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The impact of pressure on β-Cyclodextrin•acetaminophen inclusion complexes

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Cyclodextrins (CDs) have attracted considerable interest as model systems in supramolecular host-guest chemistry. They are described as hollow truncated cones with a hydrophilic outer surface and a nonpolar inner cavity suitable for small molecules' encapsulation.[1] By virtue of their character, CDs are used as excipients to improve the aqueous solubility of active pharmaceutical ingredients (APIs). High-pressure crystallisation techniques have been established as a suitable tool for exploring the phenomenon of polymorphism and solvate formation of pharmaceutical compounds throughout numerous examples reported in the literature.[2] Thus, exploring the inclusion-complex formation and the polymorphic behaviour of CDs with APIs at high pressure would be an interesting extension of the technique. The present work describes the attempt of an in-situ crystallisation of β-CD•acetaminophen inclusion complex and compression studies of the known β-CD•acetaminophen complex[3] in different crystallisation media at pressures up to 1.0 GPa. A new high-pressure crystal form observed at 0.8 GPa as well as unexpected results are presented herein. The crystals have been characterised by means of polarised optical microscopy, Raman spectroscopy and single-crystal X-ray diffraction using both home and synchrotron sources.

[1] *W. Saenger, J. Jacob, K. Gessler, et al, Chem Rev, 1998, 98, 1787–1802,* ***[2]*** *F. P. A. Fabbiani, C. R. Pulham, Chem Soc Rev, 2006, 35, 932–942,* ***[3]*** *M. R. Caira, D. R. Dodds, J Incl Phenom Macrocycl Chem, 2000, 38, 75–84*

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