Supporting Information

The Wondrous World of ABX_3 Molecular Perovskites

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Source Data for Literature Survey

Table S1. Columns in order: reference, year of publication, sum formula, A-site cation, space-group.

X = $(C_2N_3)^-$

1	2020	$(ASU)Cd(C_2N_3)_3$	azaspiroundecanium	$Pna2_1$ 100 K
2	2003	$(BeTriBu)B(C_2N_3)_3$ ($B = Mn^{2+}, Co^{2+}$)	benzyltributylammonium	*Pnma* RT
2	2003	$(BeTriEt)B(C_2N_3)_3$ ($B = Mn^{2+}, Fe^{2+}$)	benzyltriethylammonium	*Pnma* RT
3	2005	$(Cp^*{}_2Co)B(C_2N_3)_3$ ($B = Mn^{2+}, Co^{2+}, Ni^{2+}$)	decamethylcobaltocenium	*Im*-3 123 K
3	2005	$(Cp^*{}_2Fe)B(C_2N_3)_3$ ($B = Mn^{2+}, Fe^{2+}, Co^{2+}, Ni^{2+}, Cd^{2+}$)	decamethylferrocenium	*Im*-3 123 K
4	2024	$(DEP)Ni(C_2N_3)_3$	diethylpiperidinium	$P2_1/c$ RT
4	2024	$(DIP)Ni(C_2N_3)_3$	diisopropylpiperidinium	$P2_1/c$ RT
4	2024	$(DPP)Ni(C_2N_3)_3$	dipropylpiperidinium	$C2/c$ RT
5	2017	$(Et_3(CH_2CHCH_2)P)Mn(C_2N_3)_3$	allyltriethylphosphonium	$P2_1/c$ RT
6	2018	$(Et_3P(CH_2)_2Cl)Cd(C_2N_3)_3$	triethyl-(2-chloro-ethyl)-phosphonium	$P2_12_12_1$ RT
7	2019	$(Et_3P(CH_2)_2Cl)Mn(C_2N_3)_3$	triethyl-(2-chloro-ethyl)-phosphonium	$P2_1/c$ RT
6	2018	$(Et_3P(CH_2)_2F)Cd(C_2N_3)_3$	triethyl-(2-fluoro-ethyl)-phosphonium	$C2/c$ RT
7	2019	$(Et_3P(CH_2)_2F)Mn(C_2N_3)_3$	triethyl-(2-fluoro-ethyl)-phosphonium	$C2/c$ RT *Pnca* 347 K
5	2017	$(Et_3(CH_2OCH_3)P)Mn(C_2N_3)_3$	triethylmethoxy-methylphosphonium	$P2_12_12_1$ RT
8	2017	$(Et_3(n\text{-}Pr)P)Cd(C_2N_3)_3$	propyltriethylphosphonium	$P2_12_12_1$ RT
5	2017	$(Et_3(n\text{-}Pr)P)Mn(C_2N_3)_3$	propyltriethylphosphonium	$P2_12_12_1$ RT
9	2021	$(Et_4P)Mn(C_2N_3)_3$	tetraethylphosphonium	$P2_12_12_1$ RT
10	2020	$(Pr_3(CH_2CHOHCH_3)N)Mn(C_2N_3)_3$	(2-hydroxy-propyl)-tripropyl-ammonium	$P\text{-}42_1c$ 143 K
10	2020	$(Pr_3(CH_3CHCH_2OH)N)Mn(C_2N_3)_3$	(2-hydroxy-1-methyl–ethyl)-tripropyl-ammonium	$Pna2_1$ 193 K $P2_12_12_1$ 282 K
11	2004	$(SPh_3)Mn(C_2N_3)_3$	triphenylsulfonium	$P2_1/c$ RT
12	2019	$(TriBuMeN)Co(C_2N_3)_3$	tributylmethylammonium	$P2_1/n$ RT
12	2019	$(TriBuMeN)Fe(C_2N_3)_3$	tributylmethylammonium	$P2_1/n$ RT
12	2019	$(TriBuMeN)Mn(C_2N_3)_3$	tributylmethylammonium	$P2_1/n$ RT
12	2019	$(TriBuMeN)Ni(C_2N_3)_3$	tributylmethylammonium	$P2_1/n$ RT
9	2021	$(TriBuMeP)Mn(C_2N_3)_3$	tributylmethylphosphonium	$P2_1/n$ RT
13	2021	$(TriPrMeN)Co(C_2N_3)_3$	tripropylmethylammonium	*Pnma* RT
13	2021	$(TriPrMeN)Mn(C_2N_3)_3$	tripropylmethylammonium	*Pnma* RT
13	2021	$(TriPrMeN)Ni(C_2N_3)_3$	tripropylmethylammonium	*Pnma* RT
4	2024	$(PEP)Ni(C_2N_3)_3$	ethylpropylpiperidinium	$P2_1/c$ RT
14	2023	$(Pr_3NBu)Mn(C_2N_3)_3$	tripropylbutylammonium	*Pbcn* RT
15	2018	$(Pr_4N)Cd(C_2N_3)_3$	tetrapropylammonium	$P\text{-}42_1c$ RT
16,17	2016	$(Pr_4N)Co(C_2N_3)_3$	tetrapropylammonium	$P\text{-}42_1c$ 200 K
16,17	2016	$(Pr_4N)Fe(C_2N_3)_3$	tetrapropylammonium	$P\text{-}42_1c$ 200 K
18,17,19	2005	$(Pr_4N)Mn(C_2N_3)_3$	tetrapropylammonium	$P\text{-}42_1c$ RT
18,16	2005	$(Pr_4N)Ni(C_2N_3)_3$	tetrapropylammonium	$P\text{-}42_1c$ 160 K

