

Accurate Analytic Potential Energy Function and Spectroscopic Study for $G^1\Pi_g$ State of Dimer ${}^7\text{Li}_2$

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Abstract: The reasonable dissociation limit for the $G^1\Pi_g$ state of dimer ${}^7\text{Li}_2$ is determined. The equilibrium internuclear distance, dissociation energy, harmonic frequency, vibrational zero energy, and adiabatic excitation energy are calculated using a symmetry-adapted-cluster configuration-interaction method in complete active space in Gaussian03 program package at such numerous basis sets as 6-311++G, 6-311++G(2df,2pd), 6-311++G(2df,p), cc-PVTZ, 6-311++G(3df,3pd), CEP-121G, 6-311++G(2df,pd), 6-311++G(d,p), 6-311G(3df,3pd), D95(3df,3pd), 6-311++G(3df,2p), 6-311++G(2df), 6-311++G(df,pd) D95V++, and DGDZVP. The complete potential energy curves are obtained at these sets over a wide internuclear distance range and have least squares fitted to Murrell-Sorbie function. The conclusion shows that the basis set 6-311++G(2df,p) is a most suitable one for the $G^1\Pi_g$ state. At this basis set, the calculated spectroscopic constants T_e , D_e , E_0 , R_e , ω_e , $\omega_e x_e$, α_e , and B_e are of 3.9523 eV, 0.813 06 eV, 113.56 cm^{-1} , 0.320 15 nm, 227.96 cm^{-1} , 1.6928 cm^{-1} , 0.004 436 cm^{-1} , and 0.4689 cm^{-1} , respectively, which are in good agreement with measurements whenever available. The total 50 vibrational levels and corresponding inertial rotation constants are for the first time calculated and compared with available RKR data. And good agreement with measurements is obtained.

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Key words: vibrational frequency, dissociation energy, Li_2 , ab initio calculations

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