

THE PROTEIN DATA BANK  
NEWSLETTER

Number 9

July 1979

We are pleased to announce that Enrique Abola, presently of the University of Utah, will be joining the Brookhaven Protein Data Bank staff next month to fill the position formerly held by Graheme Williams. We wish to thank Graheme for his efforts on behalf of the Data Bank over the past four years. Graheme will be returning to full-time experimental research; fortunately, he is remaining at Brookhaven and will be available to provide his expertise on matters concerning the Data Bank when needed. Enrique Abola has extensive experience in protein crystallography, and we look forward to his arrival in August.

Thomas Koetzle and Frances Bernstein will be attending the Boston ACA Meeting August 12-17, where there will be a poster describing the Data Bank. We will be delighted to discuss the Data Bank with users and are especially interested in receiving suggestions for improvements and new services. Along this line a questionnaire has just been sent to our more recent Brookhaven customers. We wish to encourage recipients to complete and return this questionnaire.

At the Southeastern Macromolecular Structure Meeting held recently at Duke University, participants asked many questions about the Data Bank, and we therefore felt it would be useful to present a general overview of our services in this Newsletter. Also included are the usual Tables (1-5) describing current holdings and information available for distribution, Table 6 listing substantive corrections for the period Dec 78-July 79, and a newly revised request form.

#### Data Input

The Protein Data Bank collects and stores two classes of information: atomic coordinates and structure factor-phase data. Also available are a number of computer programs that operate on the atomic coordinate entries. All data should be sent to Brookhaven in machine-readable form, preferably magnetic tape. Contributed computer programs of general interest will be accepted for distribution, provided adequate machine-readable documentation accompanies the source code.

Atomic coordinate data are processed into the standard Data Bank format, and returned to depositors for checking and approval before entries are released for public distribution. Corrections are applied when errors become known and are documented in remarks carried at the head of each entry. Of course, the contents of an entire entry may be replaced by newer, more accurate data at any time. Early deposition is valuable: a number of fairly preliminary sets of C<sup>α</sup> coordinates have been contributed, and user demand for these has been quite high. The C<sup>α</sup> data sets generally are replaced by complete atomic coordinate information, when it becomes available.

Structure factor-phase data are stored in the format in which they are received. We urge contributors to include this information for native structures and heavy-atom derivatives as well. These primary crystallographic data should be preserved for possible future use, and the Data Bank has the mechanisms to carry out this vital archival function.

For mutual convenience, we have prepared a deposition form that we will gladly supply to all potential depositors. The Bank can also provide a magnetic tape for data transcription. In cases where depositors of atomic coordinate information have provided their own tapes, these are returned containing copies of the processed data entries.

Worldwide distribution for the Protein Data Bank is handled through four centers, as listed below. The request form included with this Newsletter may be used to order data from Brookhaven or Cambridge; users in Japan or Australia should contact their centers for detailed information.

### Data Distribution

From Brookhaven, data normally are distributed on magnetic tape or microfiche, as indicated in Tables 1 and 2 below. Requests for the standard data tape (DATAPRTP) usually are filled within a day or so unless new data are being added or corrections applied. It is simpler for us to send all current atomic coordinate entries and programs than to select a few entries, and the cost to the user is the same in any case. The other items in Tables 1 and 2 are requested less frequently and are generated as needed; this can cause a delay of up to one week. The latest available data are always sent, and the complete fiche of corrections are of interest only to people holding older data tapes.

### Charges

A revised schedule of charges for requests to Brookhaven is given in the request form. To ensure proper payment and prompt distribution, please use this current form. Data preparation charges for distributions on magnetic tape have risen slightly (from \$51.00 to \$55.20 per tape for non-U.S. Government users). The larger increase in charges for microfiche preparation (Table 2) reflects the fact that we have found fiche preparation to be quite time consuming.

