TOO SHORT CN BOND LENGTHS EXPERIMENTALLY FOUND IN COBALT CYANIDE: AN *AB INITIO* MOLECULAR ORBITAL STUDY

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In the previous Ohio meeting, we pointed out that the CN bond lengths experimentally found for FeNC, CoCN, and NiCN are too-short.[a] The CN bond lengths in these radicals found by spectroscopy are shorter in this order than those predicted by high-level *ab initio* molecular orbital calculations. The tendency is in parallel with the expected ionicity for the metal-N or metal-C bond, and hence is in parallel with the floppiness in bending motion.

Recently submillimeter spectra of $\tilde{X}\,^3\Phi_i$ has been published by Sheridan, Flory, and Ziurys, and the CN bond length r_0 derived for the $\tilde{X}\,^3\Phi_{\Omega=4}$ is reported to be 1.1313(10) Å.[b] Our r_e value for the CN bond predicted at the level of the MR-SDCI+Q+Relativistic-correction/Roos ANO(Co, C, N) is 1.171 Å, which is in the normal range observed and predicted for many CN-containing molecules. The difference in r_0 and r_e shows how floppy CoCN is for the bending vibration mode.

[a] T. Hirano, R. Fukui, and U. Nagashima, *59th Ohio State Univ. Internat. Sympo. Mol. Spectrosc.*, RF05 (2004).
[b] P. M. Sheridan, M. A. Flory, and L. M. Ziurys, *J. Chem. Phys.*, **121**, 8360-8368 (2004).