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Molecular potential energy surfaces for interstellar chemistry and fusion applications[1] BASTIAAN J. BRAAMS[2], XINCHUAN HUANG, ZHONG JIN, ZHEN XIE, XIUBIN ZHANG, JOEL M. BOWMAN[3], Emory University, AMIT RAJ SHARMA, RALF SCHEIDER, MPI for Plasma Physics, Greifswald, Germany — In the Born-Oppenheimer approximation the electronic Schrödinger equation is solved given the nuclear positions as parameters, and this defines the potential energy surface. We have used computational invariant theory and the MAGMA computer algebra system as an aid to develop representations for the potential energy and dipole moment surfaces that are fully invariant under permutations of like nuclei, extending an approach that for 3-body and 4-body systems has a long history, e.g. [J. N. Murrell et al. Molecular Potential Energy Functions, Wiley, 1984]. A many-body (cluster) expansion is used to describe reaction complexes. The methods have been applied in an almost routine way for systems of up to 7 nuclei, including several molecules that are of interest for interstellar chemistry and for the issue of hydrocarbon breakdown in fusion edge plasma: H_5^+, CH_5, CH_5^+, $C_2H_3^+$, and their fragments, with $C_2H_5^+$ on the way. The mathematical and computional methods and the hydrocarbon applications will be presented.

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