THE ORIGIN OF ANOMALOUS ELECTRONIC CIRCULAR DICHROISM SPECTRA OF $[RuPt_2(tppz)_2Cl_2]^{4+}$ IN ACETONITRILE

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The $[RuPt_2(tppz)_2Cl_2]^{4+}$ (tppz=2,3,5,6-tetra(2-pyridyl)pyrazine) is a potential material for water photo-oxidation to produce oxygen molecules. Recent experiments found that it has anomalous electronic circular dichroism (ECD) spectra in acetonitrile. In order to explain the ECD spectra, we have carried out a detailed study using a hybrid density functional theory (DFT), together with the Stuttgart/Dresden effective core potentials (MWB) for the metal and P atoms. The solvation effects in acetonitrile were taken into account in terms of the conductor polarizable continuum model (C-PCM) with the universal force field (UFF) approach. The UV-vis spectra of the complexes were calculated using the time-dependent DFT (TDDFT) method on the optimized geometry of individual system. In this talk, we will discuss the DFT/TDDFT calculations and propose a mechanism for the abnormal ECD spectra.

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