Atomic Displacement Parameters and Specific Heat of *p*-Dichlorobenzene Polymorphs between 10 and 230 K

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Synchrotron data for the α- and β-polymorphs of *p*-dichlorobenzene (*p*-DCB) between 10 and 230 K were collected to 0.5 Å resolution at the ESRF and refined with a multipole model in order to deconvolute thermal motion from valence bonding density. Sealed tube data of the γ-polymorph were collected between 100 and 180 K to 0.7 Å resolution and refined with a spherical atom model. The multi-temperature atomic displacement parameters (ADPs) were analyzed in terms of libration and translation frequencies [1]. From the six external vibration frequencies and the intramolecular vibration frequencies from high-level DFT calculations heat capacities C_v were calculated with molecular Einstein and Debye models and found to be in fair agreement with C_p from calorimetric measurements [2].

[1] Bürgi H.-B., Capelli S.C., Birkedal H., *Acta Cryst*., 2000, A**56**, 425. [2] Dworkin A., Figuière P., Ghelfenstein M., Szwarc H., *J. Chem. Thermodyn.* 1976, **8**, 835.

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