



Experiment title: Gas-phase X-ray Raman scattering study of carbon and nitrogen oxides	Experiment number: HE-3035	
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Shifts: 18	Local contact(s): Dr. S. Huotari	<i>Received at ESRF:</i>
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Report:

We have carried out an X-ray Raman scattering (XRS) experiment on gaseous N₂, N₂O, CO₂ and He samples. This experiment offers us important insights into future experimental studies on gas-phase chemical reactions and stands as a feasibility test for extending the XRS method to gaseous samples in general. Moreover, the experimental results provide an important testing ground for a newly developed computational method for studying the electronic structure of molecular materials [1].

We used the Maxipix detector and the 9-analyzer array to collect the data. All analyzer crystals employed the Si (660) reflection and consequently a monochromatic incident energy in the range of 9.7 – 10.3 keV was utilized. Due to the near point-to-point focussing geometry of each analyzer scattering from the sample, sample container and air was easily discriminated. We achieved an energy resolution of 0.5 eV and a typical peak count rate of 50 cps with a background of 10 cps.

The sample environment is shown schematically in Figure 1. This setup enabled us to carry out several fill-evacuation cycles before commencing with the measurement. The data collection was carried out with all valves closed in order to confine the possible gas leakage in case of malfunction. The sample chamber consisted of a commercially available quartz capillary (Hilgenberg GmbH) having a diameter of 2 mm and wall thickness of 10 μ m. The capillary was reinforced by coating it with epoxy glue except for a 2 cm long part used in the data collection. The capillary was tilted along the direction of the incident beam in order to increase the irradiated sample volume and thus the observed count rate.

For N_2 , N_2O and CO_2 we collected the XRS data near each elemental K-edge using two scattering angles. The momentum transfer dependence was found to be small within the q -range covered by the multi element analyzer array at a fixed value of the scattering angle. Thus we could sum the data from each analyzer together. For He we collected data only at a small scattering angle and found a large momentum transfer dependence.

The N and O K-edge XRS data, together with our theoretical calculations for N_2O are shown in Figure 2. We successfully collected good quality data on the momentum transfer dependence from all samples. A manuscript describing our findings is currently under preparation.

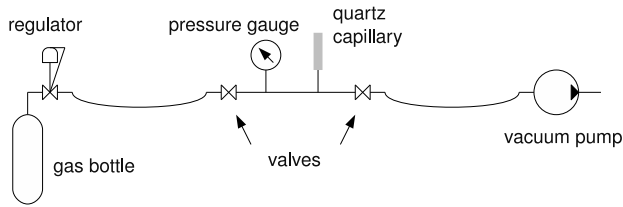


FIGURE 1. The schematic view of the sample setup.

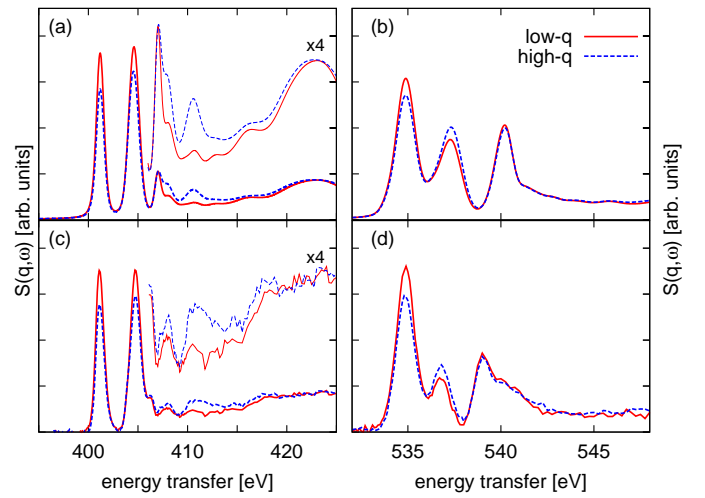


FIGURE 2. (a),(b) The theoretically calculated and (c),(d) experimental momentum transfer dependence of the XRS spectra of gaseous N_2O . The left-hand-side show the results for the N K-edge. On the right the data for the O K-edge is shown.

[1] A. Sakko, M. Hakala, J. A. Soininen, and K. Hämäläinen, Phys. Rev. B 76, 205115 (2007)