Abstract Submitted for the DAMOP14 Meeting of The American Physical Society

New *ab initio* potential curves for the ground and low-lying excited states in NaCa<sup>+</sup> and LiBe<sup>+</sup> molecular ions<sup>1</sup> DI SHU, SANDIPAN BANER-JEE, JOHN A. MONTGOMERY JR., ROBIN CÔTÉ, Department of Physics, University of Connecticut — We report new accurate *ab initio* calculations for the ground and low-lying excited states in NaCa<sup>+</sup> molecular ion and the lowest singlet and triplet states in LiBe<sup>+</sup>. Preliminary results of the corrections due to the nuclear hyperfine interactions in the lowest singlet and triplet states for NaCa<sup>+</sup> are also reported. The *ab initio* calculations were performed using valence multireference configuration interaction (MRCI) with complete active space self consistent field (CASSCF) orbitals.

<sup>1</sup>Partially supported by the National Science Foundation.

Di Shu University of Connecticut

Date submitted: 30 Jan 2014

Electronic form version 1.4