X = $(N_3)^-$

20	2017	$(CPrN)Mn(N_3)_3$	cyclopropylammonium	*Pbca* 296 K
21	1986	$(Et_4N)Ca(N_3)_3$	tetraethylammonium	$P2/m$ 293 K
22	2013	$(MeN)Mn(N_3)_3$	methylammonium	$P2_1/c$ 173 - 320 K
23	2019	$(Me_2EtN)Mn(N_3)_3$	dimethylethylammonium	*Cc* 296 K
24	2014	$(Me_2N)Cd(N_3)_3$	dimethylammonium	*P-1* 296 K *R*-3 203 - 273 K
22	2013	$(Me_2N)Mn(N_3)_3$	dimethylammonium	$P2_1$ 173 K *Cmca* 323 K
25	2015	$(Me_3N)Cd(N_3)_3$	trimethylammonium	$P2_1/c$ 283 K $C2/c$ 348 K

[22]	2013	$(Me_3N)Mn(N_3)_3$	trimethylammonium	*P*2$_1$/*c* 173 - 298 K *C*2/*c* 330 - 350 K *R*-3*m* 360 - 393 K
[26]	1988	$(Me_4N)Ca(N_3)_3$	tetramethylammonium	*P*4/*nmm* RT
[27,28]	2000	$(Me_4N)Cd(N_3)_3$	tetramethylammonium	*C*2/*c* 220 K *P*2$_1$/*m* 300 K *Pm*-3/*m* 350 K
[22]	2013	$(Me_4N)Mn(N_3)_3$	tetramethylammonium	*P*2$_1$/*m* 173 K *Pm*-3*m* 333 K

