前手性硅甲基的非等时性,分子结构对化学位差值的影响

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摘要 具有手性基团的二甲基二烷氧基硅烷的前手性硅甲基的 1 H NMR化学位移有差别, 其差值 \triangle χ随着非手性取代基的电负性成比例的改变。 \triangle χ与分子结构对Si-O间蝗(p-d)x相互作用的影响, 以及取代芳环的各向异性有关。

 关键词
 分子结构
 硅氧烷
 质子磁共振谱法
 化学位移
 手征性
 各向异性
 相互作用
 等时性

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Anisochronous prochiral silylmethyl groups: the effect of molecular structure on difference in chemical shifts

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Abstract Chem. shift nonequivalence was found in prochiral silylmethyl groups of chiral dimethylsilyl acetals. The difference in chem. shifts between the silylmethyl protons varied proportionally with the electronegativity of the chiral substituents. If the achiral part was an aryl group, the dimethylsilyl acetals containing electron-withdrawing substituents on the aryl ring had smaller differences. The important factor contributing to the magnitude of the differences was (p-d)p interaction between the empty d-orbit of the silicon atom and the lone-pair electrons of the oxygen atom and the anisotropy of the aromatic ring.

Key words MOLECULAR STRUCTURE SILOXANE PROTON MAGNETIC RESONANCE SPECTROMETRY CHEMICAL SHIFT CHIRALITY ANISOTROPY INTERACTIONS ISOCHRONISM

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