

Effective April 1, 1984 we will no longer distribute magnetic tapes written in 7-track format. Anyone who would be adversely affected by this decision should inform Brookhaven as soon as possible.

As we previously announced, we are now distributing two new products, a "yearly tape (fiche)" and a "current tape (fiche)". These are referred to as YEAR83TP, YEAR83FI, PART84TP, and PART84FI in our order form. Our October 1983 Newsletter has the details on these products. To aid our users in deciding which tape service to use, a new directory-producing program called DRCTRY has now been included on our distribution tape. This program produces a table of contents of our tapes which includes the dates of accession and latest revision (for those entries with the REVDAT records). To receive a printout of the latest directory, check the appropriate box on the order form (page 5).

The Cambridge Data Centre has announced that they would prefer that no check be enclosed with orders. Inclusion of a purchase order is desirable but not mandatory. A reminder to this effect has now been included in our order form.

Inquiries and suggestions 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 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	03-418-7333
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2, Suita, Osaka 565 Japan	N. Yasuoka	(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, 18-JAN-84 (NO. TAPES 800, 1600, 6250), AVAILABILITY (US, UK, JA, AUS). Rows include DATAPRTP, YEAR83TP, PART84TP, NONST1TP, NONST2TP, BENDERTP, BLKDT1TP, CONECTCTP, DGPLDTTP, DIHDLRTP, DSTNCEP, FISPLP, PHIPSIPT, etc.

* NEW OR REPLACEMENT ENTRY SINCE OCT-83 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

Table with columns: CODE, ITEM, 18-JAN-84, AVAILABILITY (US, UK, JA, AUS). Rows include DATAPRF1, YEAR83F1, PART84F1, NONST1F1, NONST2F1, CORR13F1, BENDERF1, BLKDT1F1, CONECTCF1, DGPLDTF1, DIHDLRF1, DSTNCF1, FISPLF1, PHIPSIF1, etc.

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TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

Table with columns: NAME, PURPOSE, AUTHOR(S), 18-JAN-84, REV DATE/SUPPORTED. Rows include BENDER, BLKDT, CHIRAL, CONNECT, CONTACT, DGPLDT, DIHDLR, DRCTRY, DSSP, DSTNCE, FISPL, LSH, NAMOD, PHPSI, REFMTE, STEREO, TAPDIR, THEOD, TORSRU, TOTALS, etc.

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

TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 1, SEE ALSO TABLE 6)

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/ CODE. Rows include R1ACTSF, CHYMF, RCARPO4, RCARPO5, R2B5CSF, R3CYT5F, R4CYT5F, R5CYT5F, R6CYT5F, R7ZNASF, R8ZNASF, R9BNA5F, R10BNA5F, R11BNA5F, R12BNA5F, R13BNA5F, R14BNA5F, R15BNA5F, R16BNA5F, R17BNA5F, R18BNA5F, R19BNA5F, R20BNA5F, R21BNA5F, R22BNA5F, R23BNA5F, R24BNA5F, R25BNA5F, R26BNA5F, R27BNA5F, R28BNA5F, R29BNA5F, R30BNA5F, R31BNA5F, R32BNA5F, R33BNA5F, R34BNA5F, R35BNA5F, R36BNA5F, R37BNA5F, R38BNA5F, R39BNA5F, R40BNA5F, R41BNA5F, R42BNA5F, R43BNA5F, R44BNA5F, R45BNA5F, R46BNA5F, R47BNA5F, R48BNA5F, R49BNA5F, R50BNA5F, R51BNA5F, R52BNA5F, R53BNA5F, R54BNA5F, R55BNA5F, R56BNA5F, R57BNA5F, R58BNA5F, R59BNA5F, R60BNA5F, R61BNA5F, R62BNA5F, R63BNA5F, R64BNA5F, R65BNA5F, R66BNA5F, R67BNA5F, R68BNA5F, R69BNA5F, R70BNA5F, R71BNA5F, R72BNA5F, R73BNA5F, R74BNA5F, R75BNA5F, R76BNA5F, R77BNA5F, R78BNA5F, R79BNA5F, R80BNA5F, R81BNA5F, R82BNA5F, R83BNA5F, R84BNA5F, R85BNA5F, R86BNA5F, R87BNA5F, R88BNA5F, R89BNA5F, R90BNA5F, R91BNA5F, R92BNA5F, R93BNA5F, R94BNA5F, R95BNA5F, R96BNA5F, R97BNA5F, R98BNA5F, R99BNA5F, R100BNA5F, etc.

