MS22-P09 | Polymorphism and the Role of F…F Interactions in Crystal Packing of Fluorinated Tosylates

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The peculiarities of interatomic interactions formed by fluorine atoms were studied in four tosylate derivatives p-$CH_3C_6H_4OSO_2CH_2CF_2CF_3$ and p-$CH_3C_6H_4OSO_2CH_2(CF_2)_nCHF_2$ (n = 1, 5, 7) using X-ray diffraction and quantum chemical calculations (Arkhipov *et al.*, 2019). Compounds p-$CH_3C_6H_4OSO_2CH_2(CF_2)_nCHF_2$ (n = 1, 5) were crystallized in several polymorph modifications. Analysis of intermolecular bonding was carried out using QTAIM approach, NCI method and energy partitioning scheme implemented in Crystal Explorer program (CE-B3LYP/6-31G(d,p)). All compounds are characterized by crystal packing of similar type and the contribution of intermolecular interactions formed by fluorine atoms to lattice energy is raised along with the increase of their amount. The energy of intra- and intermolecular F…F interactions is varied in range 0.5–13.0 kJ/mol. Total contribution of F…F interactions to lattice energy does not exceed 40%. Crystal structures of studied compounds are stabilized mainly by C-H…O and C-H…F weak hydrogen bonds. The analysis of intermolecular interactions and lattice energies in polymorphs of p-$CH_3C_6H_4OSO_2CH_2(CF_2)_nCHF_2$ (n = 1, 5) has shown that most stabilized ones are characterized by the least contribution of F…F interactions.

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[1]Arkhipov, D. E., Lyubeshkin, A. V., Volodin, A. D. & Korlyukov, A. A. (2019). *Crystals*. **9**, 242.