EXPERIMENTAL AND THEORETICAL STUDIES OF DIATOMIC IRIDIUM COMPOUNDS

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High resolution laser induced fluorescence spectra of iridium carbide (IrC) and nitride (IrN) in the spectral region between 400nm and 500nm have been recorded and analyzed. New electronic transitions: $^2\Pi_{3/2}$ - $X^2\Delta_{5/2}$ of IrC and $^1\Sigma^+$ - $X^1\Sigma^+$ of IrN have been observed. Isotopic relationship confirmed the vibrational quantum number assignment. Molecular constants for the new electronic states will be reported. Potential energy curves and spectroscopic constants of the low-lying electronic states of iridium boride (IrB) have been investigated using the complete active space self-consistent field (CASSCF) followed by complete active space second-order perturbation theory (CASPT2) with relativistic effects taken into account. On the basis of our computed results, we assign the ground state as $^3\Delta_3$ with equilibrium bond length equal to 1.7678 $\AA$, which is in very good agreement with our earlier experimental measurement. Calculated molecular constants such as excitation energies, equilibrium bond lengths, vibrational frequencies and rotational constants of the low-lying states will be reported. In addition, the bonding nature in IrB is discussed using Mulliken populations.
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