CODES
SF STRUCTURE FACTORS

TABLE 6. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 2, SEE ALSO TABLE 5)

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/ CODE. Rows include R11CBSF, R12CPSF, R13CPSF, R14CPSF, R15CPSF, R16CPSF, R17CPSF, R18CPSF, R19CPSF, R20CPSF, R21CPSF, R22CPSF, R23CPSF, R24CPSF, R25CPSF, R26CPSF, R27CPSF, R28CPSF, R29CPSF, R30CPSF, R31CPSF, R32CPSF, R33CPSF, R34CPSF, R35CPSF, R36CPSF, R37CPSF, R38CPSF, R39CPSF, R40CPSF, R41CPSF, R42CPSF, R43CPSF, R44CPSF, R45CPSF, R46CPSF, R47CPSF, R48CPSF, R49CPSF, R50CPSF, R51CPSF, R52CPSF, R53CPSF, R54CPSF, R55CPSF, R56CPSF, R57CPSF, R58CPSF, R59CPSF, R60CPSF, R61CPSF, R62CPSF, R63CPSF, R64CPSF, R65CPSF, R66CPSF, R67CPSF, R68CPSF, R69CPSF, R70CPSF, R71CPSF, R72CPSF, R73CPSF, R74CPSF, R75CPSF, R76CPSF, R77CPSF, R78CPSF, R79CPSF, R80CPSF, R81CPSF, R82CPSF, R83CPSF, R84CPSF, R85CPSF, R86CPSF, R87CPSF, R88CPSF, R89CPSF, R90CPSF, R91CPSF, R92CPSF, R93CPSF, R94CPSF, R95CPSF, R96CPSF, R97CPSF, R98CPSF, R99CPSF, R100CPSF, etc.

* NEW OR REPLACEMENT ENTRY SINCE OCT-83 NEWSLETTER

CODES
SF STRUCTURE FACTORS

TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

18-JAN-84

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR(S), DATE/STATUS, and a list of protein entries including LEHEMOGLOBIN(AQUO MET), LEHEMOGLOBIN(CYANO MET), LEHEMOGLOBIN(CYANO MET), etc.

* NEW OR REPLACEMENT ENTRY SINCE OCT-83 NEWSLETTER
STATUS CODES
BLANK STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A ALPHA CARBON ATOMS ONLY
B BACKBONE ONLY
N NEW ENTRY AWAITING APPROVAL BY DEPOSITOR
P IN PREPARATION
R RECENT (1982-1984) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE B. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