X = (B*M*$_4$)$^-$ with *M* = F and H

[29]	2019	$(H_2dabco)Na(BF_4)_3$	dabconium	*Pa*-3 293 K *Pm*-3*m* 408 K
[30]	2017	$(H_2dabco)K(BF_4)_3$	dabconium	*Pa*-3 293 K
[30]	2017	$(H_2pz)Na(BF_4)_3$	piperazinium	*P*4$_3$ 293 K
[30]	2021	$(MedabcoF)Rb(BF_4)_3$	fluoromethyldabconium	*P*2$_1$/*c* 168 K *P*4$_2$/*mbc* 253 K *Fm*-3*c* 315 K *Pm*-3*m* 353 K
[31]	2015	$(NH_4)Ca(BH_4)_3$	ammonium	*Pm*-3*m* RT

X = (CN)$^-$

[32]	2016	$(Ac)_2KFe(CN)_6$	acetamidinium	*C*2/*m* 150 K *R*-3*m* RT *Fm*-3*m* 395 K
[33]	2016	$(Az)_2KCo(CN)_6$	azetidinium	*Fm*-3*m* 113 K
[34]	2022	$(Az)_2KCr(CN)_6$	azetidinium	*Fm*-3*m* 210 K
[34]	2022	$(Az)_2KFe(CN)_6$	azetidinium	*Fm*-3*m* 240 K
[32]	2016	$(Gua)_2KFe(CN)_6$	guanidinium	*R*-3*c* RT *R*-3*m* 425 K *Fm*-3*m* 455 K
[35]	2015	$(Im)_2KCo(CN)_6$	imidazolium	*R*-3*m* 293 K
[36]	2010	$(Im)_2KFe(CN)_6$	imidazolium	*C*2/*c* 83 K *R*-3*m* 173, 293 K
[37]	2013	$(Me_2N)_2KCo(CN)_6$	dimethylammonium	*P*4/*mnc* 113, 280, 293 K
[38]	2015	$(Me_2N)_2KFe(CN)_6$	dimethylammonium	*P*4/*mnc* 165 K, RT
[39]	2019	$(Me_2N)_2KCr(CN)_6$	dimethylammonium	*P*4/*mnc* 140, 230 K
[40]	2016	$(MeN)_2KCo(CN)_6$	methylammonium	*C*2/*c* 293 K *Fm*-3*m* 463 K
[38]	2016	$(MeN)_2KFe(CN)_6$	methylammonium	*C*2/*c* 193 K *Fm*-3*m* 443 K
[40]	2016	$(MeN)_2NaCo(CN)_6$	methylammonium	*Fm*-3*m* 293 K
[41]	1994	$(MeN)_2NaFe(CN)_6$	methylammonium	*Fm*-3*m* 295 K
[40]	2016	$(MeN)_2RbCo(CN)_6$	methylammonium	*C*2/*c* 293 K
[42]	2018	$(Me_3N)_2KFe(CN)_6$	trimethylammonium	*C*2/*c* 113 K *Fm*-3*m* 350 K
[43]	2022	$(Me_3FMeN)_2KFe(CN)_6$	Trimethylfluoromethylammonium	*C*2/*c* 243 K
[44]	2020	$(Me_3NOH)_2KCo(CN)_6$	Trimethylhydroxylammonium	*Cc* 100 K *Fm*-3*m* 440 K
[45]	2017	$(Me_3NOH)_2KFe(CN)_6$	Trimethylhydroxylammonium	*Cc* RT *Fm*-3*m* 408 K
[41]	1994	$(Me_4N)_2CsCo(CN)_6$	tetramethylammonium	*I*2/*m* 295 K
[46]	2000	$(Me_4N)_2CsCr(CN)_6$	tetramethylammonium	*C*2/*c* RT
[46]	2000	$(Me_4N)_2KCr(CN)_6$	tetramethylammonium	*Fm*-3*m* RT
[38]	2016	$(Me_4N)_2KFe(CN)_6$	tetramethylammonium	*I*4/*m* RT *Fm*-3*m* 373 K
[47]	1997	$(Me_4N)_2RbCr(CN)_6$	tetramethylammonium	*R*-3*m* RT
[47]	1997	$(Me_4N)_2RbFe(CN)_6$	tetramethylammonium	*R*-3*m* RT
[47]	1997	$(Me_4N)_2TlCr(CN)_6$	tetramethylammonium	*R*-3*m* RT
[47]	1997	$(Me_4N)_2TlFe(CN)_6$	tetramethylammonium	*C*2/*c* RT
[48]	2021	$(Pyr)_2KCr(CN)_6$	pyrrolidinium	*Fm*-3*m* 295 K

