Poster Presentation

MS42.P02

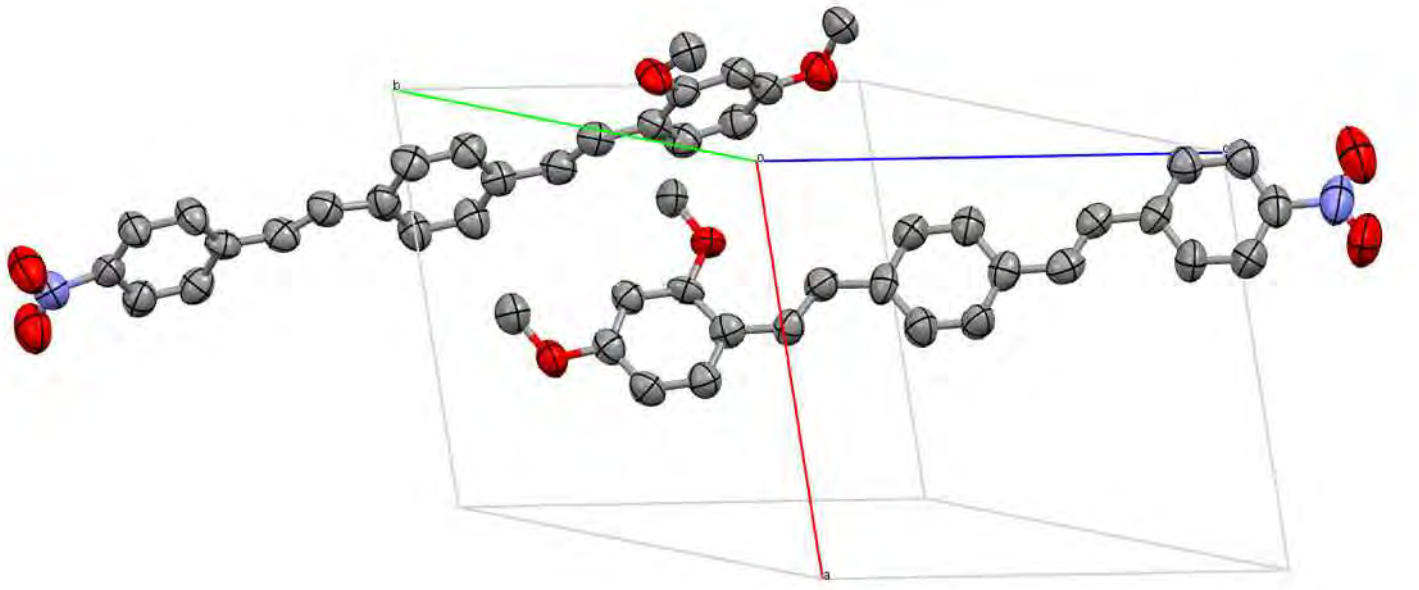
Twin Tandem Bicycle Pedal Motion - Using X-rays to Resolve Disorder Thermodynamic Parameters

C. Vande Velde[1], A. Collas[2], M. Zeller[3], F. Blockhuys[2]

[1]University of Antwerp, Faculty of Applied Engineering, Hoboken, Belgium, [2]University of Antwerp, Dept. of Chemistry, Antwerpen, Belgium, [3]Youngstown State University, Dept. of Chemistry, Youngstown, Ohio, USA

During our research into polar crystals for organic electronic applications, we synthesized E,E-1-[2-(4-nitrophenyl)ethenyl]-4-[2-(2,4-dimethoxyphenyl)ethenyl]benzene, which has a polar crystal structure (space group Pc) and displays the typical bicycle pedal motion, as studied in detail by Harada and Ogawa [1], in one of its ethenylic links. A van 't Hoff plot of the logarithm of the population ratio versus 1/T, however, showed a kink instead of being a straight line, which led us to conclude that an unusual phase transition was occurring in this material [2]. In the mean time we have crystallized the same material in a second, centrosymmetric polymorph (space group P-1). There, the asymmetric unit consists of two complete molecules, and they display the same kind of bicycle pedal motion, but this time in all four different ethenylic linkers. Every one of these population differences increases with temperature, so that four van 't Hoff plots can be constructed for this structure. Two of these behave normally, the other two display a kink, just like the van 't Hoff plot of the pedaling ethenylic link in the other polymorph of this molecule. This is, to the best of our knowledge, the first instance of a structure where four different dynamic equilibria can be resolved simultaneously, and only the second example in which van 't Hoff plots for the thermodynamics of dynamic disorder are not linear, indicating an unusual type of phase transition linked only to the dynamics of the molecules in the crystal.

[1] *Harada & Ogawa, J. Am. Chem. Soc., 2001, 123 (44), pp 10884–10888,* ***[2]*** *Vande Velde et al., Chem. Eur. J., 2010, 17(3), pp 912–919*



Keywords: bicycle pedal motion, phase transition, distyrylbenzene