ESRF	Compton scattering from N_2	**Experiment number:** HE-783
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Report:

We have studied the Compton scattering cross-section of gaseous and liquid N_2 using high-energy synchrotron radiation at the ESRF beamline ID15B.

The Compton profiles were measured in a 173° scattering angle using photons with an incident energy of 60 keV. The spectra of scattered radiation was measured using the scanning crystal spectrometer installed at the beamline. As the sample we used commercially available N_2 gas in a medium pressure (50 bar) gas cell and standard liquid N_2 in a thermally isolated gasket. The pressure of the gaseous sample was applied to increase the count rate as it is proportional to the density of the sample; this moderate pressure does not affect the electronic structure of the system under study.

Most of the recent Compton scattering experiments have been done to study the electronic properties of solid state systems. The aim of this experiment was to investigate the electronic properties of a simple molecule and to compare the Compton profiles of calculated N, N_2 and experimental N_2 to understand the underlying covalent bond, because the properties that depend on the anisotropy of the electron momentum distribution even in N_2 are not easy to calculate accurately.

Extreme caution had to be taken in order to minimize multiple scattering events in both gaseous and liquid systems as this constitutes a non-linear background that can affect the results greatly. With very carefully designed sample cells for both the gaseous and liquid samples and proper alignment of the cells ensured minimal background effects in the measured spectra. We were also able to measure the background due to the walls of the chambers by applying a vacuum to the gas cell and room air in the liquid N_2 cell. Typical count rates with 50 bar gaseous N_2 were 500 cps at the peak of the Compton profile whereas in the liquid N_2 this figure was 4000 cps. Within the beam time available, we were able to collect 80,000 counts at the peak of the Compton profile of the gaseous phases and 340,000 counts at the peak of the profile of the liquid sample. This resulted in statistical uncertainties of 0.36 % and 0.17 %, respectively.

The difference between the Compton profiles of liquid and gaseous samples is small but distinguishable and still not completely understood. Calculations to describe the difference between gaseous and liquid systems are currently being done. The profiles clearly differ from atomic Roothan-Hartree-Fock calculated profiles for N (Fig.1). A LCAO-SCF calculation for N_2 molecule clearly fits better to the measured data, but the agreement is still not perfect. More accurate calculations for the molecule are also currently being done. We also made preliminary tests for measurements for other gaseous materials as interest to go deeply into even more simple systems, like noble gases, is arising.

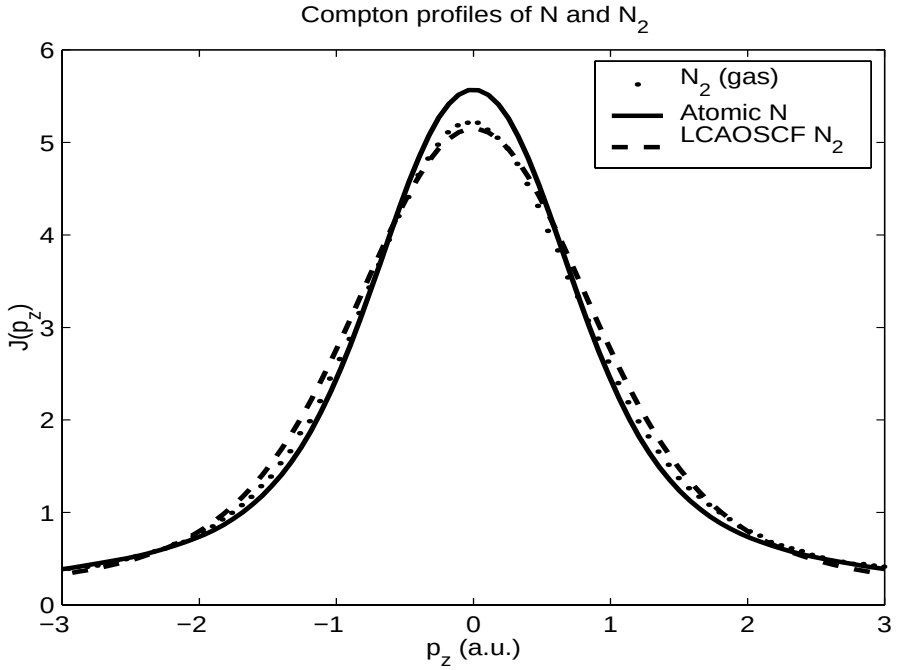

Figure 1. Roothan-Hartree-Fock (atomic) Compton profile of nitrogen (solid line), compared to experimental Compton profiles of gaseous N_2 (dots) and liquid N_2 (stars), as well as a LCAO-SCF-approximation based N_2 Compton profile (dashed line).