

Abstract Submitted
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***Ab initio* electronic structure calculations of spectroscopic constants and vibrational state lifetimes of diatomic alkali molecules** DMITRY FEDOROV, Department of Chemistry, University of Nevada, Reno, 1664 N. Virginia St., Reno, Nevada 89557-0216, USA, ANDREI DEREVIANKO, Department of Physics, University of Nevada, Reno, 1664 N. Virginia St., Reno, Nevada 89557-0220, USA, SERGEY VARGANOV, Department of Chemistry, University of Nevada, Reno, 1664 N. Virginia St., Reno, Nevada 89557-0216, USA — The diatomic alkali molecules have been proposed as possible candidates for applications in ultracold chemistry, quantum computing, and for high-precision measurements of fundamental constants. We calculate accurate potential energy and permanent dipole moment curves and the lifetimes of the ground and excited vibrational states of the heteronuclear alkali dimers XY (X, Y = Li, Na, K, Rb, Cs) using the coupled cluster with singles doubles and triples (CCSDT) method. The inclusion of the coupled cluster non-perturbative triple excitations is shown to be crucial for obtaining the accurate potential energy curves. The dissociation energies are overestimated by only 14 cm^{-1} for LiNa and by no more than 114 cm^{-1} for the other molecules. The discrepancies between the experimental and calculated harmonic vibrational frequencies are less than 1.7 cm^{-1} , and the discrepancies for the anharmonic correction are less than 0.1 cm^{-1} . The transition dipole moments between all vibrational states, the Einstein coefficients, and the lifetimes of the vibrational states are calculated. We analyze the decay rates of the vibrational states in terms of spontaneous emission, and stimulated emission and absorption induced by black body radiation.

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