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Thermodynamic Stability of $ThMn_{12}$ -type CeFe₈M₄ Magnetic Compounds J.F. HERBST, GM R&D Center, CHEN ZHOU, MEDA Engineering and Technical Services LLC, F.E. PINKERTON, GM R&D Center — Rare earth (R) elements such as Nd and Dy are critical constituents of high-performance $Nd_2Fe_{14}B$ -type permanent magnets. Ongoing economic uncertainties have stimulated great interest in magnets that use alternative R materials, Ce in particular since it is the most abundant R element. While the intrinsic magnetic properties of known Ce-based compounds are inferior to those of their Nd-based cognates, they nevertheless offer the prospect of developing magnets with technical characteristics intermediate between those of Nd-Fe-B and ferrites. Moreover, there is ample opportunity to identify novel Ce systems. As a means of guiding the synthesis of new $CeFe_{12-x}M_x$ phases we have assessed the thermodynamic stability of ThMn₁₂-type $CeFe_8M_4$ compounds with 26 different elements M via density functional calculations. Compounds of this class are attractive since they can have larger Fe:R ratios than $R_2Fe_{14}B$, and in some cases additional processing such as nitriding, hydriding, or carbiding can substantially improve the magnetic properties. We critically compare the theoretical results with experiment.

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