

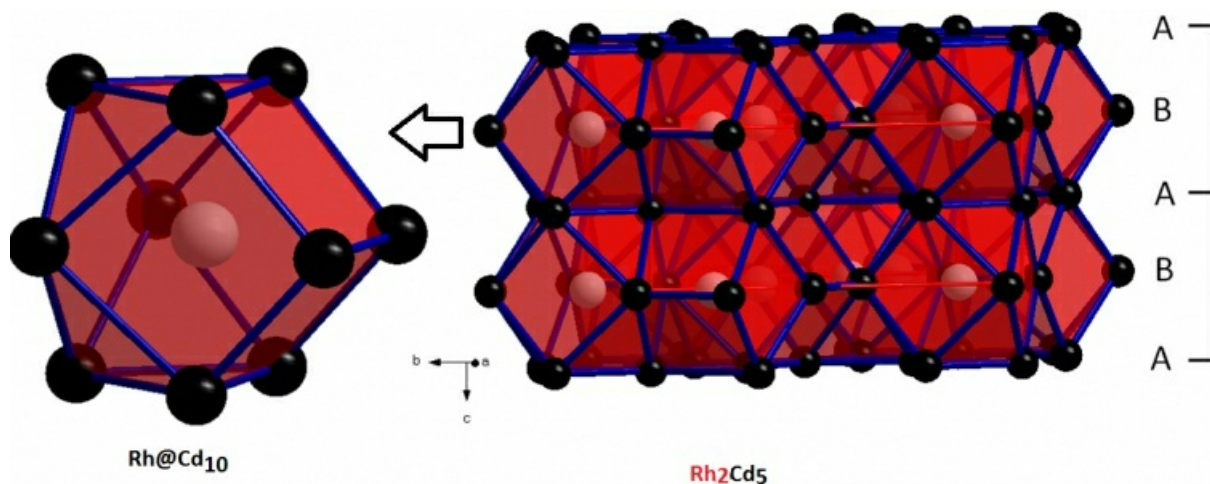
*Rh<sub>2</sub>Cd<sub>5</sub>: a defect In<sub>3</sub>Pd<sub>5</sub>-type structure*Biplab Koley<sup>1</sup>, Swastika Chatterjee<sup>2</sup>, Partha Pratim Jana<sup>1</sup><sup>1</sup>Department of Chemistry, Indian Institute of Technology, Kharagpur, India, <sup>2</sup>Department of Physics, Indian Institute of Technology, Kharagpur, India  
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Binary transition metal (TM) bearing Zn or Cd compounds have attracted considerable interest as these compounds show complex structures as well as fascinating chemical and physical properties. The search for new Rh-based intermetallics has generated much attention as such compounds have been identified as potential heterogeneous catalysts for chemoselective hydrogenation, electrocatalytic oxidation and selective isomerisation, etc. Our recent investigation on the Cd rich region of the Rh-Cd system has revealed a new compound with the c.a. 29 at% of Rh. The new phase in the Rh-Cd binary system - Rh<sub>2</sub>Cd<sub>5</sub> has been characterized by single crystal X-ray diffraction and Energy dispersive X-ray analysis. The site preference of rhodium in the structure of Rh<sub>2</sub>Cd<sub>5</sub> has been addressed by quantum mechanical first principle total energy calculations. The stoichiometric compound Rh<sub>2</sub>Cd<sub>5</sub> crystallizes in the orthorhombic space group Pbam (55) with 14 atoms/ unit cell. The structure contains 4 independent crystallographic sites of which three are occupied by cadmium and one by rhodium. The crystal structure of Rh<sub>2</sub>Cd<sub>5</sub> can be described as a defect form of the In<sub>3</sub>Pd<sub>5</sub> structure with ordered vacancies, formed of two 2D atomic layers with the stacking sequence: ABAB. The A layer consists of (3.6.3.6)-Kagomé nets of Cd atoms while the B type layers consist of (35) (37)- nets of both atomic species (Cd and Rh). The structure of Rh<sub>2</sub>Cd<sub>5</sub> can be described by one type of coordination polyhedron-RhCd<sub>10</sub>. RhCd<sub>10</sub> polyhedra are connected to each other by sharing square faces and form quasi-infinite ab-slabs with thickness of one unit cell along c direction.

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