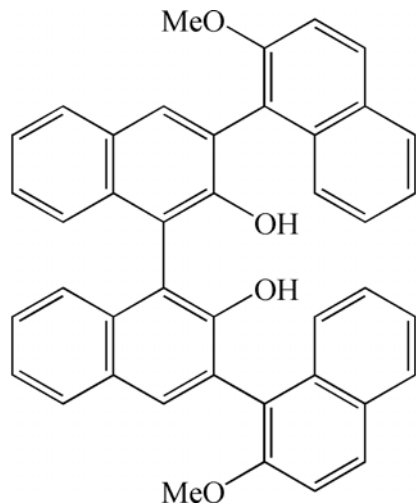


W0252

The Absolute Structure of 2,2''-Dimethoxy-[1,2';4',1'';3'',1''']quarter-naphthalene-3',2''-diol, C₄₂H₃₀O₄•(EtOAc): A Merohedrally Twinned and Disordered Structure. Michal Sabat, Marilise A. Hyacinth, Dept. of Chemistry, Univ. of Virginia, McCormick Rd., Charlottesville, VA 22904, Charles F. Campana, Bruker AXS Inc., 5465 East Cheryl Parkway, Madison, WI 53711, George M. Sheldrick, Univ. Göttingen, Inst. für Anorganische Chemie, Tammannstr. 4, D-37077 Göttingen, Germany.

An enantiomerically pure specimen of 2,2''-dimethoxy-[1,2';4',1'';3'',1'''] quarternaphthalene-3',2''-diol, C₄₂H₃₀O₄•(EtOAc) was prepared as part of our research project on the asymmetric catalysis by 1,1'-binaphthyl compounds [1]. Preliminary characterization indicated the structure to be:



A precise single crystal analysis was carried out in order to confirm the absolute stereochemistry of the molecule. A high-quality dataset was collected at 140K on a Bruker SMART 6000 system equipped with a Cu sealed tube X-ray source. The structure was solved in the trigonal space group P3₂21 using a dual-space recycling method and refined as a merohedral twin to R1 = 0.032. The refinement also includes two types of disorder. The refinement unequivocally confirms the absolute structure. Details of the methods used to solve and refine this structure will be presented.

[1] D.L. Simonson, K. Kingsbury, M.-H. Xu, Q.-S. Hu, M. Sabat and L. Pu, *Tetrahedron*, 58, 8189 (2002).