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| Title: | HeH2+: structure and dynamics |
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| Abstract: | Although the reaction He+ + H2 → He + H2+ is highly exothermic and the reaction He + H2+ → HeH+ + H is endothermic, the latter reaction occurs more readily than the former because of orbital symmetry considerations. For the same reasons, the dissociative charge transfer process He+ + H2 → He + H + H+ is more likely to occur. Availability of highly accurate ab initio potential-energy surfaces for the ground electronic state of (He, H2+) has enabled dynamical studies, classical as well as quantum mechanical. While the experimentally observed vibrational enhancement of the exchange reaction and the collision-induced dissociation process has been well accounted for by theory, the narrow sharp reactive-scattering resonances reported in quantum mechanical scattering studies have eluded experimental verification. The isotope effect in (He, HD+) collisions seems to be a sensitive probe of the interaction potential. Although the possible role of the first excited electronic state of (He, H2+) in the collision-induced dissociation process has been discussed in the literature, the role of nonadiabatic coupling terms between different electronic states in influencing the dynamics in the system remains to be investigated fully. |
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