Electronic Supplementary Information

Host-Guest Complexes of Cucurbit[6]uril with Phenethylamine-Type Stimulants

Oksana Danylyuk

Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland; E-mail: odanylyuk@ichf.edu.pl

Distortion of CB6 molecule: the highest possible symmetry of the **CB6** molecule is 6/*mmm* (D_{6h}). Such high symmetry is fulfilled only in few crystal structures of **CB6** complexes.[1] The degree of the distortion from the perfect D_{6h} symmetry can be expressed as the difference of the *max* and *min* distances between opposite carbon atoms of the **CB6** methine groups. In the ideal D_{6h} structure of **CB6** the distance between opposite CH carbon atoms is of 10.16 Å. Interestingly, the highest distortion of 13% (the difference in the *max* and *min* distances is 1.31 Å) was observed in the **CB6** inclusion complex with 4-methylpyridinium guest.[2] In the two studied complexes of **CB6** with octopamine the difference between *max* and *min* distances is of 0.33 Å (complex **3**) and 0.75 Å (complex **4**), corresponding to 3 and 7% distortion from the ideal D_{6h} symmetry.

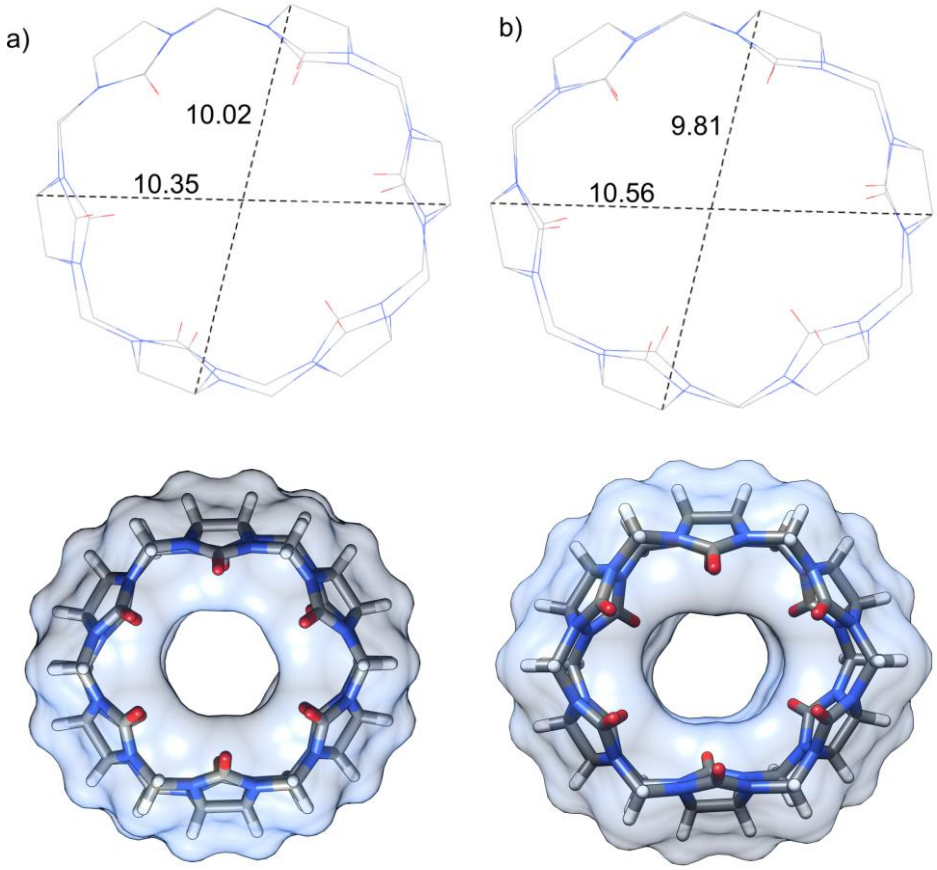

Fig. ESI-1 The distortion of **CB6** macrocycle from the perfect D_{6h} symmetry in the complexes **3** (a) and **4** (b), the *max* and *min* distances between opposite carbon atoms of the **CB6** methine groups are shown.