In spite of the recent growth in our holdings and the number of users, the Protein Data Bank is making every effort to be responsive to individual users' needs. Please feel free to write or telephone us if you need something special, or if you have questions.

<u>Area</u>	<u>Address of Center</u>	<u>Name</u>	<u>Telephone</u>
The Americas	Chemistry Department	F. C. Bernstein	516-345-4382
	Brookhaven National Laboratory Upton, New York 11973 USA	T. F. Koetzle	516-345-4384
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, ENGLAND	O. Kennard S. Bellard	0223-66499
Australia	CSIRO Div. of Chemical Physics P. O. Box 160 Clayton, Victoria 31368 AUSTRALIA	B. J. Poppleton	
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, INFORMATION AVAILABLE ON MAGNETIC TAPE

CODE	ITEM
DATAPRT	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 3,4)
NONSTDP	ALL STRUCTURE FACTOR HOLDINGS (TABLE 5)
BENDERT	PARAMETERS FOR BENT-WIRE MODELS
CONNECT	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS
DGPLOT	DIAGONAL PLOTS (LINE PRINTER)
DSTNCTP	*CONNECTIVITY SPECIFICATIONS WITH DISTANCES
FIS1PLT	PHI/PSI PLOTS (LINE PRINTER)
PHI5IF1	LISTS OF PHI/PSI/OMEGA VALUES

\* NEW OR REPLACEMENT ENTRY SINCE DEC-78 NEWSLETTER

ITEM DSTNCTP REQUIRES TWO TAPES AT 800CPI, OTHER ITEMS COMPRISE ONE TAPE EACH

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	NO. OF FICHE	PRICE
DATAPRF	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 3,4)	12	\$69.96
NONSTDF	ALL STRUCTURE FACTOR HOLDINGS (TABLE 5)	11	\$68.73
CORR04F	*LIST OF CORRECTIONS NO. 4 (DEC/78-JUL/79)	1	FREE
BENDRF1	PARAMETERS FOR BENT-WIRE MODELS	2	\$57.66
CONNECTF	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	10	\$67.50
DGPLOTF	DIAGONAL PLOTS (LINE PRINTER)	4	\$60.12
DSTNCF1	*CONNECTIVITY SPECIFICATIONS WITH DISTANCES	20	\$79.80
FIS1PLF1	PHI/PSI PLOTS (LINE PRINTER)	1	\$56.43
PHI5IF1	LISTS OF PHI/PSI/OMEGA VALUES	5	\$61.35

\* NEW OR REPLACEMENT ENTRY SINCE DEC-78 NEWSLETTER

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

TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

NAME	PURPOSE	AUTHOR(S)	REV DATE/ SUPPORTED
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	1/79 YES
CONNECT	GENERATE CONNECTIVITY	F.BERNSTEIN	4/79 YES
DGPLOT	DIAGONAL PLOTS ON PRINTER	E.SHANSON,F.BERNSTEIN	3/79 YES
DSTNCE	*CALC DISTANCES FROM CONNECT RECORDS	F.BERNSTEIN	3/79 YES
FIS1PL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79 YES
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78 NO
PHI5I	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	2/79 YES
STEREO	*EXTRACT X,Y,Z FROM STEREO DIAGRAMS	M.ROSSMANN	6/79 NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	5/78 YES

