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.