

Please note that there has been a small change in the prices listed in the order form on pages 5-6. These new prices are effective immediately and are expected to be valid through September 30, 1988.

The Protein Data Bank continues to receive large quantities of new data. Newly released entries and replacements are noted in Table 5, while Table 6 lists entries in preparation which will be made available for distribution as soon as possible.

Some suggestions for citing data obtained from the Protein Data Bank are given below:

1. The original authors and publication should be cited. Each entry has one or more AUTHOR records with the official author list for the entry. If there is a paper describing exactly the coordinates deposited with the Protein Data Bank, this paper is presented on JRNL records. If there are no JRNL records the entry should be cited as a "private communication".
2. The Protein Data Bank should be cited. The appropriate references are F. C. Bernstein, T. F. Koetzle, G. J. B. Williams, E. F. Meyer, Jr., M. D. Brice, J. R. Rodgers, O. Kennard, T. Shimanouchi, and M. Tasumi, *J. Mol. Biol.*, 112, 535-542 (1977) and E. E. Abola, F. C. Bernstein, S. H. Bryant, T. F. Koetzle, and J. Weng, in *Crystallographic Databases - Information Content, Software Systems, Scientific Applications*, eds. F. H. Allen, G. Bergerhoff, and R. Sievers, Data Commission of the Int'l Union of Crystallography, Bonn/Cambridge/Chester, 1987, pp 107-132.

We would appreciate receiving reprints of all publications making use of data from the Protein Data Bank. Please send these to Ms. Frances C. Bernstein.

Inquiries may be addressed to any of the persons listed below. The order form on pages 5-6 of this newsletter may be used to order data from Brookhaven. It is possible to place a standing order for each quarterly DATAPRTP release; anyone interested in placing such a standing order should contact F. C. Bernstein. Please note that the order form on pp. 5-6 should be used only for Brookhaven orders; users in Japan or Australia should contact their centers for detailed information.

<u>Area</u>	<u>Address of Center</u>	<u>BITNET (BNL Only)</u>	<u>Name</u>	<u>Phone</u>
Worldwide except Australia and Japan	Protein Data Bank	PDB@BNLCHM	Inquiries	516-282-4382
	Chemistry Department	ABOLA@BNLCHM	E. E. Abola	516-282-4383
	Brookhaven National Laboratory	BERNSTEIN@BNLCHM	F. C. Bernstein	516-282-4382
	Upton, NY 11973	BRYANT@BNLCHM	S. H. Bryant	516-282-4375
USA		KOETZLE@BNLCHM	T. F. Koetzle	516-282-4384
		WENG@BNLCHM	J. C. Weng	516-282-4382
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002, Australia		T. Graddon	03-418-7266
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2, Suita, Osaka 565, Japan		Y. Katsube	(06) 877-5111 ext. 3912

Supported by the U. S. National Science Foundation and U. S. National Institutes of Health.

TABLE 1. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MAGNETIC TAPE

Table with columns: CODE, ITEM, AVAILABILITY (USA, JAP, AUS). Rows include DATAPRTP, YEAB97PT, PART8BPT, PDBPGMTP, NONST1TP, NONST2TP, etc.

* NEW OR REPLACEMENT ENTRY SINCE OCT-87 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

Table with columns: CODE, ITEM, AVAILABILITY (USA, JAP, AUS). Rows include DATAPRF1, YEAB97F1, PART8BF1, CORR2F1, etc.

* NEW OR REPLACEMENT ENTRY SINCE OCT-87 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, COMPUTER PROGRAMS AND MISCELLANEOUS FILES

Table with columns: NAME, PURPOSE, AUTHOR(S), REV DATE/SUPPORTED. Rows include PART A - AVAILABLE ON DATAPRTP, BENDER, BLDKIT, BRUKTP, etc.

* NEW OR REPLACEMENT ENTRY SINCE OCT-87 NEWSLETTER

SUPPORTED PROGRAMS ARE THOSE FOR WHICH STAFF OF THE PROTEIN DATA BANK WILL PROVIDE CORRECTIONS FOR DEMONSTRATED ERRORS.

