Sizes of Molecules in Organic Crystals: the Voronoi-Dirichlet Approach

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Crystallographic data on 69011 molecular compounds were selected from the CSD by means of the program package TOPOS [1]. All the compounds are completely refined structures without metal atoms. The sizes of molecules have been calculated as the volumes of molecular Voronoi-Dirichlet polyhedra (VDPs) [2]. To construct molecular VDPs, the method by Peresypkina & Blatov [2] implemented in the ADS program (part of the TOPOS package) was used. After calculation 100632 molecules have been detected and volume distributions were constructed for the most frequent molecules.

The conclusions from the data obtained are that the volume of a molecule is rather constant and that variations follow a normal distribution and the mean volume value is almost coincident with the volume of a molecule in a homomolecular crystal. The last conclusion follows from the fact that almost all molecular volumes in the homomolecular crystals lie within the 95% confidence intervals, whose half-width is *ca* 10% of the mean value. This means that the influence of a crystal field on the size of a molecule is found to be slight and nearly equal in homo- and heteromolecular crystals. This trend can be violated if a molecule is surrounded by a good deal of highly polarized atoms or if a molecule is disordered or surrounded by disordered molecules.

The results obtained show that molecular VDPs can be used to model molecular domains and to reveal factors causing variations in domain sizes. These results can be useful, *e.g.*, for predicting organic substrates that can occupy the receptor cavity [3].

[1] Blatov V.A., Shevchenko A.P., Serezhkin V.N., *J. Appl. Cryst.*, 2000, **33,** 1193. [2] Peresypkina E.V., Blatov V.A., *J. Mol. Struct. (Theochem)*, 1999, **489**, 245-236. [3] Virovets A.V., Blatov V.A., Shevchenko A.P., *Acta Cryst.*, 2004, **B60**, 350-357.

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