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Title:	Efficiency of rovibrational cooling of HeH ⁺ by collisions with He: Cross sections and rate coefficients from quantum dynamics
Authors:	Sathyamurthy, Narayanasami (/jspui/browse?type=author&value=Sathyamurthy%2C+Narayanasami)
Keywords:	HeH ⁺ quantum dynamics
Issue Date:	2021
Publisher:	AIP Publishing
Citation:	The Journal of Chemical Physics, 155(15), 154301.
Abstract:	By extending an earlier study [Gianturco et al., J. Chem. Phys. 154, 054311 (2021)] on the purely rotational excitation of HeH ⁺ by He atoms, we report in this paper integral cross sections and rate coefficients for rovibrational excitation and de-excitation processes in HeH ⁺ due to collisions with He. The data were obtained using a new ab initio potential energy surface that includes the vibrational degree of freedom. The results are compared with those computed using the earlier potential energy surface by Panda and Sathyamurthy [J. Phys. Chem. A 107, 7125 (2003)] that additionally accounts for the proton-exchange reaction between HeH ⁺ and He. It is shown that the exchange channel contributes nearly as much as the inelastic channel to the vibrational excitation and de-excitation processes and that the total rate constants pertaining to the purely inelastic processes are largely of the same magnitude as those obtained when both inelastic and reactive channels are included in the dynamics. The inelastic rovibrational rate coefficients involving this astrophysical cation are also found to be much larger than those obtained for anions present in similar interstellar environments.
Description:	Only IISER Mohali authors are available in the record.
URI:	https://pubs.aip.org/aip/jcp/article/155/15/154301/199744/Efficiency-of-rovibrational-cooling-of-HeH-by (https://pubs.aip.org/aip/jcp/article/155/15/154301/199744/Efficiency-of-rovibrational-cooling-of-HeH-by) http://hdl.handle.net/123456789/4932 (http://hdl.handle.net/123456789/4932)
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