

# Tetragonal $\text{Mg}_3\text{RuD}_3$ , Containing Ruthenium with three Terminal Deuterium Ligands\*

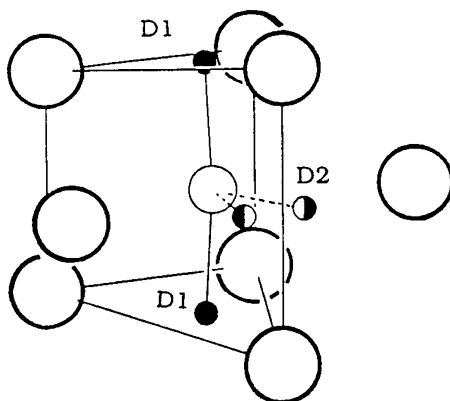
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Trimagnesium ruthenium trideuteride,  $\text{Mg}_3\text{RuD}_3$ , was synthesized by reaction of magnesium and ruthenium powders at  $610^\circ\text{C}$  at a deuterium pressure of 9 bar for 7 days; its structure was determined by X-ray and neutron powder diffraction at room temperature. The structure can be described with the tetragonal space group  $P4_2/mnm$  ( $a = 7.2729(4)$  Å,  $c = 6.9302(7)$  Å,  $Z = 4$ ), has an  $\text{IrIn}_3$ -type metal atom arrangement and contains two symmetry independent deuterium sites, of which one has an apparent disorder with 50% occupancy.



Ru environment in  $\text{Mg}_3\text{RuD}_3$ . Large circles: magnesium, medium circle: ruthenium, small circles: deuterium (filled: D1 100% occupancy, half-filled: D2 50% occupancy).  $[\text{D2-D2}] = 0.87$  Å.

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The transition metal atom is surrounded by 8 magnesium atoms in a bicapped trigonal prismatic configuration with bond distances in the range Ru-Mg = 2.73–2.75 Å, and by 3 deuterium atoms with bond distances Ru-D1 = 1.712(4) Å, Ru-D2 (disordered) = 1.709(9) Å and bond angles D1-Ru-D1 = 170.3(3)°, D1-Ru-D2 = 94.7(2)°.