LASER SPECTROSCOPY OF NICKEL CYANIDE, NiCN, IN THE VISIBLE REGION

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The electronic spectrum of NiCN has been observed in the visible region following the reaction of laser-ablated nickel with either $(CN)_2$ or CH_3CN under supersonic jet-cooled conditions. High resolution LIF experiments have shown that the ground state is $^2\Delta_{5/2}$, with B_0 = 0.1444334(30) cm^{-1}; using data taken with $CH_3C^{15}N$, the bond lengths are found to be r_0 (Ni-C) = 1.8292(37) Å and r_0 (C-N) = 1.1591(52) Å. The vibrational structure of the ground state is an excellent example of strong Fermi resonance. Four excited electronic states have been identified. They are assigned as $\tilde{A}^2\Delta_{5/2}$ at 16607 cm^{-1}, $\tilde{B}^2\Pi_{3/2}$ at 16686 cm^{-1}, $\tilde{C}^2\Phi_{7/2}$ at 17813 cm^{-1} and $\tilde{D}^2\Phi_{5/2}$ at 19129 cm^{-1}. The electronic structure of NiCN turns out to be remarkably similar to that of NiH [a].

[a] S.A. Kadavathu, R. Scullman, R.W. Field, J.A. Gray and M. Li, J. Mol. Spectrosc. 147, 448 (1991)