Dipole moments, structure, and transannular interactions in silatranes containing planar fragments

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Abstract

The method of dipole moments and theoretical calculations (DFT B3LYP/6-31G*) were used for structural assessment of silatranes N[CH2(RMeC6H2)O]3SiR1 containing planar fragments in the six-membered semirings. They are endo structures with transannular N \rightarrow Si interaction which involves, along with nitrogen and silicon, oxygen atoms adjacent to silicon. © 2008 MAIK Nauka.

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