



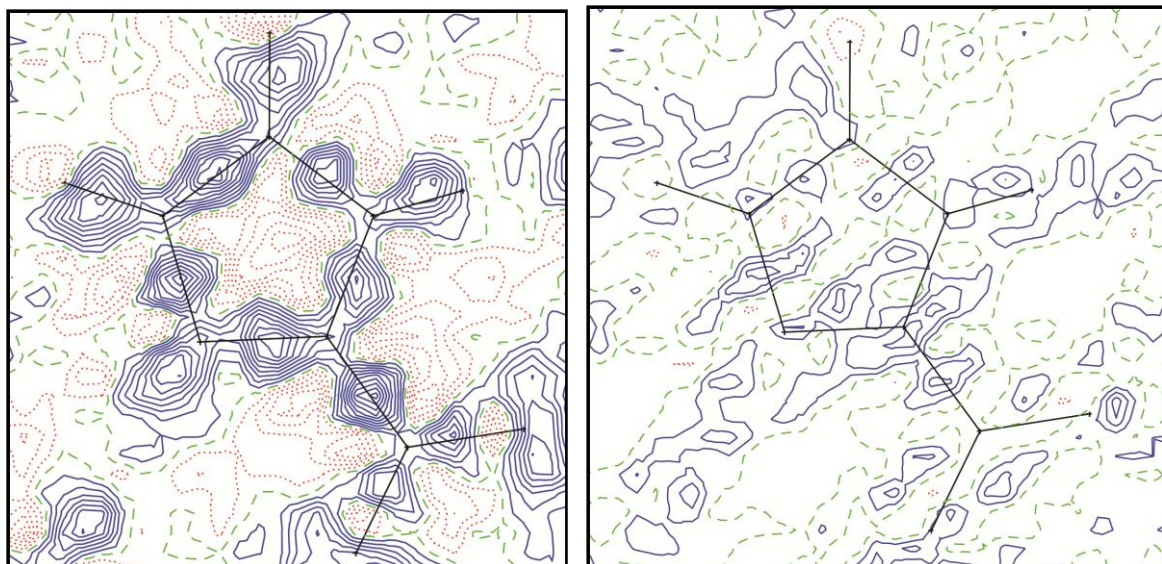
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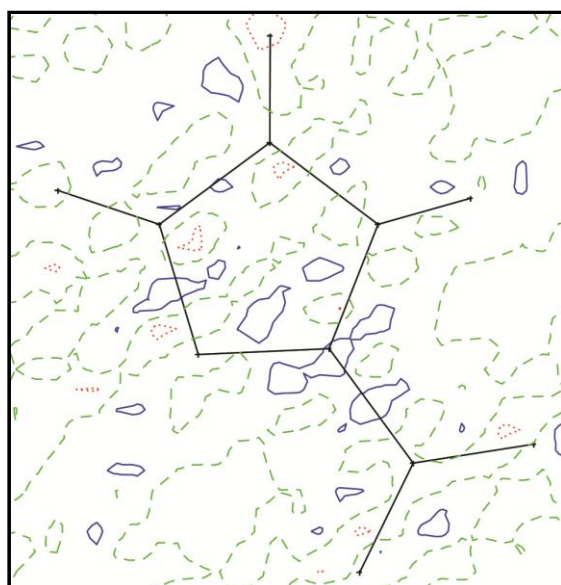
Topological characterization of electron density, electrostatic potential and intermolecular interactions of 2-nitroimidazole: An experimental and theoretical study

Chinnasamy Kalaiarasi, Mysore S Pavan and Poomani Kumaradhas

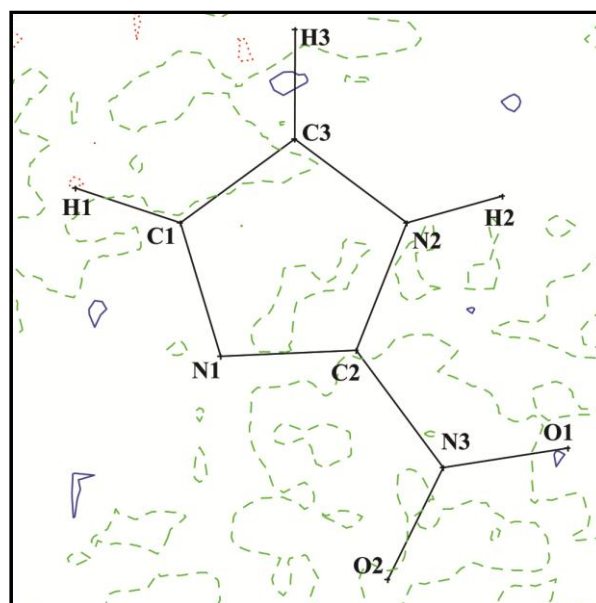


(a)

(b)



(c)



(d)

Fig S1: Residual maps of nitroimidazole molecule (a) monopole (b) dipoles (c) quadrupoles (d) octapoles. The solid blue lines represent positive contours, dotted red lines represent negative contours and dashed green lines represents zero contours. The contour lines drawn at the step size $0.1 \text{ e}\text{\AA}^{-3}$.