.64410	1.000	1.000	1a	1

3 H	H_3	0.92203	0.50939	0.71293	1.000	1.000	1a	1
4 H	H_4	0.92203	0.83046	0.71293	1.000	1.000	1a	1
5 H	H_5	0.28590	0.66992	0.88716	1.000	1.000	1a	1
6 H	H_6	0.99594	0.66992	0.45003	1.000	1.000	1a	1
7 Ce	Ce_1	0.58011	0.16992	0.14834	1.000	1.000	1a	1
8 C	C	0.00862	0.66992	0.64073	1.000	1.000	1a	1
9 N	N	0.26175	0.66992	0.70751	1.000	1.000	1a	1
10 Cl	Cl_1	0.54954	0.16992	0.64279	1.000	1.000	1a	1
11 Cl	Cl_2	0.54851	0.66992	0.17965	1.000	1.000	1a	1
12 Cl	Cl_3	0.07921	0.16992	0.11311	1.000	1.000	1a	1

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Title CH_6NEuCl_3 ($MAEuCl_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.50847	5.47507	5.61640	90.0000	87.5800	90.0000

Unit-cell volume = 169.235389 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.35063	0.51503	0.68662	1.000	1.000	1a	1
2 H	H_2	0.35063	0.82481	0.68662	1.000	1.000	1a	1
3 H	H_3	0.91129	0.50522	0.65929	1.000	1.000	1a	1
4 H	H_4	0.91129	0.83462	0.65929	1.000	1.000	1a	1
5 H	H_5	0.22277	0.66992	0.91431	1.000	1.000	1a	1
6 H	H_6	0.05413	0.66992	0.41421	1.000	1.000	1a	1
7 Eu	Eu_1	0.58835	0.16992	0.15991	1.000	1.000	1a	1
8 C	C	0.01472	0.66992	0.60755	1.000	1.000	1a	1
9 N	N	0.24657	0.66992	0.73019	1.000	1.000	1a	1

10 Cl	Cl_1	0.55793	0.16992	0.65840	1.000	1.000	1a	1
11 Cl	Cl_2	0.56051	0.66992	0.19094	1.000	1.000	1a	1
12 Cl	Cl_3	0.08666	0.16992	0.11605	1.000	1.000	1a	1

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Title CH_6NNdCl_3 ($MANdCl_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.49908	5.54919	5.59087	90.0000	87.1600	90.0000

Unit-cell volume = 170.398319 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.35615	0.51785	0.62815	1.000	1.000	1a	1
2 H	H_2	0.35615	0.82199	0.62815	1.000	1.000	1a	1
3 H	H_3	0.91694	0.50754	0.71050	1.000	1.000	1a	1
4 H	H_4	0.91694	0.83231	0.71050	1.000	1.000	1a	1
5 H	H_5	0.28852	0.66992	0.88028	1.000	1.000	1a	1
6 H	H_6	0.99719	0.66992	0.43950	1.000	1.000	1a	1
7 Nd	Nd_1	0.56835	0.16992	0.16363	1.000	1.000	1a	1
8 C	C	0.00644	0.66992	0.63535	1.000	1.000	1a	1
9 N	N	0.26447	0.66992	0.69647	1.000	1.000	1a	1
10 Cl	Cl_1	0.55993	0.16992	0.66357	1.000	1.000	1a	1
11 Cl	Cl_2	0.55572	0.66992	0.17186	1.000	1.000	1a	1
12 Cl	Cl_3	0.06870	0.16992	0.15539	1.000	1.000	1a	1

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Title CH_6NSmCl_3 ($MASmCl_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.44183	5.48218	5.51968	90.0000	86.7300	90.0000

