THE PROTEIN DATA BANK

NEWSLETTER

Number 7 December 1978

Brookhaven, Cambridge, Melbourne, Tokyo

The six months which have passed since our last newsletter have been a time of steady activity, with data acquisition, standardization and distribution continuing as usual. Current holdings are listed in Table 1. All but the most recent one of the thirteen coordinate sets for globular proteins which have been received since May are available for distribution, and two sets have already been superseded by newer data. In addition, much groundwork has been done preparatory to processing nine new polysaccharide structures and we expect that these entries will soon become available.

Four new computer programs written at Brookhaven, which will run against the Data Bank's distributable files, have been added to the list of programs (Table 2). We hope that they will be found generally useful. Prof. Y. Beppu of Nagoya University has kindly provided a molecular display program that was written with machine independence kept in mind and including features useful for macromolecules. This is now available. We are happy to accept depositions of suitable computer programs and anyone wishing to deposit code should contact us (at Brookhaven) regarding this. Another program, which is soon to become available, will perform an efficient search for intermolecular contacts. This type of search may be a major computing job for some structures, and the code in question could offer important savings.

For three years now the Protein Data Bank has been fortunate in having an Advisory Board consisting of Dr. D. R. Davies (NIH), Prof. K. R. Neet (Case Western Reserve), and Prof. F. M. Richards (Yale) to provide advice, support, and perspective for our activities. Prof. Richards is the first of this group to step down and we wish to express our warm appreciation of his work on behalf of the Bank. Prof. M. G. Rossmann of Purdue University has agreed to serve on our Board for a three-year term and we look forward to his joining us.

Because of factors beyond the control of our depositors, we have decided to award two prizes for the 100th coordinate entry rather than the single prize we announced in the May newsletter. Prof. S. Arnott of Purdue University has provided the depositions with (approximate) serial numbers 97-105 and so will receive the special prize of M. C. Escher's "Fantasy and Symmetry". The 100th distributable entry is the second of two coordinate sets for cytochrome C_{551} and we are happy to award Drs. R. J. Almassy and J. L. Chambers and Prof. R. E. Dickerson a gold-plated bent-wire model of their newest structure.

ANNOUNCEMENT

PLEASE POST

A staff position with the Protein Data Bank at Brookhaven will become available in early 1979. Persons with knowledge of macromolecular structure analysis and computer programming who wish to become involved in the solicitation and standardization of new data as well as in the writing of programs to extract useful information from the Bank are invited to apply. A limited amount of time would be available for independent research. Contact Dr. T. F. Koetzle, Department of Chemistry, Brookhaven National Laboratory, Upton, New York 11973. An equal opportunity employer, male/female.

A position on the Data Bank staff at Brookhaven will become available early next year since G.J.B. Williams has received a research grant and will be devoting most of his time to a new project. Persons wishing to learn more about the Data Bank opening should contact T. F. Koetzle (see the announcement included in this newsletter).

Table 3 lists the available files of structure factors and Tables 4 and 5 detail the items obtainable on tape and microfiche. Very few significant errors have been found in the Data Bank's files during the last six months and the few substantive corrections which have been applied are given in Table 6. As always the full list of corrections is available free of charge on microfiche, and this may be of interest to users who are not requesting new data tapes. Other items are also available on microfiche (Table 5) and individuals interested in obtaining the atomic coordinates, torsion angles, diagonal plots, bender angles, etc. on fiche should contact their proper distribution center. The last page of this newsletter may conveniently be used to make requests for magnetic tapes, microfiche or documentation.

Area	Address of Center	Name	Telephone
The Americas	Chemistry Department Brookhaven National Laboratory Upton, New York 11973 USA	F. C. Bernstein T. F. Koetzle G.J.B. Williams	516-345-4382 516-345-4384 516-345-4383
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, ENGLAND	O. Kennard S. Bellard	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	640251
Japan	Department of Chemistry Faculty of Sciences The University of Tokyo Bunkyo-ku, Tokyo, JAPAN	M. Tasumi	(03)812-2111

