Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Lattice phonons of coronene single crystal polymorphs: a theoretical approach NICOLA BANNISTER, ENRICO DA COMO, SIMON CRAMPIN, Univ of Bath — Coronene, a polyaromatic carbon based molecule of disk shape, exhibits a range of peculiar physical properties from room temperature phosphorescence [1] to superconductivity [2]. The fundamental interest in this molecule is linked to its diamagnetism, originating from the delocalized pi electrons. Recently, we reported the discovery of a new crystal structure of coronene, the beta phase, apparently favoured by the presence of an external magnetic field during crystal growth [3]. Ab-initio density functional theory (DFT) calculations of the lattice energy for the two coronene polymorphs, the known gamma and the new beta phase, indicate that the latter has a lower energy minimum and thus should be favoured. Instead experimentally we find that the gamma phase is stable at room temperature and converts into beta at 150K. This observation calls for a more complete description of the relative energetic stability of the polymorphs including the role of phonons. We present our efforts in describing the lattice phonons of the two structures by performing DFT simulations and comparing them with data from low frequency Raman spectroscopy. [1] Mieno et al. Adv. Opt. Mat. 4, 1015 (2016) [2] Kubozono et al. Phys Chem Chem Phys 13, 16476 (2011) [3] Potticary et al. Nature Comm. 7, 11555 (2016)

Nicola Bannister
Univ of Bath

Date submitted: 11 Nov 2016 Electronic form version 1.4