化学学报 2002 60 (6): 1011-1016 ISSN: 0567-7351 CN: 31-1320/06

扩展功能

本文信息

Supporting info

PDF(0KB)

[HTML全文](0KB)

参考文献

服务与反馈

把本文推荐给朋友

加入我的书架

加入引用管理器

复制索引

Email Alert

文章反馈

浏览反馈信息

相关信息

本刊中 包含“从头计算法”的相关文章

本文作者相关文章

- 张愚
- 史鸿运
- 王伟周

Rg—HX(Rg=He,Ne;X=F,Cl,Br)分子间势的精确量子化学从头计算研究**III.He—HBr**

张愚,史鸿运,王伟周

贵州大学化学系,贵阳(550025)

收稿日期 修回日期 网络版发布日期 接受日期

摘要 在用非迭代的三重激发项来校正CCSD的CCSD（T）理论水平下，采用aug-cc- pVQZ基函数对He—HBr的分子间势进行了系统的研究。结果表明：He—HBr以线型结 构存在。在极限基的情况下，复合物两种线型极小点结构He—H—Br和He—Br—H势 阱深分别为28.792 cm~(-1)和35.707 cm~(-1)，对应He原子到HBr分子质心的距离 R分别为0.407 nm和0.343 nm。讨论了不同的基函数和理论方法在研究此类弱束缚 态复合物的分子间势时的可靠性及其对结果的影响，同时也给出了热函数的解析形 式。

关键词 从头计算法 氦 氖 溴化氢 氟化氢 氯化氢

分类号 0641

High Level ab initio Study of Intermolecular Potential for the Rg— HX (Rg = He, Ne; X = F, Cl, Br) Complexes III. He—HBr

Zhang Yu,Shi Hongyun,Wang Weizhou

Department of Chemistry, Guizhou University,Guiyang(550025)

Abstract The potential energy surfaces of ground state of He—HBr complex have been calculated at several levels of theory, including the single and double excitation coupled-cluster method with noniterative perturbation treatment of triple excitation CCSD(T). Calculations have been performed using the augmented correlation-consistent polarized quadruple zeta basis set (aug-cc-pVQZ). Using the complete basis set (CBS), the global minimum with a well depth of approximately 28.792 cm~ (-1) has been found for the linear He—H—Br geometry (θ = 0.0°) with the distance R between the He atom and the center of mass of the HBr molecule equal to 0.407 nm. In addition to the global minimum, there is a second minimum at R = 0.343 nm and θ = 180°(a well depth of 35. 707 cm~(-1)). Finally the effects of the basis sets and theoretical methods on the intermolecular potential are discussed and a simple analytic form employing 17 adjustable parameters for fitting to the calculated PES is given.

Key words AB INITIO CALCULATION He Ne HBr HF HCl

DOI:

通讯作者