高等学校化学学报 2009, 30(9) 1851-1855 DOI: ISSN: 0251-0790 CN: 22-1131/O6

论文

Ne-CO_2的从头算势能面及微波光谱

谢长建[1], 陈容[1], 朱华[1,2], 谢代前[3]

1. 四川大学化学学院,
2. 生物治疗国家重点实验室, 成都 610064;
3. 南京大学化学化工学院, 理论与计算化学研究所, 南京 210093

摘要:

采用三重激发校正的耦合簇[CCSD(T)]方法和大基组计算了范德华复合物Ne-CO_2的分子间势能面. 分子间相互作用能的计算采用考虑了基组重叠误差修正的超分子方法. 计算结果表明, 该势能面有两个极小值点, 分别对应T形构型和线性Ne-OCO构型. 采用离散变量表象(DVR)方法及Lanczos算法计算了Ne-CO_2的振转能级. 计算结果表明, 体系势能面支持22个振动束缚态. 计算得到的微波光谱的跃迁频率与实验值吻合得很好.

关键词: Ne-CO_2; 势能面; 微波光谱; 三重激发校正的耦合簇方法

Ab initio Potential Energy Surface and Microwave Spectra of Ne-CO_2

XIE Chang-Jian[1], CHEN Rong[1], ZHU Hua[1,2*], XIE Dai-Qian[3]

1. Department of Chemistry,
2. State Key Laboratory of Biotherapy, Sichuan University, Chengdu 610064, China;
3. School of Chemistry and Chemical Engineering, Institute of Theoretical and Computational Chemistry, Nanjing University, Nanjing 210093, China

Abstract:

An *ab initio* potential energy surface for the Ne-CO_2 complex was calculated using the coupled-cluster singles and doubles with noniterative inclusion of connected triple [CCSD(T)] with a large basis set. The interaction energies were obtained by supermolecular approach with the full counterpoise correction for the basis set superposition error. The CCSD(T) potential energy surface was found to have two minima corresponding to the T-shaped and the linear structures. The two-dimensional discrete variable representation method was employed to calculate the rovibrational energy levels of Ne-CO_2. The calculated transition frequencies of microwave spectra are in good agreement with the experimental values.

Keywords: Ne-CO_2; Potential energy surface; Microwave spectrum; CCSD(T)

收稿日期 2008-08-20 修回日期 网络版发布日期

DOI:

基金项目:

国家自然科学基金(批准号: 20403011)资助.

通讯作者: 朱华, 女, 博士, 副教授, 主要从事量子化学研究. E-mail: zhuhua@scu.edu.cn

作者简介:

参考文献:

[1]Randall R. W., Walsh M. A., Howard B. J.. Faraday Discuss. Chem. Soc. [J], 1988, 85: 13—21

[2]Fraser G. T., Pine A. S., Suenram R. D.. J. Chem. Phys. [J], 1988, 88 (10): 6157—6167

[3]Iida M., Ohsbima Y., Endo Y.. J. Phys. Chem.
[J], 1993, 97 (2): 357—362

[4]Negri F., Ancilotto F., Mistura G., et al.. J. Chem. Phys.
[J], 1999, 111(14): 6439—6445

[5]Marshall P. J., Szczesniak M. M.. J. Chem. Phys.
[J], 1996, 104(17): 6569—6576

[6]Jacob C. R., Wesolowski T. A., Visscher L.. J. Chem. Phys.
[J], 2005, 123(17): 174104-1—174104-11

[7]Steed J. M., Dixon T. A., Klemperer W.. J. Chem. Phys.
[J], 1979, 70 (9): 4095—4100

[8]Roche C. F., Ernesti A., Hutson J. M.. J. Chem. Phys.
[J], 1996, 104(6): 2156—2166

[9]Yan G. S., Yang M. H., Xie D. Q.. J. Chem. Phys.
[J], 1998, 109(23): 10284—10292

[10]Ran H., Xie D. Q.. J. Chem. Phys.
[J], 2008, 128(12): 124323-1—124323-10

[11]Xu Y. J., J ger W.. J. Mol. Spectrosc.
[J], 1998, 192: 435—440

[12]WANG Song(王嵩), YU Jian-Kang(于健康), DING Da-Jun(丁大军), et al.. Chem. J. Chinese Universities(高等学校化学学报)
[J], 2008, 29(1): 170—173

[13]Woon D. E., Dunning T. H.. J. Chem. Phys.
[J], 1993, 98(2): 1358—1371

[14]Widmark P., Malmqvist P., Roos B. O.. Theor. Chim. Acta
[J], 1990, 77: 291—306

[15]Tao F. M., Pan Y. K.. J. Chem. Phys.
[J], 1992, 97(7): 4989—4995

[16]Boys S. F., Bernadi F.. Mol. Phys.
[J], 1970, 19: 553—566

[17]Werner H. J., Knowles P. J., Amos R. D., et al.. MOLPRO, Version 2000.1
[CP], Cardiff: University College Cardiff Consultants Limited, 2000

[18]Choi S. E., Light J . C.. J. Chem. Phys.
[J], 1990, 92(4): 2129—2145

[19]Cullum J., Willoughby R. A.. J. Comput. Phys.
[J], 1981, 44: 329—358

[20]Nauts A., Wyatt R. E.. Phys. Rev. Lett.
[J], 1983, 51(25): 2238—2241

[21]Misquitta A. J., Bukowski R., Szalewicz. J. Chem. Phys.
[J], 2000, 112(12): 5308—5319

[22]Watson J. K. G.. J. Chem. Phys.
[J], 1967, 46(5): 1935—1949

[23]ZHOU Yan-Zi(周燕子), ZHU Hua(朱华), XIE Dai-Qian(谢代前), et al.. Chem. J. Chinese Universities(高等学校化学学报)
[J], 2004, 25(6): 1081—1084

本刊中的类似文章

文章评论

序号	时间	反馈人	邮箱	标题

mer

wome

I