MS26-P16 **A supramolecular 2:1 guanidinium-carboxylate-based building block for generation of extensive water channels and tetrameric water clusters in an organic material.** Vitthal N. Yadav,[a] Carl Henrik Görbitz,[a] [a]*Department of Chemistry, University of Oslo, Norway*
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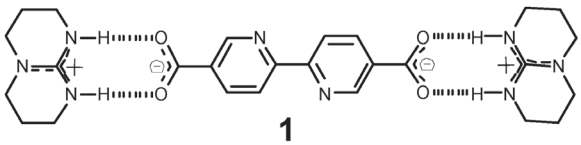
A bicyclic guanidine derivative is used here to form a hydrogen-bonded 2:1 complex with bipyridine dicarboxylic acid (**1**). The linear, rigid and charge assisted supramolecular building block has numerous additional hydrogen bond acceptors on the *anti* lone pairs of carboxylate O atoms and hence could be expected to display high propensity for inclusion of water molecules in the solid state [1]. We here show that, depending on the initial crystallization, it is in fact possible to utilize this property not only to build layered structures with clusters of water tetramers [2], [3], but also structures with extensive, unidirectional water channels [4] with a solvent accessible volume close to 20 % of the unit cell volume.



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Keywords: water channels; supramolecular chemistry; organic material

MS27-P1 **Structural Analysis and DFT Calculations of (Z)-1-[(5,6,7,8-tetrahydronaphthalen-1-ylamino)-methylene]naphthalen-2(1*H*)-one** Ahmet Erdönmez,[a] Gökhan Alpaslan,[a] Mustafa Macit,[b] Orhan Büyükgüngör,[a] [a]*Ondokuz Mayýs Univ., Department of Physics, Samsun-Turkey.* [b]*Ondokuz Mayýs Univ., Department of Chemistry, Samsun-Turkey.*
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The keto-enol tautomerism observed in *o*-hydroxy Schiff bases has received much experimental and theoretical attention in recent years [1,2].

The molecular and crystal structure of the title compound, $C_{21}H_{19}NO$, has been determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group $P2_1/c$ with unit cell dimensions a=17.8355(12)Å, b=5.9089(3)Å, c=14.8969(11)Å, β=93.449(6)°, V= 1567.11(18)Å^3, Z=4, R_1=0.047 and wR_2=0.115. The molecule adopts a keto-amine form, stabilized by an intramolecular N-H...O type hydrogen bond.

Molecular geometry of the title compound in the ground state have been calculated using the density functional method (DFT) with 6-31G(d,p) basis set and compared with the experimental data. The calculated results show that the optimized geometry can well reproduce the crystal structure.

In addition, DFT calculations of the compound, total energy and molecular electrostatic potential (MEP) were performed at B3LYP/6-31G(d,p) level of theory.

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