Synthesis and DFT calculations of new ruthenium(II) nitrosyl complexes using cis-fac dichlorotetrakis(dimethylsulfoxide)ruthenium(II) precursor and different oximes as sources of nitrosyl ligand

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Abstract:

Three NO+-ruthenium(II) complexes were prepared by using cis-[RuCl2(DMSO)4] as precursor, P, and the compounds benzohydroxamic acid (BHA), 1, anti-diphenylglyoxime (H2dpg), 2, and dimethylglyoxime (H2dmg), 3, as sources of NO moiety. The three complexes [RuCl2(DMSO)3(NO)]+(BA)−, 1, [RuCl2(DMSO)3(NO)]+(Hdpg)−, 2, and [RuCl2(DMSO)3(NO)]+(Hdmg)−, 3, were characterized by (FT-IR, NMR, UV-Vis) spectroscopy, thermogravimetry, and microanalysis. From FT-IR spectral data, two modes of coordination of DMSO to Ru atom through both S and O atoms were detected for 1 and 2. For 3, only S coordination was reported. Computational studies on the [RuCl2(DMSO)3(NO)]+ cationic parts, 1″, 2″ and 3″, of the investigated complexes 1, 2 and 3 were carried out by DFT. The molecular geometry and mode of attachment of Ru(II) with DMSO were performed with the B3LYP/LANL2DZ level of theory and basis set. Theoretical to the experimental agreement was achieved for analysis of IR data of the investigated complexes. Additional information about binding between the ruthenium atom and the DMSO ligand has been obtained by NBO analysis.

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