ELECTRONIC GROUND AND EXCITED STATES OF CoN: AN *AB INITIO* MOLECULAR ORBITAL STUDY

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Based on the information from Tanaka group of Hokkaido University,[a] we have studied the $^1\Sigma^+$ and $^5\Delta$ states of CoN by *ab initio* molecular orbital methods as an extension of our previous work on FeN.[b] The MR-SDCI+Q+E_{rel}/[Roos ANO(Co), aug-cc-pVQZ(N)] calculations[c] with full-valence plus Co $3s$ and $3p$ electron correlations predicted that the $^5\Delta$ level should be located by about 4300 cm^{-1} higher than the $^1\Sigma^+$ state. Hence, the electronic ground state is $^1\Sigma^+$. The equilibrium bond lengths for the $^1\Sigma^+$ and $^5\Delta$ states at this level of calculation are 1.5621 and 1.5945 Å, respectively. The first order relativistic correction E_{rel} increases linearly with the Co-N bond length, with steeper gradient for $^1\Sigma^+$ than $^5\Delta$ states as is expected. The resultant shortening of the Co-N bond due to the relativistic effect is 0.016 and 0.005 Å for the $^1\Sigma^+$ and $^5\Delta$ states, respectively.

[a] K. Tanaka and M. Sekiya, Division of Chemistry, Graduate School of Science, Hokkaido University, Sapporo 060-0808, Japan.

[b] M. Amano, S.S Itono, T. Hirano, U. Nagashima, M. Sekiya, and K. Tanaka, *The 57th Ohio State University International Symposium on Molecular Spectroscopy*, **FB06**, 255 (2002)

[c] Q: Davidson's correction; E_{rel}: Relativistic correction