X = [Au(CN)$_2$]$^-$ and **[Ag(CN)$_2$]$^-$**

[49]	2016	$(PPN)Cd(Au(CN)_2)_3$	bistriphenlyphosphineiminium	*I*2/*a* 291 K
[50]	2007	$(PPN)Co(Au(CN)_2)_3$	bistriphenlyphosphineiminium	*R*-3*c* RT
[49]	2016	$(PPN)Mn(Au(CN)_2)_3$	bistriphenlyphosphineiminium	*I*2/*a* 150 K
[50]	2007	$(PPN)Ni(Au(CN)_2)_3$	bistriphenlyphosphineiminium	*R*-3*c* RT

X = (HCOO)$^-$

[51]	2017	$(Ac)Mn(HCOO)_3$	acetamidinium	*P*2$_1$/*n* 100 K *Imma* 320 K
[52]	2011	$(Az)Cu(HCOO)_3$	azetidinium	*P*2$_1$/*c* 123, 280, 243, 260 K *Pnma* 300, 333 K
[53]	2004	$(Az)Mn(HCOO)_3$	azetidinium	*P*2$_1$/*c* 180 K, *Pnma* 290 K
[54]	2012	$(Az)Zn(HCOO)_3$	azetidinium	*Pnma* RT
[55]	2011	$(DMe_2N)Co(DCOO)_3$	perdeuterodimethylammonium	*Cc* 93 K, *R*-3*c* 293, 373 K
[56]	2015	$(EtN)Cu(HCOO)_3$	ethylammonium	*Pna*2$_1$ 93, 180, 291, 320, 340 K *P*2$_1$2$_1$2$_1$ 360 K
[57]	2014	$(EtN)Mg(HCOO)_3$	ethylammonium	*Pna*2$_1$ 93, 280, 292, 363 K *R*-3 378 K *Imma* 430 K
[53]	2004	$(EtN)Mn(HCOO)_3$	ethylammonium	*Pna*2$_1$ 180, 290 K
[58]	2016	$(EtN)Na_{0.5}Al_{0.5}(HCOO)_3$	ethylammonium	*Pn* 270 K *P*2$_1$/*n* 375 K
[58]	2016	$(EtN)Na_{0.5}Al_{0.475}Cr_{0.025}(HCOO)_3$	ethylammonium	*Pn* RT
[58]	2016	$(EtN)Na_{0.5}Cr_{0.5}(HCOO)_3$	ethylammonium	*Pn* 297 K *P*2$_1$/*n* 400 K
[59]	2015	$(EtN)Na_{0.5}Fe_{0.5}(HCOO)_3$	ethylammonium	*Pn* 297 K *P*2$_1$/*n* 377 K
[60]	2015	$(Fmd)Co(HCOO)_3$	formamidinium	*Pnna* 295 K
[61]	2017	$(Fmd)Cu(HCOO)_3$	formamidinium	*Pnna* 173 K
[60]	2015	$(Fmd)Fe(HCOO)_3$	formamidinium	*Pnna* 294 K
[62]	2012	$(Fmd)Mg(HCOO)_3$	formamidinium	*Pnna* 120 K
[63]	2014	$(Fmd)Mn(HCOO)_3$	formamidinium	*C*2/*c* 110, 295 K *R*-3*c* 355 K
[64]	1986	$(Fmd)Zn(HCOO)_3$	formamidinium	*Pnna* 295 K
[65]	2009	$(Gua)Co(HCOO)_3$	guanidinium	*Pnna* 293 K
[65]	2009	$(Gua)Cu(HCOO)_3$	guanidinium	*Pna*2$_1$ 293 K
[66]	2016	$(Gua)Cd(HCOO)_3$	guanidinium	*R*-3*c* 150, 250, 300, 450 K
[65]	2009	$(Gua)Fe(HCOO)_3$	guanidinium	*Pnna* 293 K
[62]	2012	$(Gua)Mg(HCOO)_3$	guanidinium	*Pnna* 298 K

