Phosphorus, Sulfur and Silicon and the Related Elements 2009 vol.184 N6, pages 1406-1412

Polarity and structure of silatranes with planar fragments

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Abstract

The structure of silatranes N[CH2(RMeC6H2)O]3SiR1 with planar fragments in six-membered semi-rings was established by the methods of dipole moments and density functional theory calculations. They are endo-structures with transannular interaction N→Si in which the oxygen atoms located adjacent to the silicon participate besides the nitrogen and silicon atoms.

http://dx.doi.org/10.1080/10426500902947500

Keywords

Density functional theory, Dipole moments, Silatranes, Transannular interaction