18-JAN-84

TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

18-JAN-84

OEAP ACID PROTEINASE (ENDOTHTA PARASITICA)
OADC ADH-NADH-DIMETHYLSULFOXIDE COMPLEX
OAF1 APOFERRITIN (HORSE)
OHAA MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE
OAZA AZURIN(ALCALIGENES DENITRIFICANS)
ORNB BARNASE (BACILLUS AMYLOLIQUEFACIENS)
ORND CALOTROPIN DI (CALOTROPIS GIGANTEA)
OPTF D-ALANYL-CARBOXYPEPTIDASE-TRANSEPTIDASE
OZGF D-ALANYL-D-ALANINE PEPTIDASE (ZN2+ G PEPTIDASE)
OCTS CITRATE SYNTHASE (PIG)
OCN2 CONCANAVALLIN A (DEMETALLIZED)
OCRO CRO REPRESSOR
OCCR GAMMA-CRYSTALLIN II (CALF)
OCYP CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)
OCYS CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)
OUC1 CYTOCHROME C555 (CHLOROBIUM THIOSULFATOPHILUM)
OC3A DES-ARG77-CA3 ANAPHYLATOXIN
OCDF DIHYDROFLATE REDUCTASE (CHICKEN LIVER)
DANB DNA(GGTATACC)
DANB DNA(GGUA+UACC)
DESZ ELASTASE COMPLEX (PIG)
DETU ELONGATION FACTOR TU COMPLEX (E. COLI)
DEBX ERABUTOXIN B
DFX1 FLAVODOXIN (DESULFOVIBRIO VULGARIS)
DFX2 FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)
OG8P D-GALACTOSE-BINDING PROTEIN(ESCHERICHIA COLI)
OGAP CATABOLITE GENE ACTIVATOR PROTEIN
OGPI GLUTATHIONE PEROXIDASE (BOVINE)
GGD1 D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)
DHMG HEMAGGLUTININ
DDCH HEMOGLOBIN (COBALT DEOXY)
DH8G HEMOGLOBIN (GLYCERA DIBRANCHIATA)
OPHH P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)
DAU1 IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU
DROY IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (V-MONOMER,KAPPA) ROY
DMCP IMMUNOGLOBULIN FAB (KAPPA) MCP603
OIG1 IMMUNOGLOBULIN G1 (KAPPA) DOB
DINI INSULIN (PORCINE)
DIN2 INSULIN (PORCINE)
OPKA KALLIKREIN A (PORCINE)
OKA1 KALLIKREIN A/BOVINE PANCREATIC INHIBITOR
OLRF N-TERMINAL DOMAIN OF LAMBDA REPRESSOR
OGLM *LYSOZYME (EMBDEN GOOSE)
DLZ1 LYSOZYME (HUMAN)
DLZ5 LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)
DLZ7 *LYSOZYME (HEN EGG-WHITE, HIGH-TEMPERATURE)
DLZ6 LYSOZYME (STREPTOMYCES ERYTHRAEUS)
OTEL *LYSOZYME (TORTOISE EGG-WHITE)
OCTF L7/L12 (E. COLI, C-TERMINUS)
OMBA MYOGLOBIN (APLYSIA LIMACINA)
OMBM MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)
OMB3 MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)
OPFK PHOSPHOFUCTOKINASE (BACILLUS STEAROTHERMOPHILUS)
OPP2 PHOSPHOLIPASE A2 (RATTLESNAKE)
OPPA PHOSPHORYLASE A (RABBIT)
OPB1 PHOSPHORYLASE B (RABBIT)
ORX5 RELAXIN (PORCINE, MODEL)
ORSA RIBONUCLEASE A (BOVINE)
ORST RIBONUCLEASE ST (STREPTOMYCES ERYTHREUS)
ORNT RIBONUCLEASE T1-2(PRIME)-GUANYLIC ACID (ASPERGILLUS ORYZAE)
OSDE *FE-SUPEROXIDE DISMUTASE (ESCHERICHIA COLI)
OSDP *FE-SUPEROXIDE DISMUTASE (PSEUDOMONAS OVALIS)
OT4H THIOREDOXIN REDUCTASE (BACTERIOPHAGE T4)
OFMT INITIATOR TRANSFER RNA (E. COLI, F/MET)
OTA1 TRANSFER RNA (YEAST, ASP. A FORM)
OTA2 TRANSFER RNA (YEAST, ASP. B FORM)
OTR1 TRANSFER RNA (YEAST, PHE)
OMTS METHIONYL TRANSFER RNA SYNTHETASE
OYP1 TRIOSE PHOSPHATE ISOMERASE (SACCHAROMYCES CEREVISIAE)
OGN5 GENE 5 DNA-UNWINDING PROTEIN (E. COLI)
OUTG UTEROGLOBIN (RABBIT)
OSTV VIRUS (SATELLITE TOBACCO NECROSIS)
OTMV VIRUS PROTEIN DISK (TOBACCO MOSAIC)
OTBV VIRUS (TOMATO BUSHY STUNT)

