Electrohydrocyclodimerization of Dimethyl Benzene-1,2-diacylate; Correction of the Structure of the Hydrocyclodimer

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We have recently 1 commented upon the fact that the cathodic reduction of dimethyl benzene-1,2-diacylate (1) seems to yield a single isomer of the hydrocyclodimer 2, in spite of the fact that it, in principle, can exist in twenty isomeric forms (sixteen enantiomeric pairs and four meso forms). This prompted us to perform an X-ray crystallographic study 2 in order to establish the stereostructure of the hydrocyclodimer. It appeared that the previous structural assignment, based on NMR data, was wrong and that the correct structure is the even more interesting one of 3 (tetramethyl cis - 4b,5,6,10b,11,12 - hexahydrochrysene - cis-5,11-carboxylate-6,12-diacetate) which is indeed not easily distinguishable from 2 on the basis of the usual array of spectroscopic techniques.

In the course of preparing crystals suitable for X-ray analysis two other hydrodimers (comprising 38 % of the total amount of hydrodimer; see Ref. 1) were isolated and subjected to an X-ray crystallographic study. 3 The one obtained from fractionated crystallization from ethyl acetate turned out to be 4 in which one ring closure has occurred whereas the one obtained from methanol had the structure of the simple hydrodimer, 5, as the meso form.


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