

Crystal-field electronic structure in CeMg₃, CeIn₃ and PrO₂

R. J. Radwanski,^{1,2} D. M. Nalecz,¹ and Z. Ropka²

¹*Institute of Physics, Pedagogical University, 30-084 Krakow, Poland*

²*Center of Solid State Physics, S^{mt} Filip 5, 31-150 Krakow, Poland*

We have analyzed magnetic and electronic properties of three compounds, CeMg₃, CeIn₃ and PrO₂, with an aim to compare their low-energy discrete electronic structure and the underlying charge distribution. In all these compounds rare-earth ions have one f electron - due to this fact these compounds can be treated as good examples from a pedagogical point of view. All of them form a cubic structure. Two cerium compounds have Γ_7 Kramers doublet ground state and the excited quartet Γ_8 . In PrO₂, the quartet Γ_8 is the lowest. By analysis of the strength of the fourth-order CEF interactions (B_4) we would like to answer about i) the origin of the crystal-field splitting, and ii) the role played by conduction electrons. We have got consistent understanding of magnetic and electronic properties of CeMg₃ including the theoretical description of the λ -type peak at T_N and the value and the direction of the Ce magnetic moment. We try to determine the charge distribution in the unit cell. Our atomistic approach offers consistent theoretical description of paramagnetic and (antiferro)magnetic state of these compounds being the atomic-scale basis for heavy-fermion and/or Kondo phenomena.