عنوان مقاله:

Investigation of NMR Parameters of para-Sulfonato-calix[۴]arene by HF Calculation

محل انتشار:

نشریه متدهای شیمیایی, دوره 2, شماره 3 (سال: 1397)

تعداد صفحات اصل مقاله: 8

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خلاصه مقاله:

Conformationally-rigid para-sulfonato-calix[۴]arene ($C_{۲۸}H_{۲۴}O_{۱۶}S_{۴}$) was isolated. The NMR parameters of the structure of calix[۴]arenes have been compared. The study of organic structures to form nanoporous materials is a well-known chemical phenomena (supermolecular chemistry) that is necessary for finding the crystal forms of calix[۴]arenes. We investigated and compared the hydrogen bonding, oxygen, and sulfur atom effects on calix[۴]arene via Hartree-fock(HF) theory by the Gaussian ۹۸ of program package.

کلمات کلیدی:

Calix[۴]arene, DFT, HF, Hydrogen bonding, Nanostructure, Chemical shift