# Photophysics and Bonding Properties of *trans*-$[RuCl(NO)(NH_3)_4]^{2+}$

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Due the importance of the nitric oxide (NO) to the human biology, the development of transition-metal nitrosyl complexes able to release NO in a controlled manner is desirable.[1,2] Better control of sustainable and site-specific NO delivery has been achieved by photoNORMs, systems that release NO when triggered with light. Ruthenium nitrosyl (RuNO) compounds, in special, has received growing attention because its potential as NO delivery agent.[2] Understanding the electronic structure and properties of such molecular systems is essential toward designing new potential RuNO candidates. In this context, the current work employs computational chemistry tools to explore ground and excited electronic states and Ru-NO bonding properties of the *trans*-$[RuCl(NO)(NH_3)_4]^{2+}$ and others related systems. The novel embedding approach, referred as WFT-in-DFT and implemented in the MOLPRO program package,[3,4] was used to perform a CASSCF(18,14)-in-B97 calculation. The lowest-lying singlet and triplet electronic states were characterized and the electronic absorption spectrum obtained at the CASSCF(18,14)-in-B97/cc-pVDZ level of theory was compared to the experimental one, **Figure 1**. The CASSCF wavefunction revealed the dominant configurations of the electronic states and the need of multiconfigurational methods to simulate the electronic absorption spectrum. Additional insights into the Ru-NO bonding were provided by the QTAIM analysis.

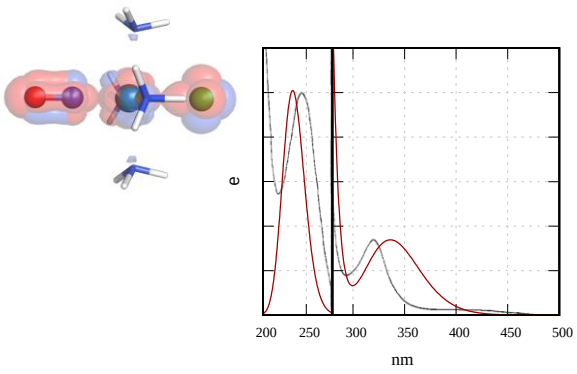


**Figure 1**. Electronic absorption spectrum of *trans*-$[RuCl(NO)(NH_3)_4]^{2+}$ obtained at the CASSCF(18,14)-in-B97/cc-pVDZ level of theory (red line) and the experimental one (black line).

**References**

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