Unit-cell volume = 164.401018 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.35618	0.51615	0.63033	1.000	1.000	1a	1
2 H	H_2	0.35618	0.82369	0.63033	1.000	1.000	1a	1
3 H	H_3	0.91172	0.50557	0.70968	1.000	1.000	1a	1
4 H	H_4	0.91172	0.83428	0.70968	1.000	1.000	1a	1
5 H	H_5	0.28323	0.66992	0.88509	1.000	1.000	1a	1
6 H	H_6	0.99706	0.66992	0.43552	1.000	1.000	1a	1
7 Sm	Sm_1	0.57320	0.16992	0.16259	1.000	1.000	1a	1
8 C	C	0.00309	0.66992	0.63407	1.000	1.000	1a	1
9 N	N	0.26215	0.66992	0.69865	1.000	1.000	1a	1
10 Cl	Cl_1	0.56456	0.16992	0.66250	1.000	1.000	1a	1
11 Cl	Cl_2	0.56258	0.66992	0.17131	1.000	1.000	1a	1
12 Cl	Cl_3	0.07381	0.16992	0.15361	1.000	1.000	1a	1

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Title CH_6NTmCl_3 ($MATmCl_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.30155	5.32332	5.32963	90.0000	84.4100	90.0000

Unit-cell volume = 149.696699 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.35863	0.51170	0.65161	1.000	1.000	1a	1
2 H	H_2	0.35863	0.82814	0.65161	1.000	1.000	1a	1

3 H	H_3	0.90046	0.50070	0.68803	1.000	1.000	1a	1
4 H	H_4	0.90046	0.83915	0.68803	1.000	1.000	1a	1
5 H	H_5	0.24528	0.66992	0.90812	1.000	1.000	1a	1
6 H	H_6	0.02835	0.66992	0.41127	1.000	1.000	1a	1
7 Tm	Tm_1	0.57800	0.16992	0.16369	1.000	1.000	1a	1
8 C	C	0.00320	0.66992	0.61831	1.000	1.000	1a	1
9 N	N	0.25388	0.66992	0.71321	1.000	1.000	1a	1
10 Cl	Cl_1	0.57409	0.16992	0.66452	1.000	1.000	1a	1
11 Cl	Cl_2	0.57484	0.66992	0.17283	1.000	1.000	1a	1
12 Cl	Cl_3	0.07969	0.16992	0.15212	1.000	1.000	1a	1

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Title CH_6NYbCl_3 ($MAYbCl_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.37451	5.33509	5.45456	90.0000	86.4500	90.0000

Unit-cell volume = 156.101178 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.34648	0.51110	0.70677	1.000	1.000	1a	1
2 H	H_2	0.34648	0.82875	0.70677	1.000	1.000	1a	1
3 H	H_3	0.90493	0.50073	0.63589	1.000	1.000	1a	1
4 H	H_4	0.90493	0.83911	0.63589	1.000	1.000	1a	1
5 H	H_5	0.18811	0.66992	0.92872	1.000	1.000	1a	1
6 H	H_6	0.07994	0.66992	0.39879	1.000	1.000	1a	1
7 Yb	Yb_1	0.59344	0.16992	0.16280	1.000	1.000	1a	1
8 C	C	0.01586	0.66992	0.59366	1.000	1.000	1a	1
9 N	N	0.23573	0.66992	0.74219	1.000	1.000	1a	1

10 Cl	Cl_1	0.56231	0.16992	0.66077	1.000	1.000	1a	1
11 Cl	Cl_2	0.58566	0.66992	0.17794	1.000	1.000	1a	1
12 Cl	Cl_3	0.09163	0.16992	0.13317	1.000	1.000	1a	1

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Title $CsEuBr_3$

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.75496	5.75496	5.75507	90.0000	89.9800	90.0000

Unit-cell volume = 190.605412 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 Eu	Eu_1	0.49997	0.25000	0.25142	1.000	1.000	1a	1
2 Cs	Cs	0.00002	0.75000	0.74770	1.000	1.000	1a	1
3 Br	Br_1	0.50001	0.25000	0.75163	1.000	1.000	1a	1
4 Br	Br_2	0.49997	0.75000	0.24890	1.000	1.000	1a	1
5 Br	Br_3	0.99996	0.25000	0.24894	1.000	1.000	1a	1

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Title $CsEuCl_3$

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.46914	5.46920	5.46946	90.0000	89.9800	90.0000

