

ion than, but do not differ significantly from, the conventional data results. All parameters are consistent with expectations based on neutron powder diffraction results (Kasper & Waterstrat, Acta Cryst. (1956), 9, 289; Algie & Hall, Acta Cryst. (1966), 20, 142).

$$\text{g}(51.8\text{Fe}, 48.2\text{Cr})$$

Site	No. Fe		SR	Coord.
	Random	Mo K $\alpha$		
A(2a)	1.04	1.8(1)	1.80(3)	12
B(4f)	2.07	1.3(1)	1.09(3)	15
C(8i)	4.14	3.0(2)	3.05(7)*	14
D(8i)	4.14	7.0(2)	7.14(5)	12
E(8j)	4.14	2.5(2)	2.46(5)	14

Conventional Mo K $\alpha$  data comprising over 1200 observations of about 500 independent diffraction maxima were collected from a crystal of the  $\tau$  carbide ( $\text{Fe}_7\text{Cr}_{16}$ )C $_6$  ( $a_0=1.0595(1)\text{nm}$ ). Precisions of measurement averaged  $\sim 3\%$  or better. Least-squares refinements of these data in S.G.Fm3m included occupation parameters for 3 of the 4 metal atom sites in the unit cell. Final values and their associated errors are listed below. SR diffraction data from this crystal have not yet been collected; based on the results of the  $\sigma$ -phase experiment, improved precisions but few significant differences would be anticipated in the occupation parameters derived from them.

$$(\text{Fe}_7\text{Cr}_{16})\text{C}_6$$

Site	No. Fe		Coord.
	Random	Mo K $\alpha$	
4a	1.22	4.0(2)	12 (Cubo-octahedron)
8c	2.43	2.9(3)	16 (Friauf Polyhedron)
48h	14.61	15.8(7)*	12 + 2C
32f	9.74	5.2(4)	10 + 3C

\* Fixed by composition and other occupation parameters.

**15.4-02** X-RAY INTERFEROMETRY AT THE DARESBURY SYNCHROTRON RADIATION SOURCE. By M. Hart and D.P. Siddons, Wheatstone Laboratory, King's College, Strand, London WC2R 2LS, UK.

A new X-ray interferometric spectrometer has been constructed to exploit the properties of the radiation from the newly-commissioned SRS. The instrument is capable of high resolution in both energy and phase. It is built around a versatile diffractometer having three precision rotation axes. They are arranged as two identical high-resolution axes, with the third axis coincident with one of the other two. This third axis has lower resolution than the other two, but a wider range of rotational adjustment. This arrangement is suitable for a very wide range of X-ray optical experiments, and provides ample scope for adjusting the parameters of the optical system to suit the particular problem.

Provision is made for placing a solid-state detector in the final diffracted beam. In all the optical systems under consideration, this beam is in the same orientation as the primary beam, and so the SSD need only be translated. In the event of it proving desirable to detect off-axis X-ray beams, provision has been made for a second low-resolution axis to be placed coincident with the second fine axis so that a scintillation counter or other small detector may be rotated about this second axis.

The instrument is arranged primarily for diffraction in the vertical plane, but operation in the horizontal plane is possible, as are combinations of the two.

Initial operational experience with the diffractometer will be presented, including assessment of the relative merits of the various possible optical systems and some preliminary dispersion data.

**15.4-03** THE CONFIGURATION OF THE FOUR IRON ATOMS IN DISSOLVED HUMAN HEMOGLOBIN AS STUDIED BY ANOMALOUS DISPERSION. By H.B. Stuhmann and H. Notbohm, European Molecular Biology Laboratory, EMBL-Outstation Hamburg, c/o DESY, Notkestrasse 85, 2000 Hamburg 52, West-Germany; Medizinische Hochschule Lübeck, Inst.f. Medizinische Molekularbiologie, Ratzeburger Allee 160, 2400 Lübeck 1, West-Germany.

The anomalous dispersion of iron at its K-absorption edge in small angle scattering of an aqueous solution of hemoglobin has been used to establish the geometrical arrangement of the four iron atoms in this protein. Though the anomalous contributions are about 0.001 to 0.01 of the total scattering, experiments with synchrotron radiation from the storage ring DORIS have shown that these effects can be measured with an average precision of about 10% at each of the 50 points of the scattering curve.

The anomalous scattering represents the convolution of the whole structure with the configuration of the four iron atoms of hemoglobin. The analysis in terms of multipoles suggests that tetrahedral symmetry of both the subunit arrangement and the iron structure is a dominant feature. The mean distance between the iron atoms of 26 Å as derived from this experiment compares well with those of crystallographic data.

**15.4-04** PARTIAL OR COMPLETE CIRCUMVENTION OF THE PHASE PROBLEM IN CRYSTAL STRUCTURE DETERMINATION USING SYNCHROTRON RADIATION. By Karl F. Fischer, Institute of Crystallography, Universitaet des Saarlandes, D 6600 Saarbruecken, Germany (BRD).

Intensity differences taken at two or three wavelengths in the neighbourhood of an atomic absorption edge are used for determination of the sign or phase of single reflections (e.g. "Anomalous Scattering", edited by Ramaseshan and Abrahams, Copenhagen, 1975).  $F^2$ -differences taken at two appropriately selected wavelengths around the absorption edge of one kind of atoms ("edge atoms") permit computation of a difference Patterson function  $L(u)$ . Its real part  $L_c(u)$  contains main peaks corresponding to vectors between these edge atoms (e.g. Sakamaki, Hosoya, Fukamachi, Acta Cryst. (1980) A 36, 183). For an acentric crystal (space group P1) with  $k$  edge atoms and  $n$  "normal atoms" per unit cell, the imaginary part  $L_s(u)$  of  $L(u)$  yields  $k$  images of the normal atoms exhibiting the correct enantiomer and/or polarity of the structure. Measurements with a third wavelength eliminate problems caused by the anti-centrosymmetry of  $L_s(u)$  and permit application to centrosymmetric crystal structures.

Detailed formalism, a computer program for this technique ("Lambda Method") and examples of applications are presented.