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Theoretical calculations on the OSiS molecule and its interstellar relevance

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Abstract:

One of the most abundant elements in the universe is silicon, and several studies have already been performed on their silicate forms. Nevertheless, few species with the SiO bond have been detected in the interstellar space [1][2]. Recently, spectroscopic techniques have detected SiS in some interstellar clouds, and SiO in minor amounts. These two diatomic molecules can be related to a depletion of silicon atoms in interstellar clouds, a fact that needs explanation and possibly is linked to formation of derivative compounds like OSiS and SiOS [1][3].

OSiS was first observed in 1981, consisting of silicon bound to one atom of oxygen and sulfur. This molecule is very little studied and can present information to create a mechanism for explaining how SiS exists in the interstellar environment and if it can evolve to SiO. Some recent publications have shown that OSiS molecule may be observed in interstellar clouds and may be a target for promising studies on stability patterns and chemical kinetics of formation of molecules in space [4] [5].

The goal of this work is to perform a theoretical study of OSiS molecule and its isomers, analysing its stability and kinetics of formation in space. For this purpose, we performed calculations in the MOLPRO package at CASSCF and MRCI level with quadruple zetta Dunning-type basis set.

The first results confirm the existence of the linear OSiS molecule as a global minimum, with inter-atomic distances for the singlet state of 1.508 and 1.907 angstrom for silicon-bound oxygen and sulfur respectively. These distances are close to the values found in the literature employing less accurate methods [4][5]. Several singlet excited eletronic states were also calculated and analysed.

The results for the triplet state showed transition states for both SiS+O reation (250 kJ . mol^{-1}) and SiO+S (50 kJ . mol^{-1}) and a non linear SSiO structure, with SiO bond length of 1.531 angstrom SiS of 2.136 angstrom and angle of 120.9 degrees. The calculations showed that the triplet state is the most probable path for the S+SiO → SSi + O reation. We have verified the existence of a singlet-triplet crossing that may be relevant for the dynamics, and futher calculations are being performed.

Calculations for the constitutional isomers were also performed showing stability patterns for the SiOS molecule with oxygen between silicon and sulfur atom. In the case of these isomers the molecules are not as stable as OSiS, but are possible to form at more energetic conditions.

Key-words: Interstellar, SSiO, silicon, ab initio.
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