

## MS28-P4 Crystal structure and DFT calculations of 2-naphthalenecarboxamide, 3-hydroxy-N(2-methylphenyl)

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The structure of title compound 2-Naphthalenecarboxamide, 3-Hydroxy-N(2-methylphenyl)  $C_{18}H_{15}NO_2$ , has been synthesized. The Schiff base compound has been characterized by single-crystal X-ray diffraction technique. The compound crystallizes in the monoclinic space group P21/c with the following unit-cell dimensions  $a=15.1334(13)\text{Å}$ ,  $b=7.0994(4)\text{Å}$ ,  $c=12.7712(12)\text{Å}$ ,  $\alpha=90.000(0)^\circ$ ,  $\beta=97.221(7)^\circ$ ,  $\gamma=90.000(0)^\circ$ ,  $V=1361.23(19)\text{Å}^3$ ,  $Z=4$ . The crystal structure contains intramolecular N-H...N hydrogen bond. X-ray measurements was carried out on a STOE IPDS II diffractometer with MoK $\alpha$  radiation. The molecular structure was solved by direct method using SHELXS97 and refinement by full-matrix least-squares on  $F^2$  using SHELXL97 program. An Ortep-3 view of the molecule of title compound is shown in Fig. 1.

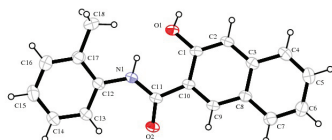


Figure 1. Ortep-3 diagram of the title compound

**Keywords:** Schiff base, tautomeric effect, DFT Calculations

## MS28-P5 Free energy determination applied for gallic acid monohydrate polymorphs

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The contribution of both entropy and enthalpy in crystal structure relative stability determination play an important role in understanding the formation and behaviour of a specific polymorph. Investigating the effects of vibrational entropy is a key factor in achieving a better understanding the relative stability of polymorphic materials. Due to low-frequency molecular vibrations, it is rather difficult to estimate vibrational entropy accurately. Therefore, the thermodynamic contribution should be extracted by combining the calculated vibration entropy with temperature-controlled crystallographic measurements. The kinetic contribution will be as well estimated by combining the calculated vibrational energies with crystallographic measurements. Gallic acid monohydrate has been shown to crystallise into five different polymorphs and it was rather difficult to obtain meaningful crystal structure prediction.<sup>1</sup> Hence, we considered is a good candidate for free energy investigation. Single crystal X-ray diffraction experiments were carried out at four different temperatures (10 K, 95 K, 123 K, and 175K) at a relatively high diffraction angle. The data obtained was then used in an aspherical atom refinement implemented in XD software<sup>2</sup> in order to obtain accurate atomic and anisotropic displacement parameters (adps). In a subsequent step the aspherical atom refinement data together with periodic ab-initio calculations were used in a normal mode refinement for gaining the vibrational entropy. The entropy was calculated using the periodic ab-initio calculations for each form. The 10K data collection for form III reveal a change in the unit cell parameters with  $Z'=3$  for the asymmetric unit. The volume is three times expanded and the molecules in the asymmetric unit show *pseudo* symmetry. Therefore, the structure can be defined from only one molecule with *pseudo*- $Z'=1$  as in case of the room temperature data of this form. Some of the H atoms involved in the (8) ring were found to show disorder. This is a possible explanation of the lack in H atom positions determination in the previous crystal structure prediction of gallic acid monohydrate polymorphs.<sup>1</sup>

### Reference:

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