Unit-cell volume = 163.601502 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1	Eu Eu_1	0.49997	0.25000	0.25139	1.000	1.000	1a	1
2	Cs Cs	0.00002	0.75000	0.74766	1.000	1.000	1a	1
3	Cl Cl_1	0.50001	0.25000	0.75142	1.000	1.000	1a	1
4	Cl Cl_2	0.49997	0.75000	0.24905	1.000	1.000	1a	1
5	Cl Cl_3	0.99997	0.25000	0.24908	1.000	1.000	1a	1

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Title $CsEuI_3$

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
6.19868	6.19861	6.19865	90.0000	89.9800	90.0000

Unit-cell volume = 238.171939 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1	Eu Eu_1	0.49997	0.25000	0.25204	1.000	1.000	1a	1
2	Cs Cs	0.00001	0.75000	0.74782	1.000	1.000	1a	1
3	I I_1	0.50002	0.25000	0.75169	1.000	1.000	1a	1
4	I I_3	0.49997	0.75000	0.24851	1.000	1.000	1a	1
5	I I_2	0.99996	0.25000	0.24854	1.000	1.000	1a	1

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Title $CH_5N_2EuBr_3$ (FAEuBr3)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.89446	5.87872	5.84302	86.0600	83.8400	86.9600

Unit-cell volume = 200.613908 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.60717	0.85373	0.23473	1.000	1.000	1a	1
2 H	H_2	0.48277	0.09877	0.36832	1.000	1.000	1a	1
3 H	H_4	0.18025	0.12843	0.14040	1.000	1.000	1a	1
4 Eu	Eu_1	0.87636	0.43280	0.61440	1.000	1.000	1a	1
5 C	C	0.31173	0.98956	0.11719	1.000	1.000	1a	1
6 N	N	0.47931	0.97934	0.24800	1.000	1.000	1a	1
7 Br	Br_1	0.83750	0.46323	0.11589	1.000	1.000	1a	1
8 Br	Br_2	0.87546	0.93334	0.61364	1.000	1.000	1a	1
9 Br	Br_3	0.37560	0.41173	0.61280	1.000	1.000	1a	1
10 N	N_2	0.28799	0.84482	0.96187	1.000	1.000	1a	1
11 H	H_6	0.40186	0.70976	0.93012	1.000	1.000	1a	1
12 H	H_7	0.15259	0.86591	0.86244	1.000	1.000	1a	1

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Title $CH_5N_2EuCl_3$ ($FAEuCl_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.63069	5.60698	5.57930	86.0600	83.0200	86.4000

Unit-cell volume = 174.162505 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.60892	0.83821	0.24794	1.000	1.000	1a	1
2 H	H_2	0.48846	0.10834	0.37650	1.000	1.000	1a	1
3 H	H_4	0.18521	0.15213	0.12574	1.000	1.000	1a	1
4 Eu	Eu_1	0.87848	0.43592	0.61074	1.000	1.000	1a	1
5 C	C	0.31178	0.99476	0.11496	1.000	1.000	1a	1
6 N	N	0.48260	0.97887	0.25498	1.000	1.000	1a	1

7 Cl	Cl_1	0.83699	0.46935	0.11337	1.000	1.000	1a	1
8 Cl	Cl_2	0.88387	0.93622	0.60853	1.000	1.000	1a	1
9 Cl	Cl_3	0.37801	0.40806	0.61603	1.000	1.000	1a	1
10 N	N_2	0.28091	0.83774	0.96052	1.000	1.000	1a	1
11 H	H_6	0.38813	0.68428	0.93956	1.000	1.000	1a	1
12 H	H_7	0.14523	0.86755	0.85093	1.000	1.000	1a	1

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Title $CH_5N_2EuI_3$ ($FAEuI_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
6.24548	6.23562	6.20891	86.0800	84.4900	87.4500