\* NEW OR REPLACEMENT ENTRY SINCE DEC-78 NEWSLETTER

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

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
RIACTSF	ACTINININ	E.BAKER	7/77 SF
CHYMOF	ALPHA-CHYMOTRYPSIN (TOSYL)	D.BLOW	4/73 SF
RCARPO4	CALCIUM-BINDING PARVALBUMIN	R.KRETSINGER	2/74 SF
RCARPO5	CALCIUM-BINDING PARVALBUMIN	R.KRETSINGER	2/74 SF
R2B5CF	CYTOCHROME B5	F.S.MATHEWS	12/77 SF
RTUNOX201	CYTOCHROME C (ALBACORE, OXIDIZED)	R.DICKERSON	5/76 SF
RTUNRD201	CYTOCHROME C (ALBACORE, REDUCED)	R.DICKERSON	5/76 SF
RCY5501	CYTOCHROME C550	R.TIMKOVICH	4/76 SF
R151CF	CYTOCHROME C551	R.DICKERSON	8/78 SF
ROPD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTRIM)	M.ROSSMANN	9/75 SF
RHUMDCH02	HEMOGLOBIN (HUMAN, DEOXY)	M.PERUTZ,G.FERMI	5/75 SF
LAMPY1	HEMOGLOBIN (LAMPREY)	HENDRICKSON,LOVE,KARLE	5/73 SF
RLDH07	LACTATE DEHYDROGENASE	M.ROSSMANN	5/75 SF
RLDH08	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M.ROSSMANN	9/75 SF
RMEYHSF1	MYOGLOBIN (SPERM WHALE, MET)	T.TAKANO	6/76 SF
RDEHYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T.TAKANO	9/76 SF
RBU0Y02	RUBREDOXIN	L.JENSEN	3/74 SF

