ELECTRONIC SPECTROSCOPY OF NICKEL MONOCARBIDE

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Laser vaporization of pure nickel metal in the throat of a supersonic expansion of He doped with about 3% CH_4 has produced NiC in high yield. When the molecules were interrogated via resonant two-photon ionization spectroscopy between $19\,000\ \mathrm{cm}^{-1}$ and $27\,000\ \mathrm{cm}^{-1}$ with ArF excimer radiation for photoionization, nearly 50 bands, some exceptionally intense, were observed. The densest portion of the spectrum is to the blue of $24\,500\ \mathrm{cm}^{-1}$. All of the 31 bands that were rotationally resolved appear to be $\Omega = 0 \leftarrow 0$ transitions. The $\delta^3\sigma^1$, $^3\Delta_3$ ground state of FeC[a] and the $\delta^4\sigma^1$, $^2\Sigma^+$ ground state of CoC[b] leads one to expect that the ground state of NiC will be $\delta^4\sigma^2$, $^1\Sigma^+$. Our observation that all transitions originate from an Ω= 0 state is consistent with the assignment of the ground state of NiC as $^1\Sigma^+$. Five distinct excited electronic states have been tentatively identified based upon isotope shift data collected from the rotationally resolved bands and from some of the bands that could not be resolved. Three of the rotationally resolved bands were identified as the first two hot bands as well as the v = 0-0 band of an $\Omega = 0 \leftarrow 0$ system. Uncharacteristic of a jet-cooled R2PI experiment, this has allowed us to determine the ground state vibrational frequency to be $\omega_e'' = 875.3\ \mathrm{cm}^{-1}$ with $\omega_e x_e'' = 5.4\ \mathrm{cm}^{-1}$. The rotational constant for the ground state has been determined to be $0.637396 \pm 0.000059\ \mathrm{cm}^{-1}$, corresponding to a ground state bond length of 1.631095 ± 0.000076 Å.

[a] W. J. Balfour, J. Cao, C. V. V. Prasad, C. X. W. Qian, *J. Chem. Phys.* 103, 4046 (1995).
[b] M. Barnes, A. J. Merer, G. F. Metha, *J. Chem. Phys.* 103, 8360 (1995).