A DFT Study of the Structure and Relative Stability of 1,3-Thiasilacycloalkanes and Their S-Functional Derivatives

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Abstract - A series of 1,3-thiasilacycloalkanes and their *S*-oxides, *S*,*S*-dioxides, and sulfonium salts were studied by the DFT (B3LYP/6-31G*) method. In six-membered sulfoxides, the oxygen atom preferentially occupies the axial position, whereas in the corresponding sulfonium salts the *S*-alkyl group occupies the equatorial position. The calculation results explain the lower hydrolytic stability of the five-membered rings compared to the six-membered analogs and the lower stability of sulfoxides compared to sulfones.