Theoretical Study of the Absorption Spectrum and the Thermochemistry of the CF_3OSO_3 Radical

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Z. Naturforsch. **65a,** 720 – 724 (2010); received June 29, 2009 / revised November 23, 2009

The UV-visible absorption spectrum of the recently reported CF_3OSO_3 radical has been studied by using the time-dependent generalization of the density functional theory (TDDFT). For this a set of eleven hybrid functionals combined with the 6-311+G(3df) basis set were employed. The main features of the three experimental absorption bands of CF_3OSO_3 recorded over the 220 – 530 nm range are well reproduced by the calculations. A dissociation enthalpy for the CF_3O-SO_3 bond of 19.1 kcal mol^{-1} is predicted at the BAC-G3MP2//B3LYP/6-311+G(3df) level of theory.

Key words: CF_3OSO_3; Absorption Spectra; Bond Dissociation Energy; Time-Dependent Density Functional Theory