Title:	Energy-transfer quantum dynamics of HeH+ with He atoms: Rotationally inelastic cross sections and rate coefficients
Authors:	Sathyamurthy, Narayanasami (/jspui/browse?type=author&value=Sathyamurthy%2C+Narayanasami)
Keywords:	Quantum mechanical principles Reaction rate constants,
Issue Date:	2021
Publisher:	AIP Publishing
Citation:	The Journal of Chemical Physics, 154(5), 054311.
Abstract:	Two different ab initio potential energy surfaces are employed to investigate the efficiency of the rotational excitation channels for the polar molecular ion HeH+ interacting with He atoms. We further use them to investigate the quantum dynamics of both the proton-exchange reaction and the purely rotational inelastic collisions over a broad range of temperatures. In current modeling studies, this cation is considered to be one of the possible cooling sources under early universe conditions after the recombination era and has recently been found to exist in the interstellar medium. The results from the present calculations are able to show the large efficiency of the state-changing channels involving rotational states of this cation. In fact, we find them to be similar in size and behavior to the inelastic and reaction rate coefficients obtained in previous studies, where H atoms were employed as projectiles. The same rotational excitation processes, occurring when free electrons are the collision partners of this cation, are also compared with the present findings. The relative importance of the reactive, proton-exchange channel and the purely inelastic channels is also analyzed and discussed. The rotational de-excitation processes are also investigated for the cooling kinetics of the present cation under cold trap conditions with He as the buffer gas. The implications of the present results for setting up more comprehensive numerical models to describe the chemical evolution networks in different environments are briefly discussed.
Description:	Only IISERM authors are available in the record.
URI:	https://pubs.aip.org/aip/jcp/article/154/5/054311/562799/Energy-transfer-quantum-dynamics-of-HeH-with-He (https://pubs.aip.org/aip/jcp/article/154/5/054311/562799/Energy-transfer-quantum-dynamics-of-HeH-with-He) http://hdl.handle.net/123456789/4942 (http://hdl.handle.net/123456789/4942)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need To Add…Full Text_PDF (/jspui/bitstream/123456789/4942/1/Need%20To%20Add%e2%80%a6Full%20Text_PDF)		15.36 kB	Unknown	View/Open (/jspui/b

Show full item record (/jspui/handle/123456789/4942?mode=full)

(/jspui/handle/123456789/4942/statistics)