65	2009	$(Gua)Mn(HCOO)_3$	guanidinium	*Pnna* 293 K
65	2009	$(Gua)Ni(HCOO)_3$	guanidinium	*Pnna* 293 K
65	2009	$(Gua)Zn(HCOO)_3$	guanidinium	*Pnna* 293 K
67	2016	$(Im)Mg(HCOO)_3$	imidazolium	$P2_1/n$ 296 K
68	2013	$(Im)Mn(HCOO)_3$	imidazolium	$P2_1/n$ 293 K $P\text{-}42_1m$ 453 K
69	2017	$(Hym)Co(HCOO)_3$	hydrazinium	$Pna2_1$ 100, 298 K *Pnma* 353, 393 K
70	2016	$(Hym)Fe(HCOO)_3$	hydrazinium	$Pna2_1$ 290 K *Pnma* 360 K
71	2014	$(Hym)Mg(HCOO)_3$	hydrazinium	$P2_12_12_1$ 110, 200, 292 K $P6_3$ 400 K
71	2014	$(Hym)Mn(HCOO)_3$	hydrazinium	$Pna2_1$ 110, 200, 290 K *Pnma* 400 K
71	2014	$(Hym)Zn(HCOO)_3$	hydrazinium	$Pna2_1$ 110, 200, 290 K *Pnma* 375 K
72	2021	$(Me_2Hym)Mn(HCOO)_3$	dimethylhydrazinium	$P2_1/n$ 99.9, 299.9 K
73	2017	$(MeHym)Fe(HCOO)_3$	methylhydrazinium	*R*-3*c* 200, 280, 330 K
73	2017	$(MeHym)Mg(HCOO)_3$	methylhydrazinium	*R*-3*c* 240, 280, 345 K
73	2017	$(MeHym)Mn(HCOO)_3$	methylhydrazinium	*P*1 100 K *R*-3*c* 230, 290, 330 K
73	2017	$(MeHym)Zn(HCOO)_3$	methylhydrazinium	*R*-3*c* 180, 300, 350 K
74	2010	$(Me_2N)Cd(HCOO)_3$	dimethylammonium	*R*-3*c* 293 K
75	2004	$(Me_2N)Co(HCOO)_3$	dimethylammonium	*R*-3*c* 297 K
76	1973	$(Me_2N)Cu(HCOO)_3$	dimethylammonium	*I*2/*c* 295 K
77	2009	$(Me_2N)Fe(HCOO)_3$	dimethylammonium	*R*-3*c* 273 K
78	2008	$(Me_2N)Mg(HCOO)_3$	dimethylammonium	*R*-3*c* 293 K
53	2004	$(Me_2N)Mn(HCOO)_3$	dimethylammonium	*R*-3*c* 180, 290 K
79	2015	$(Me_2N)Na_{0.5}Cr_{0.5}(HCOO)_3$	dimethylammonium	*R*-3 115, 302 K
80	2014	$(Me_2N)Na_{0.5}Fe_{0.5}(HCOO)_3$	dimethylammonium	*R*-3 115, 293 K
75	2004	$(Me_2N)Ni(HCOO)_3$	dimethylammonium	*P*-1 110 K *R*-3*c* 297 K
81	2008	$(Me_2N)Zn(HCOO)_3$	dimethylammonium	*R*-3*c* 273 K
72	2021	$(Me_2Hym)Mn(HCOO)_3$	dimethylhydrazinium	$P2_1/n$ 100, 300 K
82	2016	$(MeN)Co(HCOO)_3$	methylammonium	*Pnma* 100 K
66	2016	$(MeN)Cd(HCOO)_3$	methylammonium	*Pnma* RT
66	2016	$(MeN)Fe(HCOO)_3$	methylammonium	*Pnma* RT
66	2016	$(MeN)Mg(HCOO)_3$	methylammonium	*Pnma* RT
53	2004	$(MeN)Mn(HCOO)_3$	methylammonium	*Pnma* 180, 290 K
66	2016	$(MeN)Zn(HCOO)_3$	methylammonium	*Pnma* RT
83	2014	$(Me_4N)Mn(HCOO)_3$	tetramethylammonium	*Pnma* RT
83	2014	$(NH_4)Mn(HCOO)_3$	ammonium	*Im*-3 RT
84,85	1983	$(NH_4)Cd(HCOO)_3$	ammonium	$Pna2_1$ 100, 295, 350 K

