Abstract Submitted
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Calculation of *ab initio* potential curves for ground and low lying excited states of heteronuclear alkaline earth dimers $BeCa^+$, $BeMg^+$ and $MgCa^+$[1] SANDIPAN BANERJEE, JOHN MONTGOMERY, ROBIN CÔTÉ, Dept. of Physics, University of Connecticut — We report *ab initio* calculations on the ground and low lying excited states of $^2\Sigma$ and $^2\Pi$ symmetry for $BeCa^+$, $BeMg^+$ and $MgCa^+$. Valence multireference configuration interaction (MRCI) calculations were performed using complete active space self consistent field (CASSCF) orbitals. We use augmented correlation consistent valence quintuple zeta (aug-cc-pV5Z) basis set for our valence calculations. Core-valence and scalar relativistic effects are included at the CCSDT/cc-pwCVTZK level of theory. Spectroscopic constants and bound vibrational levels are calculated, as well as Frank-Condon factors and electronic dipole transition moments between the dipole–allowed states. The static dipole and quadrupole polarizabilities, along with long range expansion coefficients are also reported.

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