ESRF	**Experiment title:** Rubredoxin oxygen oxidoreductase (ROO)	**Experiment number:** LS-626
Beamline: BM14	**Date of experiment:** from: 05-Apr-97 07:00 to: 07-Apr-97 7:00	**Date of report:** 20-August-97
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Report:

Crystals of ROO were obtained in space group $P2_12_12$ with cell dimensions a=98.4Å, b=100.1 Å, c=91.1 Å, $\alpha=\beta=\gamma$=90°. Diffraction data were collected using a 180 mm MAR scanner. Four wavelengths were chosen near the Fe absorption edge, for the frozen, carefully aligned crystal.

The diffraction images were processed with DENZO and the resulting intensities scaled with SCALEPACK in such a way as to preserve the multiple observations of all the measured Bijvoet mates. The CCP4 program suite was used to merge the scaled data (programs ROTAPREP, AGROVATA and TRUNCATE) and to scale together the different wavelength data (SCALEIT). The crystallographic R_{merge}(I) for the different data sets varied within the 3.4 to 5.2% range. The $R_{anomalous}$ was maximal for the λ_3=1.7365 Å wavelength data set (|f´| maximum effect) with an overall value of 4.2%.

The accumulated Wilson distribution shows a small twin component (estimated as 0.04:0.96), which was tentatively attributed to a pseudo merohedric effect, possible due to the very similar dimensions of the ***a*** and ***b*** axes. Such a pseudo-merohedric twinning had been previously detected for cold room grown crystals, and led eventually to pseudo-hemi-merohedric twins (twin ratio of 0.5:0.5). However, for crystals grown at room temperature, such as that used in this experiment, there was no previous evidence for such a twin effect.

The anomalous Patterson synthesis led to some peaks, that were interpreted as possible Fe atom sites. A model of Fe atom sites, with a distribution in accordance with the native self rotation function, together with the anomalous dispersion data, led to electron density maps. These clearly show recognisable features of proteic secondary structure. The maps, which were obtained by using the programs SHARP, SOLOMON and DM, are being analysed with program 0, in order to fit the recently obtained ROO amino acid sequence.

Wavelength (Å)	Resolution range (A)	R_{merge} (%)	R_{anom} (%)	Complete (%)	Redundancy
1.7365 peak	24-2.70	5.2	4.2	96.8	4.0
1.7393 'i-p'	24-2.70	5.5	4.1	96.8	4.0
1.7400 i-p	24-2.70	4.5	3.3	96.3	4.0
1.0331 remote	24-2.70	3.4	2.2	98.4	3.6