**Abstract**

Two mononuclear Re(v) complexes [ReO(OMe)(PPh3)2 (Alizarin)2] and [ReO(OMe)2(PPh3)2 (Alizarin)] where Alizarin is 3-((3-nitrophenyl)hydrazinylidene)-6-oxidanylidene-cyclohexa-1,4-diene-1-carboxylate, have been prepared and characterized by elemental analysis, FT-IR and UV-Vis methods.

The structures of the complexes were optimized by Gussian09 at the semi-empirical PM6 level of theory the computational part also consists of Mulliken atomic charges, dipole moment and HOMO and LUMO energies.

Also, the electrocatalytic reduction of CO2 to CO by [ReO(OMe)(PPh3)2(Alizarin)2] and [ReO(OMe)2(PPh3)2(Alizarin)] were investigated using cyclic voltammetry technique. The CV data showed that the multi-electron reduction of CO2 was catalyzed by the metal complexes and two mechanisms were proposed for this multi-step reduction.

Key words

Rhenium complexes; Alizarin yellow GG; Cyclic voltammetry; Electrocatalytic reduction; Optimization