On the Symmetry of (-)-1,3,5,7-Tetrakis[2-(1S,3S,5R,6S,8R,10R)- D_3 trishomocubanylacetoxymethyl]adamantane

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Summary The highest symmetry attainable by the title compound is D_2 , not T as previously claimed.

In a recent report¹ describing the synthesis of the title compound, it was asserted that the latter represented the first optically active organic molecule with T symmetry. However, the interposition of the acetoxymethyl (CH₂CO₂CH₂) groups destroys all threefold symmetry inherent in the four $2-D_3$ -trishomocubanyl groups and in the adamantane skeleton, and T symmetry is ipso facto unattainable for any conceivable conformation. The title compound therefore belongs in the same class with McCasland's pentaerythritol tetra-(-)-menthyloxyacetate:2 in both molecules, four asymmetric units (menthyloxyacetoxymethyl groups in McCasland's compound and 2-D3-trishomocubanylacetoxymethyl groups in the title compound) of like chirality and of known absolute configuration are attached at the four vertices of a tetrahedral frame (methane in McCasland's compound and adamantane in the title compound), and the highest attainable symmetry is D_2 . Although neither molecule possesses T symmetry, when viewed as non-rigid systems both belong to the molecular symmetry group $(C_1)^4 \wedge T$, a group of order 12 which is isomorphic to the point group T,4 and which may be represented by the alternating group of permutations A_4 .

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M. Nakazaki and K. Naemura, J. Chem. Soc., Chem. Commun., 1980, 911; J. Org. Chem., 1981, 46, 106.
G. E. McCasland, R. Horvat, and M. R. Roth, J. Am. Chem. Soc., 1959, 81, 2399.
M. Farina and C. Morandi, Tetrahedron, 1974, 30, 1819.

⁴ L. D. Iroff and K. Mislow, J. Am. Chem. Soc., 1978, 100, 2121.