MAGNETIC g_e-FACTORS AND ELECTRIC DIPOLE MOMENTS OF LANTHANIDE MONOXIDES: PrO

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The very complex optical spectra of the lanthanide monoxides are caused by the insensitivity of the electronic energies to the numerous possible arrangements of the Ln^{2+} electrons in the 4f and 6s orbitals. Disentangling the complex optical spectra may be aided by using simple Ligand Field Theory(LFT) to establish the global electronic structure for the low-lying electronic states. A comparison of experimentally determined permanent electric dipole moments, μ_{el}, and magnetic dipole moments, μ_m, is an effective means of sorting this myriad of states and assessing the quality of LFT and other electronic structure methodologies. Here we report on the determination of the permanent electric dipole moments, μ_{el}, and magnetic g_e-factors for the $X_2(\Omega = 4.5)$ and [18.1] ($\Omega = 5.5$) states of PrO from the analysis of the optical Stark and Zeeman spectra. The g_e-factors are compared with those computed using wavefunctions predicted from ligand field theory[a]. The μ_{el} value for the $X_2(\Omega = 4.5)$ state is compared to *ab initio*[b], and density functional[c] predictions and with the experimental values of other lanthanide monoxides. A phenomenological fit of μ_{el} for the entire series of LnO is used to predict μ_{el} for the isovalent actinide monoxide series.

[a]Carette, P.,; Hocquet,A.*J. Mol. Spectrosc.***131** 301, 1988.
[b]Dolg, M.; Stoll, H. *Theor. Chim. Acta.* **75**,369, 1989.
[c]Wu, Z.; Guan, W. Meng, J. Su, Z. *J. Cluster Science* **18** 444, 2007.