DEHYDRATION OF CYCLOPENTYLCARBINOL-1-^{13}C

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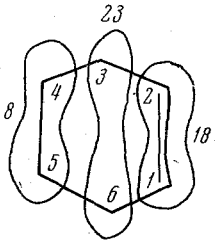
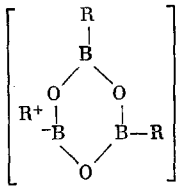
Continuing work on the study of the isomerization of cyclohexane derivatives, formed as a result of ring expansion of cyclopentylcarbinyl compounds, we studied the dehydration of cyclopentylcarbinol labelled with ^{13}C in the methylene group (enrichment 50%). Dehydration was carried out by heating the carbinol with boric acid at 340°C, analogously to the conditions of dehydration of cyclohexylcarbinol [1]. A mixture of olefins was obtained as a result of the reaction consisting of, from GLC data (polyethylene glycol 2000, Chromosorb W, 80°, helium) 70% cyclohexene, 14% 1-methylcyclopentene, 12% methylenecyclopentane, and 4% an unidentified hydrocarbon. The difference in chemical shifts of cyclohexene and the accompanying olefins made it possible to take NMDR spectra without separating cyclohexene from the mixture. The ^{13}C content in cyclohexene (%) was calculated from spectral data.



The presence of a label in positions 4 and 5 (8%) indicates that approximately 30-35% cyclohexene formed in the process of dehydration is isomerized. In agreement with data of Chapman [1], dehydration of cyclohexylcarbinol under the indicated conditions proceeds through a stage of formation of the borate ester of the carbinol and further, of an ion pair



The isomerized reaction products are formed by isomerization of the R^+ cation. An analogous mechanism can be proposed also in the case of dehydration of cyclopentylcarbinol. But the possibility of isomerization by double-bond migration in the formed cyclohexene is not excluded.

LITERATURE CITED

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Institute of Heteroorganic Compounds, Academy of Sciences of the USSR. Institute of Cybernetics, Academy of Sciences of the Estonian SSR. Translated from Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, No. 3, p. 726, March, 1970. Original article submitted December 1, 1969.