Classical and quantum theoretical studies of the Si + OH → SiO + H reactive collision.

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The SiO molecule is the most widespread silicon-bearing molecule in the interstellar medium. The largest abundances of SiO are found in shocked layers of molecular outflows associated with regions of star formation. The model currently adopted to explain the production of SiO invokes the erosion of interstellar dust grains made of silicates by shock waves [1]. The subsequent release of silicon atoms or SiO molecules into the gas phase can lead to the formation of SiO through Si + OH → SiO + OH reaction.

This work presents the first theoretical dynamics calculations on the reactive collision between Si and OH using a recently developed 3D potential energy surface. For this purpose, three theoretical methods have been used (QCT, MPPST, TDWP). The results show that the barrierless studied reaction occurs with a probability less than 0.6 for collision energies between 1-1000 meV. The reaction proceeds through an indirect mechanism involving a long life complex. The products energy distributions show a mix between statistical and not statistical behaviour. The computed thermal rate constant show strong temperature dependence for temperatures between 10-1000 K. This feature is quite different from the constant value of 10^{-10} $cm^3.s^{-1}$ which is currently adopted by the astrophysical chemical reaction network [2].

This work is the first contribution to the understanding of the mechanism of the SiO production via Si + OH → SiO + OH reaction. In the absence of experimental results, our findings can serve as a basis for future works in this area of study. Also, the thermal rate constants reported for a large range of temperatures could be introduced in the astrophysical models currently in use.

References

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