

[s2.m1.p27.la] Weak Interactions in Dipicrylamine. K. Wozniak,¹ P.R. Mallinson,² C.C. Wilson,³ E. Hovestreydt,⁴ E. Grech⁵. ¹*Chemistry Department, Warsaw University, 02 093 Warszawa, ul. Pasteura 1, Poland.* ²*Chemistry Department, University of Glasgow, Glasgow G12 8QQ, UK.* ³*ISIS Facility, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 0QX, U.K.* ⁴*Brucker AXS GMBH., Östl., Rheinbrückenstr. 50, D-76187 Karlsruhe, Germany.* ⁵*Institute of Chemistry and Environmental Protection, Technical University of Szczecin, Piastów 42, 71 065 Szczecin, Poland.*

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A low-temperature high resolution X-ray and neutron diffraction study of charge distribution in the superacid dipicrylamine (DPA) has been carried out. This structure exhibits interesting weak interactions including bifurcated N-H...O and C-H...O H-bonds which consolidate it. The corresponding interaction lines appear to be modified in the vicinity of the CPs of the covalent bonds of the hydrogen atoms.

The presence of six nitro groups generates some short N...O contacts. On the basis of the experimental interaction paths an attractive interaction is found, in agreement with the prediction of such an effect from earlier model ab-initio calculations performed for simple dimers.

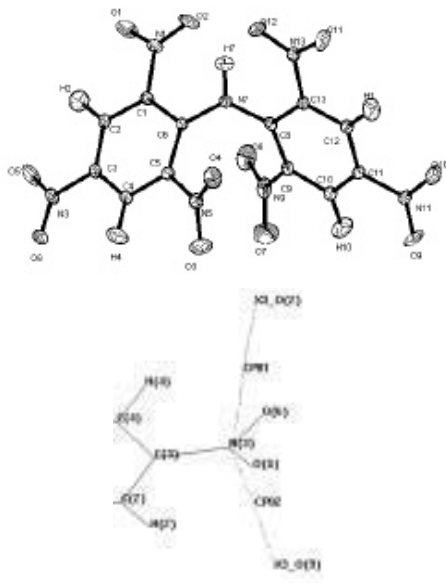


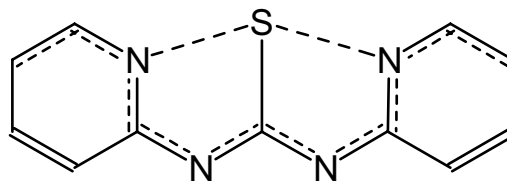
Fig. 1. Definition of the DPA molecule and a $-\text{NO}_2$ group interacting with the closest oxygen atoms.

[s2.m1.p28.la] Topological Analysis of the Electron Density in a Resonance Structure. S.J. Coles, S.M. Cafferkey and M.B. Hursthouse.

Keywords: charge spin densities.

Recent developments in supramolecular chemistry suggest the development of enantioselective receptors capable of strongly binding substrates as an alternative approach to the resolution of racemates. Thiourea derivatives have been synthesised as carboxylic acid binding sites during a scheme of research investigating the separation of racemic mixtures of carboxylic acid derivatives. Attempts to prepare N, N'-di-pyridyl thiourea resulted in the formation of (2)-pyridin-2-yl-[1,2,4]thiadiazolo[2,3a]pyridin-2-ylidene-amine.

This compound has been reported previously [1] where spectroscopic data were interpreted in terms of a resonance structure (figure 1) which is now confirmed by a routine structure determination [2].



The symmetrical resonance structure has both pyridyl nitrogen atoms interacting with the sulfur atom forming hemi-bonds, which also results in the formation of a delocalised diimine core and disturbance of the aromaticity in the pyridyl rings.

In order to describe the electronic configuration a high angle dataset was collected and multipole analysis performed to accurately determine the charge density. Topological analysis then allows a much clearer understanding of the charge distribution and hence the nature of the bonding in the molecule by means of location of bond critical points and examination of interatomic surfaces.

[1] R. L. N. Harris (1972) *Aust. J. Chem.*, 25, 993-1001.

[2] S. J. Coles, D. Douheret, M. B. Hursthouse and J. D. Kilburn (2000) *Acta Cryst. C*, submitted.