Supporting Information for:

Electronic structure analysis of the difference between Cs_2AgF_4 and Rb_2MnF_4 in their magnetic properties and single crystal structure determination of Rb_2MnF_4

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Table S1. Anisotropic displacement parameters [pm^2] of Rb_2MnF_4 ^a

atom	U_{11}	U_{22}	U_{33}
Rb	167(9)	167(9)	331(13)
Mn	92(15)	92(15)	331(20)
F(1)	220(50)	220(50)	270(60)
F(2)	200(70)	50(6)	370(60)

^a $U_{23} = U_{13} = U_{12} = 0$.

Table S2. Exponents ζ_i and valence shell ionization potentials H_{ii} of Slater-type orbitals χ_i used for extended Hückel tight-binding calculation ^a

atom	χ_i	H_{ii} (eV)	ζ_i	C^b	ζ'_i	C'^b
Cu	4s	-11.4	2.151	1.0		
Cu	4p	-6.06	1.370	1.0		
Cu	3d	-14.0	7.025	0.4473	3.004	0.6978
Ag	5s	-9.24	2.288	1.0		
Ag	5p	-3.54	1.490	1.0		
Ag	4d	-13.2	4.989	0.5798	2.584	0.5756
F	2s	-40.0	3.136	0.6737	1.945	0.4144
F	2p	-18.1	4.184	0.3546	1.851	0.7279

^a H_{ii} 's are the diagonal matrix elements $\langle \chi_i | H^{\text{eff}} | \chi_i \rangle$, where H^{eff} is the effective Hamiltonian. In our calculations of the off-diagonal matrix elements $H^{\text{eff}} = \langle \chi_i | H^{\text{eff}} | \chi_j \rangle$, the weighted formula was used. See: Ammeter, J.; Bürgi, H.-B.; Thibeault, J.; Hoffmann, R., *J. Am. Chem. Soc.* **1978**, *100*, 3686.

^b Contraction coefficients used in the double-zeta Slater-type orbital.