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Modeling Reactivity under Interstellar Conditions

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The detection of complex organic molecules in the interstellar medium raises fundamental questions about how chemistry can proceed under the extreme conditions of very low temperatures, low densities, and intense radiation.[1] In this environment, conventional chemical intuition breaks down, and a molecular-level description becomes essential. Computational chemistry has therefore become a key tool for identifying viable reaction pathways and providing the kinetic data required for astrochemical models.[1-4]
This overview talk will present recent progress in the quantum-chemical exploration of reactive potential energy surfaces relevant to interstellar chemistry.[2-5] Modern electronic-structure methods, combined with automated reaction-discovery workflows,[5] allow the systematic identification of barrierless or low-barrier processes consistent with interstellar conditions. The resulting energetic information can be coupled with kinetic simulations to derive temperature-dependent rate coefficients and branching ratios, revealing how small energetic differences can strongly affect reaction rates at cryogenic temperatures.[1] Finally, we will discuss advances in modeling chemistry on interstellar grain analogues, where surface and ice chemistry plays a crucial role in the formation of complex and prebiotic molecules.[6]
Together, these developments highlight how the integration of quantum chemistry, automated reaction discovery, and kinetic modeling is making astrochemistry an increasingly predictive and quantitatively grounded field.

References:

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