TABLE 1. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

01-DEC-78

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/ STATUS
1ACT	ACTINIDIN	E. BAKER	7/77
2ADK	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77 R
1AGA *AGAROSE		S. ARNOTT	5/78 P
1WGA	AGGLUTININ (WHEAT GERM)	C. S. WRIGHT	2/78 A
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C.-I.BRANDEN	8/76
2ADH	ALCOHOL DEHYDROGENASE (ORTHOPHEN)	C.-I.BRANDEN	8/76
1BCL	BACTERIOCHLOROPHYLL A-PROTEIN(CORE ONLY)	H. MATTHEWS	3/77
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	8/74
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	R. KRETSINGER	8/74
1CAP *CAPSULAR POLYSACCHARIDE (E. COLI K41)		S. ARNOTT	5/78 P
1CAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	6/76
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K. KANNAN	5/76
1CPA	CARBOXYPEPTIDASE A (BOVINE)	H. LIPSCOMB	2/73
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M. SCHMID, J. HERRIOTT	9/76 A
1CAR *CARRAGEENAN		S. ARNOTT	5/78 P
1C4S *CHONDROITIN-4-SULFATE		S. ARNOTT	5/78 P
2C4S *CHONDROITIN-4-SULFATE (CA SALT)		S. ARNOTT	5/78 P
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	1/75 R
3CHA	ALPHA-CHYMOTRYPSIN	A. TULINSKY	8/76
1GCH	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	2/77
1CHG	CHYMOTRYPSINOGEN	J. KRAUT, J. BIRKTOFT	3/75
2CNA	CONCANAVALIN A	REEKE, BECKER, EDELMAN	4/75
3CNA	CONCANAVALIN A	K. HARDMAN	9/76 R
2B5C	CYTOCHROME B5 (OXIDIZED)	F. S. MATHEWS	12/77 R
1CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	R. DICKERSON	9/76
2CYT	CYTOCHROME C (ALBACORE, REDUCED)	R. DICKERSON	9/76
1CYC	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	8/76
1C2C	CYTOCHROME C2	J. KRAUT	3/73
155C	CYTOCHROME C550	R. TIMKOVICH	8/76
251C *CYTOCHROME C551		R. DICKERSON	8/78 R
1EST	ELASTASE (PORCINE, TOSYL)	H. WATSON	5/76
1FDX	FERREDOXIN	ADMAN, SIEKER, JENSEN	8/76
3FXN	FLAVODOXIN (CLOSTRIDIUM MP,OXIDIZED)	M. LUDWIG	12/77 R
4FXN	FLAVODOXIN (CLOSTRIDIUM MP,SEMIQUINONE)	M. LUDWIG	12/77
1GCN	GLUCAGON	T. BLUNDELL	10/77
1PGI	GLUCOSE-6-PHOSPHATE ISOMERASE	H. MUIRHEAD	7/77
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M. ROSSMANN	7/75
1HRB *HEMERYTHRIN B		W. HENDRICKSON	6/76 A
2HHB	HEMOGLOBIN (HORSE, AQUO MET)	LADNER, HEIDNER, PERUTZ	2/77 R
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	11/73
1HHB	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	4/75
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	8/76
1LHB	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	3/73
2YHX	HEXOKINASE (YEAST) FORM B(II	STEITZ,ANDERSON,STENKAMP	3/78 R
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	4/75
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HEL(X)	S. ARNOTT	11/77
2HYA *HYALURONIC ACID (NA SALT, 4-FOLD HEL(X)		S. ARNOTT	5/78 P
3HYA *HYALURONIC ACID (NA SALT, 2-FOLD HEL(X)		S. ARNOTT	5/78 P
4HYA *HYALURONIC ACID (CA SALT, 3-FOLD HEL(X)		S. ARNOTT	5/78 P
1FAB	IMMUNOGLOBULIN FAB (NEW)	R. POLJAK	8/76
1MCG *IMMUNOGLOBULIN B-J MCG		SCHIFFER,EDMUNDSON ET AL.	5/78 A
1REI	IMMUNOGLOBULIN B-J FRAGMENT REI	O. EPP, R. HUBER	3/76
1RHE	IMMUNOGLOBULIN B-J FRAGMENT RHE	WANG, YOO, SAX	12/77 A
1KGA *KDPG ALDOLASE		A. TULINSKY	8/78 A
1KES *KERATAN SULFATE		S. ARNOTT	5/78 P
4LDH	LACTATE DEHYDROGENASE	W. EVENTOFF, M. ROSSMANN	4/77 R
