Title:	Study of Conical Intersections and Non-adiabatic effects for HeH+2 molecular ion
Authors:	Gupta, Ankur Kumar (/jspui/browse?type=author&value=Gupta%2C+Ankur+Kumar)
Keywords:	Chemistry
Issue Date:	10-Jul-2015
Publisher:	IISER M
Abstract:	HeH+2 has been the subject of much research for the past 4-5 decades. We are interested in studying the potential energy surfaces and locating the associated conical intersections for this molecular system. Therefore, it is imperative to have a thorough understanding of the coupling between electronic and nuclear motion and conical intersections which we have explained in detail in Chapter 1. One of the most important properties of conical intersections is that they show geometric phase e ect (sign ip of electronic wavefunctions) which we have used to our advantage to derive conditions to con rm the presence of an intersection between potential energy surfaces. We then applied this theory to HeH+2 and obtained the corresponding results which we have discussed in Chapter 2.
Description:	MS10056
URI:	http://hdl.handle.net/123456789/499 (http://hdl.handle.net/123456789/499)
Appears in Collections:	MS-10 (/jspui/handle/123456789/447)

Files in This Item:

File	Description	Size	Format	
MS-10056.pdf (/jspui/bitstream/123456789/499/3/MS-10056.pdf)		2.1 MB	Adobe PDF	View/Open (/jspui/bitstream/123456789/499/3/MS-10