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Experimental Charge Density Study of Co(III) Complex with Famotidine. Bojana M. Drašković^a, Sladjana B. Novaković^a, Goran A. Bogdanović^a, Bernard Fraisse^b. ^aVINČA Institute of Nuclear Sciences, Laboratory of Theoretical Physics and Condensed Matter Physics, Belgrade, Serbia. ^bLaboratoire „Structures Propriétés et Modélisation des Solides“, UMR 8580 du CNRS, Ecole Centrale Paris, 92295 Châtenay-Malabry, France.
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Famotidine belongs to a class of the stress-ulceration inhibitors, known to exhibit excellent histamine H2 blocking effect [1,2]. As a specific competitive histamine H2-receptor antagonist, famotidine inhibits the secretion of histamine-stimulated gastric fluids. Famotidine offers a set of potential coordination sites for metal ions and it is an efficient chelating agent. It has been shown that in coordination it involves the guanidine and thiazole nitrogen, as well as the thioether sulphur and amine group nitrogen [3, 4]. The experimental electron density distribution in (famotidine) ethylenediamine cobalt(III) chloride monohydrate has been determined from high-resolution X-ray diffraction data collected at a temperature of 100 K. After classical spherical refinement, the multipole refinement of the Co(III) complex was performed using the Hansen–Coppens model [5]. A great number of H-bonds as well as C–H... π and π ... π interactions were observed in the crystal packing of this compound. In order to determine quantitative parameters of the chemical bonds and nonbonded interactions in this compound we have carried out topological analysis of total electron density according to Bader’s quantum theory of atoms in molecules [6].

Experimental details: The data were collected on a Bruker-SMART diffractometer equipped with a SMART 1000 CCD area detector using monochromated Mo $K\alpha$ X-ray radiation ($\lambda = 0.71073$ Å). Maximal resolution $(\sin\theta/\lambda)_{\max} = 1.10$ Å⁻¹. The total number of the reflections collected was 86400. The data sorting and averaging led to a 19124 unique reflections with a final $R_{\text{int}} = 2.02$ %.

Crystallographic data: formula C₁₀H₂₃ClCoN₉O₃S₃, triclinic crystal system, space group P-1, $a = 9.0922(1)$, $b = 9.2850(1)$, $c = 12.3436(2)$ Å, $\alpha = 86.058(1)$, $\beta = 77.715(2)$, $\gamma = 73.977(1)^\circ$, $V = 978.59(8)$ Å³.

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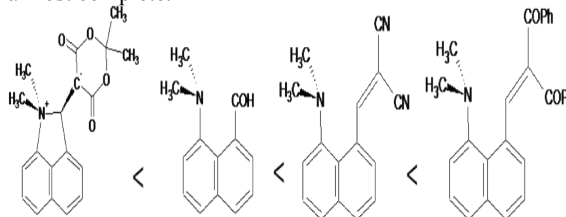
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Probing Chemical Bonds: X-Ray Charge Density Studies on Bond Formation and Interactions in Peri-Substituted Naphthalenes. Mateusz Pitak^a, Simon J. Coles^a, John D. Wallis^b. ^aSchool of Chemistry, University of Southampton, UK. ^bDepartment of Chemistry and Physics, Nottingham Trent University, UK.
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Our present studies are focused on a solid state experimental characterisation of the correlation between the bond formation and bond breaking processes in the addition reaction of the nucleophilic Me₂N group and different electron deficient alkenes located in the *peri* positions of naphthalenes [1,2]. This type of reaction is significant in the organic area of synthesis and a full understanding of the mechanism is crucial for influencing the outcome of these reactions.

In our system, the two terminal groups can a) be splayed outwards with a Me₂N...C separation distance in the range of ~2.4–3.2 Å or b) arranged inward (~1.6 Å), where the nucleophilic addition of the Me₂N group to the alkene is almost complete.



The orientation of the dimethylamino group is such that a lone pair of electrons is directed towards the reacting adjacent carbonyl group. The strength of an interaction between a pair of atoms is considered to be an indicator of the formation and reactivity of a chemical bond and is defined by their separation. Greater insight into electronic structure of those compounds with emphasis put on attractive/repulsive interactions and reactivity can be obtained by analysis of the experimental charge density using Bader’s ‘Theory of Atoms in Molecules [3], in which bonding interactions are characterized by topology of the total electron density.

Analysis of the Laplacian $\nabla^2\rho(r)$ and local kinetic (G^{CP}) and potential (V^{CP}) energy densities [4], calculated at the bond critical point (BCP) describes quantitatively how the nature of the Me₂N...C=C interaction changes from electrostatic (closed-shell) to covalent (shared) as a function of distance between interacting atoms [5].

This work aims to adopt a systematic approach to understanding and quantifying the electronic properties of the studied system and employ those properties to characterise the kinetics and mechanism of the bond formation/breaking process. Results obtained for different electronic models will be presented on this poster.

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