\* NEW OR REPLACEMENT ENTRY SINCE DEC-78 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/ STATUS
1ACT	ACTINININ	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.WRIGHT	8/76
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C.-I.BRANDEN	8/76
2ADH	ALCOHOL DEHYDROGENASE (ORTHOPHOS)	C.-I.BRANDEN	8/76
3ADH	*ALCOHOL DEHYDROGENASE (APO)	C.-I.BRANDEN	6/79 N
1ALP	*ALPHA LYTC PROTEASE	BRAYER,DELBAERE,JAMES	6/79
2BCL	*BACTERIOCHLOROPHYLL A-PROTEIN	B.MATTHEWS	1/79 RA
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 M41)	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)	W.LIFSCHOMB	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
1GCB	CHYMOTRYPSINOGEN	J.KRAUT,J.BIRKHOFF	3/75
2CNA	CONCANAVALIN A	G.REEKE,J.BECKER,G.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
1B5C	CYTOCHROME C550	R.TIMKOVICH	8/76
2B5C	CYTOCHROME C551	R.DICKERSON	8/78 R
1EST	ELASTASE (PORCINE, TOSYL)	H.WATSON	5/76
1ECD	*ERYTHROCUORIN (REDUCED, DEOXY)	W.STEIGEMANN,E.WEBER	3/79
1ECO	*ERYTHROCUORIN (CARBONMONOXIDE)	W.STEIGEMANN,E.WEBER	3/79
1ECN	*ERYTHROCUORIN (AQO, MET)	W.STEIGEMANN,E.WEBER	3/79
1ECM	*ERYTHROCUORIN (CYANO, MET)	W.STEIGEMANN,E.WEBER	2/79
1FDX	FERREDOXIN	E.ADMAN,L.SIEKER,L.JENSEN	6/76
3FXN	FLAVODOXIN (CLOSTRIDIUM MP, OXIDIZED)	M.LUDWIG	12/77 R
4FXN	FLAVODOXIN (CLOSTRIDIUM MP, SEMIQUINONE)	M.LUDWIG	12/77
1GCL	GLUCAGON	T.BLUNDELL	10/77
1PGI	GLUCOSE-6-PHOSPHATE ISOMERASE	H.MUIRHEAD	7/77
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTRIM)	M.ROSSMANN	7/76
1HRB	HEMERYTHRIN B (HUMAN, MET)	H.HENDRICKSON	6/76 A
1HMN	*HEMERYTHRIN (MET, AQUO)	R.STENKAMP ET AL.	1/79 A
2HMB	HEMOGLOBIN (HORSE, AQUO MET)	R.LADNER,HEIDNER,PERUTZ	2/77 R
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M.PERUTZ,G.FERMI	11/73
1HMB	HEMOGLOBIN (HUMAN, MET)	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 B111	STEITZ,ANDERSON,STENKAMP	3/78 R
1H1P	HIGH POTENTIAL HYPOHETICAL	S.ARNOTT	4/75
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S.ARNOTT	11/77
2HYA	HYALURONIC ACID (NA SALT, 4-FOLD HELIX)	S.ARNOTT	5/78 P
3HYA	HYALURONIC ACID (NA SALT, 2-FOLD HELIX)	S.ARNOTT	5/78 P
4HYA	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S.ARNOTT	5/78 P
2FAB	*IMMUNOGLOBULIN FAB NEW	R.DOLJAK	6/79 R
1MCG	IMMUNOGLOBULIN B-J	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	B.WANG,C.YOO,M.SAX	12/77 A
1KGA	KOPF ALDOLASE	A.TULINSKY	8/78 A
1KES	KERATAN SULFATE	S.ARNOTT	5/78 P
4LDH	LACTATE DEHYDROGENASE	M.EVENTOFF,M.ROSSMANN	4/77 R
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M.ROSSMANN	11/74
1LDK	LACTATE DEHYDROGENASE (HOUSE TESTES)	H.MUSICK,M.ROSSMANN	3/79
1HBL	LECHEMOGLOGIN	VAINSSTEIN,HARUTYUNYAN	1/78
1LZM	LYSOZYME (BACTERIOPHAGE T4)	B.MATTHEWS	3/77
1LYZ	LYSOZYME (HEN EGG-WHITE, SET W2)	R.DIAMOND,D.PHILLIPS	2/75
2LYZ	LYSOZYME (HEN EGG-WHITE, SET R55D)	R.DIAMOND,D.PHILLIPS	2/75
3LYZ	LYSOZYME (HEN EGG-WHITE, SET R56A)	R.DIAMOND,D.PHILLIPS	2/75
4LYZ	LYSOZYME (HEN EGG-WHITE, SET R59A)	R.DIAMOND,D.PHILLIPS	2/75
5LYZ	LYSOZYME (HEN EGG-WHITE, SET R512A)	R.DIAMOND,D.PHILLIPS	2/75
6LYZ	LYSOZYME (HEN EGG-WHITE, SET R516)	R.DIAMOND,D.PHILLIPS	2/75
7LYZ	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	A.YONATH	5/77
8LYZ	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S.OLATEY	9/77
1MDH	MALATE DEHYDROGENASE	L.BANASZAK	6/76 A
1MLP	MUREIN LIPOPROTEIN (HYPOTHETICAL)	A.MCLACHLAN	8/75
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
1MBS	MYOGLOBIN (SEAL, MET)	H.SCOLLUDU	3/79
1MHR	MYOHEMERYTHRIN	H.HENDRICKSON	6/76 A
6PAP	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
1PER	PEPSIN (PORCINE)	M.ANDREVA ET AL.	7/78 A
1PKK	PHOSPHOGLYCERATE KINASE (YEAST)	H.WATSON	5/76 A
2PKK	PHOSPHOGLYCERATE KINASE (HORSE)	P.EVANS,C.BLAKE	9/76 B
1PGM	PHOSPHOGLYCERATE MUTASE	CAMPBELL,WATSON,HODGSON	8/75 A
2PAB	PREALBUMIN (HUMAN, PLASMA)	S.OLATEY,C.BLAKE	9/77 R
1RLX	RELAXIN(MODEL, CONFORMATION A, UNREFINED)	A.EVANS,A.NORTH	3/78
2RLX	RELAXIN(MODEL, CONFORMATION B, UNREFINED)	A.EVANS,A.NORTH	3/78
3RLX	RELAXIN(MODEL, CONFORMATION A, REFINED)	A.EVANS,A.NORTH	3/78
4RLX	RELAXIN(MODEL, CONFORMATION B, REFINED)	A.EVANS,A.NORTH	3/78
1RHD	RHODANSE	H.HOL	12/77
2RSA	*RIBONUCLEASE A	A.WLODAHER	6/79
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
2SGB	*STREPTOMYCES GRISEUS PROTEASE B	DELBAERE,BRAYER,JAMES	6/79 R
1SBT	SUBTILISIN BPN	J.KRAUT	8/76
2SBT	SUBTILISIN NDQ	J.DRENTH	9/76
1SSI	*SUBTILISIN INHIBITOR (STREPTOMYCES)	Y.MITSUI ET AL.	1/79 A
1SOD	SUPEROXIDE DISMUTASE	J.RICHARDSON,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
4TNA	TRANSFER RNA (YEAST, PHE)	A.JACK,J.LADNER,A.KLUG	4/78 R
6TNA	TRANSFER RNA (YEAST, PHE)	S.-H.KIM ET AL.	11/78 R
6TNA	TRANSFER RNA (YEAST, PHE)	M.SUNDARANGAM	2/79 R
1TIP	TRIOSE PHOSPHATE ISOMERASE	H.HILSON,D.PHILLIPS	9/76
1PTN	TRYP SIN (NATIVE, PHB)	FEHLHAMMER,BODE,SCHWAGER	1/77
2PTB	TRYP SIN(BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER,BODE,SCHWAGER	1/77 R
1PTC	TRYP SIN/TRYP SIN INHIBITOR COMPLEX	R.HUBER,W.BODE	11/76
3PTI	TRYP SIN INHIBITOR (BOVINE, PANCREAS)	R.HUBER,J.DEISENHOFER	11/76 R
3PTP	TRYP SIN (DIP INHIBITED)	J.CHAMBERS,R.STROUD	12/77 R
1TGP	*TRYP SINOGEN/TRYP SIN INHIBITOR	W.BODE,P.SCHWAGER,R.HUBER	3/79
1TPI	*TRYP SINOGEN/TRYP SIN INHIBITOR/ILE-VAL	W.BODE,P.SCHWAGER,R.HUBER	3/79
1TPI	TRYP SINOGEN (MGSO4, WITHOUT CA)	BODE,FEHLHAMMER,HUBER	3/79
1TGB	*TRYP SINOGEN (WITH CA, FROM PEG)	BODE,FEHLHAMMER,HUBER	3/79

