

Effective immediately we will no longer distribute DATAPRTP (all current coordinate entries, bibliographic entries, programs) on one tape at 1600 cpi. We are virtually at the end of the tape and expect to be adding more entries within the next month. DATAPRTP is available on one tape at 6250 cpi, and on two tapes at 1600 cpi or 800 cpi. Please be careful to specify the desired density and correct number of tapes when filling out the order form.

We are pleased to announce that Jan Hermans is joining Jane Richardson and Wayne Hendrickson on the Protein Data Bank Advisory Board. At this time we would like to thank Harold Scheraga for his valuable assistance in three years of service on the Board.

Those of you who read Table 3 closely should be aware that we have changed the meaning of the status flag R. Until now it has identified all entries which were replacements of previous data sets. With the passage of time an increasing proportion of data sets had been flagged with R. It therefore seemed sensible to reserve R status to indicate that the data set is a replacement received within the past two years (1982-1983), and we will use this convention henceforth. We will naturally continue to retain all data sets, including those for which replacements have been received, in our archival storage.

Inquiries and suggestions are welcomed and 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 Upton, New York 11973 USA	T. F. Koetzle	516-282-4384
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
DATAPRTP	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			
BLDKITTP	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			
DIHDLRTP	COMPLETE TORSION ANGLES	2	1	1	X			
DSTNCTTP	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 JAN-83 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	AVAILABILITY			
		US	UK	JA	AUS
DATAPRFI	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	X	X	X	
NONST1FI	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	X	X	X	
NONST2FI	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	X	X	X	
CORR11FI	LIST OF CORRECTIONS NO. 11 (JUL/82 - JAN/83)	X	X	X	X
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	X			
BLDKITFI	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER			
CONECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X			
DGPLOTFI	DIAGONAL PLOTS (LINE PRINTER)	X			
DIHDLRFI	COMPLETE TORSION ANGLES	X			
DSTNCFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X			
FISIFLFI	PHI/PSI PLOTS (LINE PRINTER)	X			
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	X			

\* NEW OR REPLACEMENT ENTRY SINCE JAN-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 (October 1982)  
 ( ) Sources of Visual Aids for Macromolecular Structure (May 1982)  
 ( ) Atomic Coordinate Entry Format Description for DATAPRTP and  
 DATAPRFI (December 1981)  
 ( ) Non-Standard Entries (Structure Factors) format description for  
 NONST1TP and NONST1FI (October 1982)  
 ( ) Non-Standard Entries (Structure Factors) format description for  
 NONST2TP and NONST2FI (January 1983)  
 ( ) Data Deposition form

## 3. Please send the following magnetic tape items (from Table 1). Each 1-tape item costs \$181 (£106 from Cambridge); each 2-tape item costs \$220 (£129). 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
( ) 9 track, 6250 cpi, EBCDIC	yes	yes
( ) 9 track, 1600 cpi, EBCDIC	yes	yes
( ) 9 track, 800 cpi, EBCDIC	yes	yes
( ) 9 track, 6250 cpi, ASCII	yes	yes
( ) 9 track, 1600 cpi, ASCII	yes	yes
( ) 9 track, 800 cpi, ASCII	yes	yes
( ) 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 \$111 (£65), postage included. Correction fiche are free.

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

6. Please send the following printed listings. Each listing costs \$70, (£41), postage included.

<u>Ident Code (From Table 3)</u>	<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 (£9) is required per magnetic tape (not per item).

Number of tapes x \$15.00 (£9) = \_\_\_\_\_

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