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First Principles Study of Thermal and Vibrationalfrequencies and Bonding Analysis in Oxides (M2O) Superosides (MO2) and Ozonides (MO3); (M=Li, Na, K)

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First-principles calculations in order to study the stability of oxides, superoxide and ozonide of alkali metals (Li, Na, K) has been performed by HF cluster procedure implemented by Gaussian 09 sets of programs with the choice of basis set 6-31G*. The correlation effects in the calculations have been accounted by applying Moller-Plesset second order perturbation approximations (MP2). Our calculation shows that when increasing the bond length between atoms of molecules, the binding energy of the corresponding system decreases, i.e. the stability of the studied system is inversely proportional to the bond length between the atoms of the corresponding system. Quantum Theory of Atoms In Molecule (QTAIM) approach has been adopted for bonding analysis for studied systems and this study shows that the bonding in all studied systems are of closed shell type at all. Our study for the variation of the real space function with bond length finds that with increase in bond length the real space function values at BCP (ρ and 2ρ) found to be decrease, which are in close agreement with the previously reported calculations. The electrostatic potential within the molecular surface of the studied systems has been systematically analysed. The study of the HOMO-LUMO gap on the alkali metal oxide, superoxide and ozonide shows that the calculated value is higher for ozonide and lower for oxides. Calculations have been also performed to estimate the frequency of vibration and force constant of the studied systems and then we study the variation of the frequency of vibration with the corresponding masses. Further calculation is extended to study some thermal behaviour of studied systems with and without isotropic substitution of oxygen as well as non- bonded Lenard-Jones parameters for lithium oxide.

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