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Supporting information for article:

Chain caesium borophosphates with B:P ratio 1:2: synthesis, structure relationships and low-temperature thermodynamic properties

Larisa Shvanskaya, Olga Yakubovich, Polina Krikunova, Evgeny Ovchenkov and Alexander Vasiliev

Table S1 Chemical composition of sample (II)* determined by EDS analysis

Element (in atomic %)		B	O	P	Mn	Cs
	Point 1	8,7(2)	67,2(2)	13,2(1)	7,5(1)	3,5(1)
	Point 2	6,5(2)	68,4(2)	13,7(1)	7,8(1)	3,6(1)
	Point 3	7,1(2)	68,1(2)	13,5(1)	7,7(1)	3,6(1)
Average value		7.4	67.9	13.5	7.7	3.6

*Chemical formula, calculated from EDS results: $Cs_{0.53}Mn_{1.14}B_{1.09}P_2O_{10.05}$.

Chemical formula from results of single crystal structure determination: $Cs_{0.51}Mn_{1.17}B_{1.00}P_2O_{10.45}$

Table S2 Bond valence data for $Cs[BP_2O_6(OH)_2]$ (I)

Atom	Cs	B	P1	P2	H1	H2	H3	Σ
O1	0.097	0.791	1.179					2.067
O2	0.032	0.763		1.238				2.033
O3	0.069; 0.060	0.763		1.202				2.094
O4	0.131; 0.101		1.350			0.42		2.002
O5	0.073	0.776	1.154					2.003
O6	0.131		1.350		0.50			1.981
O7	0.138; 0.033			1.258		0.58		2.009
O8	0.096			1.346			0.50	1.942
Σ	0.961	3.093	5.033	5.044	0.50	1.00	0.50	

Table S3 Composition, crystallographic parameters and selected geometric characteristics for the Mn members of $A_xM_y(H_2O)_2[BP_2O_8]\bullet z(H_2O)$ family.

Formula	*a*	*c*	*c*/*a*	*V*	Space group	Mn2–O, average, (Å)	Reference
$(H)_{0.5}Mn_{1.25}(H_2O)_{1.5}[BP_2O_8]\cdot H_2O$	9.6547(12)	15.791(3)	1.64	1274.7	P6122	2.28	Yimaz *et al.,* 2005
$LiMn(H_2O)_2[BP_2O_8]\cdot H_2O$	9.5765 (4)	15.857 (1)	1.66	1259.4	P6522	-	Zhuang *et al.,* 2008
$NaMn(H_2O)_2[BP_2O_8]\cdot H_2O$	9.589(5)	15.939(9)	1.66	1269	P6122	-	Kniep *et al.,* 1997
$NaMn(H_2O)_2$ $[BP_2O_8)H_2O$	9.6023(14)	16.037(3)	1.67	1280.5	P6522	-	Yakubovich *et al.,* 2009
$(NH_4)_{0.50}Mn_{1.25}(H_2O)_2[BP_2O_8]\cdot 0.3H_2O$	9.6559(3)	15.7939(6)	1.64	1275.3	P6522	2.25	Li *et al.,* 2017
$KMn(H_2O)_2[BP_2O_8]H_2O$	9.683(4)	16.139(6)	1.67	1310.5	P6522	-	Wang, 2012
$KMn(H_2O)_2[BP_2O_8]H_2O^*$	9.639(1)	15.931(2)	1.65	1281.8	P6122	-	Kniep *et al.,* 1997
$Cs_{0.51}Mn_{1.17}(H_2O)_2[BP_2O_8]\bullet 0.45H_2O$	9.6292(3)	15.8051(5)	1.64	1269.1	P6122	2.17	Our work

*powder data

Table S4 Bond valence data for $CsMn[BP_2O_8(OH)]$ (III)

Atom	Cs	Mn	B	P1	P2	H	Σ
O1	0.090	0.607			1.296		1.993
O2	0.108; 0.105		0.761	1.154			2.128
O3	0.129	0.692		1.310			2.131
O4	0.136		0.741		1.192		2.069
O5	0.078	0.692		1.252			2.022
O6	0.140; 0.134	0.414		1.350			2.038
O7			0.729		1.192		1.921
O8	0.112	0.654			1.321		2.087
O9	0.118		0.808			1.00	1.926
Σ	1.150	3.059	0.039	5.066	5.001	1.00	