

October marks the beginning of our new fiscal year, and we are making a very small increase in our charges to users. This increase for orders to Brookhaven is approximately 2%. The cost of all coordinate entries and programs (DATAPRTP) on one tape at 6250 cpi is increasing from \$181 to \$184 and on two tapes at 1600 or 800 cpi from \$220 to \$225. The charges for other services are detailed on the request form.

We are initiating two new tape services starting January, 1984. We will be offering a "yearly tape" which will contain only new and significantly revised entries, including computer programs, for each calendar year. A "current tape" will also be available, containing similar information applicable to the current year, and updated in a timely manner. The new services should provide an efficient way for users who have received tapes in the past to stay current, and we expect that these updates will easily fit on one reel of tape at either 800 or 1600 cpi. The usual full DATAPRTP tape will, of course, still be available.

In connection with these new services, we are inserting three new record types (OBSLTE, SPRSDE and REVDAT) in our entries, where applicable. The OBSLTE record will be used to identify entries which have been replaced by newer data: This record type will be included in our archived entries. A new entry will also be generated for our distribution tape which will contain all OBSLTE records found in the database. SPRSDE will be used to identify the entries which have replaced older ones. This record will be inserted after the AUTHOR record of entries superseding older ones. REVDAT records will describe revisions made to an entry. A full description of OBSLTE, SPRSDE and REVDAT will appear in our "Atomic Coordinate Entry Format Description" document.

Inquiries and suggestions may be addressed to any of the persons listed below. The request form on pages 5-6 of this Newsletter may be used to order data from Brookhaven or Cambridge; users in Australia or Japan should contact their centers for detailed information.

Area	Address of Center	Name	
The Americas	Protein Data Bank	E. E. Abola	516-282-4383
	Chemistry Department	F. C. Bernstein	516-282-4382
	Brookhaven National Laboratory	T. F. Koetzle	516-282-4384
	Upton, New York 11973 USA		
Europe and Worldwide	University Chemical Laboratory	O. Kennard	0223-66499
	Lensfield Road Cambridge CB2 1EW, England	S. Bellard	
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002 Australia	C. Garrow	03-419-1333
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2, Suita, 565 Japan	N. Yasuoka	(06) 877-5111 ext. 3912

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

CODE	ITEM	NO. TAPES			AVAILABILITY		
		800	1600	6250	US	UK	JA AUS
		07-OCT-83					
DATAPRT	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	2	2	1	X	X	X X
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	2	1	1	X	X	X X
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	2	1	1	X	X	X X
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	1	1	1	X		
BLDK1ITP	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER					
CONECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	1	X		
DGPLOTTTP	DIAGONAL PLOTS (LINE PRINTER)	1	1	1	X		
DIHORLTP	COMPLETE TORSION ANGLES	2	1	1	X		
DSTNCETP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	2	1	1	X		
FISIPLTP	PHI/PSI PLOTS (LINE PRINTER)	1	1	1	X		
PHIPSITP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	1	X		

\* NEW OR REPLACEMENT ENTRY SINCE JUL-83 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	AVAILABILITY		
		US	UK	JA AUS
		07-OCT-83		
DATAPRF	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)		X	X X
NONST1F	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)		X	X X
NONST2F	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)		X	X X
CORR12F	LIST OF CORRECTIONS NO. 12 (JAN/83 - JUL/83)		X	X X X
BENDERF	PARAMETERS FOR BENT-WIRE MODELS		X	
BLDK1TF	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER		
CONECTF	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS		X	
DGPLOTF	DIAGONAL PLOTS (LINE PRINTER)		X	
DIHORLF	COMPLETE TORSION ANGLES		X	
DSTNCEF	CONNECTIVITY SPECIFICATIONS WITH DISTANCES		X	
FISIPLF	PHI/PSI PLOTS (LINE PRINTER)		X	
PHIPSIF	LISTS OF PHI/PSI/OMEGA VALUES		X	

\* NEW OR REPLACEMENT ENTRY SINCE JUL-83 NEWSLETTER





REQUEST FORM (Please include a self-addressed label)

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

2. Documentation desired (no charge).
- Latest Newsletter
  - Introduction to The Protein Data Bank (July 1982)
  - Sources of Visual Aids for Macromolecular Structure (May 1982)
  - Atomic Coordinate Entry Format Description for DATAPRTP and DATAPRFI (October 1983)
  - Non-Standard Entries (Structure Factors) Format Description for NONST1TP and NONST1FI (April 1983)
  - Non-Standard Entries (Structure Factors) Format Description for NONST2TP and NONST2FI (October 1983)
  - Data Deposition form

3. Please send the following magnetic tape items (from Table 1). Each 1-tape item costs \$184 (£123 from Cambridge); each 2-tape item costs \$225 (£150). Domestic postage is included.

<u>Item</u>	<u>Number of Tapes</u>	<u>Cost</u>
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Total \_\_\_\_\_

Special Instructions (to be completed for Brookhaven requests only).  
Please check the appropriate box.

We are especially interested in the pending entries with the following Ident Codes: \_\_\_\_\_ . Please delay shipment until the date \_\_\_\_\_ if any of these entries are expected to be available by that date.

Normal order-will be processed as soon as possible.

4. Tape format desired (all tapes are unlabelled)

	Availability	
	US	UK
<input type="checkbox"/> 9 track, 6250 cpi, EBCDIC	yes	yes
<input type="checkbox"/> 9 track, 1600 cpi, EBCDIC	yes	yes
<input type="checkbox"/> 9 track, 800 cpi, EBCDIC	yes	yes
<input type="checkbox"/> 9 track, 6250 cpi, ASCII	yes	yes
<input type="checkbox"/> 9 track, 1600 cpi, ASCII	yes	yes
<input type="checkbox"/> 9 track, 800 cpi, ASCII	yes	yes
<input type="checkbox"/> 7 track, 800 cpi, BCD	yes	please inquire

All tapes are distributed in blocked form with fixed record length and block size. Brookhaven normally uses a block size close to, but less than, 5120 characters. Please indicate here any difficulties this might cause.

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$122 (£81), postage included. Correction fiche are free.

<u>Item</u>	<u>Cost</u>
	Total _____

6. Please send the following printed listings. Each listing costs \$71, (£47), postage included.

<u>Ident Code</u> (From Table 3)	<u>Cost</u>
	Total _____

7. Foreign air mail postage from Brookhaven to destinations outside the U. S. and Canada or from Cambridge to destinations outside the United Kingdom. A postage surcharge of \$15 (£10) is required per magnetic tape (not per item).

Number of tapes x \$15.00 (£10) = \_\_\_\_\_

8. Total charges

Magnetic tape charges (3 above)	_____
Microfiche charges (5 above)	_____
Printed listing charges (6 above)	_____
Foreign air mail postage charges (7 above)	_____
Total	_____

For Brookhaven only:

Brookhaven requires that either a check or actual purchase order be received before data are shipped. Inclusion of check with order will expedite processing.

Payment to the order of Brookhaven National Laboratory

by ( ) check is ( ) enclosed  
( ) purchase order number \_\_\_\_\_ ( ) sent separately to the Protein Data Bank

Please return to

Ms. F. C. Bernstein  
Chemistry Department  
Brookhaven National Laboratory  
Upton, New York 11973 USA

or  
Dr. S. Bellard  
University Chemical Laboratory  
Lensfield Road  
Cambridge CB2 1EW, England

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