Experimental Electron Density Distribution of the Antithyroid Drug 1-Methyl-2-mercaptoimidazole (MMI)

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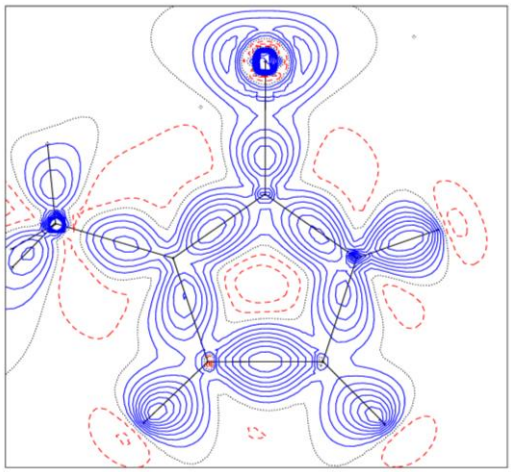
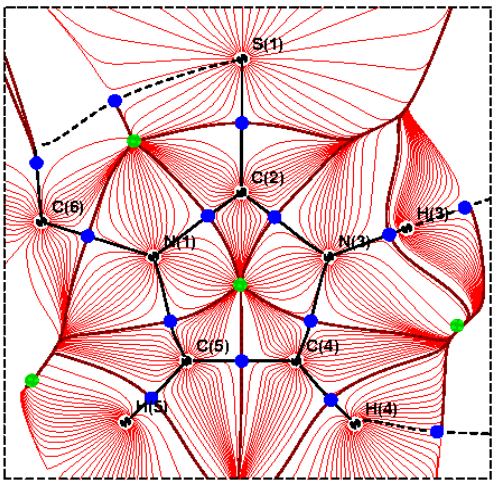
Hyperthyroidism is a medical condition resulting from over activity of the thyroid gland, producing an excess of thyroid hormones. Current methods for treating hyperthyroidism involve administering an antithyroid drug such as the title compound, also known as 1-methyl-2-mercaptoimidazole (MMI). This compound blocks the production of thyroid peroxidase, an enzyme involved in the synthesis of thyroid hormones. The experimental electron density distribution of MMI has been determined from high-resolution x-ray intensity measurements from a single crystal of MMI cooled to 120 K. MMI crystallizes in a triclinic structure with two independent molecules in the asymmetric unit, yielding two determinations of the electron distribution of the molecule in very similar, but not identical, crystal environments. Multipole refinement of the x-ray data yield very similar static deformation densities for both molecules, and topological analysis of the density using the Quantum Theory of Atoms in Molecules show clear evidence of bond paths corresponding to N-H ⋯ S and weaker C-H⋯S hydrogen bonds.



Static Deformation Density of MMI at 120 K. Contours plotted at 0.1 e/Å^3 intervals.



Gradient trajectory plot of the total electron density with bond paths corresponding to hydrogen bonds shown as dashed lines.