THE PERMANENT ELECTRIC DIPOLE MOMENT OF 3D-MONOHYDRIDES: CrD^a.

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

A description of the bonding in the ground and low-lying electronic states of the first-row transition metal monohydrides becomes complicated because of the simultaneous involvement of the $3d^n 4s^2$, $3d^{n+1} 4s^1$ and, to some extent, $3d^n 4s^1 4p^1$ electron configurations of the metal. The permanent electric dipole moment can provide insight into this complicated bonding. Here we report on the determination of μ_e for chromium CrD. A number of low-N lines of the $X^6\Sigma - A^6\Sigma$ (0,0) band of chromium monodeuteride, CrD, have been recorded at near the natural line width limit by combining a supersonic molecular beam with high resolution laser excitation spectroscopy. The analysis gives the permanent electric dipole moment of the $X^6\Sigma$ (v=0) state as 3.51(3)D and 1.152(5)D for the $A^6\Sigma$ (v=0) state can be measured with higher precision because of some interesting near degeneracies in its level structure. A comparison with theoretical predictions for CrH^{b,c,d,e} and experimental values other 3d transition metal monohydrides will be given.

^aSupported by DoE-Basic Energy Sciences

^bD.P.Chong, S.R.Langhoff, C.W.Bauschlicher, Jr., S.P.Walch and H. Partridge, J. Chem. Phys. (85), 2850(1986).

^cD.Dai, K. Balasubramanian, J. Mol. Spectrosc. 161, 455(1993).

^dS.Koseki, T. Matsushita, and M.S. Gordon, J. Phys. Chem, 110, 2560(2006).

^eG.Ghigo, B.O.Roos, P.C.Stancil, and P.F. Weck, J. Chem. Phys. 121, 8194(2004).