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Title:	Non-adiabatic coupling and conical intersection(s) between potential energy surfaces for HeH2+
Authors:	Gupta, A.K. (/jspui/browse?type=author&value=Gupta%2C+A.K.) Dhindhwal, V. (/jspui/browse?type=author&value=Dhindhwal%2C+V.) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Nonadiabatic coupling conical intersection; HeH2 +
Issue Date:	2020
Publisher:	Taylor and Francis
Citation:	Molecular Physics, 118(12)
Abstract:	By computing the non-adiabatic coupling terms and the adiabatic-to-diabatic transformation angle along closed contours in nuclear configuration space using the CASSCF method and the aug-cc-pVTZ basis set for the lowest three electronic states of HeH2 +, we explore the conical intersection between states in near collinear and noncollinear geometries, particularly in the C 2v geometry.
Description:	Only IISERM authors are available in the record.
URI:	https://www.tandfonline.com/doi/full/10.1080/00268976.2019.1683243 (https://www.tandfonline.com/doi/full/10.1080/00268976.2019.1683243) http://hdl.handle.net/123456789/3334 (http://hdl.handle.net/123456789/3334)
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