UC分子基态~3Π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MP2方法计算得到势能曲线,由此导出基电子状态的Murrell-Sorbie势能函数,并计算出能量,光谱和热力学性质,气态UC(X3Π)的标准生成焓ΔHf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 X3Π 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 X3Π, 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.