THE PERMANENT ELECTRIC DIPOLE MOMENTS OF THE $^3\Pi$ and $^3\Delta$ STATES OF RUTHENIUM MONOCARBIDE, RuC

WILTON L. VIRGO, TIMOTHY C. STEIMLE AND LAURA E. AUCOIN, *Department of Chemistry and Biochemistry, Arizona State University, Tempe, AZ 85287-1604*; JOHN M. BROWN, *Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, Oxford, England OX1 3QZ.*

Elucidating the structure and function of the chemically pervasive transition metal-carbon bond is a problem of both fundamental and applied scientific interest. Recent insight into the nature of the metal-carbon bond has been due to high-resolution gas-phase spectroscopy of the diatomic monocarbides, where measurement of permanent electric dipole moments and hyperfine structure are particularly informative. Ruthenium monocarbide has garnered recent interest[a b c d e f] due to its ease of production, intense visible electronic transitions and large magnetic hyperfine structure. We report on the investigation of the (0,0) $\{12.7\}^3\Pi_2 - \{0.1\}^3\Delta_3$ and (0,0) $\{13.9\}^3\Pi_1 - \{0.9\}^3\Delta_2$ band systems using high-resolution laser induced fluorescence spectroscopy. Stark shifts of the ^{102}RuC and ^{104}RuC isotopomers were analyzed to produce the magnitude of the permanent electric dipole moments for the $^3\Delta_3$, $^3\Delta_2$, $^3\Pi_2$ and $^3\Pi_1$ states. The measured moments prompt a discussion of the electronic structure and bonding in the $^3\Delta$ and $^3\Pi$ electronic states. Dipole moment trends are most informative when coupled to molecular orbital correlation diagrams. The measured dipole moments can be used as true benchmarks for rigorous electronic structure calculations. A comparison with isovalent FeC is made. [g]

[a] T. C. Steimle and W. L. Virgo *J. Chem. Phys.* **118**, 2620 (2003).
[b] I. Shim and K. A. Gingerich *Chem. Phys. Lett.* **317**, 338 (2000).
[c] J. D. Langenberg, R. S. DaBell, L. Shao, D. Dreessen and M. Morse *J. Chem. Phys.* **109**, 7863 (1998).
[d] R. S. DaBell, R. G. Meyer and M. D. Morse *J. Chem. Phys.* **114**, 2938 (1998).
[e] I. Shim, H. C. Finkbeiner and K. A. Gingerich *J. Phys. Chem.* **91**, 3171 (1987).
[f] R. Scullman and B. Thelin *Phys. Scr.* **3**, 19 (1971).
[g] T. C. Steimle, W. L. Virgo and D. A. Hostutler *J. Chem. Phys.* **117**, 1511 (2002).