Neue Strukturverfeinerung und Eigenschaften von Cr_3C_2

Structure Refinement and Properties of Cr_3C_2

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Cr_3C_2 was obtained from arc-melting of pellets made of carbon and chromium. The structure of Cr_3C_2 was determined by single crystal X-ray diffraction (*Pnma*, Z = 4, a = 553.99(6), b = 283.27(4), c = 1149.4(1) pm, R_1 = 0.019 and wR_2 = 0.037 for all collected reflections). The crystal structure contains isolated carbon atoms which reside inside of trigonal prismatic voids of metal atoms. The compound exhibits temperature independent paramagnetism. The electronic structure of Cr_3C_2 has been investigated using extended Hückel calculations.

Key words: Chromium Carbide, Magnetic Properties, Electronic Structure