* NEW OR REPLACEMENT ENTRY SINCE OCT-83 NEWSLETTER

THE CORRECTIONS IN THIS TABLE ARE GIVEN IN THE FORM OF 'UPDATE' MODIFICATIONS, AND CONSIST OF 'UPDATE' DIRECTIVES PLUS NEW DATA RECORDS THAT ARE TO BE INSERTED OR THAT REPLACE ERRONEOUS RECORDS IN CERTAIN DATA BANK ENTRIES. 'UPDATE' IS THE CDC LIBRARY-FILE MANAGEMENT SYSTEM UNDER WHICH THE MASTER PROTEIN DATA BANK FILE IS MAINTAINED. FOR A DESCRIPTION OF 'UPDATE' USERS ARE REFERRED TO THE 'UPDATE REFERENCE MANUAL' PUBLICATION NUMBER 603R2500, CONTROL DATA CORPORATION, ARDEN HILLS, MN, 1974. BRIEFLY, EACH DATA ENTRY IS GIVEN AN IDENTIFICATION CODE WHICH ALSO SERVES AS THE 'UPDATE' 'DECK' NAME. EACH RECORD IN THE FILE IS IDENTIFIED WITH TWO TAGS. THE FIRST TAG IS SIMPLY THE 'DECK' NAME (OR AN 'IDENT' NAME -SEE BELOW) AND THE SECOND IS A CHARACTER WITHIN THE 'DECK' (OR 'IDENT'). THESE TAGS ARE INCLUDED IN CHARACTERS 73-80 OF THE RECORDS IN EACH DATA ENTRY AS DISTRIBUTED.

