MS43-P13 **Carbamates I: Structural and conformational study of eight methoxyphenyl-*N*-pyridinylcarbamates.**
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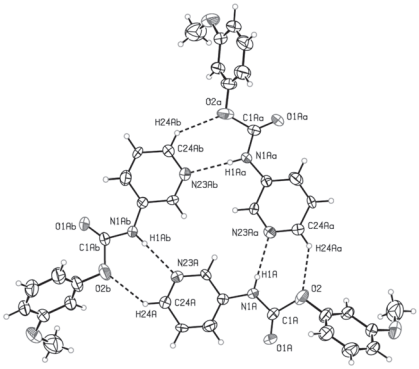
A 3×3 isomer grid of nine methoxyphenyl-*N*-pyridinylcarbamates ($C_{13}H_{12}N_2O_3$) as **CxxOMe** (**x** = *para*-/*meta*-/*ortho*-) was synthesized and studied to determine the crystal structures and correlate structural relationships from both *ab initio* calculations and the solid-state using conformational analysis. Eight of nine isomers crystal structures were determined using single crystal X-ray diffraction. All isomers form N-H…N hydrogen bonds as primary interaction, with one isomer (**CmmOMe**) forming a relatively unusual disordered hydrogen bonded trimer *via* the N-H…N interactions, while the **CoxOMe** isomers form the N-H…N hydrogen bonded dimers. In all isomers additional C-H…O interactions aid aggregation, whereas in most of isomers the methoxy group is engaged in important C-H…O hydrogen bonding patterns.



The solid state and the modelled conformations are mismatched in 3 of 8 molecules in which methoxy groups and *meta*-methoxyphenyl rings (**mOMe**) of the solid state structures adopt *meta*-stable or unstable conformations as compared to the optimised computational models.

Keywords: carbamates, conformational analysis, ab initio

MS43-P14 **(*E*)-2-[(2,4-dimethylphenylimino)methyl]-6-ethoxyphenol and (*E*)-2-[(2,4-dichlorophenyl imino)methyl]-6-ethoxyphenol**
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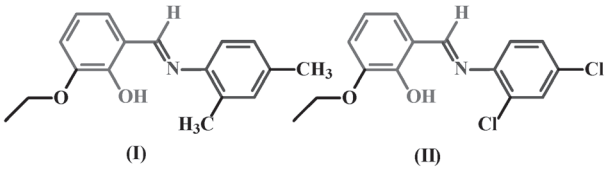
In industry, azomethine dyes have a wide range of application such as dyes and pigments with luminescent properties [1]. These dyes are known to be among most important dyes because of their wide applications, including color photographic system, dye diffusion thermal transfer print system and others [2]. In addition, azmethine dyes have been used widely as ligands in the field of coordination chemistry [3]. o-Hydroxy azomethine dyes that have a strong intra-molecular hydrogen bond. These compounds are of interest because of their thermochromism and photochromism in the solid state, which can involve reversible intra-molecular proton transfer from an oxygen atom to the neighboring nitrogen atom [4]. Taking into account these important features of the azomethine dyes, we aimed to investigate the conformation of the (I) and (II) by X-ray crystallography.



The crystal structure of the (I) exhibit O-H…N, C-H…O hydrogen bonds and C-H…π interactions. There are two symmetry-independent molecules in the asymmetric unit. The dihedral angle between the aromatic rings in (I) are 4.95(2)° and 13.72(2)°. The crystal structure of the (II) has O-H…N, O-H…Cl and C-H…π interactions. The dihedral angle between the aromatic rings in (II) is 12.47(3)°.

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Keywords: Schiff's base, Azomethine dye, Salicyl aldehyde