X = $(H_2POO)^-$

86	2017	$(Fmd)Mn(H_2POO)_3$	formamidinium	$P2_1/c$ 115 K *C*2/*c* RT
87	2022	$(Gua)Cd(H_2POO)_3$	guanidinium	*R*-3*c* 293 K
87	2022	$(Gua)Co(H_2POO)_3$	guanidinium	*I*2/*m* 293 K
86	2017	$(Gua)Mn(H_2POO)_3$	guanidinium	*I*2/*m* 298 K *P*-1 302 K
88	2021	$(HyEt)Mn(H_2POO)_3$	hydroxyethylammonium	$P2_1/n$ RT
87	2022	$(Im)Cd(H_2POO)_3$	imidazolium	$P2_1/c$ RT
87	2022	$(Im)Co(H_2POO)_3$	imidazolium	*Pbca* 295 K
86	2017	$(Im)Mn(H_2POO)_3$	imidazolium	$P2_1/c$ RT
89	2020	$(MeHym)Mn(HCOO)_3$	methylhydrazinium	*Pnma* 100, 295 K
90	2018	$(Me_2N)Mn(H_2POO)_3$	dimethylammonium	$P2_1/c$ RT
87	2022	$(Pyr)Cd(H_2POO)_3$	pyrrolidinium	*Aea*2 295 K
88	2021	$(Pyr)Mn(H_2POO)_3$	pyrrolidinium	$P2_1/n$ RT
86	2017	$(Trz)Mn(H_2POO)_3$	triazolium	$P2_1/c$ RT

X = $(SCN)^-$

91	2021	$(Me_2N)_2CdNi(SCN)_6$	dimethylammonium	*P*-1 293 K
91	2021	$(Me_2N)_2CdMn(SCN)_6$	dimethylammonium	*P*-1 293 K
91	2021	$(Me_3S)Cd(SCN)_3$	trimethylsulfonium	*Pa*-3 RT
92	2016	$(NH_4)_2CdNi(SCN)_6$	ammonium	$P2_1/c$ 90 K, RT

X = $(ClO_4)^-$

30	2017	$(H_2dabco)K(ClO_4)_3$	dabconium	*Pa*-3 293 K
30	2017	$(H_2dabco)Na(ClO_4)_3$	dabconium	*Pa*-3 293 K
93	2018	$(H_2dabco)Rb(ClO_4)_3$	dabconium	*Pa*-3 293 K
94	2018	$(H_2dabco)K(ClO_4)_3$	hydroxydabconium	$P2_1/c$ 223 K *Fm*-3*c* RT
95	2017	$(H_2hpz)K(ClO_4)_3$	homopiperazinium	*Pbca* RT
30	2017	$(H_2pz)Na(ClO_4)_3$	piperazinium	$P2_1/c$ RT, 378 K

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