Electronic structure and molecular properties of the octacyanorhenate [Re(CN)8]3- and [Re(CN)8]2- complexes

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We report scalar and four component relativistic density functional calculations on octacyanorhenate [Re(CN)8]2- and [Re(CN)8]3- complexes. The relativistic calculations predict that the molecular g-tensor of the paramagnetic [Re(CN)8]2- complex is isotropic. The calculated optical electronic transitions for both complexes with a polarizable continuum model using a time dependent density functional (TDDFT)/B3LYP formalism suggest that the [Re(CN)8]3- complex may distort towards dodecahedral geometry in solution. The electronic excitations of LMCT type of [Re(CN)8]2- are displaced at very high wavelengths with significant oscillator strength values which is characteristic of Re compounds having luminescent behaviour. Thus, our calculations predict that [Re(CN)8]2- could be luminescent.