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Synthesis and crystal structure of a new rhenium scandium oxide, Sc_6ReO_{12}

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A number of Ln_6MO_{12} phases, where Ln = rare earth cation and M = Mo, W, Re or U, crystallizes in a distorted rhombohedral fluorite structure with space group R-3 [1, 2]. The same crystal structure is observed for Sc_6MO_{12} compounds, where M = Mo and W [3]. In our work a new complex rhenium scandium oxide, Sc_6ReO_{12}, has been synthesized as a single phase in a sealed silica tube and by high-pressure high-temperature synthesis, and its crystal structure has been determined by single crystal X-ray diffraction. This compound crystallizes in a rhombohedral structure (space group R-3, a = 9.248(2) Å, c = 8.720(2) Å, Z = 3). Figure 1 demonstrates the dependence of the cell parameters ”a” and ”c” on the ionic radius of the trivalent cations in the isostructural compounds Ln_6ReO_{12} (Ln = Sc, Ho, Er, Tm, Yb and Lu). This structure represents a three-dimensional framework formed by ReO_6 and ScO_7 polyhedra connected via edges and corners. ReO_6 octahedra are undistorted, the Re-O interatomic distance $d_{Re\text{-}O}$ = 1.926 Å is in a good agreement with the Re-O distances observed for other Re containing oxides with a formal rhenium oxidation state +6. ScO_7 polyhedra represent capped prisms with six close oxygens ($d_{Sc\text{-}O}$ = 2.027 - 2.230 Å, in agreement with average Sc-O distances in other Sc-containing oxides), and one more distant oxygen ($d_{Sc\text{-}O}$ = 2.67 Å), which is included in the coordination sphere due to calculated bond-valence parameters. The synthesis of Sc_6ReO_{12} under high pressure indicates the stability of its structure up to 50 kbar and 1300 °C. The magnetic properies of Sc_6ReO_{12} were also investigated.

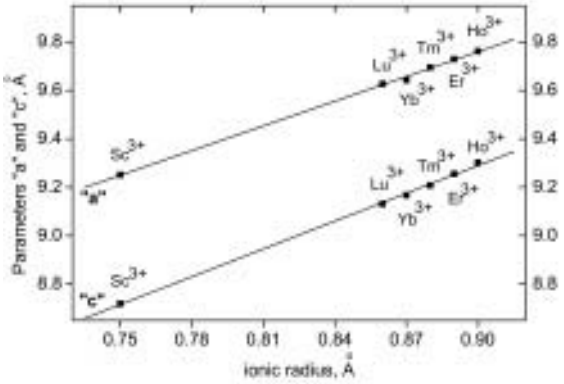

Figure1. ”a” and ”c” cell parameters dependence on the ionic radius for Ln_6ReO_{12} (Ln = Ho, Er, Tm, Yb, Lu) and Sc_6ReO_{12}.

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