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	11/74
1LDX *LACTATE DEHYDROGENASE (MOUSE TESTES)		M. MUSICK, M. ROSSMANN	9/78
1HBL *LEGHEMOGLOGIN		VAINSHTEIN,HARUTYUNYAN	11/78 N
1L2M	LYSOZYME (BACTERIOPHAGE T4)	B. MATTHEWS	3/77
1LYZ	LYSOZYME (HEN EGG-WHITE, SET H2)	R. DIAMOND, D. PHILLIPS	2/75
2LYZ	LYSOZYME (HEN EGG-WHITE, SET RS5D)	R. DIAMOND, D. PHILLIPS	2/75
3LYZ	LYSOZYME (HEN EGG-WHITE, SET RS6A)	R. DIAMOND, D. PHILLIPS	2/75
4LYZ	LYSOZYME (HEN EGG-WHITE, SET RS9A)	R. DIAMOND, D. PHILLIPS	2/75
5LYZ	LYSOZYME (HEN EGG-WHITE, SET RS12A)	R. DIAMOND, D. PHILLIPS	2/75
6LYZ	LYSOZYME (HEN EGG-WHITE, SET RS16)	R. DIAMOND, D. PHILLIPS	2/75
7LYZ	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	A. YONATH	5/77
8LYZ	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S. OATLEY	9/77
1MDH	MALATE DEHYDROGENASE	L. BANASZAK	6/76 A
1MLP *MUREIN LIPOPROTEIN (HYPOTHETICAL)		A. MCLACHLAN	8/78
1MBN	MYOGLOBIN (SPERM WHALE, MET)	H. WATSON	4/73
2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	9/76
3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	9/76
1MHR *MYOHEMERYTHRIN		H. HENDRICKSON	6/76 A
8PAP	PAPAIN (NATIVE)	J. DRENTH	11/76 R
1PAD	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)	J. DRENTH	11/76 R
2PAD	PAPAIN (CYS DERIV OF CYS-25)	J. DRENTH	11/76 R
3PAD	PAPAIN (OXIDIZED CYS-25)	J. DRENTH	11/76 R
4PAD	PAPAIN (TOS-LYS, CYS-25)	J. DRENTH	11/76 R
5PAD	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)	J. DRENTH	11/76 R
6PAD	PAPAIN (BZOXY-PHE-ALA, CYS-25)	J. DRENTH	11/76 R
1PEP *PEPSIN (PORCINE)		N. ANDREEVA ET AL.	7/78 A
1PGK	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON	5/76 A
2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, C. BLAKE	9/76 B
1PGM	PHOSPHOGLYCERATE MUTASE	CAMPBELL,WATSON,HODGSON	8/75 A
2PAB	PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, C. BLAKE	9/77 R
1RLX	RELAXIN(MODEL,CONFORMATION A,UNREFINED)	A. EVANS, A.C.T. NORTH	3/78
2RLX	RELAXIN(MODEL,CONFORMATION B,UNREFINED)	A. EVANS, A.C.T. NORTH	3/78
3RLX	RELAXIN(MODEL,CONFORMATION A,REFINED)	A. EVANS, A.C.T. NORTH	3/78
4RLX	RELAXIN(MODEL,CONFORMATION B,REFINED)	A. EVANS, A.C.T. NORTH	3/78
1RHD	RHODANESE	W. HOL	12/77
1RNS	RIBONUCLEASE S	H. WYCKOFF, F. RICHARDS	4/73
2RXN	RUBREDOXIN	L. JENSEN	1/75
1SNS	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN	4/73
1SGA *STREPTOMYCES GRISEUS PROTEINASE A		BRAYER,DELBAERE,JAMES	6/78
1SGB	STREPTOMYCES GRISEUS PROTEINASE B	M. JAMES	5/76 A
1SBT	SUBTILISIN BPN'	J. KRAUT	8/72
2SBT	SUBTILISIN NOVO	J. DRENTH	9/76
1SOD	SUPEROXIDE DISMUTASE	J. AND D. RICHARDSON	8/75 A
1TLN	THERMOLYSIN (UNREFINED)	B. MATTHEWS	4/75
2TLN	THERMOLYSIN (REFINED)	B. MATTHEWS	4/75
1SRX	THIOREDOXIN (E. COLI, OXIDIZED)	B.-O. SODERBERG	5/76 A
2TNA	TRANSFER RNA (YEAST, PHE)	M. SUNDARALINGAM	5/76
4TNA	TRANSFER RNA (YEAST, PHE)	JACK, LADNER, KLUG	4/78 R
6TNA *TRANSFER RNA (YEAST, PHE)		S.-H. KIM ET AL.	11/78 RN
1TIM	TRIOSE PHOSPHATE ISOMERASE	J. WILSON, D. PHILLIPS	9/76
1PTN	TRYPSIN (NATIVE, PH8)	FEHLHAMMER, BODE, SCHWAGER	1/77
2PTB	TRYPSIN(BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER, BODE, SCHWAGER	1/77 R
1PTC	TRYPSIN/TRYPSIN INHIBITOR COMPLEX	R. HUBER, W. BODE	11/76
3PTI	TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	11/76 R
3PTB	TRYPSIN (DIP INHIBITED)	J. CHAMBERS, R. STROUD	12/77 R

* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER (MAY/78)

STATUS CODES

BLANK	STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
N	NEW ENTRY WITH DEPOSITOR FOR APPROVAL
P	IN PREPARATION
R	REPLACES AN OUT-OF-DATE PARAMETER SET

TABLE 2. PROTEIN DATA BANK, AVAILABLE PROGRAMS

01-DEC-78

NAME	PURPOSE	AUTHOR(S)	REV DATE/ SUPPORTED
BENDER	*PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	11/78 YES
CONECT	*GENERATE FULL CONNECTIVITY	F.BERNSTEIN	10/78 YES
DGPLOT	*DIAGONAL PLOTS ON PRINTER	E.SWANSON,F.BERNSTEIN	10/78 YES
FISIPL	*PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	11/78 YES
NAMOD	*BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78 NO
PHIPSI	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	11/78 YES
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	5/78 YES

* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER

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

TABLE 3. PROTEIN DATA BANK, NON-STANDARD ENTRIES

01-DEC-78

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
RIACTSF	ACTINIDIN	E. BAKER	7/77 SF
CHYMOF	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	4/73 SF
RCARP04	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
RCARP05	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
RCYTB5D2	CYTOCHROME B5	F. S. MATHEWS	5/73 TA
R2B5CSF	CYTOCHROME B5	F. S. MATHEWS	12/77 SF
RTUNOX20	CYTOCHROME C (ALBACORE, OXIDIZED)	R. DICKERSON	5/76 SF
RTUNRO20	CYTOCHROME C (ALBACORE, REDUCED)	R. DICKERSON	5/76 SF
RCYC550I	CYTOCHROME C550	R. TIMKOVICH	4/76 SF
R151CSF	*CYTOCHROME C551	R. E. DICKERSON	8/78 SF
RGPD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M. ROSSMANN	8/75 SF
RHUMDEH02	HEMOGLOBIN (HUMAN,DEOXY)	M. PERUTZ, G. FERMI	5/75 SF
LAMPRY1	HEMOGLOBIN (LAMPREY)	HENDRICKSON,LOVE,KARLE	5/73 SF
RLDH06	LACTATE DEHYDROGENASE	M. ROSSMANN	8/75 SF
RLDH07	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	8/75 SF
RMETMYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76 SF
RDEMYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76 SF
RRUBY02	RUBREDOXIN	L. JENSEN	3/74 SF
TORSNAD1	TORSION ANGLES (11 PROTEINS)	T. WU, E. KABAT	5/73 TA

* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER (MAY/78)

CODES

SF	STRUCTURE FACTORS
TA	TORSION ANGLES

NOTE IN SOME CASES, MORE RECENT TORSION ANGLES THAN THOSE CONTAINED IN THE ABOVE ENTRIES MAY BE CALCULATED FROM THE APPROPRIATE ATOMIC COORDINATE ENTRIES LISTED IN TABLE 1.