Unit-cell volume = 239.946985 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.60060	0.86879	0.22655	1.000	1.000	1a	1
2 H	H_2	0.47913	0.09566	0.35112	1.000	1.000	1a	1
3 H	H_4	0.18550	0.10887	0.14469	1.000	1.000	1a	1
4 Eu	Eu_1	0.87176	0.42892	0.61033	1.000	1.000	1a	1
5 C	C	0.31409	0.98367	0.11921	1.000	1.000	1a	1
6 N	N	0.47644	0.98243	0.23831	1.000	1.000	1a	1
7 I	I_1	0.84132	0.46032	0.11088	1.000	1.000	1a	1
8 I	I_2	0.86999	0.93028	0.61708	1.000	1.000	1a	1
9 I	I_3	0.37043	0.41635	0.61104	1.000	1.000	1a	1
10 N	N_2	0.29292	0.84760	0.97209	1.000	1.000	1a	1
11 H	H_6	0.40621	0.72850	0.93417	1.000	1.000	1a	1
12 H	H_7	0.16019	0.86002	0.88431	1.000	1.000	1a	1

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Title CH_6NEuBr_3 ($MAEuBr_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.77933	5.73877	5.87569	90.0000	88.1800	90.0000

Unit-cell volume = 194.776263 Å^3

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.34719	0.52007	0.67165	1.000	1.000	1a	1
2 H	H_2	0.34719	0.81523	0.67165	1.000	1.000	1a	1
3 H	H_3	0.92760	0.51040	0.64332	1.000	1.000	1a	1
4 H	H_4	0.92760	0.82490	0.64332	1.000	1.000	1a	1
5 H	H_5	0.22613	0.66765	0.88907	1.000	1.000	1a	1
6 H	H_6	0.06262	0.66765	0.40997	1.000	1.000	1a	1
7 Eu	Eu_1	0.59488	0.16765	0.14433	1.000	1.000	1a	1
8 C	C	0.02595	0.66765	0.59463	1.000	1.000	1a	1
9 N	N	0.24795	0.66765	0.71308	1.000	1.000	1a	1
10 Br	Br_1	0.56609	0.16765	0.64290	1.000	1.000	1a	1
11 Br	Br_3	0.56783	0.66765	0.17757	1.000	1.000	1a	1
12 Br	Br_2	0.09259	0.16765	0.09976	1.000	1.000	1a	1

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Title CH_6NEuI_3 ($MAEuI_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
6.15939	6.12197	6.24635	90.0000	87.7500	90.0000

Unit-cell volume = 235.353282 Å^3

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1	H H_1	0.33808	0.52925	0.67169	1.000	1.000	1a	1
2	H H_2	0.33808	0.80605	0.67169	1.000	1.000	1a	1
3	H H_3	0.94389	0.52005	0.64616	1.000	1.000	1a	1
4	H H_4	0.94389	0.81525	0.64616	1.000	1.000	1a	1
5	H H_5	0.22310	0.66765	0.87697	1.000	1.000	1a	1
6	H H_6	0.07197	0.66765	0.42609	1.000	1.000	1a	1
7	Eu Eu_1	0.58387	0.16765	0.13832	1.000	1.000	1a	1
8	C C	0.03636	0.66765	0.59999	1.000	1.000	1a	1
9	N N	0.24426	0.66765	0.71090	1.000	1.000	1a	1
10	I I_1	0.56262	0.16765	0.63808	1.000	1.000	1a	1
11	I I_3	0.56516	0.66765	0.17558	1.000	1.000	1a	1
12	I I_2	0.08233	0.16765	0.09963	1.000	1.000	1a	1

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Title $CsYbBr_3$

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.03064	5.03076	5.03210	90.0000	89.9800	90.0000

Unit-cell volume = 127.352093 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1	Yb Yb_1	0.49996	0.25000	0.25184	1.000	1.000	1a	1
2	Cs Cs	0.00002	0.75000	0.74750	1.000	1.000	1a	1
3	Br Br_2	0.50001	0.25000	0.75088	1.000	1.000	1a	1
4	Br Br_1	0.49997	0.75000	0.24917	1.000	1.000	1a	1
5	Br Br_3	0.99998	0.25000	0.24921	1.000	1.000	1a	1

