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ESRF	**Experiment title:** Crystal structure of the Semliki Forest Virus E1 envelope Glycoprotein	**Experiment number:** LS-1237
Beamline: ID14-EH3	**Date of experiment:** from: 25-Sept-1998 to: 27-Sep-1998	**Date of report:** 26-Feb-1999
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Report:

We used the 6 shifts to collect several data-sets from different heavy atom derivatives. Screening for putative heavy atoms had been done previously on beam-line W32 at LURE-DCI (Orsay, France) to about 6Å resolution. Only derivatives that showed enoguh intensity differences at low resolution were then collected in ID2. These are:
Ta_6Cl_{14} at 1mM, $OsCl_6^{=}$0.5mM, $ReCl_6^{3-}$ 0.1mM, $AuCl_4^{-}$ 0.1mM.
In each case, a native data set was collected from a crystal of the same drop, since crystals from different drops are often non-isomorphous to each-other. The results show that although there is binding from these compounds, the phasing power from each of these derivatives is significant only at low resolution. These data contributed, however, to the determination of a reasonable envelope for the molecule. It was found that crystals soaked in 1mM Ta_6Cl_{14} diffracted better than native crystals, but gave a Native/derivative Rmerge of close to 50% (for the amplitudes) with changes in cell parameters in the order of 3-4%. In particular, the diffraction pattern is less anisotropic (see experience report LS-1332, reverse page, for anomalous data collected at the Ta edge from this derivative).
The ensemble of these data (except for Ta which could not be merged) was combined to previous data collected on a Uranyl and a Pt derivative. The highest phasing power comes from the anomalous signal of U collected at the U edge (λ=0.72Å) at beam line BW7A from

Synchrotron DESY (Hamburg, Germany). These data extend to about 4Å resolution.

The figure shows a stack of sections of our current 4Å resolution electron density map, obtained after solvent flattening. There are 30 sections superposed spanning 28Å along the c axis of the hexagonal unit cell. The 6_2 axis is at the center, so that there are 4 consecutive unit cells in the figure (x going from -1 to 1 and y from –1 to 1). We used all of the derivatives collected at ID14 described above and previous data from a uranyl derivative collected at beam line ID2 plus the anomalous data collected at DESY. An additional derivative, $PtCl_4^{=}$, collected previously at beam-lines ID2, BM2 and BM14, was added as well. The problem is that the main Pt position is unfortunately on a 2-fold axis, and a second position has very low occupancy, making it not suitable for facing. It contributes somewhat, nevertheless, to the overall phasing.