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T_2分子$X^1\Sigma_g^+$,$B^1\Sigma_u^+$和$C^1\Pi_u$态的势能函数

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Analytical potential energy functions for the electronic states $X^1\Sigma_g^+$,$B^1\Sigma_u^+$ and $C^1\Pi_u$ of molecule T_2

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摘要 使用SAC/SAC-CI和D95++**,6-311++g**及cc-PVTZ基组,分别对T_2分子的基态$X^1\Sigma_g^+$、第2激发态$B^1\Sigma_u^+$和第3简并激发态$C^1\Pi_u$的平衡结构和谐振频率进行优化计算.对所有计算结果进行比较,得出cc-PVTZ基组为最优基组.运用cc-PVTZ基组和SAC方法对基态$X^1\Sigma_g^+$,SAC-CI方法对激发态$B^1\Sigma_u^+$和Cu 进行单点能扫描计算,并用正规方程组拟合Murrell-Sorbie函数,得到相应电子态的势能函数解析式,由得到的势能函数计算了与$X^1\Sigma_g^+$,$B^1\Sigma_u^+$和$C^1\Pi_u$态相对应的光谱常数,结果与实验数据吻合.

关键词: 分子结构与势能函数 激发态 Murrell-Sorbie函数

Abstract: The energies,equilibrium geometries and harmonic frequencies of the ground state $X^1\Sigma_g^+$,the second state $B^1\Sigma_u^+$ and the third degenerate state $C^1\Pi_u$ of molecule T 2 have been calculated using the method Group Sum of Operators of SAC/SAC-CI with the basis sets D95++**,6-311++g** and cc-PVTZ.Comparing the three basis sets above mentioned,the conclusion was gained that the basis set cc-PVTZ was the most suitable for the energy calculation of molecule T 2.The whole potential curves for these three electronic states were further scanned adopting SAC/cc-PVTZ method for the ground state and SAC-CI/cc-PVTZ method for the excited states,then a least square was fitted to Murrell-Sorbie function,and last the spectroscopy constants were calculated,which are in better agreement with the experimental data.It was believed that Murrell-Sorbie function form and SAC/SAC-CI method were suitable not only for the ground state,but also the low-lying excited states.

Key words: molecular structure and potential function excited state Murrell-Sorbie function

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