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【144】 Computational study of Y NMR shielding in intermetallic Yttrium compounds

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In this work, we present calculation of the Y NMR shielding in intermetallic compounds. (YM, YMX, YM_2X , YM_2X_2 , Y_2MB_6 and Y_2MSi_3 where M represents various transition metals and X refers to Si, Ge, Sn). The total shift σ of this selection varies by about 2500 ppm and correlates very well with the experimentally observed shielding except for YMg and YZn. The diamagnetic contribution σ_o (chemical shift) is not constant and varies up to 1700ppm. Half of our compounds have a paramagnetic (negative) σ_c due to reoccupation of the valence Y-5s electrons, while for others the induced Y-4d magnetic moment induces diamagnetic core contributions.

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