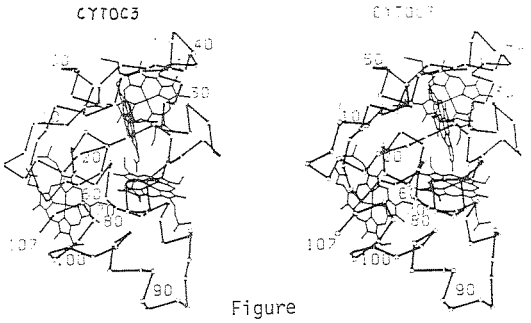
shown in the Figure. The overall dimensions of the molecule are approximately 33 X 39 X 34 Å. The heme-heme distances and angles are listed in the Table.

The structure of cytochrome c3 from D. desulfuricans, Norway, has been reported by Haser et al. Since they did not give any stereo drawing, precise comparison of our structure to theirs was not possible. It seems that the peptide back-bone of these two proteins differs significantly. This would be the reflection of only 27.7 % homology between them. Nevertheless, the overall shapes, especially the relative orientations of four hemes, resemble each other. It could be reasonable to assume that only the conformation of hemes is important in the structures of cytochrome c3 family, and the variations of amino acid residues, or even the deletion and insertion of peptides are allowable as long as the relative heme orientations are kept unchanged. This assumption could be confirmed if more structural information on other cytochrome c3 family proteins became available.

Table	Heme	Distance (Å) 1	2	3	4
Heme-Heme Distances	1	-	16.3	18.1	12.8
(upper right) and	2	71	-	12.4	16.2
Heme-Heme Angles	3	22	89	-	11.3
(lower left)	4	80	64	82	-

Angle (°)



Figure

02.1-21 THE STRUCTURE OF A BACTERIAL CYTOCHROME C_4 AND ITS RELATION TO OTHER CYTOCHROMES. By L. Sawyer and C.L. Jones, Napier College, Colinton Road, Edinburgh, A.M. Damas and R.O. Gould, Chemistry Department, Edinburgh University, and M.M. Harding, I.P.I. Chemistry Department, University of Liverpool, U.K.

The bacterial cytochrome c_4 from *Pseudomonas aeruginosa* has 181 amino acids, two haem groups, and a sequence which suggests that it is a 'covalent dimer' of two typical, 'short' cytochrome c segments. A crystal structure determination should show the relation of the protein chain folding of these parts to each other and to that of other cytochromes.

Hexagonal crystals of cytochrome c_4 were obtained from 2M ammonium sulphate with a = 62.38, c = 174.4 Å, space group $P6_522$ (see below), Z = 12. An electron density map at 5 Å resolution has been calculated using intensity data (CAD_4 diffractometer), including anomalous differences, from the native crystal, a $UO_2(NO_3)_2$ derivative (one site, 2 Å from a crystallographic 2-fold axis, occupancy 0.32), and a $K_2Pt(NO_2)_4$ derivative (three sites, occupancies 0.42, 0.15, 0.11). The U atom site was found from the Patterson series using $|F_{HLE}|^2$ as coefficients and the Pt sites from difference Fourier series. Peak heights in difference Fouriers and figures of merit for the derived phases favour the space group $P6_522$ but do not exclude $P6_122$. In the electron density map the molecular boundary can be seen, and within it there are two lobes of electron density; there are similarities in the chain folding in the two lobes, and a similarity to the patterns seen in other cytochromes. A 3 Å resolution electron density map is being prepared.

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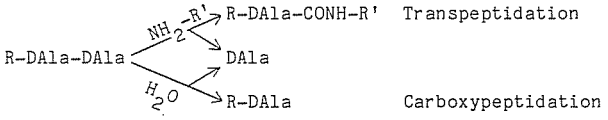
02.1-22 CRYSTAL STRUCTURE DETERMINATION OF A DD CARBOXYPEPTIDASE AT 2.5 A RESOLUTION. By O. Dideberg and P. Charlier, Institut de Physique B5, Université de Liège au Sart Tilman, B - 4000 Liège, Belgique.

The exocellular DD-carboxypeptidase of Streptomyces albus G is a metallo (Zn^{2+}) enzyme. The cofactor is required for activity on substrate analogues (e.g., Ac_2-L-Lys-D-Ala-D-Ala) and for binding of β-lactam antibiotics. We have obtained a 2.5A resolution map using the method of multiple-isomorphous replacement supplemented by anomalous-scattering information. Three heavy-atom derivatives were used; K_2AuCl_4, $K_3UO_2F_5$ and $K_2Pt(C_2O_4)_2$. For 6.700 reflections the figure of merit was 0.66. The electron density map allowed a tracing of almost all the polypeptide chain. The molecule is divided into two domains. The smallest one (71 residues) consists of three helices and random coil regions. The other domain (105 residues), where the zinc ion (catalytic site) is located, consists of two parallel strands and two α-helices, and possesses the only two disulfide bridges. No conformational similarities exist between this DD carboxypeptidase and other Zn^{++} metallopeptidases such as carboxypeptidase A and thermolysin. Ligand binding studies and high resolution map are currently under investigation, details and implications of the protein-drug interactions will be reported.

02.1-23 X-RAY CRYSTAL STRUCTURE OF A PENICILLIN TARGET: STREPTOMYCES R61 DD-TRANSPEPTIDASE-CARBOXYPEPTIDASE. By Judith A. Kelly, Paul C. Moews, James R. Knox, Biological Sciences Group and Institute of Materials Science, University of Connecticut, Storrs, Ct. 06268 U.S.A.

The DD-transpeptidase-carboxypeptidase from S. R61 is an exocellular, penicillin sensitive enzyme (MW 38,000 daltons). The reactions catalyzed are:



These reactions are critical in the growth and maintenance of the bacterial cell wall and are inhibited by beta-lactam antibiotics.

The crystal structure of this enzyme is being determined in order that we may visualize its interactions both with cell-wall substrates and with beta-lactam inhibitor molecules.

The crystals of the DD-transpeptidase are orthorhombic ($P2_12_12_1$) with unit cell dimensions a = 51.1, b = 67.5 and c = 102.9 A (Phil. Trans. R. Soc. Lond. B 289, 361 (1980); J. Molec. Biol. 124, 217 (1979)). The structure has been solved to 2.8 A resolution using three heavy atom derivatives, Na_2PtCl_6, $K_3UO_2F_5$ and CH_3HgCl. The binding site of ortho-iodophenylpenicillin has been located in a well-defined cleft in the molecule.

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