TABLE 4. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/ CODE. Rows include PART 1 - AVAILABLE ON NONST1TP, R1ACTSF, CHYMOF, etc.

PART 2 - AVAILABLE ON NONST2TP, NONST2F1

Table with columns: CODE, ITEM, AVAILABILITY (USA, JAP, AUS), AUTHOR(S), REV DATE/SUPPORTED. Rows include R1CCRSF, R351CSF, R451CSF, etc.

PART 3 - AVAILABLE ON NONST3TP, NONST3F1

Table with columns: CODE, ITEM, AVAILABILITY (USA, JAP, AUS), AUTHOR(S), REV DATE/SUPPORTED. Rows include R1CATSF, R4CHASF, R2C0H5F, etc.

PART 4 - AVAILABLE ON NONST4TP, NONST4F1

Table with columns: CODE, ITEM, AVAILABILITY (USA, JAP, AUS), AUTHOR(S), REV DATE/SUPPORTED. Rows include R2APRSF, R3AGASF, R2AZASF, etc.

CODES
SF STRUCTURE FACTORS

BROOKHAVEN ORDER FORM (Please include a self-addressed label)

1. Name _____ Date _____
Address _____ Telephone _____

2. Documentation desired (no charge).

- Introduction to The Protein Data Bank (June 1986)
- Latest Newsletter
- Atomic Coordinate and Bibliographic Entry Format Description for DATAPRTP and DATAPRFI (January 1985)
- Current DATAPRTP Directory
- Sources of Visual Aids for Macromolecular Structure (September 1986)
- Non-Standard Entries (Structure Factors) Format Description
- Data Deposition form

3. Please send the following magnetic tape items (from Table 1).

	6250 cpi	1600 cpi	TK50
DATAPRTP (coordinate tape)			
VAX/VMS BACKUP	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	<input type="checkbox"/> \$283
VAX/VMS COPY	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	<input type="checkbox"/> \$283
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	
PDBPGMTP			
VAX/VMS COPY	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	<input type="checkbox"/> \$283
NONST1TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST2TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST3TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST4TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST5TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	

Special order items (described in Table 1):

Please inquire at Brookhaven for availability and price.

YEAR86TP	CONECTTP	DSTNCETP
PART87TP	DGPLOTP	FISIPLTP
BENDERTP	DIHDLRTP	PHIPSITP

(CONTINUED)

4. Foreign air mail postage for tape items listed in 3 above mailed from Brookhaven to destinations outside the U. S. and Canada. A postage surcharge of \$19 is required per item.

Number of items x \$19.00 = _____

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$292, postage included. Correction fiche are free.

Items: _____ Total Cost: _____

6. Please send the following printed listings. Each listing costs \$95, postage included.

Ident Code(s) (From Table 5): _____ Total Cost: _____

7. **Total charges - All prices are expected to be valid through September 30, 1988. After that date please confirm prices.**

Magnetic tape charges (3 above)	_____
Foreign air mail postage charges (4 above)	_____
Microfiche charges (5 above)	_____
Printed listing charges (6 above)	_____
Bank charge	_____
No charge for checks drawn in US dollars on US bank, otherwise \$10	_____
Total	_____

Method of Payment:

Brookhaven requires that either a check or written purchase order payable to Brookhaven National Laboratory be received before service is provided. Order forms and purchase orders may be sent by facsimile to (United States) 516-282-3000. The original order forms and purchase orders should also be sent to Brookhaven by mail.

() check is () enclosed
() purchase order number _____ () sent separately

Please return to

Ms. F. C. Bernstein
Chemistry Department
Brookhaven National Laboratory
Upton, New York 11973 USA
(516-282-4382)

It is advisable to send a photocopy of this order form directly to Brookhaven; experience shows that purchasing departments often do not forward this form with the order.