TABLE 4. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MAGNETIC TAPE

01-DEC-78

CODE	ITEM
DATAPRTP	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 1,2)
NONSTDTP	ALL NON-STANDARD ENTRIES (TABLE 3)
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS
CONECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS
DGPLOTTP	DIAGONAL PLOTS (LINE PRINTER)
FISIPLTP	PHI/PSI PLOTS (LINE PRINTER)
PHIPSITP	LISTS OF PHI/PSI/OMEGA VALUES

EACH OF THESE ITEMS IS CONSIDERED TO COMPRISE ONE MAGNETIC TAPE

TABLE 5. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

01-DEC-78

CODE	ITEM	NO. OF FICHE	PRICE
DATAPRF1	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 1,2)	10	$37.50
NONSTDF1	ALL NON-STANDARD ENTRIES (TABLE 3)	11	$38.70
CORR03F1	LIST OF CORRECTIONS #3 (MAY-NOV 1978)	1	FREE
BENDERF1	PARAMETERS FOR BENT-WIRE MODELS	3	$29.10
CONECTF1	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	9	$36.30
DGPLOTF1	DIAGONAL PLOTS (LINE PRINTER)	4	$30.30
FISIPLF1	PHI/PSI PLOTS (LINE PRINTER)	1	$26.70
PHIPSIF1	LISTS OF PHI/PSI/OMEGA VALUES	4	$37.50

PRICES QUOTED ARE IN U.S. DOLLARS FOR DISTRIBUTIONS FROM BROOKHAVEN. REQUESTORS FROM OTHER CENTERS SHOULD INQUIRE FOR AVAILABILITY AND PRICES.

TABLE 6. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

01-DEC-78

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*IDENT,IFDHC
*INSERT,IFDHB.26
REMARK   7
REMARK   7 CORRECTION. CHANGE NAME OF ATOM OH OF RESIDUE ARG A 141
REMARK   7  TO OXT.  RENUMBER AND REORDER IT AND ADJACENT ATOMS TO
REMARK   7  ACHIEVE PROPER ORDER. 20-JUL-78.
*DELETE,IFDH.1140,1142
ATOM   1067  NH1 ARG A 141      -8.602   8.795  -4.282  1.00  0.00
ATOM   1068  NH2 ARG A 141     -10.097   7.962  -5.830  1.00  0.00
ATOM   1069  OXT ARG A 141      -8.973  13.984  -8.310  1.00  0.00
*DELETE,IFDHB.28
MASTER       42    0    2   15    0    0    0    9 2288    2   90   23

*IDENT,IHHBC
*INSERT,IHHBB.2
REMARK  11
REMARK  11 CORRECTION. FIX HELIX AH, BH RECORDS. 15-AUG-78.
*DELETE,IHHB.72
HELIX    8  AH THR A  118  SER A  138  1
*DELETE,IHHB.80
HELIX   16  BH THR B  123  HIS B  143  1
*DELETE,IHHBB.12
MASTER       68    0    2   16    0    0    0    9 2278    2   90   23

*IDENT,IHGAA
*INSERT,IHGA.38
REMARK   5
REMARK   5 CORRECTION. CORECT Y-COORDINATE OF ATOM 147. 24-OCT-78.
*DELETE,IHGA.230
ATOM    147  CA  CYS   147      19.000  -6.000  12.400  1.00  0.00
*DELETE,IHGA.248
MASTER       29    0    0    0    0    0    0   15  164    0    0   13

