$MgRhD_{1-x}$, A New Interstitial Deuteride Containing Square Planar $[Rh_4D_4]$ Rings with Nearly Linear Rh-D-Rh Bridges*

By F. Bonhomme, K. Yvon

Laboratoire de Cristallographie, Université de Genève, 24, Quai E. Ansermet, CH-1211 Genève 4, Switzerland

and P. Fischer

Labor für Neutronenstreuung, ETH Zürich, CH-5232 Villigen PSI, Switzerland

The title compound was investigated by neutron powder diffraction at various deuterium pressures. It has metallic character and crystallizes with a tetragonally deformed CsCl-type metal arrangement (MgRhD_{0.94(2)}: space group P 4/mmm; Z = 4, a = 6.395(1) Å, c = 3.2368(7) Å at p = 39 bar D₂ and T = 298 K). The rhodium atoms are connected to four-membered

Structure of MgRhD_{1-x} projected along the tetragonal axis; large circles: magnesium at z = 0; small circles: rhodium and deuterium at z = 1/2. The occupancy of the deuterium site is 94% (p = 39 bar), 86% (p = 2.5 bar), 61% ($p = 10^{-5}$ bar).

^{*} Presented at the International Symposium on Metal – Hydrogen Systems, Fundamentals and Applications, Uppsala, Sweden, June 8 – 12, 1992.

planar rings via deuterium atoms with bond distances [Rh-D] = 1.708(4) Å and bond angles $[D-Rh-D] = 87.5(7)^{\circ}$ and $[Rh-D-Rh] = 177.5(9)^{\circ}$. Two thirds of the magnesium atoms are bonded to deuterium at distances in the range [Mg-D] = 2.23-2.33 Å.