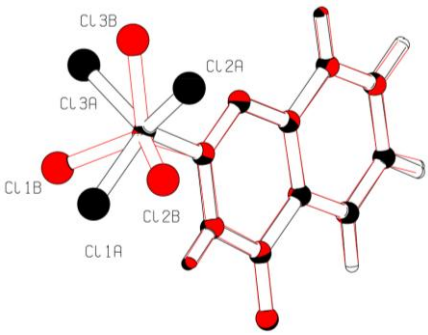
Charge density study on 3-trichloromethylquinazoline

Agnieszka Rybarczyk-Pirek[1], Magdalena Małecka[1], Lilianna Chęcińska[1], Carsten Paulmann[2]

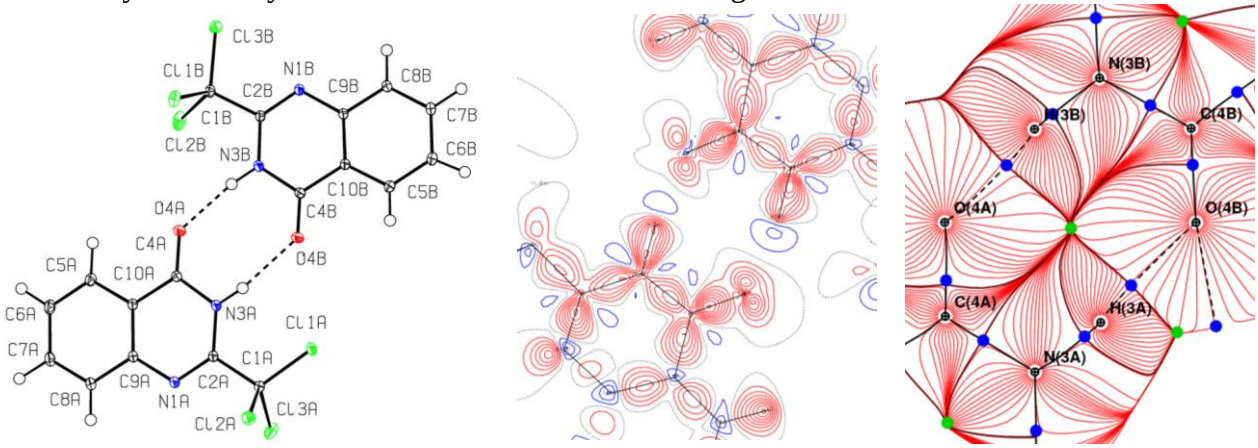
[1]Department of Structural Chemistry and Crystallography, University of Lodz, Pomorska 163/165, 90 236 Lodz, Poland
[2]Mineralogisch-Petrographisches Institut, Universität Hamburg, Grindelalleee 48, 20146 Hamburg, Germany

Efficient crystal engineering needs a hierarchy of supramolecular synthons of hydrogen bonding to be established. Our project is aimed to resonance assisted intra- and intermolecular hydrogen bonds [1,2]. The presented study focus on intermolecular well recognized $R^2_2(8)$ synthoms of N-H…O heteronuclear hydrogen bonding, which is observed in the title crystal structure.



The high resolution X-ray data were measured at beamline F1 at Hasylab. The set of 22154 unique reflections of was collected with synchrotron radiation of the wavelength λ=0.6 Å. For the data reduction the XDS [3] program package was used. The title compound crystallizes in triclinic system, space group *P* -1 with Z'= 2. Two independent molecules, designated as A (black) and B (red), differ each other by conformation of trichloromethyl group as presented above. The spherical model of molecule obtained from SHELXL was used for aspherical atom multipole formalism using the XD2006 [4] package program. The preliminary multipole refinement on hexadecapolar level of gave $R(F)$ = 0.0247, $R(F^2)$ = 0.0376.

The X-ray study confirmed the existence of intermolecular hydrogen N-H…O bonds and geometry analysis confirmed the contribution of electron resonance in the formed $R^2_2(8)$ ring system. The preliminary calculation of experimental electron density indicated the existence of N-H…O bond critical points between two neighboring molecules A and B, while topological parameters based on AIM theory let classify these interactions as medium strength ones.



Molecular structure of dimer formed by title molecules A and B with labeling scheme and 50% atomic displacement ellipsoids (left), static deformation density maps in the plane of hydrogen bonded $R^2_2(8)$ ring; positive, negative and zero contours are represented by blue solid, red solid and black dotted lines, respectively, contour intervals are drawn at 0.1 $Å^{-3}$ (middle); electron density gradient trajectories in the N-H…O intermolecular hydrogen bond region (right).

References:

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