*IDENT,PHIPS12
*INSERT,PHIPS11.23
C
C     CORRECTION.  MAKE SURE THAT AN ANGLE OF -180 IS NEVER PRODUCED.
C     CHANGE IT TO 180.  ALSO ACCEPT HETATM RECORDS AS WELL AS ATOM
C     RECORDS.  10-NOV-78.
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*INSERT,PHIPS1.329
      DATA HETA/4HHETA/
*INSERT,PHIPS1.351
      IF (IDEN(REC(1),HETA,1).EQ.0) GO TO 30
*INSERT,PHIPS1.457
      IF (IPH(IENTER).EQ.-180) IPH(IENTER)=180
      IF (IPS(IENTER).EQ.-180) IPS(IENTER)=180
      IF (IOMEGA(IENTER).EQ.-180) IOMEGA(IENTER)=180
```

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 ATOMIC COORDINATE 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 60342500, 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 SEQUENCE NUMBER 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 '1MBNA' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK '1MBN' FOR SPERM-WHALE MYOGLOBIN, '1MBNB' 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.

ANNOUNCEMENT:

A special volume: Guide to the Literature 1935-76 (303 x 225 mm, 660 pp. + xxiii) has recently been published by the International Union of Crystallography and the Cambridge Crystallographic Data Centre. This volume represents a comprehensive key to the literature of structural chemistry and will be of interest to all scientists whose work involves molecular structures or interactions.

The "Guide" comprises a set of six indexes to the 15,933 organic, organometallic, and metal-complex structures published during the 41 year period covered by MSD Bibliographic Volumes 1-8. The indexes are:

- Compound Name Index (Organic): a permuted KWIC index ordered alphabetically by keyword. The most significant parts of each name are displayed with maximum retention of context. There are 21,238 index entries for 11,116 names.
- Compound Name Index (Organometallics and Metal Complexes): constructed as above but with the 12,897 index entries grouped under 54 metal-name sub-headings.
- Formula Index: conventional C,H-ordered listing.
- Permuted Formula Index: display of rarer elements using a permuted element-in-context layout. The 7,842 entries are grouped under 70 rare-element sub-headings.
- Author Index: 43,039 citations to 10,362 authors.
- Literature Index: covering 260 primary sources.

The volume provides bibliographic search facilities based on chemical names or name fragments, formulae, elements and authors names. The indexes yield entry numbers which key into the MSD Bibliographies 1-8, where complete information is listed, or into the Literature Index of the "Guide" for rapid retrieval of references.

The "Guide" is available from Bohn, Scheltema and Holkema Publishing Co., Emmalaan 27, Postbus 13079, Utrecht, The Netherlands and Polycrystal Book Services, P. O. Box 11567, Pittsburgh, PA. 15238, U.S.A. The cost (exclusive of postage) is 150 Netherland Guilders (approx. $66) with a 25% reduction for personal copies.

Volume 9 of the MSD bibliographic series is available for $45 (approx.) with a similar personal discount. Earlier volumes are available at much reduced prices and those interested should contact either "Polycrystal" or Bohn et. al.

REQUEST FORM

1. Name _____ Date _____

   Address _____ Telephone _____

   _____

   _____

   _____

2. Send the following information (please check):

   ( ) description of atomic coordinate entries (no charge)

   ( ) the magnetic tape items listed below (from Table 4)

   _____ _____ _____ _____ _____

   (Item "DATAPRTP" comprises all atomic coordinate sets and programs)

   ( ) the microfiche items listed below (from Table 5)

   _____ _____ _____ _____ _____

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

4. Tape format desired:

( ) 7 track	( ) 556 cpi	( ) BCD-7 track only	( ) Unlabelled (preferred)
( ) 9 track	( ) 800 cpi	( ) ASCII-9 track only	( ) Labelled, - User's label
	( ) 1600 cpi	( ) EBCDIC-9 track only	_____ Retained

NOTE: All current coordinate entries and programs can be written to one 2400' reel of magnetic tape for one unit charge (see over) if some space economies are achieved by blocking the records. Please indicate here the maximum block size permitted if this is less than 5120 characters (bytes)_____.

(Please complete reverse side)

REQUEST FORM

5. Charges

(i) For requests to Brookhaven

A. Data preparation (unit charge per magnetic tape) $_____

Employee of U.S. Department of Energy	$40.25	( )
Employee of other U.S. Federal Agency	$47.45	( )
All others	$51.00	( )

B. Magnetic Tape (charge per tape) $ 8.85 $_____
(please check if answer to 3 above was NO)

C. Postage (per magnetic tape) $_____

U.S. and Canada	$ 2.00	( )
Air Mail to Other Countries	$17.00	( )

D. Microfiche items (Price from Table 5) $_____

E. Total Charge $_____

F. Payment to the order of Brookhaven National Laboratory

by ( ) check is ( ) enclosed

( ) purchase order number _____ ( ) sent separately to the Protein Data Bank

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

(ii) For requests to Cambridge

A. Data preparation and postage (per user-supplied tape) ≠_____

Within United Kingdom	≠27.50	( )
Elsewhere	≠35.00	( )

B. Magnetic tape ≠ 8.00 ( )
(Please check if NO was checked on 3 above) ≠_____

C. Microfiche (please inquire for prices) ≠_____

D. Total ≠_____

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.