

We are glad to report that, in spite of the avalanche of data that the Protein Data Bank has been receiving, processing is nearly up-to-date and a total of 196 atomic coordinate data sets are presently available for distribution. Thus, although we are instituting a price increase, to \$181 (\$106) for a single magnetic tape, the unit cost remains very low at less than \$1 per coordinate entry.

In the near future, an advisory notice concerning compilation and dissemination of the material in the Protein Data Bank will appear on all Data Bank distributions. The notice will appear on each magnetic tape in machine readable form, or as text on each microfiche item or printed listing. The advisory notice provides information regarding the Federal Agencies that have supported the operation of the Protein Data Bank, as well as an indication that the goal of these Agencies is to have the information in the Data Bank disseminated as widely as possible to the scientific community. The notice concludes with the indication that the materials available from the Protein Data Bank cannot be offered for resale as commercial items by the recipients.

Brookhaven National Laboratory will be closed from December 23 to January 3 for the holidays. Any requests or data that arrive in that period will be processed in January. 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. 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

Supported by the U. S. National Science Foundation.

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

CODE	ITEM	NO. TAPES		AVAILABILITY			
		800	1600	US	UK	JA	AUS
DATAPRT	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	2	1	X	X	X	X
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	2	1	X	X	X	
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	2	1	X	X	X	
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	1	1	X			
BLDK11TP	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER					
CONNECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	X			
DSPLOTTP	DIAGONAL PLOTS (LINE PRINTER)	1	1	X			
D1HDRLTP	COMPLETE TORSION ANGLES	2	1	X			
DSTNCTTP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	2	1	X			
F1S1PLTP	PHI/PSI PLOTS (LINE PRINTER)	1	1	X			
PH1PS1TP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	X			

* NEW OR REPLACEMENT ENTRY SINCE JUL-82 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	NO. MICROFICHE		AVAILABILITY			
		800	1600	US	UK	JA	AUS
DATAPRF1	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)			X	X	X	
NONST1F1	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)			X	X	X	
NONST2F1	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)			X	X	X	
CORR10F1	LIST OF CORRECTIONS NO. 10 (JAN/82 - JUL/82)			X	X	X	X
BENDERF1	PARAMETERS FOR BENT-WIRE MODELS			X			
BLDK11F1	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER					
CONNECTF1	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS			X			
DGPL0TF1	DIAGONAL PLOTS (LINE PRINTER)			X			
D1HDRL1F1	COMPLETE TORSION ANGLES			X			
DSTNCF1	CONNECTIVITY SPECIFICATIONS WITH DISTANCES			X			
F1S1PL1F1	PHI/PSI PLOTS (LINE PRINTER)			X			
PH1PS11F1	LISTS OF PHI/PSI/OMEGA VALUES			X			

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TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

NAME	PURPOSE	AUTHOR(S)	18-OCT-82	
			REV DATE/ SUPPORTED	
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	4/82	YES
BLDKIT	MODEL BUILDER'S KIT	E.ABOLA	5/82	YES
CHIRAL	CHECK CHIRALITY	E.ABOLA	1/82	YES
CONNECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	8/82	YES
CONTC	INTERMOLECULAR CONTACTS	L.ANDREWS	9/82	NO
DGPL0T	DIAGONAL PLOTS ON PRINTER	E.SWANSON,F.BERNSTEIN	3/79	YES
D1HDRL	COMPLETE TORSION ANGLES	E.ABOLA	3/80	YES
DSTNCE	CALC. DISTANCES FROM CONECT RECORDS	F.BERNSTEIN	8/82	YES
F1S1PL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79	YES
LSM	COLOR-CODED ALPHA-CARBON MODELS	R.MATELA,R.FLETTERICK	3/82	NO
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78	NO
PH1PS1	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	2/79	YES
STEREO	EXTRACT X,Y,Z FROM STEREO DIAGRAMS	M.ROSSMANN	6/79	NO
TAPDIR	PRINT DIRECTORY OF TAPE CONTENTS	H.BERNSTEIN,F.BERNSTEIN	11/79	YES
THEOD	MEASURE COORDINATES WITH THEODOLITE	L.LEB10DA	1/82	NO
TORSRU	COMPLETE TORSION ANGLES	G.REEKE	10/79	NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	3/82	YES

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

TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

Table with columns: IDENT, MOLECULE, DEPOSITOR(S), DATE/STATUS, and protein names. Includes entries like 1AAPP ACID PROTEINASE (PENICILLIUM JANTHINELLUM), 1A9A AGAROSE, 1A9B L-ARABINOSIDE-BINDING PROTEIN, etc.

