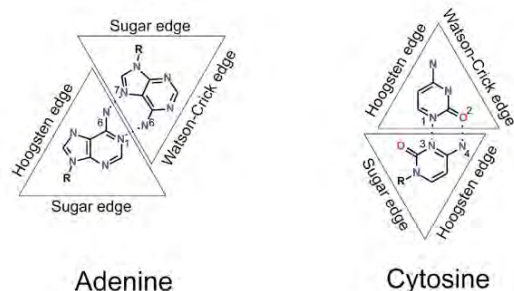


Fig. 1. Examples of homodimers of adenine and cytosine, with the naming of the edges



**Keywords:** nucleobases, hydrogen bonding

## MS10-P02

### Analysis of the hydrogen bonds in the crystal structures of the pyrrole-2-yl-dichloromethyl ketone derivatives

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Pyrroles are both important natural products and crucial starting materials for the synthesis of porphyrins. Nevertheless, a brief survey of the Cambridge Structural Database [1] shows that there are almost 500 instances of the organic structures with a 2-substituted pyrrole core and almost 100 instances with the pyrrol-2-yl carbonyl core. What is more, only a few crystal structures of aromatic N-unsubstituted monopyrroles have been reported. In crystal structures of investigated compounds, we expected the existence of the net of hydrogen and halogen bonding as it was in case of the trichloromethyl derivative of pyrroloketone [2]. However, X-ray structure determinations showed only the latter one. In an extension of ongoing studies on the hydrogen bonding patterns in porphyrins and dipyrromethanes, we were also interested in the strengths and types of hydrogen bonds of isolated pyrrole units. For initial studies we choose 2,2-dichloro-1-(*1H*-pyrrol-2-yl) ethanone and 2,2-dichloro-1-(1-methyl-*1H*-pyrrol-2-yl) ethanone. The calculations have been performed using Gaussian03 sets of codes, and by means of the density functional methods (DFT). The H-bonding characteristics of the complexes have been investigated with the use of Bader's theory QTAIM [3].

#### References:

- [1] Allen, F. H. (2002). *Acta Cryst.* B58, 380-388.  
 [2] Bilewicz, E. et al. (2007). *J. Mol. Struct.* 829, 208-211.  
 [3] Bader, R. F. W. (1990). *Atoms in Molecules: A Quantum Theory*; Oxford University Press, New York.

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