

BROOKHAVEN NATIONAL LABORATORY

PROTEIN DATA BANK

NEWSLETTER

Number 5

November, 1977

We are pleased to announce that the National Science Foundation has extended funding of primary Protein Data Bank activities for three years, starting November 1, 1977. By virtue of this ongoing financial support, the Data Bank will be able to continue to expand services to our community of users. We also have a new distribution center, C.S.I.R.O. (Melbourne), which will take over distribution of data in Australia (see addresses below).

The Bank now includes a total of 84 atomic coordinate entries, seven of which have been added since distribution of the last issue of this Newsletter (Number 4, May 1977). A list of the coordinate holdings, with identification codes to be used in requesting data, is shown in Table 1. In addition, the Bank holds 15 sets of structure factors and phases. These are listed in Table 2, along with two additional non-standard entries containing torsion angle data.

A large number of minor revisions to the atomic coordinate data have been made since distribution of the last Newsletter. The most important revisions, which involve corrections of atomic coordinates or changes in secondary structure specifications, are given in Table 3. The full listing of revisions is too bulky to reproduce here, but is available on microfiche at no charge from Brookhaven. To order this listing, please check the appropriate box on the request form attached to this Newsletter. Most changes involve corrections of typographical errors, clarifications of remarks, etc.

At this time, we wish to emphasize the advantages of including structure factor-phase information in the Protein Data Bank. Preservation and dissemination of these primary crystallographic data are an important part of the Bank's archival function. Contributors are urged to deposit structure factor-phase data, for native structures and heavy-atom derivatives. Also, receipt of atomic coordinate data for hypothetical structures, based on energy calculations or model building, will be welcomed. The methods used to derive these data will be clearly identified, and the data will be distributed in the normal fashion.

A large part of the work necessary to make the Protein Data Bank bibliographic and sequence information available for interactive search has now been accomplished, thanks to funds provided by the National Institutes of Health. We hope that within three to six months, this portion of the file will be included as part of the NIH/EPA Chemical Information System on CYPHERNET (see Science 195, 253 (1977)). In order to adapt the protein file to this interactive system, certain stylistic changes have been made to the bibliographic data, and a few additional record types included. These minor changes already are reflected in the format of some of the newest atomic coordinate entries. A revised description of file record formats will be available shortly, and can be ordered by checking the appropriate box on the request form.

A communication describing the Protein Data Bank has recently been published in J. Mol. Biol. 112, 535 (1977).

Unfortunately, due to changes in Department of Energy accounting procedures and in order to cover a higher percentage of costs, it is necessary for Brookhaven to increase charges for distribution of data. These new charges, which are effective immediately, are detailed on the request form. At this writing, Melbourne and Tokyo have set no distribution charges, but Cambridge plans to implement a small charge in 1978. If you wish to receive data, please fill out the request form and mail it, together with a new 2400 foot reel of magnetic tape, to the appropriate center listed below. (Note: Brookhaven finds it convenient to supply a new tape for this purpose, and will do so for a small additional charge.) Users' comments and suggestions are always welcome.

AREA	ADDRESS OF CENTER	NAMES
The Americas	Chemistry Department Brookhaven National Laboratory Upton, New York 11973 USA	F. C. Bernstein (tel. 516-345-4382) T. F. Koetzle (tel. 516-345-4384) G.J.B. Williams (tel. 516-345-4383)
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, England	O. Kennard (tel. (0223)66499)
Australia	C.S.I.R.O. Division of Applied Organic Chemistry Box 4331 G.P.O. Melbourne, Victoria 3001 Australia	B. J. Poppleton
Japan	Department of Chemistry Faculty of Science The University of Tokyo Bunkyo-ku, Tokyo, Japan	M. Tasumi





REQUEST FORM

1. Name: \_\_\_\_\_ Date: \_\_\_\_\_  
 Address: \_\_\_\_\_ Telephone: \_\_\_\_\_  
 \_\_\_\_\_  
 \_\_\_\_\_

2. Send the following information (please check):
- ( ) all current coordinate entries
  - ( ) parameter sets listed (complete 3. below)
  - ( ) description of file record formats
  - ( ) list of revisions on microfiche

3. Parameter sets requested (by ident code please):

_____	_____	_____	_____	_____	_____	_____
_____	_____	_____	_____	_____	_____	_____
_____	_____	_____	_____	_____	_____	_____

4. Tape: I am sending a new 2400 foot reel of magnetic tape ( ) yes ( ) no.

5. Tape format desired:

- ( ) 7 track ( ) 556 bpi ( ) ASCII ( ) Unlabelled (preferred)
- ( ) 9 track ( ) 800 bpi ( ) BCD ( ) Labelled-user's label
- ( ) 1600 bpi ( ) EBCDIC \_\_\_\_\_ retained

Tape copies are normally blocked since otherwise the entire contents will not fit on a 2400 foot reel of tape. Indicate the maximum block size allowed if blocks of 5120 characters (bytes) cannot be handled,

\_\_\_\_\_

Please complete reverse side.

REQUEST FORM

6. Charge (Brookhaven requests only)		Enter Amount
A. Data preparation (unit charge per magnetic tape)		\$ _____
U. S. Department of Energy	\$40.25 ( )	
Other U. S. Federal Agencies	\$47.45 ( )	
All others	\$51.00 ( )	
B. Magnetic tape	\$ 8.59 ( )	\$ _____
(please check if answer to 4. above was <u>NO</u> )		
C. Postage		\$ _____
U. S. and Canada	\$ 2.00 ( )	
Air Mail to other countries	\$17.00 ( )	
D. Total charge (A + B + C)		\$ _____
E. Payment to the order of Brookhaven National Laboratory		
by ( ) check		is ( ) enclosed
( ) purchase order number _____		( ) sent separately

Mail this completed form to the appropriate center (Brookhaven, Cambridge, Melbourne or Tokyo) at the address listed in the body of the Newsletter.

It is expected that the Protein Data Bank be acknowledged in publications which result from work making use of the Bank's services. We would appreciate receiving reprints of any such publications.