An Assessment of Long-Range Corrected Density Functional Approximations in the Calculation of the Reduction Potentials of Ni(S2C2H2)2, Ni(Se2C2H2)2, Ni(S2C2H2)(N2C2H4), and Ni(Se2C2H2)(N2C2H4) Complexes

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Abstract

Herein an assessment of several Long Range Corrected (LRC) Density Functional Theory (DFT) methods for the calculation of reduction potentials of the ([Ni(X2C2H2)2]n/[Ni(X2C2H2)2]n-1), and ([Ni(X2C2H2)(N2C2H4)]n/[Ni(X2C2H2)(N2C2H4)]n-1) and (where X= S or Se and n = 0, or -1) redox couples was done. From the results the values of ω that provide best agreement with CCSD(T) for the tested LRC DFT methods are 0.05 bohr-1, 0.15 bohr-1, 0.05 bohr-1, and 0.20 bohr-1 for ω-B97XD, LC-BLYP, CAM-B3LYP, and ω-B97, respectively. With these values the unsigned average in error was 0.12 V with a standard deviation of 0.13 V for ω-B97XD. For LC-BLYP, CAM-B3LYP, and ω-B97 the unsigned averages in relative errors were 0.12 V, 0.11 V, and 0.13 V, respectively, with respective standard deviations of 0.11 V, 0.12 V and 0.13 V.

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