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Title $CsYbCl_3$

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.29124	5.29125	5.29162	90.0000	89.9800	90.0000

Unit-cell volume = 148.150930 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1	Yb	Yb_1	0.49997	0.25000	0.25140	1.000	1.000	1a	1
2	Cs	Cs	0.00002	0.75000	0.74767	1.000	1.000	1a	1
3	Cl	Cl_1	0.50001	0.25000	0.75120	1.000	1.000	1a	1
4	Cl	Cl_2	0.49997	0.75000	0.24915	1.000	1.000	1a	1
5	Cl	Cl_3	0.99997	0.25000	0.24918	1.000	1.000	1a	1

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Title $CsYbI_3$

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
6.03180	6.03177	6.03171	90.0000	89.9800	90.0000

Unit-cell volume = 219.448261 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1	Yb	Yb_1	0.49997	0.25000	0.25145	1.000	1.000	1a	1
2	Cs	Cs	0.00001	0.75000	0.74778	1.000	1.000	1a	1
3	I	I_1	0.50001	0.25000	0.75160	1.000	1.000	1a	1
4	I	I_3	0.49997	0.75000	0.24887	1.000	1.000	1a	1
5	I	I_2	0.99996	0.25000	0.24890	1.000	1.000	1a	1

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Title $CH_5N_2YbBr_3$ ($FAYbBr_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.77653	5.74321	5.74534	85.5700	83.3400	86.9900

Unit-cell volume = 188.571901 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.60572	0.84611	0.24795	1.000	1.000	1a	1
2 H	H_2	0.48640	0.10519	0.36964	1.000	1.000	1a	1
3 H	H_4	0.18494	0.13896	0.12773	1.000	1.000	1a	1
4 Yb	Yb_1	0.87062	0.44038	0.60517	1.000	1.000	1a	1
5 C	C	0.31321	0.99060	0.11717	1.000	1.000	1a	1
6 N	N	0.48093	0.97991	0.25249	1.000	1.000	1a	1
7 Br	Br_1	0.83624	0.46482	0.10696	1.000	1.000	1a	1
8 Br	Br_2	0.88197	0.94132	0.60578	1.000	1.000	1a	1
9 Br	Br_3	0.36860	0.41980	0.60748	1.000	1.000	1a	1
10 N	N_2	0.28707	0.83537	0.96889	1.000	1.000	1a	1
11 H	H_6	0.39779	0.69178	0.94870	1.000	1.000	1a	1
12 H	H_7	0.15509	0.85718	0.86182	1.000	1.000	1a	1

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Title $CH_5N_2YbCl_3$ ($FAYbCl_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
5.50725	5.46797	5.46504	84.8100	82.5200	86.8100

Unit-cell volume = 162.341476 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.61696	0.83952	0.24970	1.000	1.000	1a	1
2 H	H_2	0.49017	0.11084	0.38107	1.000	1.000	1a	1
3 H	H_4	0.18009	0.15355	0.12482	1.000	1.000	1a	1
4 Yb	Yb_1	0.86935	0.43757	0.60967	1.000	1.000	1a	1
5 C	C	0.31222	0.99539	0.11523	1.000	1.000	1a	1
6 N	N	0.48616	0.98058	0.25769	1.000	1.000	1a	1
7 Cl	Cl_1	0.83370	0.46814	0.10974	1.000	1.000	1a	1
8 Cl	Cl_2	0.87952	0.93898	0.60796	1.000	1.000	1a	1
9 Cl	Cl_3	0.36783	0.41569	0.61062	1.000	1.000	1a	1
10 N	N_2	0.28555	0.83314	0.96092	1.000	1.000	1a	1
11 H	H_6	0.39800	0.67900	0.94455	1.000	1.000	1a	1
12 H	H_7	0.14904	0.85901	0.84782	1.000	1.000	1a	1

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Title $CH_5N_2YbI_3$ ($FAYbI_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
6.15631	6.13494	6.11064	85.8500	84.4400	87.6300

