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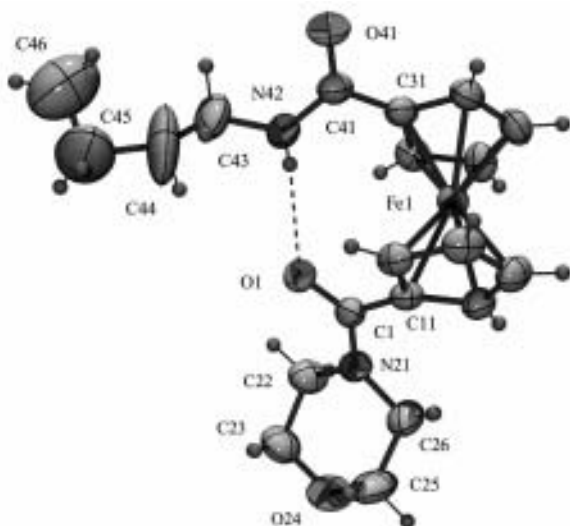
Intramolecular Hydrogen Bonds in Heterodisubstituted Ferrocene Diamides

Attila C. Bényei,^a Gábor Rangits^b, Árpád Kuik,^c
Rita Skoda-Földes, László Kollár^b

^a University of Debrecen, Department of Chemistry, Laboratory for X-ray Diffraction, Debrecen, Hungary ^b University of Pécs, Department of Inorganic Chemistry, Pécs, Hungary ^c University of Veszprém, Department of Organic Chemistry, Veszprém, Hungary. E-mail: abenyei@delfin.unideb.hu

Keywords: hydrogen bonding of coordination compounds, ferrocene compounds, homogeneous catalysis

Strong intramolecular hydrogen bond was observed in various substituted ferrocene 1,1'-diamides prepared via homogeneous catalytic carbonylation starting from 1,1'-diiodoferrocene. Structure of (N^t-butyl-carbamoyl)-morpholino ferrocene carboxamide was determined:



Formula $C_{20}H_{26}FeN_2O_3$, $M = 398.28$, monoclinic, $P2_1/n$, $a = 9.835(4) \text{ \AA}$, $b = 20.165(3) \text{ \AA}$, $c = 9.863(8)$, $\beta = 104.51(4)^\circ$, $V = 1893.7(17) \text{ \AA}^3$, $Z = 4$, $R1 = 0.0551$ and $wR2 = 0.1581$, $GOF = 1.067$, 3662 reflections, 238 parameters. Residual electron density: $0.481/-0.345 \text{ e/\AA}^3$. The H-bond is characterized by H42 ...O1 distance of $2.27(5) \text{ \AA}$, N42 ...O1 $2.938(5) \text{ \AA}$ and N42-H42...O1 $174(6)^\circ$ angle data. Rotation of the Cp ring is prevented by the H-bond and Fe-C distances are in the range of $2.01-2.05 \text{ \AA}$. Atoms C41-N42-O1-C1-Fe1 are in a plane with rms deviation of 0.055 \AA . In solution there is an equilibrium between the H-bonded and non H-bonded form by 1H NMR and IR and interesting effect of chloride ion was observed. Acknowledgements: This work was supported by the Hungarian National Scientific Research Fund (Grant No. OTKA-T043365).

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Oxovanadium(V) thiosemicarbazonato complexes

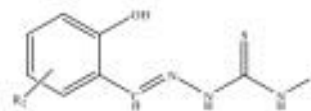
Ivica Dilović, Mirta Rubčić, Marina Cindrić

Dubravka Matković-Čalogović, Chemistry Department, University of Zagreb, Croatia.. E-mail: idilovic@chem.pmf.hr

Keywords: oxovanadium(V) complexes, thiosemicarbazones, X-ray structure

The thiosemicarbazones are interesting primarily due to their biological activities with potential use in antibacterial, antiviral and antitumor treatment. Such compounds that have N, O and S donors are good metal-chelating agents [1]. In the last few years the structure of vanadium complexes is of particular interest because of their model character for biological function of vanadium [2].

Series of ligands (scheme) and corresponding complexes with vanadium(V) ions was synthesized in order to investigate the above mentioned properties.



Existence of thione-thiol tautomeric forms is the structural characteristic of the thiosemicarbazones derived from salicylaldehyde with the thione form dominating in the solid state. In the structurally characterized complexes vanadium was found in the tetragonal-pyramidal environment with the oxo group in the apical position and thiosemicarbazone acting as a tridentate ligand. A molecule of solvent completes the coordination sphere of vanadium.

- [1] Cindrić M., Vrdoljak V., Strukan N., Kamenar B., *Polyhedron*, 2005, 24, 369-376.
[2] Wang D., Ebel M., Schulzke C., Grüning C., Hazari S.K.S., Rehder D., *Eur. J. Inorg. Chem.*, 2001, 935-942.