Cyclohexane Fatty Acids from a Thermophilic Bacterium

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Summary In the saponifiable lipids of *Bacillus acidocaldarius* the principal components are 11-cyclohexylundecanoic and 13-cyclohexyltridecanoic acids.

IT has been suggested that in thermophilic bacteria a major contribution to thermostability is made by membrane structures[1] and in this connection the composition of cell lipids in such organisms is of obvious interest. An isolate now identified with the *Bacillus acidocalderius* of Brock[1] comes from a very extreme environment (high temperature, low pH) and its lipids are under investigation. The characterization of pentacyclic triterpenes from the non-saponifiable fraction has already been reported.[2]

The lipid extract from cells grown on 0·1% glucose–0·1% yeast extract–mineral salts, adjusted to pH 3·0 with H_2SO_4 and incubated at 64°, following saponification and methylation, contained exclusively saturated esters (as shown by chromatography on SiO_2–$AgNO_3$). G.l.c. of the mixture (10% diethyleneglycol succinate at 220°) showed two unusual esters as the major components, together with about 25% of the more common iso-C_{17} and anteiso-C_{17} esters, about 5% of iso-C_{16}, and traces of n-C_{14}, iso- and anteiso-C_{15}, n-C_{16}, n-C_{17}, and n-C_{18} esters. The two major esters had equivalent chain lengths, on this column, of 19·15 (27%) and 21·15 (31%).

Larger-scale g.l.c. gave samples of both esters, $C_{18}H_{34}O_2$ (liquid at 15°) and $C_{20}H_{38}O_2$ (m.p. 28°) (both monocyclic since not unsaturated). The n.m.r. spectra of each revealed the absence of *C*-Me and an 11—13 proton signal at δ 1·65 consistent with a terminal cyclopentyl or cyclohexyl structure (the β-CH_2 group of fatty acid esters also resonates in this region). In the i.r. spectra bands at 842, 890, and 1455 cm^{-1}, not found in normal fatty acid esters, could be interpreted similarly.

For methyl 11-cyclohexylundecanoate, from a very minor component of butter-fat, g.l.c. and spectroscopic data very similar to our own for the lower homologue have been established,[3] whereas the equivalent chain length of a cyclopentyl analogue, methyl dihydrochaulmoograte, was 19·85 on our column. A sample of synthetic methyl 11-cyclohexylundecanoate† proved undistinguishable from the lower homologue in our hands, and the higher homologue must be the 13-cyclohexyltridecanoate.

The lower homologue also occurs at about 3% of the fatty acids in a rumen bacterium,[4] but in *B. acidocaldarius* the two cyclohexyl acids can comprise as much as 65%, *e.g.* from cultures grown at 50° and pH 2, or 70° and pH 5. The distribution of these acids in other bacterial species might prove to be taxonomically significant; meanwhile their biosynthesis is under investigation.

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