Unit-cell volume = 228.965068 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1 H	H_1	0.60281	0.86586	0.23037	1.000	1.000	1a	1
2 H	H_2	0.48010	0.09600	0.35702	1.000	1.000	1a	1
3 H	H_4	0.18403	0.11056	0.14537	1.000	1.000	1a	1
4 Yb	Yb_1	0.86798	0.43472	0.60655	1.000	1.000	1a	1
5 C	C	0.31422	0.98376	0.11981	1.000	1.000	1a	1
6 N	N	0.47713	0.98128	0.24234	1.000	1.000	1a	1

7	I	I_1	0.83827	0.45847	0.10758	1.000	1.000	1a	1
8	I	I_2	0.87159	0.93700	0.61492	1.000	1.000	1a	1
9	I	I_3	0.36622	0.41997	0.60742	1.000	1.000	1a	1
10	N	N_2	0.29434	0.84422	0.97155	1.000	1.000	1a	1
11	H	H_6	0.40878	0.72243	0.93833	1.000	1.000	1a	1
12	H	H_7	0.16311	0.85715	0.87854	1.000	1.000	1a	1

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Title CH_6NYbBr_3 ($MAYbCl_3$)

Space group name *P 1*

Lattice parameters

a	b	c	alpha	beta	gamma
5.63937	5.60039	5.71449	90.0000	86.9700	90.0000

Unit-cell volume = 180.226545 $Å^3$

Structure parameters

		x	y	z	Occ.	B	Site	Sym.
1	H	H_1	0.34747	0.51430	0.67614	1.000	1.000	1a	1
2	H	H_2	0.34747	0.81651	0.67614	1.000	1.000	1a	1
3	H	H_3	0.92547	0.50438	0.60542	1.000	1.000	1a	1
4	H	H_4	0.92547	0.82643	0.60542	1.000	1.000	1a	1
5	H	H_5	0.19599	0.66540	0.88684	1.000	1.000	1a	1
6	H	H_6	0.09167	0.66540	0.37944	1.000	1.000	1a	1
7	Yb	Yb_1	0.60327	0.16540	0.12998	1.000	1.000	1a	1
8	C	C	0.03142	0.66540	0.56531	1.000	1.000	1a	1
9	N	N	0.24149	0.66540	0.70892	1.000	1.000	1a	1
10	Br	Br_1	0.57591	0.16540	0.62891	1.000	1.000	1a	1
11	Br	Br_2	0.59910	0.66540	0.14678	1.000	1.000	1a	1
12	Br	Br_3	0.10171	0.16540	0.10276	1.000	1.000	1a	1

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Title CH_6NYbI_3 ($MAYbI_3$)

Space group name P_1

Lattice parameters

a	b	c	alpha	beta	gamma
6.01742	5.97497	6.07974	90.0000	86.8900	90.0000

Unit-cell volume = 218.268442 $Å^3$

Structure parameters

			x	y	z	Occ.	B	Site	Sym.
1	H	H_1	0.33672	0.52371	0.67587	1.000	1.000	1a	1
2	H	H_2	0.33672	0.80710	0.67587	1.000	1.000	1a	1
3	H	H_3	0.94058	0.51427	0.60840	1.000	1.000	1a	1
4	H	H_4	0.94058	0.81654	0.60840	1.000	1.000	1a	1
5	H	H_5	0.19319	0.66540	0.87397	1.000	1.000	1a	1
6	H	H_6	0.09776	0.66540	0.39586	1.000	1.000	1a	1
7	Yb	Yb_1	0.59542	0.16540	0.12453	1.000	1.000	1a	1
8	C	C	0.04018	0.66540	0.57069	1.000	1.000	1a	1
9	N	N	0.23663	0.66540	0.70639	1.000	1.000	1a	1
10	I	I_2	0.57468	0.16540	0.62445	1.000	1.000	1a	1
11	I	I_1	0.59930	0.66540	0.14402	1.000	1.000	1a	1
12	I	I_3	0.09467	0.16540	0.10361	1.000	1.000	1a	1

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