

# Electronic structure and molecular properties of the heptacyanorhenate

## $[\text{Re}(\text{CN})_7]^{3-}$ and $[\text{Re}(\text{CN})_7]^{4-}$ complexes

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We report scalar relativistic and Dirac scattered wave (DSW) calculations on the heptacyanorhenate  $[\text{Re}(\text{CN})_7]^{3-}$  and  $[\text{Re}(\text{CN})_7]^{4-}$  complexes. Both the ground and lowest excited states of each complex split by spin-orbit interaction by about 0.3 eV. The calculated molecular electronegativities indicate that the open-shell complex is less reactive than the closed-shell complex, in agreement with experimental observations. The calculations indicate that the ground state spin density is highly anisotropic and that spin-orbit effects are responsible for the magnetic anisotropy of the molecular g tensor of the  $[\text{Re}(\text{CN})_7]^{3-}$  complex. The calculated optical electronic transitions for both complexes with a polarizable continuum model using a time-dependent density functional (TDDFT)/B3LYP formalism are in reasonable agreement with those observed in the absorption spectrum. © 2006 American Chemical Society.