

MS40-01 Crystal structure prediction of Pyridine with four molecules in the asymmetric unit. Jacco van de Streek,^a *University of Copenhagen, Denmark*
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Pyridine is a small, rigid, symmetrical molecule, with an unexpectedly complex crystal structure. The crystal structure that is routinely obtained for pyridine has four molecules in the asymmetric unit; this occurs for less than 0.5% of all organic crystal structures [1]. A crystal-structure prediction study with up to four independent molecules in all 230 space groups was undertaken for pyridine with a dispersion-corrected density functional theory method [2] using the software *GRACE* [3]. The two known polymorphs, $P2_12_12_1$ with $Z' = 1$ and $Pna2_1$, with $Z' = 4$, were found as ranks 1 and 2 in the correct stability order at low temperature. A pressure scan correctly predicts that the $P2_12_12_1$ form is favoured under pressure. The completeness of the structure generation and the number of hypothetical crystal structures per energy interval are analysed as a function of Z' [4].

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MS40-02 Towards the computation-led design of porous molecular crystals. Graeme M. Day,^a Edward O. Pyzer-Knapp,^a Tim. G. Cooper,^b Kim. E. Jelfs,^b Andrew I. Cooper,^b *University of Cambridge, UK*, *University of Liverpool, UK*
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Microporosity in materials can lead to chemically interesting properties because pore sizes in such materials correspond to molecular dimensions. Micropores have the potential to interact in very specific ways with guest molecules and we can exploit these interactions in applications such as gas storage, molecular separations and heterogeneous catalysis. The area of microporous materials has shown incredible growth over the last 10–15 years, thanks to the development of new classes of materials, in particular crystalline porous coordination polymers such as metal-organic and covalent-organic frameworks. Porous molecular organic compounds, on the other hand, are relatively rare, due to the tendency for molecules to fill space efficiently. A recently emerging strategy is the covalent pre-fabrication of cavities within the molecules themselves – so-called porous organic molecules. However, the connectivity of the in-built void space and the resulting accessibility of the pores, is still dependent on crystal packing. Here, we show how crystal structure prediction calculations, based on global lattice energy minimisation, can be used to assess potential molecules, suggesting a computationally-led design strategy. Results will be discussed for a series of cage-like molecules formed from the condensation of aromatic aldehydes with amine linker groups [1]. These molecules crystallise as solvates, but are readily desolvated to yield porous crystals. Remarkably, the observed structures are predicted in almost all cases as the global minimum in lattice energy, without needing to include the solvent molecules in the predictions [2]. The calculations have also been applied to the prediction of two-component porous cocrystal structures. Limitations of the method, the need to accurately model crystal packing effects on molecular geometry, and the potential importance of solvent templating on the resulting structure will be discussed.

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