An Examination of All the Inter-ion Interactions in Tetraphenyl-phosphonium Squarate

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The tetraphenyphosphonium squarate salt crystallises with a hydrogen bonded dimeric squarate anion in space group $P2_1/n$ with Z = 4. X-ray data were collected on a Saturn 70 with Mo-K_α radiation to $2\theta(max) = 76^o$ at -153^oC. The multipole refinement was performed with XD [1] and all the topological interactions were then investigated. Currently of the 20 unique C-H hydrogen atoms, all but two form significant interactions either to the squarate ion (C-H…O interactions) or among the phenyl groups C-H….H-C, or C-H…π(Ph). The two remaining 'non-interacting' (C)H atoms are adjacent *ortho* hydrogen atoms, that look as though there ought to be an intramolecular H…H interaction though this has not yet been fully characterized. The remaining interactions satisfy all the eight of Koch & Popelier's criteria [2] for a weak interaction.The O-H…O classical hydrogen bond of the squarate is found to have weakened in the crystal when compared with the theoretically calculated values for an isolated dimeric anion

[1] Koritsanszky T. S., Howard S., Macchi P., Gatti, C., Farrugia L.J., Mallinson P.R., Volkov A., Su Z., Richter T., Hansen N. K., *XD (version 4.10, July): A computer program package for multipole refinement and analysis of electron densities from diffraction data*, 2003. [2] a) Koch U., Popelier P. L. A., *J. Phys. Chem.,* 1995, **99**, 9747; b) Popelier, P., *Atoms in Molecules*, Prentice Hall, UK, 2000, 151.

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