Experimental Electron Density and Topological Analysis of D- and DL- Camphoric Anhydride

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Parameter indeterminacies often encountered during pseudoatom modeling of non-centrosymmetric structures unavoidably bias the results of experimental charge density studies [1,2]. A comparative analysis of high-resolution X-ray data of both crystal forms of Camphoric Anhydride $C_{10}H_{14}O_3$ was performed to learn about model restrictions applicable to reduce correlations between least-squares parameter estimates and the transferability of experimental pseudoatoms. The title compound is an ideal candidate for such a study, since the two enantiomers have very similar crystal packing and thus density differences due to different intermolecular forces are expected to be negligible. All intensity data were collected at 100K using SMART 1K CCD area detector with Mo K_α radiation up to a resolution corresponding to $(\sin\theta/\lambda)_{max} = 1.1 Å^{-1}$. The multipole refinement and the analysis of the static densities were performed using the XD program suite. The results obtained by different constrained models will be presented in terms of local and integrated topological properties of the densities.

[1] Spackman M.A., Byrom P.G., *Acta Cryst*., 1997, **B53**, 553. [2] El Haouzi A., Hansen N.K., Le Hènaff, C., Portas L., *Acta Cryst*., 1996, **A52**, 291. [3] Koritsanszky T., Richter T., Macchi P., Volkov A., Gatti C., Howard S., Mallinson P.R., Farrugia L., Su Z., Hansen N.K, *XD: a Computer Program Package for Multipole Refinement and Topological Analysis of Electron Densities from Diffraction Data,* 2003.

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