

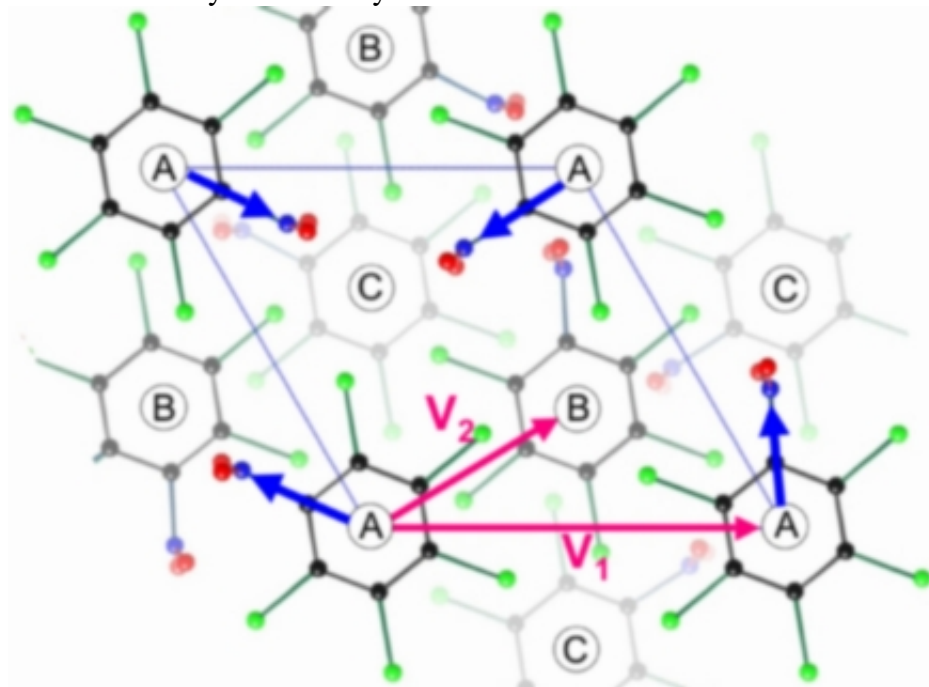
Disorder in Pentachloronitrobenzene, $C_6Cl_5NO_2$: A Diffuse Scattering Study.

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Pentachloronitrobenzene (PCNB) is one of a series of chloronitrobenzene derivatives that are currently being studied because their disordered nature and propensity to undergo phase-transitions are thought to be responsible for their anomalous dielectric properties. Disorder often strongly affects the electronic environment in such materials, and it is considered that this may be fundamental to such properties as, for example, SHG (second harmonic generation). Our goal is to quantify the disorder and short-range order as fully as possible with a view to being able to control or harness such disorder and aid the design of new functional molecular materials. We have recorded complete 3D diffuse scattering data for PCNB at the 11D-C high-energy beamline at the Advanced Photon Source (APS) and have used our latest Monte Carlo simulation methods to carry out an analysis.



Since each molecular site contains a molecule in any one of 6 different orientations as many as 36 SRO parameters are required to fully specify local ordering patterns, even when only nearest-neighbour interactions are considered. If neighbours within a single molecular plane and between neighbouring planes are both considered this number expands to 72 and this represents a formidable parameter space that needs to be explored.

In this paper we give an account of how a satisfactory solution to this problem was achieved.