ThMnPnN (Pn = P, As): Synthesis, Structure, and Chemical Pressure Effects.

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Table S1. Magnetic structure refinement with different canting models on the basis of C-type AFM state. The first column gives a brief description of the direction of the ordered Mn^{2+} moment. For example, "AF-a" means the moments only have in-plane components (lie in the ab plane), and the coupling between the nearest neighbor (in-plane) is antiferromagnetic. "AF-c" means the moments are parallel to the c-axis, and the coupling between the nearest neighbors (in-plane) is antiferromagnetic. "AF-a, F-c" represents a canted magnetic state. While the in-plane components of the moments between the nearest neighbors are antiferromagnetic, the components along the c-axis are ferromagnetically coupled with the nearest neighbors.

ThMnPN @300K	R_p	R_{wp}	R_{exp}	χ^2	Magnetic moment (μ_B)
AF-a	5.66	7.42	6.64	1.25	3.18(13)
AF-c	5.52	7.22	6.65	1.18	2.69(9)
AF-a, c	unstable				
AF-a, F-c	5.63	7.39	6.64	1.24	3.18(13)/1.61(36)
F-a, AF-c	5.52	7.21	6.64	1.18	0.62(60)/2.70(9)
ThMnPN @4K	R_p	R_{wp}	R_{exp}	χ^2	Magnetic moment (μ_B)
AF-a	6.16	8.09	6.52	1.54	4.16(15)
AF-c	5.85	7.57	6.52	1.35	3.60(10)
AF-a, c	unstable				
AF-a, F-c	6.09	8.00	6.52	1.51	4.20(15)/2.29(33)
F-a, AF-c	5.85	7.57	6.52	1.35	0.72(68)/3.61(10)
ThMnAsN @300K	R_p	R_{wp}	R_{exp}	χ^2	Magnetic moment (μ_B)
AF-a	4.76	6.15	6.69	0.845	2.82(14)
AF-c	4.77	6.15	6.69	0.845	2.30(11)
AF-a, c	unstable				
AF-a, F-c	4.77	6.15	6.68	0.845	2.83(14)/0.48(88)
F-a, AF-c	4.77	6.15	6.68	0.845	0.05(-)/2.30(11)
ThMnAsN @4K	R_p	R_{wp}	R_{exp}	χ^2	Magnetic moment (μ_B)
AF-a	4.56	5.96	6.41	0.865	4.32(13)
AF-c	4.34	5.60	6.41	0.761	3.41(8)
AF-a, c	unstable				
AF-a, F-c	4.54	5.95	6.41	0.860	4.35(13)/1.53(46)
F-a, AF-c	unstable				