[MS30-05] Structural, energetic and charge density investigations of triptycene and its selected derivatives

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Triptycene and its derivatives, due to their characteristic rigid framework with the point symmetry, play an important role in crystal engineering, and are often employed as molecular machine building blocks. New structures of chloro-, methylo- derivatives of tripytcenes are presented in details and compared to the related structures deposited in CSD. It occurred that the studied triptycene derivatives create two distinguishable network types, one of which constitutes a layered architecture. Interestingly, the 1,4,-dichloro-9,10-dimethylotriptycene (**DCDMT**) appears in two polymorphic forms. It crystallizes in the P*21/c* space group at room temperature with one molecule in the asymmetric part of the unit cell. However, when the temperature is decreased to 100 K, its symmetry is partially broken (the inversion centre vanishes). For all the measured and related CSD structures periodic *ab-initio* calculations in the *CRYSTAL09*[1] and *PIXEL*[2] packages were conducted and careful analyses of lattice and dimer interaction energies were performed. The influence of substituent on crystal packing and lattice energy stability was investigated. In the case of triptycene and 9,10-dimethylotriptycene (**DMT**), X-ray high resolution measurements and multipolar refinements were performed, and thus experimental charge density distributions were obtained and analysed by means of the AIM theory. During the refinement of DMT, it was necessary to include the anharmonic thermal motion effect for carbon atom from the methyl group. Additionally, different approaches to hydrogen atom treatment were tested.

[1] Dovesi, R., Saunders, V. R., Roetti, R., Orlando, R., Zicovich-Wilson, C. M., Pascale, F., Civalleri, B.; Doll, K., Harrison, N. M., Bush, I. J., D'Arco, P., Llunell, M. (2009) *CRYSTAL09*, University of Torino: Torino
[2] Gavezzotti, A., (2002) *J. Phys. Chem. B*, **106**, 41454154.

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