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, we have studied the $^1\Sigma^+$ and $^6\Delta$ states of CoN by ab initio molecular orbital methods as an extension of our previous work on FeN. The MR-SDCI+Q+/$[\text{Roos ANO(Co), aug-cc-pVQZ(N)}]$ calculations with full-valence plus Co $3\sigma$ and $3\pi$ electron correlations predicted that the $^6\Delta$ 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 $^6\Delta$ states at this level of calculation are 1.5621 and 1.5945 Å, respectively. The first order relativistic correction $E_{\text{rel}}$ increases linearly with the Co-N bond length, with steeper gradient for $^1\Sigma^+$ than $^6\Delta$ 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 $^6\Delta$ states, respectively.

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$^c$Q: Davidson’s correction; $E_{\text{rel}}$: Relativistic correction