

## OPTICAL STARK SPECTROSCOPY OF RHODIUM CONTAINING MOLECULES: RhN<sup>a</sup>.

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Rhodium is very important in both the homogeneous and heterogeneous catalytic induced chemical modification of nitrogen containing molecules. The only practical means of gauging the quantitative predictability of either *ab initio* and DFT computations used to model catalysis is by a comparison of experimental and predicted properties of bound Rh containing molecules. Here we report on the optical Stark effect in the Q(1) and R(0) lines of the [15.1]1 -  $X^1\Sigma^+$  (1,0) band of rhodium mononitride, RhN, which were analyzed to determine the permanent electric dipole moments,  $\mu$ , for the  $X^1\Sigma^+$  (v=0) and [15.1]1 (v=1) states to be 2.43(5)D and 1.75(1)D, respectively. The determined dipole moments are compared with predicted values obtained from DFT<sup>a</sup> and an all-electron *ab initio* calculation<sup>b</sup>. A simple molecular orbital correlation diagram is used to rationalize the relative values of  $\mu$  for RhN, isovalent IrN<sup>c</sup> and RhO<sup>d</sup>. Bonding in the 4d metal containing nitrides, as revealed from an interpretation of  $\mu$ , will be presented.

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<sup>a</sup>Stevens et al, *Chem. Phys. Lett.* **421**, 281 (2006).

<sup>b</sup>Shim et al, *J. Mol. Struct.* **293**, 127 (1997).

<sup>c</sup>A.J. Marr, M.E. Flores and T.C. Steimle, *J. Chem. Phys.* **104**, 8183 (1996).

<sup>d</sup>J. Gengler, T. Ma and T.C. Steimle, *J. Chem. Phys.* (accepted).