# Stacking interactions in cavity-containing molecular structures built from acylphloroglucinols: a computational study

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Computational studies of cavity-containing molecular structures built from acylphloroglucinol units had shown that the bowl-shaped structures are likely the deepest and most tightly-textured bowls that can be obtained from hydroxybenzenes [Mol. Phys. 17-18:2254-2266 (2017); J. Mol. Model. 26: 13. https://doi.org/10.1007/s00894-019-4208-z (2020)] and that tube-shaped structures exhibit tight texture with alternatingly higher and lower levels of the benzene rings of the building units. Because of the mutual positions of the aromatic rings in the walls of the cavity, stacking interactions can be expected to play significant roles. The current work presents the results of a computational study in which the previously calculated bowl-shaped and tube-shaped structures were recalculated using the same levels of theory (HF/6-31G(d,p) and DFT/B3LYP/6-31+G(d,p)) with the inclusion of the Grimme correction to take stacking interactions into account. The energy lowering and the changes in other molecular properties – with respect to the results of calculations without the correction – are analysed in terms of the shapes of the structures (bowl- or tube- shaped), the number of monomeric units constituting it, the symmetry type, and the conformer type. The results confirm the significance of the stacking interactions for cavity-containing structures built from acylphloroglucinols.