Infrared Spectroscopy and Quantum Dynamics of the CuNO System

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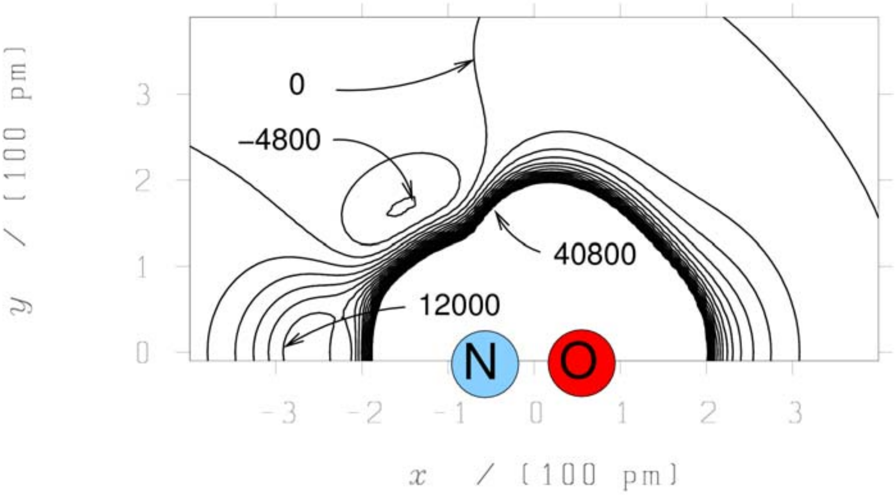
The CuNO molecule, observed in in the gas phase by neutralization-re-ionization mass spectrometry [1] as well as in matrix isolation [2], is a potentially interesting system in NOx redox chemistry, in particular for studying pathways of the reduction of NO via transition metal compounds in homogeneous catalysis. Experimental data are scarce, hence the importance of carrying out accurate calculations on this system. In this contribution we highlight results from recent accurate multireference CI and coupled cluster calculations of the electronic structure of the manifold of 12 low lying electronic states of CuNO (both with singlet and triplet spin) [3] and present an analytical, global representation of the potential energy surface for the ground state [4]. This surface is then used to calculate the infrafed spectrum as well as the wave packet dynamics of Cu + NO collisions at various initial conditions. We discuss this dynamics in comparison with the spectroscopy and make predictions for scattering cross sections. The following figure shows contour lines of the potential energy surface in the molecular plane (in units of *hc* cm^{-1}; the N-O distance being kept fixed at 115 pm).



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