Abstract Submitted
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An investigation of resonance involvement in electron circular dichroism of NMR shift reagent molecules[1] ADAM SCHEER, GORDON GALLUP, TIMOTHY GAY — We have measured the total scattering cross sections of several NMR shift reagent molecules, $X(hfc)_3$, where X = Yb, Er, Eu and Pr by means of electron transmission spectrometry (ETS) to determine their vertical attachment energies (VAEs). With the aid of restricted open-shell Hartree-Fock (ROHF) calculations on closely related molecules, we have assigned specific normally unoccupied orbitals to the resonances observed in ETS. Nolting *et al.* [J. Phys. B **30**, 5491 (1997)] have demonstrated that the NMR shift reagents exhibit electron circular dichroism (ECD) between 1-10 eV. We reexamine their asymmetry spectra and provide a set of possible orbital assignments for major ECD structures. Inconsistencies in associating asymmetry features with resonances observed in the total scattering cross section are also discussed. Specifically, significant shifts to lower energy are observed in analogous ECD features as the atomic number of the central lanthanide atom decreases. However, similar shifts in VAEs are not seen as would be expected if resonance behavior were solely responsible for asymmetry.

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