

The Effect of High Pressure on the Topology of Organic Systems

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The effect of high pressure on a crystal structure is dependent on the delicate balance of forces. Recent work has shown that in many cases the application of high pressure has the effect of compressing a structure anisotropically. This is exemplified by alanine [1], which compresses significantly in the b and c directions, but only slightly in the a-direction.

There are a range of methods for analysing the change in structure due to pressure, one which gives a useful overall picture of the molecular symmetry works by partitioning the structure into Voronoi-Dirichlet polyhedra (VDPs) [2]. It is often the case that the application of hydrostatic pressure causes the structure to become more locally symmetric. Using these VDPs it is possible to see structures tend towards standard hard-sphere packing structures such as BCC, FCC and HCP as the pressure is increased.

[1] Dawson A., *PhD Thesis*, The University of Edinburgh, 2003. [2] Blatov V. A., Shevchenko A. P., Serezhkin V. N., *J. Appl. Cryst.*, 1999, **32**, 377.

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