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Calculation of potential curves for the $X^2\Sigma_u^+$ and $A^2\Sigma_g^+$ states of Be_2^+ : Existence of a double minimum SANDIPAN BANERJEE, JOHN MONTGOMERY, JASON BYRD, HARVEY MICHELS, ROBIN CÔTÉ, Dept. of Physics, University of Connecticut, Storrs, CT 06269 — We report *ab initio* calculations performed on the ground $X^2\Sigma_u^+$ and $A^2\Sigma_g^+$ states of the Be_2^+ dimer. We have analyzed the ground $X^2\Sigma_u^+$ state and predict the location of all bound vibrational levels. We have also found two local minima, separated by a large barrier, in the otherwise expected repulsive $A^2\Sigma_g^+$ state. Bound vibrational levels have been calculated for both wells. Spectroscopic constants, Frank-Condon factors, transition dipole moments and lifetimes of these levels have also been calculated. For the *ab initio* calculations we have used a full valence CI , taking into account core-core and core-valence correction separately. We have also predicted some of the long-range van der Waals coefficients by extrapolating our *ab initio* data at large separations.

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