\* NEW OR REPLACEMENT ENTRY SINCE DEC-78 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 REPLACES AN OUT-OF-DATE PARAMETER SET

TABLE 6. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS  
20-JUL-79

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*IDENT,IMBNJ
*INSERT,IMBN1.2
REMARK 15
REMARK 15 CORRECTION. CORRECT ATOMIC NOMENCLATURE FOR 12 ATOMS IN
REMARK 15 HEME GROUP. 15-JAN-79.
*DELETE,IMBNE.21,24
HETATM 1236 C19 HEM 1 13.700 27.000 7.500 1.00 0.00
HETATM 1237 C28 HEM 1 13.100 25.800 8.100 1.00 0.00
HETATM 1238 C38 HEM 1 13.000 24.800 7.100 1.00 0.00
HETATM 1239 C48 HEM 1 13.600 25.400 5.900 1.00 0.00
*DELETE,IMBNE.28,32
HETATM 1244 C1C HEM 1 14.400 25.300 3.500 1.00 0.00
HETATM 1245 C2C HEM 1 14.500 24.600 2.300 1.00 0.00
HETATM 1246 C3C HEM 1 15.200 25.500 1.300 1.00 0.00
HETATM 1247 C4C HEM 1 15.400 26.700 2.100 1.00 0.00
*DELETE,IMBNE.37,40
HETATM 1252 C1D HEM 1 16.300 29.100 2.300 1.00 0.00
HETATM 1253 C2D HEM 1 17.000 30.200 1.700 1.00 0.00
HETATM 1254 C3D HEM 1 17.100 31.200 2.700 1.00 0.00
HETATM 1255 C4D HEM 1 16.400 30.600 3.600 1.00 0.00
*DELETE,IMBN1.5
MASTER 65 6 1 8 0 3 2 6 1260 1 46 12

