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Predicting magnetostructural trends in equiatomic FeRh-based ternary systems¹ RADHIKA BARUA, FELIX JIMENEZ-VILLACORTA, LAURA H. LEWIS, Department of Chemical Engineering, Northeastern University, NANOMAGNETISM GROUP TEAM — A phenomenological model is proposed to predict the influence of elemental substitution on the magnetostructural transition temperatures and Curie temperatures of nominally-equiatomic FeRh-based compounds with the B2 (CsCl)-type crystal structure. Clear trends in the characteristic magnetic transition temperatures, as reported in the literature, are found as a function of the averaged weighted valence band electrons ((s + d) electrons/atom) in compounds of composition $Fe(Rh_{1-x}M_x)$ or $(Fe_{1-x}M_x)Rh$ $(M = 3d, 4d \text{ or } 5d \text{ transi$ tion metals). Substitution of 3d or 4d elements (≤ 6.5 atomic %) into B2-type FeRh causes the magnetostructural transition temperature T_t to increase to a maximum around a critical valence band electron concentration of 8.5 electrons/atom and then decrease. Substitution of 5d transition metal atoms echoes this trend but shifts it to higher transition temperatures. These data and associated trends allow deductions that the stability of the ground state antiferromagnetic phase of the FeRh-based system depends both on the size of the constituent atoms as well as the character of the valence electrons.

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