

**MS41-P2** Thermal motion in the Crystals of Octamethyl-Anthracene and its Ion-Radical Salts. Sergey Lindeman,<sup>a</sup> Shriya Wadumethrige,<sup>a</sup> Rajendra Rathore,<sup>a</sup> Oleg Dolomanov.<sup>b</sup> <sup>a</sup>Marquette University, USA, <sup>b</sup>Durham University, UK

E-mail: [sergey.lindeman@mu.edu](mailto:sergey.lindeman@mu.edu)

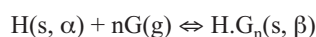
Oxidation of octamethylanthracene (OMA) – a prototypic  $\pi$ -donor substrate – results in cation-radical crystals of immediate relevance to the important class of organic conductors. The oxidation results in a distinct re-distribution of carbon-carbon bond lengths and in a noticeable distortion from molecular planarity. In order to ascertain if the observed geometrical changes are of a static (electron delocalization) or a dynamic nature (electron hopping, disorder), we undertook a multi-temperature study of OMA and its oxidation products. The crystals of OMA, its 1:1 chloranil complex and its ion-radical salt OMA<sup>+</sup>SbCl<sub>6</sub><sup>-</sup> were studied between 250 and 100K in 30K intervals. Throughout the cooling, the aromatic OMA moieties exhibited monotonically increasing deviations from rigid-body model (according to TLS test) that previously was attributed on many instances to some additional internal molecular movements. However, the corresponding high-angle refinements on experiments with 0.5 Å resolutions resulted in no perceptible deviations from the rigid-body model. Therefore we conclude that the observed deviations are a result of unaccounted asphericity of atoms rather than internal motions. An algorithm was developed to compare thermal motion of substrates in different crystallographic environments, including graphical representation. It was shown that attractive intermolecular forces can be identified from the analysis of the thermal motion.

**Keywords:** multi-temperature experiments, TLS analysis, thermal motion in crystal

**MS41-P3** How to measure the Dynamics of Solid-Gas reactions. Luigi R. Nassimbeni,<sup>a</sup> Nikoletta B. Báthori,<sup>b</sup> Ayesha Jacobs,<sup>b</sup> <sup>a</sup>Centre for Supramolecular Chemistry Research, Department of Chemistry, University of Cape Town, Rondebosch, 7701, South Africa, <sup>b</sup>Department of Chemistry, Cape Peninsula University of Technology, Cape Town, South Africa

E-mail: [luigi.nassimbeni@uct.ac.za](mailto:luigi.nassimbeni@uct.ac.za)

A solid host compound can combine with a gaseous guest to yield a solid host-guest compound:



where H is the solid host compound, in its non-porous  $\alpha$  phase (the apohost) and G is the guest. The rate constant,  $k_f$ , of the forward reaction can be measured by techniques which employ especially designed equipment. In the case where the host is an acid and the guest is a volatile base, the product is a salt. The reverse reaction, characterised by  $k_r$ , is usually carried out on commercially available Thermal Gravimetry balances. We have measured the kinetics of both salt formation and decomposition of a series of bile acids with volatile amines and have established the rate laws which control the kinetics. The structures of the ensuing crystalline products were elucidated and correlated with the activation energies of the reactions. The equipment which was employed to measure the kinetics of the salt formation reactions will be described. Results were obtained with lithocholic acid (LCA), deoxycholic acid (DCA) and cholic acid (CA) which were exposed to n-propylamine, sec-butylamine, and sec-methylbutylamine. Resolution of the later two guests occurred with DCA. The host-guest interaction were analysed with the aid of fingerprint plots generated by the program Crystal Explorer.

**Keywords:** kinetics; apparatus; bile acids