Abstract Submitted
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Comparative study of the *ab initio* potential curves for Be_2^+, Mg_2^+, Ca_2^+ and Sr_2^+ molecular ions[1] SANDIPAN BANERJEE, JOHN MONTGOMERY, ROBIN CÔTÉ, Dept. of Physics, University of Connecticut, Storrs, CT 06269 — We perform a comparative study of the X $^2\Sigma_u^+$, A $^2\Pi_u$ and B $^2\Sigma_g^+$ states in the homonuclear alkaline-earth family of molecular ions — Be_2^+, Mg_2^+, Ca_2^+ and Sr_2^+. A qualitative comparison of the "double-well" in the B $^2\Sigma_g^+$ state and interaction with the excited 2 $^2\Sigma_g^+$ state is made for all the molecular ions. Multireference configuration interaction (MRCI) calculations are performed with a complete active space (CAS) wavefunction as reference. Spectroscopic constants, bound vibrational levels, transition moments and radiative lifetimes are calculated. The static dipole and quadrupole polarizabilities, and the leading order van der Waals coefficients are also reported. We also show preliminary results for corrections to the Born-Oppenheimer Hamiltonian — non-adiabatic couplings and and hyperfine structure due to nuclear spins and electric quadrupoles.

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Sandipan Banerjee
Dept. of Physics, University of Connecticut, Storrs, CT 06269

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