ELECTRONIC SPECTROSCOPY OF MOLYBDENUM MONOCARBIDE

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In a continuing effort to understand the nature of the metal carbon bond in transition metal monocarbides we have undertaken the first spectroscopic investigation of MoC by resonant two-photon ionization spectroscopy. Molybdenum carbide was produced by laser vaporization of a Mo sample disk in a supersonic expansion of He and 3% CH_4. Using 6.42 eV photons for photoionization we have observed a number of transitions between $17\,700\,\mathrm{cm}^{-1}$ and $24\,000\,\mathrm{cm}^{-1}$. Twenty four of the observed bands have been studied at sufficient resolution (0.04 cm^{-1}) to allow the rotational structure of each transition to be resolved. An analysis of the isotope shifts has allowed a tentative identification of three band systems among the 24 observed transitions. A number of the observed bands have remained ungrouped. Every rotationally resolved band appears to be an $\Omega = 1 \leftarrow 0$ transition. Given that the ground state of NbC[a] is known to be $11\sigma^2 2\delta^1$, $^2\Delta_r$ and that of RuC[b] is known to be $11\sigma^2 2\delta^4$, $^1\Sigma^+$, it seems likely that the addition of another electron on moving from NbC to MoC yields for a ground state the $\Omega = 0^+$ component of a $^3\Sigma^-$ term. This is consistent with the observation that every transition in this study originates from an $\Omega = 0$ state. The $X^3\Sigma^-$ rotational constant for the most abundant isotope, $^{98}Mo^{12}C$, has been determined to be 0.553640 ± 0.000055 cm^{-1}. This corresponds to a ground state bond length of 1.687719 ± 0.000084 Å.

[a] B. Simard, P. I. Presunka, H. P. Loock, A. Berces, and O. Launila, submitted to *J. Chem. Phys.* (1997).

[b] J. Langenberg, R. S. Dabell, L. Shao, D. Dreessen, and M. D. Morse, in preparation.