Anisotropic Displacement Parameters for Normal Mode Analysis: Which Refinement is Needed?

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Information on low-frequency modes of molecular motion in the crystal[1] can be extracted from Anisotropic Displacement Parameters (ADPs) measured over a wide range of temperatures. Here we investigate the bias on the ADPs due to effects of deformation density and its influence on the model of motion.

Four models were refined with a data set on (*E*)-2,2'-dimethylstilbene measured at 90 K to the high resolution of 0.41 Å[2]: 1) Spherical form factors 2) Multipole Parameters (MPPs) from a library[3] 3) MPPs fitted to a calculated charge density[4] 4) MPPs fitted to the experimental charge density. The ADPs from the different refinements differ by 0.00006 - 0.0017 A^2, corresponding to 1 to 20 s.u.. The U11 and U22 components lying in the molecular plane decrease for models 2, 3 and 4 as compared to model 1. The decrease is largest for model 4. In model 2 the U33-out of plane components are becoming clearly bigger whereas they become smaller with model 4 compared to a spherical model. In the Normal Mode Analysis these differences are reflected primarily in a decrease of the temperature independent part of the model of motion [1].

[1] Bürgi H.B., Capelli S.C., *Acta Cryst*., 2000, A**56**, 403-412. [2] Ogawa K., Harada J., *unpublished results*. [3] Pichon-Pesme V., et al., *J. Phys. Chem*., 1995, **99**, 6242-6250. [4] Courtesy of T. Koritsansky, Middle Tennessee State University.

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