

Excited State of Lanthanum Dioxide

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A MO_2 molecule may be in a linear or bent structure. A linear structure could have a $D_{\infty h}$ symmetry (OMO, dioxide) or $C_{\infty v}$ (MOO, superoxide), whereas a bent structure could have a C_{2v} symmetry (OMO, dioxide; $\text{M}(\text{O}_2)$, peroxide) or C_s (MOO, superoxide). Our spectral and computational analysis shows that MO_2 ($\text{M} = \text{La}$) produced in a laser-vaporization cluster beam source has a bent C_{2v} structure in an excited state at the energy of 3.40 eV. The excited state of LaO_2 is ${}^4\text{B}_2$ formed by transferring two La electrons to O atoms and has a valence electron configuration consisting of O 2p- and La 6s-based orbitals.

