02.1-18 \textbf{THE STRUCTURE AND HEME ENVIRONMENT OF BEEF LIVER CATALASE AT 2.5 Å RESOLUTION.} By Mathur S. N. Murthy, Thomas J. Reid III, Andrew Sicignano, Nobue Okazaki, J. M. Donelan, L. E. Nakache, Michael G. Rossman, Departments of Biochemistry and Biological Sciences, Purdue University, West Lafayette, Indiana 47907, USA.

Most of the amino acid side chains of beef liver catalase were clearly identifiable in the 2.5 Å resolution electron density map and are in good agreement with the sequence (W. L. Schroeder et al., Arch. Biochem. Biophys. 131, 653-655, 1969). The tertiary structure of one subunit consists of a large antiparallel β-pleated sheet domain with helical insertions followed by a smaller domain containing four α-helices. The heme group is buried at least 20 Å below the molecular surface and is accessible by a channel lined with hydrophobic residues. The proximal ligand is cysteine 557 while histidine 74 and Asn 147 are the important residues on the distal side of the heme.

The inhibitor 3-amino-1,2,4-triazole, with its N(2) atom coordinated to the heme iron, was shown to covalently bond to His 74, can be built into the heme cavity with its N(2) atom coordinated to the heme iron.

02.1-19 \textbf{STRUCTURE OF CATALASE FROM PENCILLIUM VITACEAE AT 3.0 Å RESOLUTION.} By B.B. Vainshtein, V.R. Melik-Adamyan, V.V. Barynin, A.A. Vagin, A.I. Grebenko. Institute of Crystallography of USSR Acad.Sci., Moscow, USSR.

Catalase (H₂O₂:O₂-oxidoreductase, EC 1.11.1.6) is an enzyme responsible for decomposition of hydrogen peroxide to molecular oxygen and water. Crystals of catalase from fungus Penicillium vitaceae (MW 280,000) were grown in a preparative ultracentrifuge and belonged to space group P₃₂₁ with 1/2 molecule per asymmetric unit. The unit cell parameters are a = 69.5 Å, b = 69.5 Å, c = 133.8 Å. Intensities were collected on a four-circle diffractometer. Phase determination was based on data for two derivatives (K₂UO₂F₅, K₂Pt(NO₂)₄) up to 3.0 Å and for two others (K₂Pt(CN)₄, Fe(O₂CCH₃)₂) up to 4.5 Å. The 6 Å electron density map and heavy-atom sites have led to a recognition of 4 equivalent protein subunits related in pairs by a 2-fold non-crystallographic axis (Vainshtein et al., Dokl. Akad. Nauk S.S.S.R. 1979 246,220). After two cycles of phase refinement based on the method proposed by G. Briscoe (Acta Crystal. 1976 A32, 392) an improved electron density map was made possible to trace the polypeptide chain (Vainshtein et al., Dokl. Akad. Nauk S.S.S.R. 1980 253,242) and find preliminary co-ordinates of 584 α-carbon atoms. The polypeptide chain in the P. vitale catalase subunit forms three domains. About 350 residues starting from the N-termnus constitute the largest domain. It contains a β-sheet of 8 strands with helical insertions between them, forming a distorted barrel. An irregular region of about 60 residues forms a connection between the N-terminal domain and a smaller one of 70 residues packed in 4 successive helices. The third, C-terminal domain, comprising 160 residues, is similar in structure to chloroperoxidase.

02.1-20 \textbf{THE STRUCTURE OF CYTOCHROME C3 FROM DESULFOVIBRIO VULGARIIS, MIYAZAKI AT 2.5 Å RESOLUTION.} By J. Hayashi,*, G. Nakano,*, M. Komuro,*, M. Nakaoka,*, H. Okazaki,†, Y. Yagi,‡ and H. Iizuka.*** Institute for Protein Research, Osaka University, Suita, 565. **Faculty of Science, University of Toyonaka, Osaka, 560. ***Department of Chemistry, Faculty of Education, Shizuoka, Shizuoka University, Shizuoka, Shizuoka University, Shizuoka, 422. ****Institute for Molecular Science, Okazaki, 444, Japan.

Cytochrome C₃, an electron carrier to hydrogenase [EC1.11.2.1], in sulfate-reducing bacteria has an unusually low redox potential, which seems to be attributed to the fact that it has four heme groups. Some kinds of cytochrome C₃ have been isolated and characterized from various strains of sulfate-reducing bacteria to date. One of them, cytochrome C₃ from Desulfovibrio desulfuricans, Norway strain has been investigated by X-ray diffraction method, and the preliminary result was reported (Hase et al. 1979 Nature 282, 900).

Here, a brief description of the result of our X-ray structure determination of cytochrome C₃ isolated from Desulfovibrio vulgaris, Miyazaki at 2.5 Å resolution is presented. The amino acid sequence study has been completed (Shinkai et al. 1980 J. Biochem. 87, 1747) and the 72.3% of the sequence differs from that of Strain Norway.

The protein was isolated and purified according to the procedure of Yagi & Harayama. Crystals of good quality have been obtained by the vapor diffusion method (Hando et al. 1979 J. Biochem. 85, 269). Heavy atom derivatives were prepared by the soaking method. Several kinds of heavy atom reagents were examined, among which MgPtCl₆, K₂Pt(SCN)₆, Ag(UO₂F₅) and K₂IrCl₆ gave the best results. The Bijvoet-difference Fourier map based on an additional measurement of anomalous scattering on a native catalase crystal showed that the heme group was situated within the N-terminal domain. The distances between iron atoms in different subunits were found to be 31, 35 and 48 Å.

Crystals of P. vitale catalase inhibited by 3-amino-1,2,4-triazole (AT) were obtained and 6 Å resolution data were collected. The difference Fourier map showed that the binding site of AT is situated about 5 Å of the heme group and its center is shifted to a periphery of the porphyrin.

More detailed description of the active site could be done when the sequence is known.