



Experiment title: Directional Compton Profiles of the organic superconductor (TMTSF) ₂ ClO ₄	Experiment number: HE-450	
Beamline: ID15B	Date of experiment: from: 30.09.98 to: 04.10.98	Date of report: 01.03.99 <i>Received at ESRF:</i>
Shifts: 15	Local contact(s): Thomas Buslaps	

Names and affiliations of applicants (* indicates experimentalists):

- * Abhay Shukla, Thomas Buslaps; ESRF
- Harald Müller, ESRF
- Shoji Ishibashi, Electrotechnical Laboratory, 1-1-4 Umezono, Tsukuba, Ibaraki 305, Japan

Report:

The experiment on the organic superconductor (TMTSF)₂ClO₄ (tetramethyltetraselenafulvalene perchlorate) was motivated by two aspects related to the understanding of the anomalous low dimensional transport properties which result from its unique anisotropic crystal structure:

1. Is a molecular picture adequate to describe the ground state electron wave function like it was found in the similar charge transfer salt TTF-TCNQ (tetrathiofulvalinum tetracyanoquinodimethan) which would then allow to describe the electronic structure using TMTSF and ClO₄ molecular orbitals ?
2. The anomalous transport properties along and perpendicular to the high conductivity a-axis are not well understood in terms of conventional pictures. Different approaches exist to explain the possibility of coherent or incoherent transport between the stacks.

Therefore we measured directional Compton profiles at different temperatures along (T= 300K) and perpendicular (T= 300K and 120K) to the high conductivity a-axis. Due to the 'absorption limited count rate at 30keV, given by the selenium, we changed the experimental setup for an incident X-ray energy of 56 keV. The time needed for this explains the missing of the 'T= 120K' data set with the scattering vector parallel to the a-axis. For all data sets we could achieve sufficient statistical accuracy of ~0.14% at the Compton peak maximum (~ 5*10⁵ counts in a bin of 0.05 a.u.). The resolution in p_z-space achieved for the data sets along

the a-axis (0.25 a.u.) is larger than for the perpendicular direction (0.17 a.u.) due to the sample geometry.

The analysis of the experimental Compton profiles will be done by comparison to a theory based on a self-consistent quantum chemical calculation performed by one of the co-proposers (Shoji Ishibashi) which is available now.