OH-induced oxidative cleavage of dimethyl disulfide in the presence of NO.

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Streszczenie

We report the results of the theoretical study of $^{\bullet}$OH-induced oxidative cleavage of dimethyl disulfide (DMDS) and the experimental study of the CH_3SSCH_3 + $^{\bullet}$OH reaction in the presence of $^{\bullet}$NO. Infrared low temperature argon matrix studies combined with ab initio calculations allowed us to identify *cis*-CH_3SONO, which evidences the formation of the $CH_3SO^{\bullet}$ and CH_3SH molecules in the course of the CH_3SSCH_3 + $^{\bullet}$OH reaction. Ab initio/quantum chemical topology calculations revealed details of the oxidative cleavage of dimethyl disulfide, which is a complex multistep process involving an alteration of S–O and S–S covalent bonds as well as a hydrogen atom transfer. The ability of delocalization of the unpaired electron density by sulfur atoms and a formation of a hydrogen bond by $CH_3SO^{\bullet}$ and CH_3SH are the factors which seem to explain antiradical properties of DMDS.

Adres publiczny

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https://www.acs.org/content/acs/en.html