Ab initio potential curves for the X $^2\Sigma_u^+$, A $^2\Pi_u$ and B $^2\Sigma_g^+$ states of Ca_2^+

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Abstract

We report *ab initio* calculations for the X $^2\Sigma_u^+$, A $^2\Pi_u$ and B $^2\Sigma_g^+$ states of the Ca_2^+ dimer. Valence multireference configuration interaction (MRCI) calculations were performed using complete active space self consistent field (CASSCF) orbitals. The CASSCF calculations included all configurations with 3 electrons in 18 valence orbitals and used the aug-cc-pV5Z basis. Core-valence and scalar relativistic effects are included at the CCSDT/cc-pWCVTZ-DK level of theory. A double well, similar to that obtained in recent calculations[1] on Be_2^+ is found in the B $^2\Sigma_g^+$ state. Spectroscopic constants and bound vibrational levels are calculated, as well as Frank-Condon factors and electronic dipole transition moment between the X $^2\Sigma_u^+$ and B $^2\Sigma_g^+$ states.

[1] S. Banerjee *et al.* Chem. Phys. Lett. 496 (2010) 208.