*IDENT,BENDER1
*INSERT,BENDER.29
REMARK 12
REMARK 12 CORRECTION. DELETE BAD CARD AND REPLACE IT WITH THE CORRECT
REMARK 12 COMMENT CARD. 22-JAN-79.
*DELETE,BENDER.415
MASTER 4130

*IDENT,IHHD
*INSERT,IHHC.2
REMARK 12
REMARK 12 CORRECTION. FIX CONECT RECORDS. 05-MAR-79.
*DELETE,IHHD.5
CONECT 1814 1812 1813 2238
*DELETE,IHHD.2417
CONECT 2238 1814 2243 2254 2262
*DELETE,IHHC.5
MASTER 70 0 2 16 0 0 0 9 2278 2 90 23

*IDENT,IRHDC
*INSERT,IRHDB.17
REMARK 7
REMARK 7 CORRECTION. FIX CONECT RECORDS. 05-MAR-79.
*DELETE,IRHD.2441,2442
CONECT 1963 1962 2328
CONECT 2326 1963
*DELETE,IRHDB.18
MASTER 52 0 1 10 10 19 0 6 2326 1 2 23

*IDENT,IPTNC
*INSERT,IPTNB.58
REMARK 7
REMARK 7 CORRECTION. FIX CONECT RECORDS. 07-MAR-79.
*DELETE,IPTN.1782,1783
CONECT 397 395 1638
CONECT 421 420 1638
*DELETE,IPTN.1794
CONECT 1638 384 397 421 461
*DELETE,IPTNB.57
MASTER 57 4 1 3 0 0 0 6 1709 1 20 18

*IDENT,IHBLA
*INSERT,IHBL.149
REMARK 4
REMARK 4 CORRECTION. FIX CONECT RECORDS. 07-MAR-79.
*DELETE,IHBL.1409
CONECT 1177 1209 1221
*DELETE,IHBL.1452
CONECT 1221 1177 1220
*DELETE,IHBL.1453
MASTER 144 4 2 7 0 0 0 6 1222 1 46 12

*IDENT,ICYCE
*INSERT,ICYCD.27
REMARK 9
REMARK 9 CORRECTION. CORRECT Y-COORDINATE OF ATOM 173. 23-APR-79.
*DELETE,ICYC.217
ATOM 173 0 GLY 24 -27.186 -3.803 9.829 1.00 0.00
*DELETE,ICYCD.30
MASTER 46 0 1 5 0 3 0 9 839 1 48 8

*IDENT,IPTCC
*INSERT,IPTCB.5
REMARK 7
REMARK 7 CORRECTION. FIX NAMING OF ATOMS 2241,2246,2259,2264.
REMARK 7 25-APR-79.
*DELETE,IPTCB.160
HETATM 2241 0 HOH 567 19.898 82.629 5.944 1.00 0.00
*DELETE,IPTCB.165
HETATM 2246 02 HOH 571 -5.561 76.318 20.118 1.00 0.00
*DELETE,IPTCB.178
HETATM 2259 0 HOH 586 19.371 93.135 6.543 1.00 0.00 1
*DELETE,IPTCB.183
HETATM 2264 02 HOH 590 21.793 79.099 18.969 1.00 0.00
*DELETE,IPTCB.197
MASTER 98 9 0 4 2 0 0 6 2256 2 18 23

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*IDENT,FIS1PL1
*INSERT,FIS1PL.82
REMARK 7
REMARK 7 CORRECTION. FIX LABELLING OF PSI AXIS. 04-MAY-79.
*DELETE,FIS1PL.227
IND=185-51

