



**Experiment title:**  
**Electron momentum distribution  
of TTF-TCNQ**

**Experiment  
number:**  
HE277

**Beamline:**  
ID15 B

**Date of Experiment:**  
from: 23-Sep-97 7:00 to: 26-Sep-97 7:00

**Date of Report:**  
31-Oct-97

**Shifts:**  
9

**Local contact(s):**  
Abhay SHUKLA, P. SUORTTI

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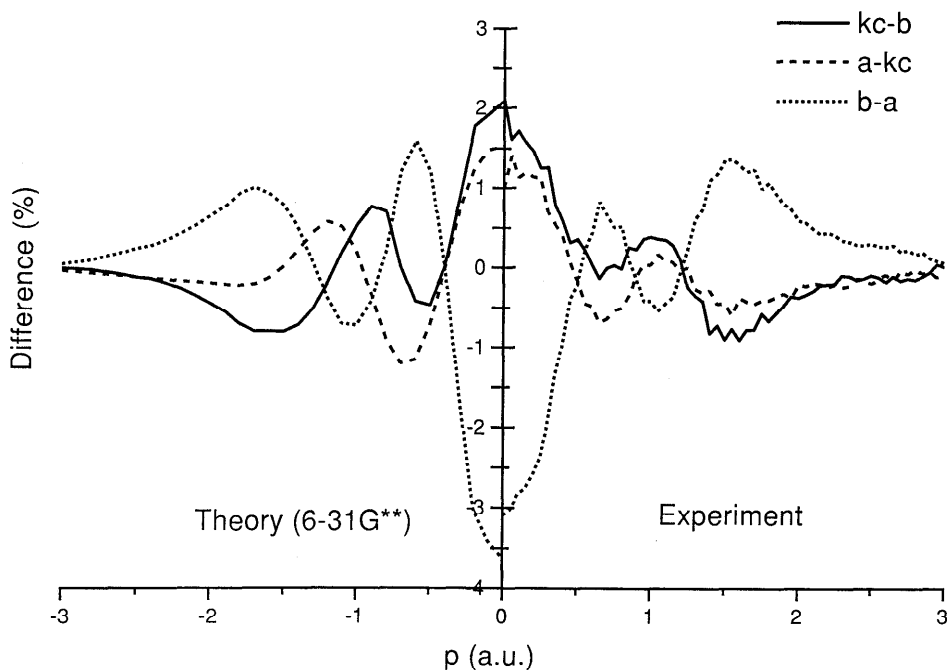
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**Report:**

We have investigated the electronic structure of TTF-TCNQ by Compton scattering using 30 keV synchrotron radiation. TTF-TCNQ is an organic conductor with a monoclinic crystal structure. It shows a one dimensional metallic conductivity along the b-axis above a temperature of 58 K.

Using the spectrometer of ID15 B, we have measured at room temperature the directional Compton profiles along three principal crystallographic directions (a, b and kc). Single crystals appropriately stacked either for the transmission or the reflection geometry were used. We have hence obtained, for the first time, high momentum resolution (0.15 a.u.) and high statistics (0.1 %) profiles, suited for comparison with theoretical simulations.

The experimental data have been corrected for absorption in the sample and analyser reflectivity. The background has been measured separately and subtracted from the profiles. In the figure, we show the calculated (left) and measured (right) directional anisotropies exhibiting the differences between the profiles along the three measured directions.



In the calculations of the Compton profiles, the electron wave functions were expressed as TTF or TCNQ molecular orbitals obtained self-consistently using GAUSSIAN 94 [1]. The agreement with the experiment depends on the basis set used. We find that 6-31G or higher is needed to describe correctly our measurements.

## References

- [1] M.J. Frisch, G.W. Trucks, H.B. Schlegel, P.M.W. Gill, B.G. Johnson, M.A. Robb, J.R. Cheeseman, T. Keith, G.A. Petersson, J.A. Montgomery, K. Raghavachari, M.A. Al-Laham, V.G. Zakrzewski, J.V. Ortiz, J.B. Foresman, C.Y. Peng, P.Y. Ayala, W. Chen, M.W. Wong, J.L. Andres, E.S. Replogle, R. Gomperts, R.L. Martin, D.J. Fox, J.S. Binkley, D.J. Defrees, J. Baker, J.P. Stewart, M. Head-Gordon, C. Gonzalez, and J.A. Pople, Gaussian 94, Revision B.3, Gaussian, Inc., Pittsburgh PA, 1995.