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STATUS CODES

- BLANK STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A ALPHA CRYSTAL ATOMS ONLY
B BACKBONE ONLY
N NEW ENTRY AWAITING APPROVAL BY DEPOSITOR
P IN PREPARATION
R REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

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

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
R1ACTSF	ACTINININ	E. BAKER	7/77 SF
CHYMOF	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	4/73 SF
RCARRP04	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
RCARRP05	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
R2B5CSF	CYTOCHROME B5	F. S. MATHEWS	12/77 SF
R3CYTSF	CYTOCHROME C (ALBACORE, OXIDIZED)	T. TAKANO, R. DICKERSON	7/80 SF
R4CYTSF	CYTOCHROME C (ALBACORE, REDUCED)	T. TAKANO, R. DICKERSON	7/80 SF
RCYCS501	CYTOCHROME C550	R. TIMKOVICH	4/76 SF
R1ZNASF	DNA (Z', CGCG, HIGH-SALT, SYNTHETIC)	H. DREW, R. DICKERSON	1/81 SF
R1BNASF	DNA (B, CCGCAATTCGCG, SYNTHETIC, 290 DEG K)	H. DREW, R. DICKERSON	1/81 SF
R9PD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	8/75 SF
R2GPOSF	APO-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79 SF
R1HMSF	HEMERYTHRIN (MET, HYDROXO)	R. STENKAMP	6/81 SF
R2HBSF	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER, HEIDNER, PERUTZ	6/80 SF
R1FDHSF	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	6/80 SF
RHUMDEH02	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	5/75 SF
LAMPYR1	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
RLSDHSF	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U. GRAU, M. ROSSMANN	1/81 SF
R1LZHSF	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	C. BLAKE, D. RICE	6/81 SF
R2LZHSF	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)	C. BLAKE, D. RICE	6/81 SF
RME1MYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76 SF
RDE1MYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76 SF
RRUB102	RUBREDOXIN	L. JENSEN	3/74 SF
R4TNSF	TRANSFER RNA (YEAST, PHE)	A. JACK, J. LADNER, A. KLUG	6/80 SF

CODES
SF STRUCTURE FACTORS

TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
OEAP	ACID PROTEINASE (ENDOTHA PARASITICA)		
OACX	*ACTINOXANTHIN (ACTINOMYCES GLOBISPORUS)		
OADC	ADH-NADH-DIMETHYLSULFOXIDE COMPLEX		
OAF1	AFERRITIN (HORSE)		
OMA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE		
ORNB	*BARNASE (BACILLUS AMYLOLIQUEFACIENS)		
OICB	CALCIUM-BINDING PROTEIN (MINOR A FORM, BOVINE)		
OCTS	CITRATE SYNTHASE (PIG)		
OCN2	CONCAVALIN A (DEMETALLIZED)		
OCRO	CRO REPRESSOR		
OGCR	GAMMA-CRYSTALLIN II (CALF)		
OCYP	CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)		
OCY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)		
OSCI	CYTOCHROME C555 (CHLOROBIVUM THIOSULFOPHILUM)		
OC3A	DES-ARG77-C3A ANAPHYLATOXIN		
OCDF	*DIHYDROFLATE REDUCTASE (CHICKEN LIVER)		
OANB	*DNA (GGTATACC)		
OANB	*DNA (GG+UA+UACC)		
OCZ	ELASTASE COMPLEX (PIG)		
OET1	ELONGATION FACTOR TU COMPLEX (E. COLI)		
OEBX	ERABUTOXIN B		
OFX1	FLAVODOXIN (DESULFOVIBRIO VULGARIS)		
OFX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)		
OGAP	CATABOLITE GENE ACTIVATOR PROTEIN		
OGP1	GLUTATHIONE PEROXIDASE (BOVINE)		
OGD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)		
OHMG	HEMAGGLUTININ		
ODCH	*HEMOGLOBIN (COBALT, DEOXY)		
OHBG	HEMOGLOBIN (GLYCERA DIBRANCHIATA)		
OPHH	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)		
OAU1	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU		
OROY	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (V-MONOMER, KAPPA) ROY		
OMCP	IMMUNOGLOBULIN FAB (KAPPA) MCP603		
OFB4	IMMUNOGLOBULIN FAB (LAMBDA) KOL		
OIG1	IMMUNOGLOBULIN G1 (KAPPA) DOB		
OIG2	IMMUNOGLOBULIN G1 (LAMBDA) KOL		
OINI	INSULIN (PORCINE)		
OIN2	INSULIN (PORCINE)		
OGF1	INSULIN-LIKE GROWTH FACTOR I (HUMAN)		
OGF2	INSULIN-LIKE GROWTH FACTOR II (HUMAN)		
OLZ1	LYSOZYME (HUMAN)		
OLZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)		
OLZ6	LYSOZYME (STREPTOMYCES ERYTHRAEUS)		
OCF	L7/L12 (E. COLI, C-TERMINUS)		
OMBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)		
OMB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)		
OSN3	SCORPION NEUROTOXIN VARIANT-3		
OPFK	PHOSPHOFRUCTOKINASE (BACILLUS STEAROTHERMOPHILUS)		
OBP1	PHOSPHOLIPASE A2 (PORCINE)		
OPP2	PHOSPHOLIPASE A2 (RATTLESNAKE)		
OPPA	PHOSPHORYLASE A (RABBIT)		
OPB1	PHOSPHORYLASE B (RABBIT)		
ORX5	RELAXIN (PORCINE, MODEL)		
ORSA	RIBONUCLEASE A (BOVINE)		
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)		
OTR1	METHIONYL TRANSFER RNA SYNTHETASE		
OGN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)		
OUTG	UTEROGLOBIN (RABBIT)		
OTMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)		
OTBV	VIRUS (TOMATO BUSHY STUNT)		

