The crystal structure of [P2.2.2. 2 protomers/asymmetric unit] of the enzyme \( \alpha \)-chymotrypsin is exposed to the solvent, but on op­
membrane-like aggregates.

Restricted.

putative interfacial recognition surface of each crys­
face

P.L.

microscopy and a model of the molecule was obtained at

molecular

the

faces cannot interact with the

stabilizes the

al. (1978)

Crystals of 18.

daltons; \( d = 1.216 \text{ g.cm}^{-3}. \)

Features of the model can be tentatively

as:YTIJ.iuetr~c

Features of the model can be tentatively

Properties of the molecule.

The preliminary results of this investigation as

rotation function studies are being carried out on the

Isolation of the major ovine neurophysin

Bovine neurophysin-II has been crystallized

Posterior pituitary hormones, oxytocin and vasopressin.

by J. Rose, C.S. Yoo, W. Furey, Jr.,

W. Furey, Jr. ,

Breslow, Department of

Biochemistry, Cornell University, New York, NY 10021.

CRYSTALLOGRAPHIC STUDIES OF NEUROPHYSIN-

DIPETIDE COMPLEXES. By J. Rose, C.S. Yoo, W. Furey, Jr.,

B.C. Wang and M. Sax Biocrystallographic Laboratory, VA

Medical Center, Pittsburgh, PA 15240 and the Department

of Crystallography, University of Pittsburgh,

Pittsburgh, PA 15260, and E. Breslow, Department of

Biochemistry, Cornell University, New York, NY 10021.

The neurophysins are known to be carriers for the

posterior pituitary hormones, oxytocin and vasopressin.

Bovine neurophysin-II has been crystallized [Yoo, et al. J.

Mol. Biol. 127, 1979] as a binary complex with \( \text{L-pha-}

L-tyr amide, a peptide known to bind neurophysin at its

active site. The crystals belong to space group

P2_{1}2_{1}2_{1}, with cell constants \( a=121.6, b=67.9, c=62.1 \text{ Å.} \)

Recently, a modified BNP-II (BNP-II'), in which the

three C terminus residues have been deleted, has been

crystallized as a binary complex with \( \text{L-pha-L-tyr amide.} \)

\( \text{McGl}_{2} \) or \( \text{(NH}_{4}\text{)}_{2}\text{SO}_{4} \) were used as the precipitating agent.

Crystals of both BNP-II and BNP-II' obtained through

the \( \text{McGl}_{2} \) precipitation belong to space group

P2_{1}2_{1}2_{1} with cell constants \( a=153.4, b=70.1, c=36.1 \text{ Å} \) and appear
to be isomorphous with porcine neurophysin-I (Blundell,
et al, FEBS Let., 121 No. 1, Nl, 1980). Crystals of

BNP-II' obtained through \( \text{(NH}_{4}\text{)}_{2}\text{SO}_{4} \) precipitation are
assumed to be isomorphous with BNP-II reported
previously.

Rotation function studies are being carried out on the

bovine neurophysin to investigate the state of

aggregation in the crystal, which should prove useful in
the crystal structure determination.

Isolation of the major ovine neurophysin (ONP-II),
which closely resembles BNP(II), has been initiated.
The preliminary results of this investigation as well as
the results from the BNP-II investigation will be
presented.

**02.1-49**

THE 6 Å STRUCTURE AND BIOLOGICAL ACTIVITY

OF CRYSTALS OF \( \delta^{3}-3\text{-KETOSTEROID ISOMERASE.} \) By E.W. West­

brook, O.E. Piro and P.B. Sigler, Department of Biophys­

ics and Theoretical Biology, University of Chicago,

Chicago, IL 60637, U.S.A.

\( \delta^{3}\text{-ketosteroid isomerase (KSI)} \) from P. testosteron
functions as an \( \alpha \) dimer having 13,400 dalton protomers.
The enzyme catalyzes intramolecular transfer of a proton
from \( \text{C}4 \) to \( \text{C}6 \) in certain \( \delta^{3}\text{-ketosteroids thereby iso­}

merizing the \( \delta^{3} \text{ double bond to } \alpha \). \) Crystals of KSI,
grown from high salt have three remarkable properties.
First, the unit cells of the \( \delta \)-dependent polymorphs
are large and the molecular packing is unusually com­
nlicated but well ordered, i.e. \( \text{P}_{2}1_{1} \), (\( \phi_{h}=5.5 \)), \( a = 140, b = 85, c = 95 \text{ Å}, \) \( s = 130.1^\circ, \) 24 protomers per unit

Second, the hexagonal form from birds

specific competitive inhibitors stoichiometrically.

Third, molecules in the hexagonal lattice are cata­
lytically active. The crystals give useful intensities to
2.7 Å.

An electron-density map of the hexagonal form was pre­
pared by multiple isomorphous replacement (MIR). The

\( 304 \text{ Å c-axis spacing was resolved by Franke's optics.} \)

As the complexity of the cell subverted the difference

Patterson analysis, the derivatives were interpreted by

applying direct methods to the difference amplitudes.
The MIR map was improved by real space direct methods

(see Schvitz et al. in these abstracts), initially by

attenuating the negative density and 'leveling' the

solvent and subsequently - after the local symmetry be­

came apparent - by averaging the four protomers of the

asymmetric unit and calculating phases from the symmetry­

averaged density. The functional dimer is characterized

by a local dyad (one of three) that relates protomers in

pairs through a substantial contact surface.

**02.1-48**

STRUCTURE OF MITOCHONDRIAL F\(_1\)-ATPase TO 9 Å

RESOLUTION. By L.H. Ansell, F. Haravanan and

P.L. Pederson. Johns Hopkins University School of

Medicine, Baltimore, Md., USA.

Crystals of F\(_1\)-ATPase from rat liver mitochondria belong to

rhombohedral space group \( B32. \) Cell data are:

\( a = b = 148, c = 368 \text{ Å (hexagonal)} \text{,} \) \( H.W. = 380,000 \)
daltons; \( \rho_{\text{app}} = 1.216 \text{ g.cm}^{-3}. \text{ With the value of 0.74 \text{ for the}

partial specific volume of the protein, the molecular

weight of asymmetric unit is 180,000 daltons. The relatively

rhombohedral unit is 3.5 Å resolution and we analyzed the structure by X-ray diffraction and electron

microscopy and a model of the molecule was obtained at

9 Å resolution. The model had been found to be a
dimer and each half appears to be composed of three

masses. Features of the model can be tentatively

correlated with known properties of the molecule.