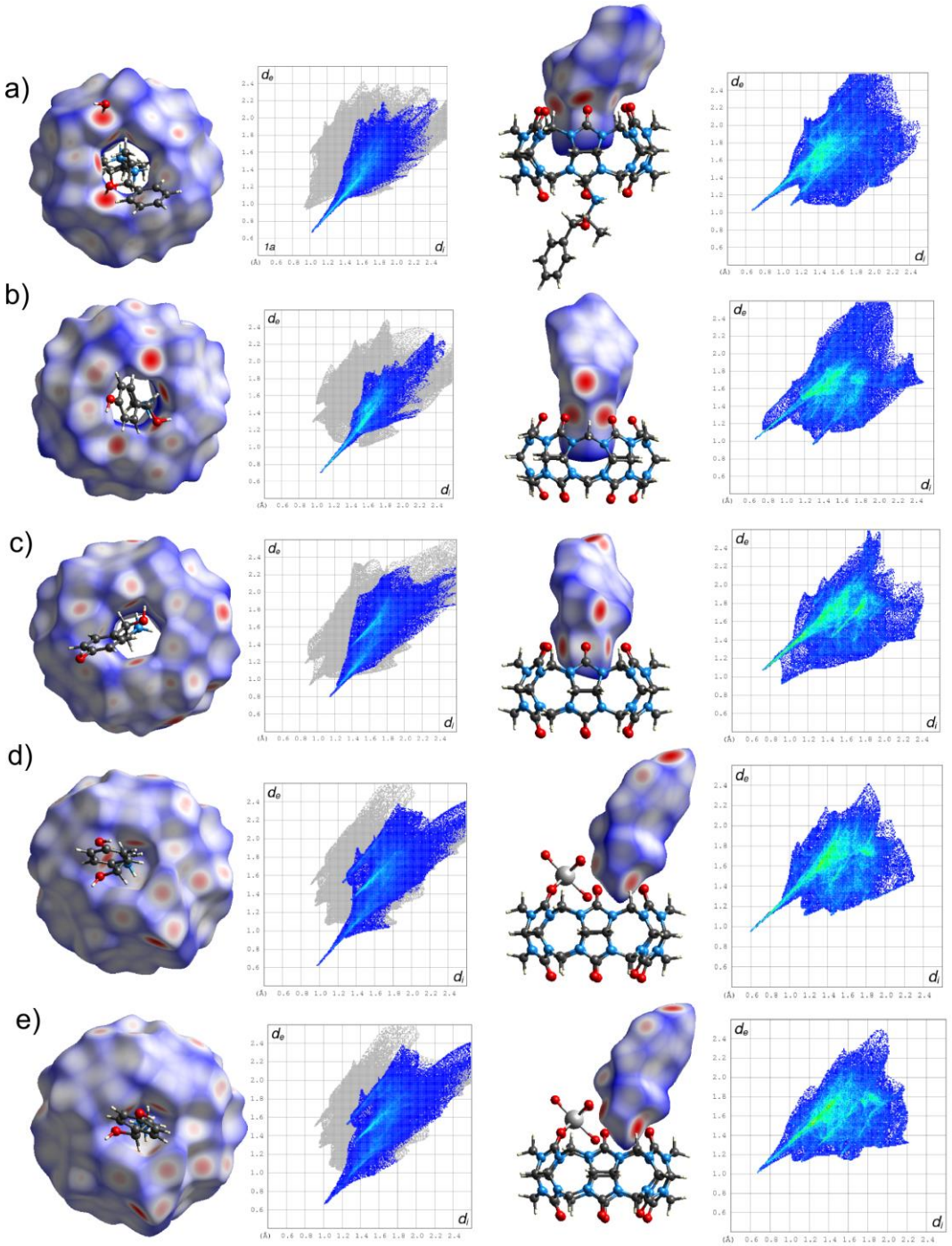

Fig. ESI-2 From left to right: the Hirshfeld surface of **CB6**, filtered fingerprint plot for **CB6** highlighting the close contacts for O atoms of **CB6** and all atoms outside the surface, Hirshfeld surface of the guest, fingerprint plot for the guest - for the complexes 1 (a), 2 (b), 3 (c), 4 (d and e, corresponding to two possible orientations of octopamine guest molecule due to structural disorder).

[1] D.G.Samsonenko, M.N.Sokolov, A.V.Virovets, N.V.Pervukhina, V.P.Fedin, *Eur.J.Inorg.Chem*., **2001**, 1, 167; D.Bardelang, K.A.Udachin, D.M.Leek, J.A.Ripmeester, *CrystEngComm*, **2007**, 9, 973.

[2] D. G. Samsonenko, A. V. Virovets, J. Lipkowski, O. A. Geras'ko, V. P. Fedin, *J. Struct. Chem*., **2002**, 43, 664.