

Recollections of Pittsburgh Diffraction Conferences Past: 1977 – 2023

Part I: William Furey

Department of Pharmacology & Chemical Biology
University of Pittsburgh, School of Medicine

What I was told (1977) and later confirmed

The Pittsburgh Diffraction Conference (PDC) had been **the premiere crystallographic meeting in the US**, attended by virtually all major crystallographers, and was the place to present and discuss major findings and advances in diffraction science!

Chronology of crystallographic organizations

PDC 1943

IUCR 1946 (first congress 1948)

ACA 1950

Diffraction Dominates the PDB both in Numbers, and Especially in Resolution

210,554 known protein structures in PDB as of Oct 12th 2023

Method	No.	%	Resolution at least	
			2.5Å	2.0Å
XRAY	178,895	85.0%	78.8%	50.5%
EM	17,103	8.1%	5.7%	1.1%
NMR	14,173	6.7%	N/A	N/A

My PDC Presentations

1. "Phase Extension and Refinement of Bence Jones Protein Rhe," **W. Furey Jr.**, B. C. Wang, C. S. Yoo and M. Sax, 36th Annual Pittsburgh Diffraction Conference, Pittsburgh, Pa, November 1978.
2. "Rotation Function Studies of Bovine Neurophysin II - Dipeptide Complex at 5.0 Å Resolution," **W. Furey Jr.**, B. C. Wang, C. S. Yoo and M. Sax, 37th Annual Pittsburgh Diffraction Conference, Purdue University, November 1979.
3. "Hydrogen Bonding and Water Structure in Bence Jones Protein Rhe at 1.6 Å Resolution," **W. Furey Jr.**, B. C. Wang, C. S. Yoo and M. Sax, 37th Annual Pittsburgh Diffraction Conference, Purdue University, November 1979.
4. "The Conservation of Solvent Structure in Proteins," M. Sax, S. Swaminathan and **W. Furey**, 43rd Pittsburgh Diffraction Conference, Pittsburgh, Pa, November 1985.
5. "Structure Determination of Cd, Zn Metallothionein Using Anomalous Scattering Data from Native Crystals," B. C. Wang, **W. Furey**, A. H. Robbins, L. L. Clancy and C. D. Stout, 43rd Pittsburgh Diffraction Conference, Pittsburgh, Pa, November 1985.
6. "Supercomputers for Crystallographic Computations," Pittsburgh Diffraction Conference, **W. Furey**, November, 1987.
7. "Recent Developments, Strategies and Algorithms for Macromolecular Structure Determination with the PHASES Program Package," **W. Furey**, 54th Annual Pittsburgh Diffraction Conference, November, 1996.
8. "Structural Studies on the Pyruvate Dehydrogenase Multienzyme Complex E1 Component," **W. Furey**, Pittsburgh Diffraction Conference, October 2002.
9. "SAD Phasing Basics: How and Why it Works, and When it's Likely to Fail," **W. Furey**, 66th Annual Pittsburgh Diffraction Conference, Pittsburgh, Pa, November 2008.
10. "The Pyruvate Dehydrogenase Multienzyme Complex: Structure-function Studies on its Components and their Interactions," **W. Furey**, 68th Annual Pittsburgh Diffraction Conference, Pittsburgh, Pa, October 2010.

My First PDC Presentation

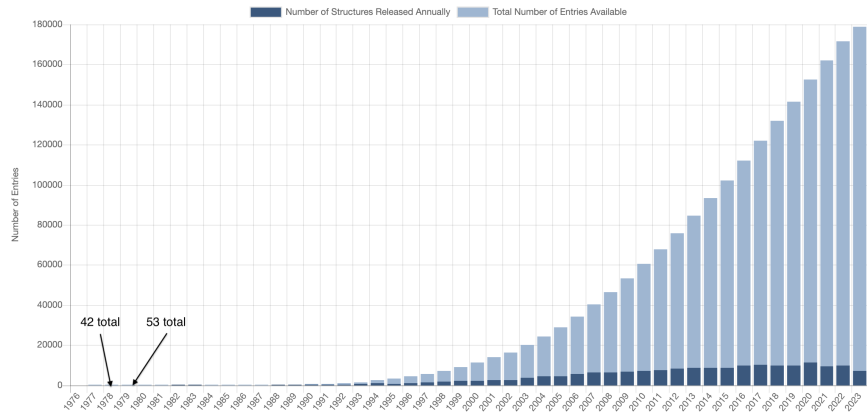
“Phase Extension and Refinement of Bence Jones Protein Rhe” 1978

PDB entry RHE1, ~ No. 50, deposited 11/28/1977, so in first 0.03%

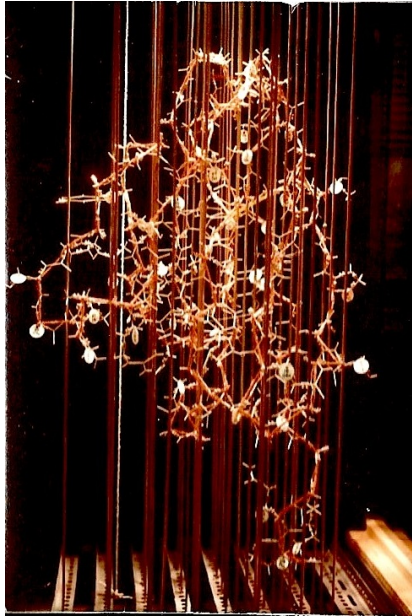
PDB Statistics: Growth of Structures from X-ray Crystallography Experiments Released per Year

