ELECTRONIC TRANSITIONS OF IRIDIUM MONOBORIDE

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Laser induced fluorescence spectrum of iridium monoboride (IrB) in the spectral region between 420 and 480nm has been studied. New electronic transition system observed at 435nm has been assigned to be the [22.3] $^3\Phi_3$ - X$^3\Delta_3$ transition. Isotopic relationship confirmed the vibrational numbering. Molecular constants obtained will be reported. Resolved fluorescence spectrum of the [22.3] $^3\Phi_3$ - X$^3\Delta_3$ transition showed that the $\Delta G_{1/2}$ of the X$^3\Delta_3$ state is 917 cm^{-1}. Theoretical study using complete active space self-consistent field (CASSCF) calculations followed by MS-CASPT2 including scalar relativistic effect has been performed to the IrB molecule; molecular bond length, electronic configurations and relative energies of the ground and low-lying electronic states have been obtained. Our computed results indicated that the ground state of IrB is an inverted X$^3\Delta$ state with a bond length, r_0, equal to1.767 $\mathring{A}$, which is in very good agreement with our experimental determination earlier. The electronic configuration giving rises to the ground state is $1\sigma^2\, 2\sigma^2 1\pi^4\, 3\sigma^1 1\delta^3$. Our calculations also showed that the earlier observed [16.5] $^3\Pi$ state and the [22.3] $^3\Phi$ state in this work are the (2)$^3\Pi$ and the (2)$^3\Phi$ states, respectively. The molecular properties obtained in our calculations agree reasonably well with those determined.
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