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

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
R351CSF	CYTOCHROME C551 (OXIDIZED)	T. TAKANO, R. DICKERSON	9/81 SF
R451CSF	CYTOCHROME C551 (REDUCED)	T. TAKANO, R. DICKERSON	9/81 SF
R1ANASF	DNA (A, D-1000-CCGG)SPACE GROUP P 43 21 2	B. CONNER, R. DICKERSON	6/82 SF
R1ANAP2	DNA (A, D-1000-CCGG)SPACE GROUP P 21	B. CONNER, R. DICKERSON	6/82 SF
R2BNASF	DNA (B, CCGCAATTCGCG, SYNTHETIC, 16 DEG K)	H. DREW, R. DICKERSON	11/81 SF
R3BNASF	DNA (B, 9-BR-CGCGAATTCGCG, 20 DEG C)	KOPKA, FRATINI, DICKERSON/82 SF	
R4BNASF	DNA (B, 9-BR-CGCGAATTCGCG, 7 DEG C)	KOPKA, FRATINI, DICKERSON/82 SF	
R2INS5F	INSULIN (BOVINE, 2-ZINC)DES-PHE B1	C. REYNOLDS, G. DODSON	5/82 SF
R1LH1SF	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH1SF	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH2SF	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH2SF	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH3SF	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH3SF	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH4SF	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH4SF	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH5SF	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH5SF	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH6SF	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH6SF	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH7SF	LEGHEMOGLOBIN (FERRO) /NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH7SF	LEGHEMOGLOBIN (FERRO) /NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LYMSF	*LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	HOGLE, RAO, SUNDARALINGAM/82 SF	
R1ML1SF	MELITTIN	TERWILLIGER, EISENBERG	8/81 SF
R1OV0SF	OVOMUCOID FRAGMENT	E. PAPAMOKOS, R. HUBER	1/82 SF
R2BP2SF	PROPHOSPHOLIPASE A2 (BOVINE)	D. J. KOSTER, HOLBRENTH	9/81 SF
R1R3SF	RIBONUCLEASE	BORKAKOTI, MOSS, PALMER	6/82 SF
R4RSASF	*RIBONUCLEASE A (XRAY)	A. WLODAWER	6/82 SF
R4RSASFN	*RIBONUCLEASE A (NEUTRON)	A. WLODAWER	6/82 SF
R3TLNSF	THERMOLYSIN (NATIVE)	B. MATTHEWS, M. HOLMES	2/82 SF
R2PTNSF	TRYPSIN (ORTHORHOMBIC, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81 SF
R1TPOSF	*TRYPSIN (ORTHORHOMBIC)	BODE, WALTER, HUBER	9/82 SF
R3PTNSF	TRYPSIN (TRIGONAL, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81 SF
R3PTBSF	*TRYPSIN (BENZAMIDINE INHIBITED)	BODE, SCHWAGER, WALTER	9/82 SF
R1TTPSF	*TRYPSIN/P-AMIDINO-PHENYL-PHYRUVATE	WALTER, BODE, HUBER	9/82 SF
R4PT1SF	*TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	9/82 SF
R2PTCSF	*TRYPSIN/TRYPSIN INHIBITOR COMPLEX	R. HUBER, J. DEISENHOFER	9/82 SF
R1TPASF	*TRYPSIN (ANHYDRO)/TRYPSIN INHIBITOR	HUBER, BODE, DEISENHOFER	9/82 SF
R2TGASF	TRYPSINOGEN (2.4M MGSO4)	J. WALTER, R. HUBER	10/81 SF
R1TGC5F	TRYPSINOGEN (.5 CH3OH, .5 HOH)	J. WALTER, R. HUBER	10/81 SF
R1TGT5F	TRYPSINOGEN (1.73 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81 SF
R2TGT5F	TRYPSINOGEN (1.03 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81 SF
R2TGPSF	*TRYPSINOGEN/TRYPSIN INHIBITOR	R. HUBER ET AL.	9/82 SF
R3TPTSF	*TRYPSINOGEN/TRYPSIN INHIBITOR/ILE-VAL	R. HUBER ET AL.	9/82 SF
R2TPTSF	TRYPSINOGEN/PTI (ILE-VAL (MERCURATED))	J. WALTER, R. HUBER	10/81 SF
R1TGS5F	*TRYPSINOGEN/PTI	R. HUBER ET AL.	9/82 SF

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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. 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) _____

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