CORRECTIONS MAY BE MADE USING 'UPDATE' DIRECTIVES TO 'INSERT' NEW RECORDS OR 'DELETE' OLD ONES. EACH CORRECTION SET BEGINS WITH A '*IDENT' DIRECTIVE. THIS IDENTIFIES THE CORRECTION SET, E.G. AS 'IMBA' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK 'IMBN' FOR SPERM-WHALE MYOGLOBIN, 'IMBNB' FOR THE SECOND CORRECTION, ETC. '*DELETE' DIRECTIVES SPECIFY A RECORD OR INCLUSIVE RUN OF RECORDS TO BE DELETED, IF DATA RECORDS OCCUR IMMEDIATELY FOLLOWING '*DELETE'. THESE ARE TO BE INSERTED IN PLACE OF THE RECORDS DELETED. '*INSERT' DIRECTIVES ARE USED TO SPECIFY A PARTICULAR RECORD AFTER WHICH INFORMATION IS TO BE INSERTED. THE RECORDS TO BE INSERTED FOLLOW IMMEDIATELY AFTER '*INSERT' IN THE CORRECTION SET. WITHIN EACH CORRECTION NEW RECORDS PLACED IN THE FILE ARE GIVEN THE 'IDENT' NAME AND NUMBERED SEQUENTIALLY.

```
*IDENT,1162B
*INSERT,1162A.4
REMARK 9
REMARK 9 CORRECTION. CORRECT (3,3) ELEMENT OF SCALE MATRIX.
REMARK 9 27-OCT-83.
*INSERT,1162.5
REVDAT 3 27-OCT-83 1162B 3 SCALE
*DELETE,1162.153
SCALE3 0.000000 0.000000 .012180 0.000000
DELETE,1162A.5
MASTER 79 8 0 0 0 0 0 6 3384 1 12 52

*IDENT,5CPAC
*INSERT,5CPAB.8
REMARK 7
REMARK 7 THE COORDINATES FOR THE SOLVENT MOLECULES GIVEN BELOW
REMARK 7 INCLUDE SOME ATOMS WHICH ARE RELATED TO OTHERS IN THE LIST
REMARK 7 BY THE CRYSTAL SYMMETRY. THIS EXPANDED LIST CONTAIN ALL
REMARK 7 THE SOLVENT MOLECULES WHICH COULD BE LOCATED IN THE FOURIER
REMARK 7 MAPS AND WHICH INTERACT WITH THE PROTEIN MOLECULE WHOSE
REMARK 7 COORDINATES ARE GIVEN IN THIS ENTRY. SOLVENT ATOMS WHICH
REMARK 7 HAVE THE SAME SEQUENCE NUMBER ARE RELATED BY SYMMETRY
REMARK 7 AND DIFFERENT INSERTION CODES HAVE BEEN ASSIGNED TO
REMARK 7 DISTINGUISH THEM. EACH *FTNOTE* RECORD GIVES THE
REMARK 7 SYMMETRY OPERATION RELATING A SOLVENT ATOM WITH INSERTION
REMARK 7 CODE *A* TO THE SOLVENT ATOM WITH THE *FTNOTE* AND THE
REMARK 7 SAME SEQUENCE NUMBER.
REMARK 8
REMARK 8 CORRECTION. REVISE COORDINATES OF WATER MOLECULES AS PER
REMARK 8 DEPOSITOR'S INSTRUCTIONS. RESTORE SEQUENCE NUMBER FOR ZN.
REMARK 8 ADD REMARK 5. 01-NOV-83.
*INSERT,5CPA.6
REVDAT 4 01-NOV-83 5CPAC 3 REMARK FTNOTE FORMUL HETATM
*INSERT,5CPA.9B
FTNOTE 2
FTNOTE 2 SEE REMARK 5. COORDINATES FOR THIS ATOM WERE SYMMETRY
FTNOTE 2 GENERATED USING THE OPERATION,
FTNOTE 2
FTNOTE 2 (XB,YB,ZB) = (-XA,YA+30.135,-ZA)
FTNOTE 2 (XB,YB,ZB) ARE THE COORDINATES OF ATOMS WITH INSERT CODE
FTNOTE 2 *B*. (XA,YA,ZA) ARE THE COORDINATES OF ATOMS WITH INSERT
FTNOTE 2 CODE *A*.
FTNOTE 3
FTNOTE 3 SEE REMARK 5. COORDINATES FOR THIS ATOM WERE SYMMETRY
FTNOTE 3 GENERATED USING THE OPERATION,
FTNOTE 3
FTNOTE 3 (XC,YC,ZC) = (-XA+5.979,YA+30.135,-ZA+46.870)
FTNOTE 3 (XC,YC,ZC) ARE THE COORDINATES OF ATOMS WITH INSERT CODE
FTNOTE 3 *C*. (XA,YA,ZA) ARE THE COORDINATES OF ATOMS WITH INSERT
FTNOTE 3 CODE *A*.
.
.
FTNOTE 12
FTNOTE 12 SEE REMARK 5. COORDINATES FOR THIS ATOM WERE SYMMETRY
FTNOTE 12 GENERATED USING THE OPERATION,
FTNOTE 12
FTNOTE 12 (XL,YL,ZL) = (XA+5.979,YA,ZA+46.870)
FTNOTE 12 (XL,YL,ZL) ARE THE COORDINATES OF ATOMS WITH INSERT CODE
FTNOTE 12 *L*. (XA,YA,ZA) ARE THE COORDINATES OF ATOMS WITH INSERT
FTNOTE 12 CODE *A*.
*DELETE,5CPA.99
FORMUL 3 HOH *192(H2 O1)
*DELETE,5CPA.259H,2873
HETATM 2439 ZN ZN 308 -3.304 26.331 -5.535 1.00 5.23
