Bulletin of the Academy of Sciences of the USSR Division of Chemical Science 1976 vol.25 N12, pages 2509-2513

Configurations and conformations of the α - and β -thiooxides of $\Delta 3$ -carene

Samitov Y., Nuretdinova O., Vul'fson S., Timosheva A., Arbuzov B. *Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

Abstract

1. Analysis of1H NMR spectra has shown that the thiooxide obtained from the α -oxide of $\Delta 3$ -carene has the two three-membered rings in the cis-configuration, while the thiooxide obtained from the β -oxide is a trans-isomer. 2. Measurements of the1H and13C NMR spectra and the Kerr effect have shown the predominant conformation of the α -thiooxide molecule to be that of the inverted boat. In the case of the β -thiooxide, a conformational equilibrium is established in which the predominant configuration is that of the inverted boat, according to the NMR data, and that of the boat itself, according to the Kerr effect measurements. © 1977 Plenum Publishing Corporation.

http://dx.doi.org/10.1007/BF00920889