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Atmospheric Chemistry: Energetic properties of Sulphur-containing species

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We have computationally studied the energetic properties of sulphur-containing organic compounds such as hydroperoxy methyl thioformate (HPTM) and methyl thiomethyl peroxy radical (MSP), which are newly discovered stable intermediates of the dimethyl sulfide (DMS) oxidation process. DMS is the most abundant biological source of sulfur of the marine atmosphere. A reliable estimation of the standard molar enthalpies of formation and the bond dissociation enthalpies, in the gas phase at 298.15 K has been performed, by means of atomization and isodesmic reactions methods using Gn (n = 3, 4) and M05-2X (DFT) levels of theory. Gn methodologies, particularly G4 have been shown to be an accurate theoretical method to provide reliable energetic values for a wide variety of organic compounds.

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