原子与分子物理学报

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UC分子基态~3Ⅲ的量子力学计算

The quantum mechanical calculation of the ground state X^3 Π for UC

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中文关键词 UC势能函数 离能解 ΔH_f C_p

英文关键词

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中文摘要

基于群论和量子力学计算,导出UC气体的基电子状态为 3Π ,其平衡核间距和离解能,分别为0. 1852nm和4. 5470eV。同时,用量子力学的MP 2方法计算得到势能曲线,由此导出基电子状态的Murrel I - Sorbi e势能函数,并计算出能量,光谱和热力学性质,气态UC(X 3Π)的标准生成烩 Δ H f为808. 06J/mol, 定容热容Cp为31. 288J/mol,绝对熵S为235. 76J/mol. K。

英文摘要

The electronic ground state of UC is derived to be X3∏ based on atomic molecular reaction statics(AMRS). Then its reasonable dissociative limit is successfully derived. Using the MP2 (The HF calculation followed by a second-order Moller-Plesset correlation) of Gaussian 94W and the RECP potentional (the relativistic effective core potential) for U and basis 6-31 G* for C, the present work has calculated the full potential energy curves for the ground state X3∏, whose equilibrium nuclear distance and dissociation energy are 0.18052 nm amd 4.5470 eV. From its Murrell-Sorbie function, the complete spectroscopic data and thermodynamic data are also derived for the first-time. The standard enthalpies of formation of UC is 808.06 kJ/mol, heat capacity at constant pressure Cp is 31.288 J/mol and entropy S is 235.76J/mol.K.

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