

MS43-P1 Unusual Ligand Coordination Effects: Crystallographic Study of $[\text{Re}(\text{CO})_3]^+$ Complexes. Alice Brink,^a Hendrik G. Visser,^a Andreas Roodt^a ^a*Department of Chemistry, University of the Free State, P.O. Box 339, Bloemfontein 9300, South Africa.*
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The momentum of research conducted on coordinated technetium(I) and rhenium(I) complexes have gained significant interest due to the remarkable synthesis of Alberto's *fac*- $[\text{Tc}(\text{CO})_3(\text{H}_2\text{O})_3]^+$ complex utilising $[\text{TcO}_4]^-$ in water and under mild conditions.[1] The intriguing feature of the *fac*- $[\text{M}(\text{CO})_3]^+$ (M = Tc(I), Re(I)) core is its d^6 low spin configuration in an octahedral field based high kinetic stability with many types of ligand. As the *fac*- $[\text{M}(\text{CO})_3]^+$ core accepts many types of ligands, it is possible to design bifunctional chelator ligand systems which may affect the hydro/lipophilicity properties of the organometallic complex. A significant amount of valuable work has been published on *fac*- $[\text{M}(\text{CO})_3]^+$ complexes coordinated to a wide variation of ligand systems as model radiopharmaceuticals with diverse biological, catalytic and crystallographic properties.[2-8] The [2+1] mixed ligand concept allows the labeling of bioactive molecules containing a monodentate or bidentate donor site [9] and is one of our research directions. The solid state behaviour and the kinetic rate of substitution is widely influenced by the charge of the coordinated ligand system and the effects of the substituted monodentate incoming ligand. Very few crystal structures of the Schiff-base synthesised salicylidene Re(I) tricarbonyl complexes have been reported and no studies have been reported on the substitutional kinetics of these complexes.

A diverse collection of crystal structures of the methanol substituted rhenium(I) tricarbonyl complexes containing the salicylidene ligand was obtained and is presented here.[10] The organometallic complexes containing aliphatic and aromatic functionalized iminomethylphenolato ligand systems experience the unusual effect of crystallizing in isomorphous space groups and significantly contributed to the pool of available crystallographic data of these systems. Furthermore the kinetic solvent substitution reaction on the "open" third position and the influence of incoming ligands with various acid/base characteristics will be highlighted.

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MS43-P2 Theoretical Modeling And Experimental Studies on (E)-2-chloro-N-((5-nitrothiophen-2-yl)methylene)aniline. Ümit Ceylan,^a Özlem Deveci,^a Sümeyye Gümüş,^b Erbil Adar^b and Orhan Büyükgüngör^a ^a*Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Kurupelit, Samsun, Turkey,* ^b*Department of Chemistry, Faculty of Arts and Science, Ondokuz Mayıs University, 55139 Kurupelit, Samsun, Turkey*
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The Schiff base compound, (E)-2-chloro-N-((5-nitrothiophen-2-yl)methylene)aniline (C₁₁H₇CIN₂O₂S), has been synthesized and characterized by IR, electronic spectroscopy, and X-ray single-crystal determination. The compound crystallizes in the monoclinic space group P 2₁/c with a= 12.0220(5) Å, b= 7.1699(4) Å, c= 15.4347(7) Å, β= 121.101(3)° and Z=4 in the unit cell. The molecular structure is stabilized by C-H...O intramolecular hydrogen bond and molecules are linked through intermolecular C-H...O type hydrogen bond and C-H...Cg (π-ring) interaction.

Schiff bases are important class of compounds in medicinal and pharmaceutical field. Schiff bases have been used extensively as ligands in the field of coordination chemistry [1]. There is considerable interest in Schiff base complexes due to their striking anti-tumour activities [2]. Besides, Schiff bases has been reported to possess antimicrobial properties [3-4] apart from other biological activities.

The molecular geometry from X-ray experiment of the title compound in the ground state have been compared using the Hartree-Fock (HF) and density functional theory (B3LYP) with 6-31G(d) basis set. The energetic behaviour of the title compound in solvent media was examined using the B3LYP method with the 6-31G(d) basis set by applying the Onsager and the polarizable continuum model (PCM). In addition, molecular electrostatic potential (MEP) and frontier molecular orbitals (FMO) analysis of the title compound were performed by the B3LYP/ 6-31G(d) level of theory.

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