Crystallographic and magnetic study of novel intermetallic compounds R_2MoSi_2C (R = Y, Gd-Tm, Lu)

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Intermetallic compounds occupy a special place among solid materials, owing to the great diversity in both their crystal chemistry and physical properties. Rare earth (R)-based intermetallics have attracted significant interest from the modern technological applications viewpoint as well as from the fundamental research side, offering a plethora of tunable structural, electronic, and magnetic properties. There is a broad range of successful utilization of intermetallics in functional applications comprising permanent magnets, magneto-mechanical sensors and actuators, magnetocalorics, superconductors, hydrogen storage, or magneto-optical recording, to name but a few [1-6]. Intermetallic materials with the most outstanding magnetic properties are enabling many functionalities in motors, generators, sensors, actuators, robotics, advanced prosthetics and energy conversion devices in general.

Here, I report the discovery of novel quaternary intermetallic compounds R_2MoSi_2C (R = Y, Gd–Tm, Lu) during a survey of the R–Mo–Si–C phase diagram. The alloys were synthetized by high frequency induction melting and subsequent appropriate annealing treatment. Their crystal structure was solved by means of single crystal and powder X-ray diffraction. The analysis of X-ray diffraction data reveals that the R_2MoSi_2C compounds crystallize in a tetragonal lattice (space group *P4/mbm*, Pearson's symbol tP12) [7] with unit-cell parameters that follow the conventional lanthanide contraction. Magnetization and specific heat measurements indicate that Y_2MoSi_2C and Lu_2MoSi_2C systems are paramagnetic (PM) over the investigated temperature range (2–300 K) whereas the compounds with R = Gd–Tm exhibit an antiferromagnetic (AFM) ground state below the Néel temperature (T_N = 2.4 – 25 K). Interestingly, the Gd-based compound undergoes a spin reorientation transition at T_{SR} =15 K. It is noteworthy that the magnetic ordering temperature T_N does not obey the de Gennes scaling. Such a breakdown can be attributed to crystal field effects on the *R* ions. It is further shown that the AFM state gets transformed into a ferromagnetic (FM) state via a magnetic-field-induced metamagnetic phase transition. Another salient feature is: the deduced saturation magnetic moment for the field-driven FM state is much smaller than the free ion saturation magnetic moment. This reduced saturation moment is most likely due to crystal field effects. The observed effective magnetic moment is higher than the theoretical μ_{eff} expected for the R^{3+} ions; this difference may reflect a contribution from the *d*-electrons. In other words, this difference may be probably ascribed to the positive spin polarization of 5*d* states.

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