PyQMMM for modelling chemical processes in the interstellar medium

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We have developed PyQMMM; [1] a Python-based interfacing software for subtractive quantum mechanics/molecular mechanics (QM/MM) calculations with the AMOEBA09 polarizable force field. PyQMMM enables calculating large molecular systems, such as interstellar ices, using the ONIOM(QM:MM) [2-7] method at a low computational cost. We have used PyQMMM, employing the ONIOM(QM:AMOEBA09) method, to calculate the binding energy of SH and OH radicals on amorphous solid water (ASW). A range of binding energies was obtained for SH radical (0.10-0.36 eV) and OH radical (0.21-0.52 eV) on ASW. Computed average binding energies, 0.22 eV of SH and 0.36 eV of OH, suggested that the SH radical binding on ASW is weak compared to that of OH. We have also rationalized the mechanism for the reaction between OH anion and CO_2 in ice using the ONIOM(wB97X-D:AMOEBA09) calculations. The computed reaction mechanism showed a very low energy path, giving rise to HO-C(O)-OH and OH anion is recovered during the reaction. Thus, for implications in astrochemistry, we propose that OH anions in interstellar ices can react with the molecules trapped in ices to synthesize organic molecules. These examples evidence that the PyQMMM is a user-friendly strategy to study chemical processes in the interstellar medium.

References

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