

# Crystal-field electronic structure in $\text{CeMg}_3$ , $\text{CeNi}_3$ and $\text{PrO}_2$

R.J. Radwanski,<sup>1,2</sup> D.M. Nalecz,<sup>1,2</sup> M. Krupska,<sup>1,2</sup> T. Piowarczyk,<sup>1,2</sup>  
Z. Ropka,<sup>2</sup> and J. Wasowicz<sup>1,2</sup>

<sup>1</sup>*Institute of Physics, Pedagogical University, 30-084 Krakow, Poland*

<sup>2</sup>*Center of Solid State Physics, S<sup>nt</sup> Filip 5,31-150 Krakow, Poland*

We have analyzed magnetic and electronic properties of three compounds,  $\text{CeMg}_3$ ,  $\text{CeNi}_3$  and  $\text{PrO}_2$ , with an aim to compare their low-energy discrete electronic structure and the underlying charge distribution. In all these compounds rare-earth ions have 1  $f$  electron - due to this fact these compounds can be treated as good examples from pedagogical point of view. All of them form a cubic structure. Two cerium compounds have  $\Gamma_7$  Kramers doublet ground state and excited quartet  $\Gamma_8$ . In  $\text{PrO}_2$ , the quartet  $\Gamma_8$  is the lowest. By analysis of the strength of the octupolar interactions 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  $\text{CeMg}_3$  including the theoretical description of the  $\lambda$ -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.