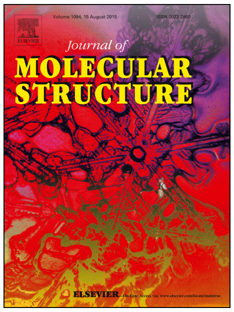

Synthesis, spectroscopic, DFT studies and biological activity of some ruthenium carbonyl derivatives of bis-(salicylaldehyde)phenylenediimine Schiff base ligand

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Synthesis, spectroscopic, DFT studies and biological activity of some ruthenium carbonyl derivatives of bis-(salicylaldehyde)phenylenediimine Schiff base ligand

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Abstract

Bis-(salicylaldehyde)phenylenediimine Schiff base (H_2salphen) reacted oxidatively with the triruthenium dodecacarbonyl complex, $[Ru_3(CO)_{12}]$ to give the dicarbonyl derivative $[Ru(CO)_2(salphen)]$, **1**. In presence of a secondary ligand L (L = pyridine, triphenyl phosphine, 2-aminobenzimidazole or thiourea), the monocarbonyl derivatives [Ru(CO)(salphen)L], **2-5**, were isolated. When the bipyridine (bpy) ligand was used as a secondary ligand, the dicarbonyl complex $[Ru(CO)_2(Hsalphen)(bpy)]$, **6**, was obtained. In complexes **1-5**, the Schiff base ligand acted as a tetradentate, while it coordinated as a bidentate in complex **6**. The structure and stoichiometry of the complexes were investigated by the conventional analytical and spectroscopic techniques, which revealed that they have several structural arrangements. The structures of ligand and complexes were verified by theoretical calculations based on accurate DFT approximations. The relative reactivities were estimated using chemical descriptors analysis. Biological activities of the complexes against the *Escherchia coli* and *Staphylococcus aureus* bacteria were screened.

Keywords: Ruthenium complexes; Schiff bases; Pyridines; Complexes; Spectra; Stereochemical studies.