## THE PERMANENT ELECTRIC DIPOLE MOMENT OF CaD<sup>*a*</sup>.

JINHAI CHEN, TIMOTHY C. STEIMLE, Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287.

In 2004 we determined from the analysis of the Stark effect in the  $A^2\Pi - X^2\Sigma^+$  (0,0) band of system the magnitude of the permanent electric dipole moment,  $|\mu|$ , of CaH to be 2.94(16) D and 2.372(12)D for the  $X^2\Sigma^2$  (v=0) and  $A^2\Pi$ (v=0) states, respectively<sup>b</sup>. The numbers in parenthesis are  $1\sigma$  error estimates. Recently, two groups have performed high-level, all-electron, *ab initio* calculation and predicted  $\mu$  values of 2.623 D<sup>c</sup> and 2.617 D<sup>d</sup> for the  $X^2\Sigma^+$  (v=0) state. Although inside a  $2\sigma$  error estimate, these values are somewhat smaller than the experimentally observed value. In an effort to improve the precision of  $|\mu|$ , the Stark effect in the  $B^2\Sigma^+ - X^2\Sigma^+$  (0,0) band system of CaD has been recorded and analyzed. As expected, the Stark effect is about four times larger in CaD compared to CaH. The analysis gives  $|\mu|$  of 2.633(27) D and 2.018(33) D for the  $X^2\Sigma^+$  (v=0) and  $B^2\Sigma^+$  (v=0) state, respectively. A discussion of the isotopic dependence of  $\mu$  and experimental systematic errors will be given. The trend in  $\mu$  for the  $X^2\Sigma^+$ ,  $A^2\Pi$  and  $B^2\Sigma^+$  is modeled using a simple molecular orbital picture.

<sup>&</sup>lt;sup>a</sup>Supported by NSF-Exp.Phys

<sup>&</sup>lt;sup>b</sup>T. C. Steimle, J. Chen, and J. Gengler, J. Chem. Phys. **121**, 829-834(2004).

<sup>&</sup>lt;sup>c</sup>F. Holka and M. Urban, Chem. Phys. Lett. **426**, 252(2006).

<sup>&</sup>lt;sup>d</sup>I. S. K. Kerkines and A. Mavridis, J. Phys. Chem. A111, 371(2007).