

s13.m42.p21 **Systematic Study into the Salt Formation of Functionalised Organic Substrates.** Suzanna Ward and Michael Hursthouse, *School of Chemistry, University of Southampton, Southampton, SO17 1BJ, UK.* E-mail: scw1@soton.ac.uk

Keywords: Salts; Pharmaceuticals; Systematic

There is currently a great amount of interest in the use of salts in the pharmaceutical industry because the physicochemical properties of the solid forms can be modified without altering the biochemical properties of the drug. Much effort has been expended in screening to select the best salt form and a number of empirical rules have been proposed such as the 'rule of three', which states that a successful salt formation generally requires a difference of three pK_a units between the conjugate acid and the conjugate base. However, this rule does not always hold and the reasons are often unclear. The idea of this project is to perform a detailed systematic study of organic salt formation through a series of designed experiments, in order to obtain a broader and better understanding of the chemical descriptors, or factors that might be involved. A set of descriptors that describe molecular properties relevant to salt formation have been identified. For the initial experiments, a collection of salt forming acids has been assembled from the Cambridge Structural Database [1], and other sources, and their descriptor values calculated. These acids define a chemical space from which the compounds for the experiments can be chosen. The experiments aim to explore this chemical space whilst building statistical models that will allow an understanding of how the descriptors affect salt formation. Findings from the chemical space investigation coupled with experimental results from this study will be presented. This work is part of the Combechem E-science project at the University of Southampton.

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s13.m42.p22 **1-{4-[(2,3-Dihydroxy-benzylidene)-amino]-phenyl}-ethanone.** Süheyla Yüce^a, Arzu Özek^a, Cigdem Albayrak^b, Mustafa Odabasoglu^b and Orhan Büyükgüngör^a, ^aDepartment of Physics, 19 Mayıs University, TR-55139, Samsun, Turkey, and ^bDepartment of Chemistry, 19 Mayıs University, TR-55139, Samsun, Turkey. E-mail: syuce@omu.edu.tr

Keywords: Schiff base; Phenol-imine tautomerization; Photochromism

The title compound, (I), adopt phenol-imine tautomerism with intramolecular O---H...N hydrogen bond (Fig. 1). The strong intramolecular hydrogen bond occurs between O1 and N1 atoms, the H atom being bonded to the O1 atom [2.5941(17)Å]. This intramolecular O1...N1 distance is comparable to those observed for conformation and structure of N-(2-hydroxyphenyl)-salicylaldimine [2.625(7)Å; Elerman *et al.*, 1995], 2-{Tris(hydroxymethyl)methyl} aminomethylene} cyclohexa-3,5-dien-1(2H)-one and its 6-hydroxy and 6-methoxy derivatives [2.556(2)Å; Odabasoglu *et al.*, 2003]. The N1--C7 bond length of 1.2772(16)Å⁰ indicates a high degree of double bond character. This double-bond distance is comparable to the conformation and structure of 3-methoxyphenyl-salicylaldimine [1.280(2)Å⁰; Elmali *et al.*, 1999]. The title compound, (I), may show photochromic property because of its non-planarity according to the Schiff bases studies that led to the proposal that molecules exhibiting photochromism are not planar, while those exhibiting thermochromism are planar. The angle between the two aromatic rings is 35.69 (5)⁰.

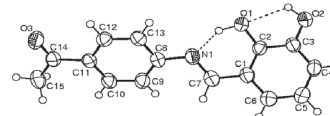


Fig.1. View of molecule (C₁₅H₁₃O₂N)

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- [3] Elmali, A., Kabak, M., Elerman, Y. (1999). *J. Mol. Struct.* **484**, 229-234.