POLYATOMIC RADICALS IN THE REACTION PRODUCTS OF LASER-ABLATED METALS WITH SIMPLE MOLECULES; SOME INTERESTING ELECTRONIC SPECTRA

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Spectra of a number of transition metal-containing radicals have been observed following the reaction of laser-ablated metals with simple molecules. Among the species we have found are hydroxides (MOH), methylidynes (MCH), carbides (MC_2), imides (MNH) and cyanides (MCN). Except for YC_2, which is T-shaped, all the molecules we have studied are linear. Because of the density of electronic states in d electron systems, vibronic coupling effects are very much more important than in light molecules. A good example is YOH, where the first order coupling between the close-lying $\tilde{B}^1\Pi$ and $\tilde{C}^1\Sigma$ states causes the molecule to become non-linear in the lower Born-Oppenheimer component of the $\tilde{B}^1\Pi$ state. Strong vibronically-induced bands occur in almost all the observed electronic transitions, and in molecules containing heavy metals (e.g. LaNH) so much spin-orbit coupling may be transferred to the $l \neq 0$ bending levels of $^2\Sigma$ electronic states that they follow case (a) coupling. Nevertheless, after all the complexities of orbital angular momentum, rotational perturbations and Fermi resonance have been taken into account, the underlying electronic structure is often very simple: the observed states of NiCN, for example, bear a surprisingly strong resemblance to those of NiH.

Nuclear hyperfine effects are important when metals with odd atomic number are present: impressive magnetic dipole splittings occur in the $\tilde{X}^3\Delta$ states of VCH and NbCH, while the $\tilde{X}^1\Sigma^+$ state of TaCH shows some of the largest electric quadrupole splittings yet found in a molecule.