[All Statistics](#)

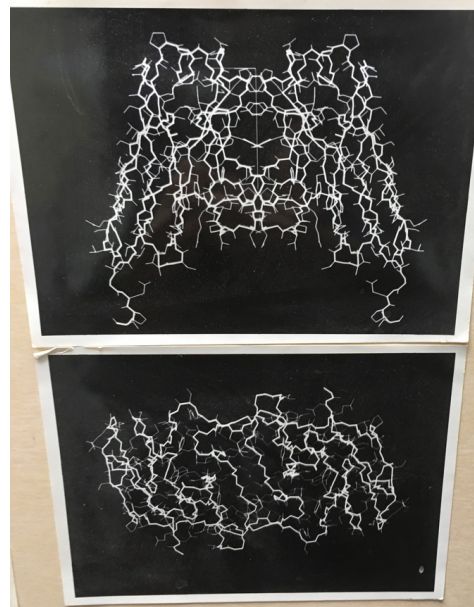
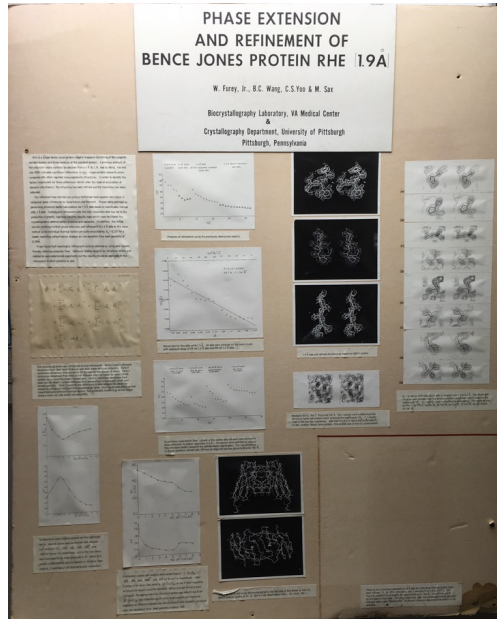
Experimental methods such as X-ray crystallography, NMR spectroscopy, and 3D electron microscopy are used to determine the location of each atom relative to each other in the molecule.



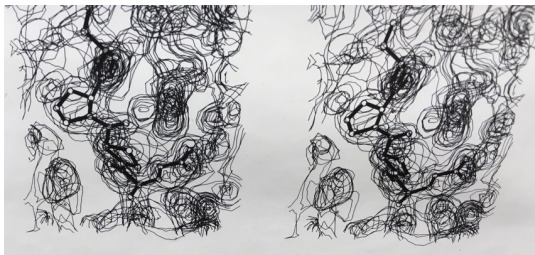
Starting model from Richards Box at 3.0Å Resolution



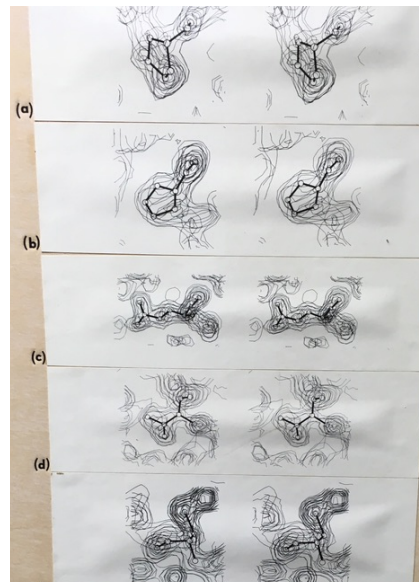
My First PDC Presentation 1978



My First PDC Presentation 1978

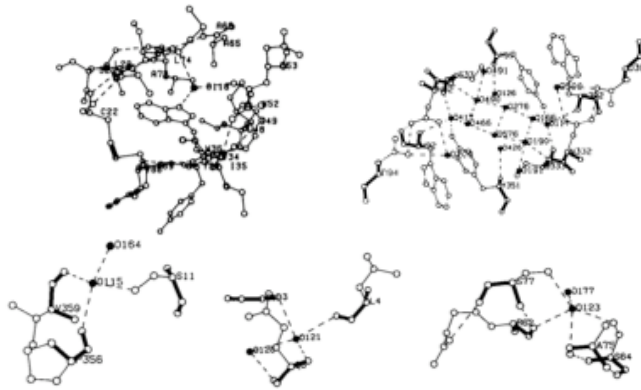


Key developments:
Stereo model/density
Chartpak Tape
Interactive graphics



PDC at Purdue (1979)

"Hydrogen Bonding and Water Structure in Bence Jones Protein Rhe at 1.6 Å Resolution"



Key recollections: The drive (A. T.)
The dinner (M. R. & P. S.) The posters and reception (J. J. & P. F)

PDC Organizational Activities

Chairman and a Local Organizer, 38th Annual PDC, 1980

Key recollections:

A lot of work!