HETATM 2440 O HOH 309A 1.940 30.255 -16.826 1.00 31.41
HETATM 2441 O HOH 310A 1.858 3.566 -13.347 1.00 31.11
HETATM 2442 O HOH 310C 4.122 33.701 -33.523 1.00 31.11 3
HETATM 2443 O HOH 311A -0.522 10.773 6.218 1.00 28.79
HETATM 2444 O HOH 311B 0.523 40.908 -6.218 1.00 28.79 2
HETATM 2445 O HOH 312A 3.364 26.638 -23.982 1.00 32.09
HETATM 2446 O HOH 313A 1.914 29.077 -11.973 1.00 15.50
HETATM 2447 O HOH 314A 0.455 30.804 -14.767 1.00 26.19
HETATM 2448 O HOH 315A 3.770 8.910 6.739 1.00 28.05
HETATM 2449 O HOH 315C 2.210 39.045 -28.922 1.00 25.56 3
HETATM 2450 O HOH 316A 2.394 21.473 -5.857 1.00 9.43
HETATM 2451 O HOH 317A 4.457 13.917 -23.326 1.00 24.26
HETATM 2452 O HOH 317C 1.523 44.052 -23.544 1.00 27.95 3
HETATM 2453 O HOH 318A 4.105 20.727 -19.441 1.00 19.32
HETATM 2454 O HOH 319A 2.617 1.885 -3.953 1.00 1.17
HETATM 2455 O HOH 319B -2.617 32.020 3.953 1.00 31.17 2
HETATM 2456 O HOH 321A 2.627 13.790 -4.834 1.00 3.00
HETATM 2457 O HOH 322A 0.560 20.655 10.858 1.00 27.95
HETATM 2458 O HOH 323A 4.426 8.977 -15.442 1.00 21.73
HETATM 2459 O HOH 323C 1.553 39.112 -31.428 1.00 21.73 3
HETATM 2460 O HOH 324A 1.098 12.393 12.691 1.00 29.93
HETATM 2461 O HOH 324B -1.098 42.518 -12.691 1.00 29.93 2
HETATM 2462 O HOH 325A 1.747 24.438 9.458 1.00 32.84
HETATM 2463 O HOH 325D -1.747 -5.697 -9.458 1.00 32.84 4
HETATM 2464 O HOH 325A 2.844 9.673 6.739 1.00 28.05
HETATM 2465 O HOH 326B -2.844 39.808 -5.739 1.00 28.05 2
HETATM 2466 O HOH 327A 6.643 28.464 -23.573 1.00 23.62
HETATM 2467 O HOH 328A 4.118 12.104 4.426 1.00 19.28
.
.
HETATM 2746 O HOH 582B 3.719 34.882 -10.076 1.00 24.11 2
HETATM 2747 O HOH 583A -0.930 13.965 -10.604 1.00 11.57
HETATM 2748 O HOH 584A -1.652 5.220 -1.479 1.00 28.71
HETATM 2749 O HOH 584B 1.652 35.355 1.479 1.00 28.71 2
HETATM 2750 O HOH 585A 0.601 9.285 -17.763 1.00 11.26
HETATM 2751 O HOH 585C 5.505 39.420 -30.099 1.00 11.26 3
HETATM 2752 O HOH 586A -2.793 17.748 9.779 1.00 25.16
HETATM 2753 O HOH 586B 2.920 47.883 -10.771 1.00 25.16 2
HETATM 2754 O HOH 587A -1.353 27.720 -2.085 1.00 23.59
*DELETE,5CPAB.9
MASTER 83 79 1 8 8 32 0 6 2753 1 6 24
```

ORDER 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 (January 1984)
 - Sources of Visual Aids for Macromolecular Structure (January 1984)
 - Atomic Coordinate Entry Format Description for DATAPRTP and DATAPRFI (October 1983)
 - Current DATAPRTP Directory
 - Non-Standard Entries (Structure Factors) Format Description for NONST1TP and NONST1FI (April 1983)
 - Non-Standard Entries (Structure Factors) Format Description for NONST2TP and NONST2FI (January 1984)
 - 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>
-------------	------------------------	-------------

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 (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 (£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 _____

Method of Payment:

Cambridge: Cambridge prefers that no check is sent with order. Inclusion of purchase order is desirable but not mandatory.

Brookhaven: Brookhaven requires that either a check or written purchase order payable to Brookhaven National Laboratory be received before service is provided.

() check
() purchase order number _____

is () enclosed
() sent separately

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.