Data were collected at the Swiss Norwegian Beam Line at the ESRF. A spherical crystal of Corundum with diameter 0.20mm, as supplied by Sandoz Fils S.A., was used to collect Bragg diffraction intensities. Intensities were collected at wavelength of 0.5500 Å using a Huber 6 circle diffractometer.

At room temperature, 5409 intensities were collected in an omega scan technique. The intensities covered a hemisphere in reciprocal space ranging from 0.70 up to 1.70 reciprocal Angstroms.

During the data reduction it was suspected that 222 reflections were affected by 'umweganregung'. Additional measurements on several of these affected reflections clearly shows the characteristics of 'umweganregung'. Rejecting these 222 reflections from the data gives 841 unique reflections with an internal agreement of $R(I) = 0.030$.

Additional data on the same crystal has been collected at room temperature at different wavelengths. A full sphere of reciprocal space was collected at a wavelength of 1.0000 Å. The data at this wavelength consists of 2988 intensities going up to 0.95 reciprocal Angstroms. Additionally an hemisphere of reciprocal space was collected at a wavelength of 0.4000 Å. The 1050 measured intensities at this wavelength cover reciprocal space up to 1.40 reciprocal Angstroms.

Data will be analyzed by Mark Spackman, University of New England, Armidale, NSW 235, Australia.

Four pentacarbonyl chromium carbene complexes, (CO)$_5$Cr(CX)R, have been studied via X-ray diffraction and molecular orbital calculations. One of the carbene complexes (X=OCH$_3$, R=C=CPH) has been investigated extensively at 110K by X-ray diffraction using MoK$_\alpha$ radiation. The electron density distribution of this compound as well as the asphericity in electron density around the Cr atom are clearly demonstrated.

The comparison between experiment and theory is made in terms of deformation density, net atomic charge, and d-orbital populations of Cr. Further chemical bond characterization is based on quantum mechanical molecular orbital calculation. The resemblances and differences between amino- (X=NR $R^+$) and oxy- (X=OR $R^+$) carbene complexes are of special interest. The results indicate that the competition between the n-character of C=C$\equiv$C and C$\equiv$CR=O bonds also exists, however the majority contribution comes from either C$\equiv$CR=O or the p$_z$ orbital of CR=O in carbene ligand.

This makes the carbene carbon an electrophilic site at the carbene carbon. For flexible molecules, one can verify that the density of the fragments linked to a single bond is invariant (to an accuracy of the order of 0.01 eÅ$^{-3}$) through rotations around the single bond.

A simple method is introduced to decompose the electronic density of a molecule into the sum of fragments. The method is based on the Hirshfeld's partitioning scheme, which is very general and independent on any basis set.

For flexible molecules, one can verify that the density of the fragments linked to a single bond is invariant (to an accuracy of the order of 0.01 eÅ$^{-3}$) through rotations around the single bond. The method has been carefully checked for alkane, acetone, urea, water dimers, alanine and glycylglycine. The invariance of the density of fragments on each side of the peptide bond is well fulfilled.

Moreover, it turns out that some fragment densities can be transferred from one molecule to a bigger one within the same limit of accuracy. This allows for the possibility of predicting electron density of complex molecules that cannot be calculated by quantum mechanical methods.

The method is compared with the Mulliken's partitioning used in recent similar studies by Mezey. Within a given molecule, the two methods lead to similar conclusions for various conformations. However, transferability, which is the key for efficient use of such schemes, is significantly better with our present approach. It is also possible to estimate the variations of energy with changes of conformational parameters, within a Density Functional