*IDENT,2ADKC
*INSERT,2ADKB.72
REMARK 7
REMARK 7 CORRECTION. FIX HELIX RECORD AND INSERT MISSING ATOM NZ
REMARK 7 OF LYS 194 AS PER AUTHOR INSTRUCTIONS OF 20-APR-77.
REMARK 7 8-JUN-79.
*DELETE,2ADK.65
HELIX 4 H ARG 53 GLU 62 1
*INSERT,2ADK.1600
ATOM 1518 NZ LYS 194 49.500 18.600 54.600 1.00 0.00
*DELETE,2ADKB.73
MASTER 96 3 0 10 5 0 0 6 1519 1 0 15

*IDENT,ITGAA
*INSERT,ITGA.60
REMARK 7
REMARK 7 CORRECTION. FIX CONECT RECORD FOR ATOM 1569. 06-JUL-79.
*DELETE,ITGA.1864
CONECT 1569 859 1568
*DELETE,ITGA.1865
MASTER 49 4 1 3 0 0 0 6 1750 1 12 18

*IDENT,ITGBA
*INSERT,ITGB.60
REMARK 7
REMARK 7 CORRECTION. FIX CONECT RECORD FOR ATOM 1569. 06-JUL-79.
*DELETE,ITGB.1864
CONECT 1569 859 1568
*DELETE,ITGB.1865
MASTER 49 4 1 3 0 0 0 6 1750 1 12 18

*IDENT,ITGPA
*INSERT,ITGP.74
REMARK 8
REMARK 8 CORRECTION. FIX NAMING OF ATOMS 1814 AND 1815. FIX CONECT
REMARK 8 RECORD FOR ATOM 1569. 06-JUL-79.
*DELETE,ITGP.1861,1862
ATOM 1814 NH1 ARG 1 17 14.260 74.206 4.561 .94 1.45
ATOM 1815 NH2 ARG 1 17 12.805 72.451 4.912 .94 1.61
*DELETE,ITGP.2388
CONECT 1569 859 1568
*DELETE,ITGP.2395
MASTER 61 9 0 4 2 0 0 6 2246 1 18 23

*IDENT,ITPIA
*INSERT,ITPI.74
REMARK 8
REMARK 8 CORRECTION. FIX CONECT RECORD FOR ATOM 1569. 06-JUL-79.
*DELETE,ITPI.2398
CONECT 1569 859 1568
*DELETE,ITPI.2405
MASTER 60 9 0 4 2 0 0 6 2256 1 18 23

```

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 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 '\*IMBN1' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK 'IMBN' FOR SPERM-WHALE MYOGLOBIN, '\*IMBN2' 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.

Molecular Structures and Dimensions: The tenth classified bibliography of organic, organometallic and crystal structures prepared by the Cambridge Crystallographic Data Centre has just been published jointly with the International Union of Crystallography. The previous nine volumes covered the years 1935-1977 and the present volume provides references principally to structure analyses reported in literature during 1977 and 1978. Volume 10 contains 3018 references to 2945 distinct chemical compounds with 147 cross-reference entries. There are extensive indices. The price of the new volume is 100 Netherland Guilders (approx. \$45) with a 25% reduction for personal copies. Orders can be placed with: Bohn, Scheltema and Holkema Publishing Co., Geert Grootestraat 4, 7411 GS, Deventer, THE NETHERLANDS or with: Polycrystal Book Service, P. O. Box 11567, Pittsburgh, Pennsylvania 15238, U. S. A.

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 1)

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

( ) the microfiche items listed below (from Table 2)

\_\_\_\_\_

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. Federal Agency \$51.40 ( ) \_\_\_\_\_  
     All others \$55.20 ( ) \_\_\_\_\_
- 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 2) \$ \_\_\_\_\_
- 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 Charge £ \_\_\_\_\_

It is expected that the Protein Data Bank be acknowledged in publications which result from work making use of the Bank's services. In citing the Protein Data Bank in print, we suggest that a reference be included to 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, 535-42 (1977).

We would appreciate receiving reprints.