Russian Journal of General Chemistry 2009 vol.79 N6, pages 1090-1096

Polarity and structure of eight-membered organosilicon compounds with planar fragments

Vereshchagina I., Gazizova A., Ishmaeva E., Timosheva A., Chachkov D., Timosheva N. *Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

Abstract

For the first time is determined the polarity of eight-membered silocyns with planar fragments. By the methods of dipole moments and theoretical calculations (DFT B3LYP/6-31G*) of 1,3,2-dioxasilocyns is established that in these compounds occurs the conformational equilibrium of the forms bath-chair and distorted bath with the predominance of the first, in this case the bonds C(sp 3)-S and C(sp 3)-H of the exocyclic MeSCH2 group are in the not eclipsed gauche orientation relative to each other. © 2009 Pleiades Publishing, Ltd.

http://dx.doi.org/10.1134/S1070363209060097