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NEW MOLECULAR DATA FOR CONFINED MOLECULAR SYSTEMS AND ASTROCHEMICAL MODELLING

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Abstract. Methods of computational chemistry have become increasingly important in the last decades for the investigation of interaction and dynamics of small molecules enclosed in larger structures (Albert et al. 2020, Reis et al. 2022). Despite their huge size, molecular clouds perform an important but little understood role in confined systems. Currently, there are a few hundred known molecular species in interstellar space, which include neutrals, cations, and anions ranging from diatomic to large ones. (Mandal & Roesky 2010). Due to scattering and absorption of interstellar radiation molecules that are deep inside molecular clouds can avoid photodissociation and/or photoionization (de Lara-Castells and Hauser 2020, Vujčić et al. 2023). Therefore, it is crucial to investigate not only radiative but also concurrent collisional processes.

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