

## MS31. Tailored physical properties in molecular crystals

Chairs: Sebastien Pillet, Pilar Gomez-Sal

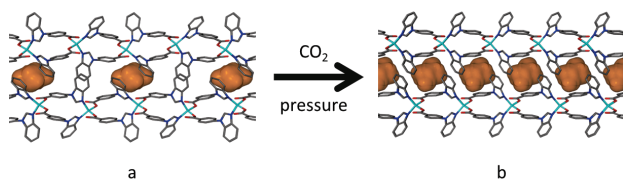
### MS31-P1 Adaptive structural changes for increased sorption capacity

Vincent J. Smith<sup>1</sup>

1. Department of Chemistry and Polymer Science, University of Stellenbosch, Stellenbosch 7600, South Africa

email: vjs@sun.ac.za

A two-dimensional (2-D) metal-organic framework  $\{[Zn(L)_4] \cdot DMF \cdot H_2O\}_n$ , (**1**), prepared by the reaction of 4-(1*H*-benzo[d]imidazol-1-yl)benzoic acid (**L**) with  $Zn(NO_3)_2 \cdot 4H_2O$  under solvothermal conditions, can adapt its structure during supercritical carbon dioxide ( $CO_2$ ) guest-exchange and  $CO_2$  sorption. The 2-D layers of the framework are associated by weak interactions that enable the framework to undergo guest-induced expansion and contraction. At high pressure, additional space is created between adjacent layers resulting in a significant increase in the  $CO_2$  sorption capacity (Figure 1). Moreover, the structural changes and gas uptake by the host occur preferentially for  $CO_2$  at 25 °C while nitrogen ( $N_2$ ) and methane ( $CH_4$ ) are not adsorbed under the same conditions. Pressure differential scanning calorimetry (PDSC) and in situ single-crystal X-ray diffraction (SCD) experiments under gas loading were carried out to obtain insight into the dynamic behaviour of the framework.



**Figure 1.** The framework viewed along [100]. a) Discrete mid-sized pockets of the structure observed at low pressure and b) the larger pockets observed at high pressure. Hydrogen atoms and guest molecules have been omitted for clarity.

**Keywords:** sorption, flexibility, carbon dioxide and hysteresis

### MS31-P2 Crystal structure and gelation properties of naphthalene bioconjugates

Zoran Kokan<sup>1</sup>, Berislav Perić<sup>1</sup>, Janja Makarević<sup>2</sup>, Goran Štefanić<sup>1</sup>, Leo Frkanec<sup>2</sup>, Srećko I. Kirin<sup>1</sup>

1. Materials Chemistry Department, Ruđer Bošković Institute, Bijenička c. 54, Croatia

2. Organic and Biochemistry Department, Ruđer Bošković Institute, Bijenička c. 54, Croatia

email: zoran.kokan@gmail.com

Low molecular mass gelators have been intensively researched in the past decade due to their ease of preparation and potential application in the field of soft and optical materials, transportation media, and as active media for organic reactions and catalysis.<sup>1</sup> Of special interests are chiral gelators where amplification of chiral or luminescent properties can be achieved via gelation.<sup>2</sup> We have successfully applied amino acid substituted benzene derivatives bearing phosphine moiety as ligands in Rh-catalyzed enantioselective hydrogenation reactions;<sup>3</sup> it was shown that the enantioselectivity is strongly dependant of the amino acids used as well as the benzene substitution (*meta*- or *para*-). As an expansion of our research towards the field of soft materials, here we present an ongoing work on amino acid disubstituted naphthalene bioconjugates where solid state and gelation properties are influenced by small modifications of the molecule. Several crystal structures of bioconjugates were obtained. All compounds exhibit hydrogen bonding in their but no  $\pi$ - $\pi$  stacking was observed. In the case of nonchiral glycine methyl ester derivative, two polymorphs were obtained by slow evaporation of different solvent solutions. It was shown by means of polycrystalline X-ray diffraction that in THF, a single phase is formed whilst in ethanol, both phases are present. The two polymorphs differ only in their characteristic torsion angles of the amide group. All derivatives were tested as gelators in various organic solvents. The results have shown that alanine derivative (Figure 1) with C6-aliphatic chains exhibit super-gelation of nonpolar aromatic solvents.

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