Abstract Submitted
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Ab initio **potential curves for the ground and low-lying excited states in $LiBe^+$ and $NaCa^+$ molecular ions**[1] DI SHU, SANDIPAN BANERJEE, JOHN MONTGOMERY, ROBIN CÔTÉ, Department of Physics, University of Connecticut, Storrs, CT, 06269 — We report accurate *ab initio* calculations for the ground and low-lying excited states in $LiBe^+$ and $NaCa^+$ molecular ions. Valence multireference configuration interaction (MRCI) calculations were performed using complete active space self consistent field (CASSCF) orbitals. Spectroscopic constants and bound vibrational levels are calculated, as well as Franck-Condon factors and dipole-allowed electronic transition moment between appropriate states. The static dipole and quadrupole polarizabilities, along with long range expansion coefficients are also calculated. Preliminary results for the hyperfine structure in the lowest singlet and triplet states are also reported.

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