PHOTODISSOCIATION SPECTRUM OF $Au_2^+N_2$

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The binding motif of nitrogen on transition metals is an interesting issue. Here we present the electronic spectrum of the $\tilde{A}^2\Sigma^+ \rightarrow \tilde{X}^2\Sigma^+$ transition of $Au_2^+N_2$, which was measured via photodissociation spectroscopy. The spectrum contains a long progression, caused by symmectric and asymmetric strech vibrations. We extract harmonic frequencies, anharmonicities and cross-anharmonicities of the excited state via a Dunham expansion and harmonic frequencies of the ground state via Franck-Condon simulations. In comparison to density functional theory calculations, the observed frequencies agree well with the theory. We also discuss the binding motif of $Au_2^+N_2$ in the ground and excited state.

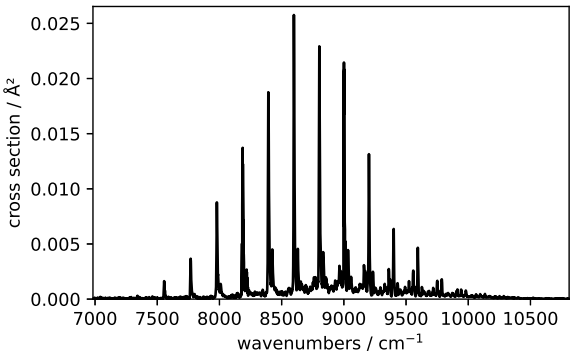

Figure 1: Electronic spectrum of $Au_2^+N_2$.

[1] M. Förstel, K. Pollow, T. Studemund, O. Dopfer, Chem. Eur. J. 2021, 27, 15075-15080.

[2] M. Förstel, K. M. Pollow, K. Saroukh, E. A. Najib, R. Mitric, O. Dopfer, Angew. Chem. Int. Ed. 2020, 123, 21587-21592.