

VIBRATIONAL AND GEOMETRIC STRUCTURES OF $\text{La}_3\text{C}_2\text{O}$ AND $\text{La}_3\text{C}_2\text{O}^+$ FROM MASSE-ANALYZED THRESHOLD IONIZATION

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$\text{La}_3\text{C}_2\text{O}$ is produced for the first time by laser vaporization in a pulsed cluster source and identified by photoionization time-of-flight mass spectrometry. Vibrationally-resolved ion spectra are obtained with mass-analyzed threshold ionization (MATI) spectroscopy. The adiabatic ionization energy of $\text{La}_3\text{C}_2\text{O}$ is measured to be $30891(5) \text{ cm}^{-1}$. The spectra display several short vibrational progressions, and these progressions are associated mainly with La-La, La-C and $\text{La}_3\text{C}_2\text{O}$ stretching excitations. The electron-spin multiplicities and molecular symmetries of $\text{La}_3\text{C}_2\text{O}$ and $\text{La}_3\text{C}_2\text{O}^+$ are determined by combining the experimental measurements with ab initio calculations at MP2 level. Preliminary data analysis shows that the ${}^1\text{A}_1 \leftarrow {}^2\text{A}_1$ transition is responsible for the observed MATI spectra. The cluster has C_{2v} symmetry with $\text{La}_3\text{C}_2\text{O}$ in a bi-pyramid structure and oxygen being attached to the La_3 plane.