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Integration of Molecular Dissociative Recombination Theoretical Data into the ACol VAMDC Node for Confined Molecular Systems

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This work enhances data interoperability for the study of confined molecular systems by integrating a high-precision theoretical dataset on molecular dissociative recombination into the Atomic and Molecular Collisions (ACol) node of the Virtual Atomic and Molecular Data Centre[a] (VAMDC). The integrated pilot data[b,c,d], generated using advanced quantum chemical methods (MQDT, R-matrix), provides critical cross-sections and rate coefficients for processes governing molecular ions in low-temperature, low-density environments, such as the interstellar medium and laboratory analogues.

The core technical achievements include mapping the dataset to the VAMDC XSAMS schema, extending the ACol[e] node's data model to support reactive collision data, and implementing a validated pilot dataset with prototype visualization tools. This integration directly supports the COST Action COSY (Confined Molecular Systems) by contributing to shared astrochemical datasets, promoting FAIR data principles, and bridging theoretical data with experimental efforts to understand molecule-environment interactions and motion in confined systems.

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