

Ternary Intermetallic Compounds $LnMn_2Al_{10}$ ($Ln = Y, La-Nd, Sm, Gd-Dy$) and $LnRe_2Al_{10}$ ($Ln = Ce, Pr, Sm$) with $CaCr_2Al_{10}$ -Type Structure

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Intermetallic Compounds, Crystal Structure, X-Ray Data

The twelve title compounds have been prepared for the first time. Their $CaCr_2Al_{10}$ -type structure ($P4/nmm$, $Z=4$) was refined from single-crystal X-ray data for the three representatives $TbMn_2Al_{10}$ ($a = 1274.3(2)$ pm, $c = 511.4(2)$ pm, $R = 0.025$ for 680 structure factors F and 43 variable parameters V), $CeRe_2Al_{10}$ ($a = 1295.5(5)$ pm, $c = 517.2(4)$ pm, $R = 0.054$ for 810 F and 46 V), and $SmRe_2Al_{10}$ ($a = 1291.5(2)$ pm, $c = 516.5(1)$ pm, $R = 0.021$ for 622 F and 46 V). The atomic positions of the lanthanoid and transition metal atoms are fully occupied. Significant deviations from the full occupancies were observed for two aluminum sites in $TbMn_2Al_{10}$ and for all five aluminum sites of the two rhenium-containing compounds, resulting in the compositions $TbMn_2Al_{9.63(2)}$, $CeRe_2Al_{9.52(8)}$, and $SmRe_2Al_{9.16(9)}$. The cell volume of $CeRe_2Al_{10}$ and to a smaller extent also that of $CeMn_2Al_{10}$ indicate mixed or intermediate +III/+IV valencies of the cerium atoms in these compounds. The structural relationships between the three closely related body-centered tetragonal structures of $ThMn_{12}$, $CeMn_4Al_8$, $DyFe_6Al_6$, and the primitive tetragonal structure of $CaCr_2Al_{10}$ are briefly discussed.

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