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研究论文

OH自由基的高精度量子化学研究

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摘要　采用内收缩MRCI方法(Internally Contracted Multiconfiguration-Reference Configuration Interaction)研究了OH自由基,计算得到其基态稳定构型的键长是0.09708 nm, 对应的实验值是0.096966 nm, 第一激发态的键长是0.10137 nm,实验值是0.10121 nm. 同时得到势能曲线PECs (Potential Energy Curve), 再分别由Murrell-Sorbie势能函数拟合计算和POLFIT程序计算得到OH自由基在基态$X^2\Pi$和第一激发态$A^2\Sigma^+$时的光谱数据：平衡振动频率ω_e, 非谐性常数$\omega_e\chi_e$以及高阶修正ω_eY_e, 平衡转动常数B_e, 振转耦合系数α_e, 解离能D_0和垂直跃迁能量v_{00}. 这些理论计算结果与最新的实验值非常吻合, 精确度比前人也有很大提高. 其中我们计算得到基态OH($X^2\Pi$)的解离能$D_0=$35568.86 cm^{-1}, 第一激发态OH ($A^2\Sigma^+$)的解离能$D_0=$18953.93 cm^{-1}, 从第一激发态$A^2\Sigma^+$ ($v=0$)到基态$X^2\Pi$ ($v=0$)的垂直跃迁能$v_{00}=$32496.42 cm^{-1}.

关键词　OH自由基　IC-MRCI方法　光谱参数　解离能D_e-

分类号

Highly Accurate Quantum Chemical Study of the OH Radical

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Abstract Two potential energy curves for the ground electronic state $X^2\Pi$ and the first excited electronic state $A^2\Sigma^+$ of OH radical have been calculated using the internally contracted multiconfiguration-reference configuration interaction (IC-MRCI) method including Davidson correction. And they were fitted to analytical potential energy functions using the Murrell-Sorbie potential function to deduce the spectroscopic parameters: equilibrium bond length R_e, rotation coupling constant ω_e, anharmonic constant $\omega_e\chi_e$, equilibrium rotation constant B_e and vibration-rotation coupling constant α_e. These constants and higher-order anharmonic constant ω_eY_e were also calculated by POLFIT. Most of the values obtained are in excellent agreement with experimental results. The calculated dissociation energy D_0 for OH($X^2\Pi$) is 35568.86 cm^{-1}, which is in excellent agreement with the recent experimental value (35565±30) cm^{-1}. The calculated dissociation energy D_0 for OH($A^2\Sigma^+$) is 18953.93 cm^{-1}. The calculated vertically excited energy from the ground state $X_2\Pi$ ($v=0$) to the first excited state $A^2\Sigma^+$ ($v=0$) is 32496.42 cm^{-1}.

Key words OH radical　IC-MRCI　spectroscopic parameter　dissociation energy

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