Crystal structure and spin-trimer magnetism of $Rb_{2.3}(H_2O)_{0.8}Mn_3[B_4P_6O_{24}(O,OH)_2]$

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Table S1. $Rb_{2.3}(H_2O)_{0.8}Mn_3[B_4P_6O_{24}(O,OH)_2]$. Atomic coordinates and equivalent isotropic displacement factors ($Å^2$)

Atom	*x/a*	*y/b*	*z/c*	U_{eq}/U_{iso}*
Rb1	0.16319(7)	0.3908(2)	0.22222(11)	0.0410(5)
Rb2	0.1483(4)	0.4742(10)	0.1958(6)	0.0410(5)
Rb3	0.0	0.6443(8)	0.25	0.059(2)
Mn1	0.42472(6)	0.4078(2)	0.48702(9)	0.0114(3)
Mn2	0.5	0.6710(2)	0.25	0.0186(6)
P1	0.29291(12)	0.2122(3)	0.45598(18)	0.0106(6)

P2	0.38004(11)	0.4722(3)	0.23048(19)	0.0121(6)
P3	0.06099(11)	0.2816(3)	0.46685(19)	0.0134(7)
B1	0.2881(5)	0.4976(13)	0.3893(8)	0.0108(19)
B2	0.1748(5)	0.1612(13)	0.5434(7)	0.0108(19)
O1	0.3198(2)	0.5482(6)	0.2858(4)	0.0088(10)
O2	0.2444(3)	0.2135(7)	0.5542(3)	0.0099(15)
O3	0.4169(3)	0.5882(8)	0.1651(3)	0.0178(16)
O4	0.3538(3)	0.3522(7)	0.1527(4)	0.0116(9)
O5	0.2758(3)	0.3390(7)	0.3765(4)	0.0110(16)
O6	0.4264(3)	0.4069(8)	0.3143(3)	0.0116(9)
O7	0.0459(3)	0.3235(7)	0.3507(4)	0.0150(17)
O8	0.3634(2)	0.2145(7)	0.4950(4)	0.0129(15)
O9	0.2776(2)	0.0700(7)	0.3923(4)	0.0116(9)
O10 (OH)	0.0333(3)	0.3984(9)	0.5472(5)	0.0210(16)
O11	0.1367(3)	0.2765(7)	0.4849(4)	0.0144(15)
O12	0.0299(2)	0.1334(6)	0.4945(4)	0.0148(16)
O13	0.3280(2)	0.5242(6)	0.4850(4)	0.0088(10)
O14 (H_2O)	0.0512(10)	0.619(3)	0.2496(18)	0.059(2)
H1	0.029(6)	0.486(5)	0.526(11)	0.08(6)*

site occupations: Rb1 0.807(4), Rb2 0.189(4), Rb3 0.135(4), O14 0.38(1)

Table S2. $Rb_{2.3}(H_2O)_{0.8}Mn_3[B_4P_6O_{24}(O,OH)_2]$. Bond-valence data

Atom	Mn1	Mn2	P1	P2	P3	B1	B2	Rb1**	Rb2**	Rb3**	H1	Σ
O1				1.195		0.723		0.057				1.98
O2			1.205				0.737	0.134	0.012			2.09
O3	0.340	0.424↓2		1.293				0.052				2.11
O4				1.208			0.780		0.006			1.99
O5			1.186			0.747		0.112				2.04
O6	0.413	0.045↓2		1.335						0.040↓2		1.83
O7		0.458↓2			1.354			0.146	0.017	0.014↓2		1.99
O8	0.371		1.394					0.113	0.023			1.90
O9			1.202			0.795		0.144	0.026			2.17
O10					1.179				0.015	0.097↓2	1.0	2.29
O11					1.241		0.733		0.007			1.98
O12	0.281; 0.372				1.262							1.92
O13	0.317					0.821	0.817					1.96
O14*								0.087	0.106			0.19
Σ	2.09	1.85	4.99	5.03	5.04	3.09	3.07	0.84	0.21	0.30		

Values marked by ↓2 contribute two times to the sum along the column by symmetry. *Without the valence contributions of hydrogen atoms. **Taking into account the sites' population.

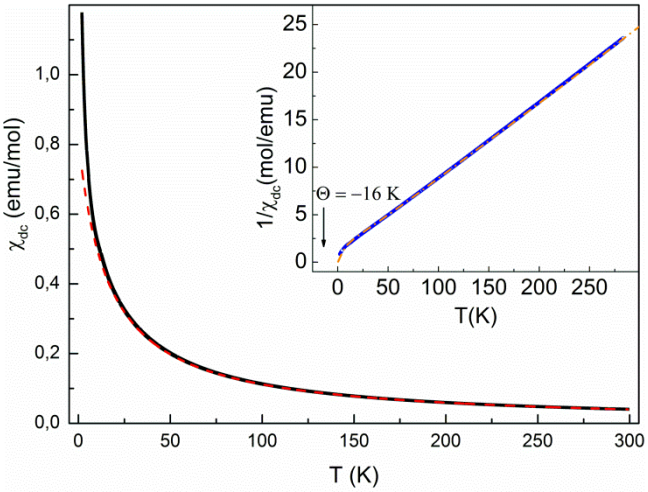

Figure S1. The temperature dependence of dc-magnetic susceptibility in $Rb_{2.3}(H_2O)_{0.8}Mn_3[B_4P_6O_{24}(O,OH)_2]$, the dashed line represents the extrapolation of high-temperature Curie-Weiss law. The inset: the temperature dependence of inverse dc-magnetic susceptibility: experimental (the straight line), calculated (the dashed line).