A NEW ONE-ELECTRON EFFECTIVE POTENTIAL FOR CaF BASED ON AB-INITIO CALCULATIONS

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The Rydberg spectrum of CaF has been extensively analyzed both theoretically and experimentally, and new QDT fit and Stark/polarization results will soon be reported. In these results, a new level of detail is achieved that enables a comparison between experimental results and reaction matrix calculations for state decompositions, and dependences on R(Ca-F), as well as energies. The most commonly used potential for the Rydberg states of CaF was presented a decade ago[a]. It has been effective in predicting energies for electronic states with R(Ca-F) near the equilibrium separation, but does not include any variation with internuclear separation, and predicts quantities such as the ion-core dipole moment that disagree with *ab-initio* results as a function of R. We have performed all-electron ccsd(T) calculations for CaF^+ and test-charge potential calculations for a wide range of R(Ca-F) values and test-charge angular positions. We will discuss the differences between these new results and the earlier potential and describe a new one-electron effective potential for CaF.

[a]M. Arif, Ch. Jungen and A. L. Roche *J. Chem. Phys.* **106**(10), 4102 (1997).