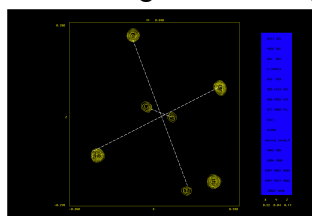
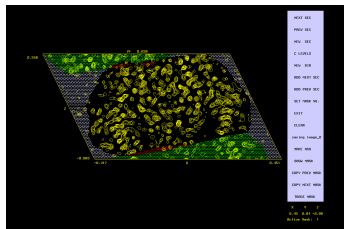
Sidhu award to Greg Petsko

**Co-chairman, Session on Supercomputers and Crystallography,
44th Annual Pittsburgh Diffraction Conference, 1986**

**Chairman, Session on Computational Methods for X-Ray
Crystallography, 45th Annual Pittsburgh Diffraction Conference, 1987**

PDC at Pittsburgh (1996)

“Recent Developments, Strategies and Algorithms for Macromolecular Structure Determination with the PHASES Program Package”

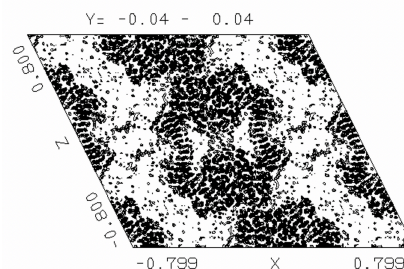


Phase Refinement Options

$$\sum W_h \sum_{\phi_p} (|FP_{hobs}|_h - |FP_{hcalc}(\phi_p)|_h)^2$$

- “Classical” - ϕ_p = centroid, $W_h = 1/E^2$, $1/\langle E^2 \rangle$ or unity, $P_{\phi_p} = 1$, use reflections with FOM > 0.4-0.6
- “Maximum Likelihood” - ϕ_p stepped over allowed phases, P_{ϕ_p} = corresponding probability, $W_h = 1/E^2$, $1/\langle E^2 \rangle$ or unity, use reflections with FOM > 0.2

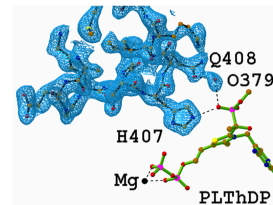
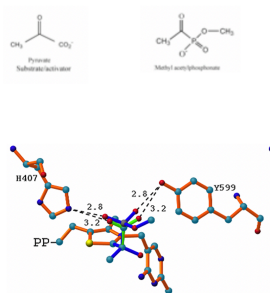
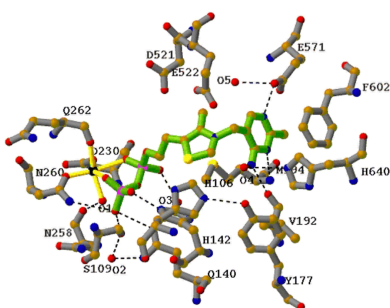
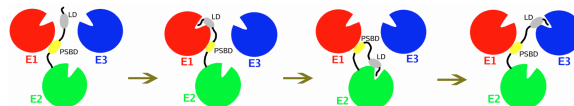
ϕ_p , P_{ϕ_p} can also come from external source, i.e. solvent flattened or NC-symmetry averaged maps.



Key recollections: M. R., M. S.

PDC at Pittsburgh (2010)

“The Pyruvate Dehydrogenase Multienzyme Complex: Structure-function Studies on its Components and their Interactions”



Two disordered loops (401-413) and (541-557) become ordered!

Remembering Chung Soo Yoo

Died August 31, 1983

KAL Passenger Flight 007 shot down by Russian pilot

Some of his key, joint publications

"Automated Interpretation of Electron Density Maps as Applied to Bence-Jones Protein Rhe," B. C. Wang, **C. S. Yoo**, W. Furey, Jr. and M. Sax, *J. Mol. Biol.* **135**, 305-308, 1979.

"Phase Extension and Refinement of Bence Jones Protein Rhe (1.9Å)," W. Furey, Jr., B. C. Wang, **C. S. Yoo** and M. Sax, *Acta Cryst.* **A35**, 810-817, 1979.

"Structure of a Novel Bence Jones Protein Fragment at 1.6Å Resolution," W. Furey, Jr., B. C. Wang, **C. S. Yoo**, M. and M. Sax, *J. Mol. Biol.* **167**, 661-692, 1983.

"Crystal Structure of a Bovine Neurophysin II Dipeptide Complex at 2.8Å Determined from the Single Wavelength Anomalous Scattering Signal of an Incorporated Iodine Atom," L. Chen, J. Rose, E. Breslow, D. Yang, W. Chang, **C. Yoo**, W. Furey, M. Sax & B. Wang, *Proc. Natl. Acad. Sci.*, **88**, 4240-4244, 1991.