The potential energy function and Vibrational energy levels of Li_2O (C_S, X^1A') molecule

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Abstract: By using density functional method, the equlibrium geometry of Li_2O has been calculated. The possible electronic state and the reasonable dissociation limit of the ground state of Li_2O molecule is determined based on atomic and molecular reaction statics. The analytic potential energy function of Li_2O (C_S, X^1A') molecule was derived by many-body expansion theory. Then, the vibrational energy levels of the ground state of Li_2O molecule are determined by both the discrete variable representation for three-dimension (DVR3D) program and modified DVR3D program. The calculated results derived from the two programs are compared with each other, as well as available experimental results for the title system.

Keywords: Potential energy function; Many-body expansion method; Discrete variable representation; Vibrational energy levels

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