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Antiferromagnetism, structural instability and frustration in intermetallic AFe_4X_2 systems[1] HELGE ROSNER, CHRISTOPH BERGMANN, KATHARINA WEBER, INGA KRAFT, N. MUFTI, Max Planck Institute for Chemical Physics of Solids, Dresden, HANS-HENNING KLAUSS, T. DELLMANN, T. WOIKE, Dresden University of Technology, CHRISTOPH GEIBEL, Max Planck Institute for Chemical Physics of Solids, Dresden — Magnetic systems with reduced dimensionality or frustration attract strong interest because these features lead to an increase of quantum fluctuations and often result in unusual properties. Here, we present a detailed study of the magnetic, thermodynamic, and structural properties of the intermetallic AFe$_4$X$_2$ compounds (A=Sc,Y,Lu,Zr; X=Si,Ge) crystallizing in the ZrFe$_4$Si$_2$ structure type. Our results evidence that these compounds cover the whole regime from frustrated AFM order up to an AFM quantum critical point. Susceptibility χ(T), specific heat, resistivity, and T-dependent XRD measurements were performed on polycrystalline samples. In all compounds we observed a Curie-Weiss behavior in χ(T) at high T indicating a paramagnetic moment of about $3\mu_B$/Fe. Magnetic and structural transitions as previously reported for YFe$_4$Ge$_2$ occur in all compounds with trivalent A. However, transition temperatures, nature of the transition as well as the relation between structural and magnetic transitions change significantly with the A element. Low T_N's and large θ_{CW}/T_N ratios confirm the relevance of frustration. The results are analyzed and discussed with respect to electronic, structural and magnetic instabilities applying DFT calculations.

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