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THE EXAFS DATABASE: PROPOSED SPECIFICATION

by

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1. Introduction

Daresbury Laboratory provides central support for the computing needs of various research projects at the SRS. EXAFS is one of the most active ones. Data reduction and analysis needs are covered by a number of programmed utilities that form part of the SRSPL [1]. In addition a database of reduced EXAFS spectra or data files needed by analysis programs has been formed.

2. Reduced data Database

The database will contain EXAFS datasets that may have been collected or analysed anywhere in the world. Each dataset will include spectral coordinates after instrumental corrections, details of sample and experimental conditions and other information supplied by authors of publications where the analysis and interpretation is described. The dataset format is described in Appendix I.

The need for an international databank has arisen from the nature of the work carried out in this field, i.e., comparison with model compounds whose structural parameters are well established by other techniques or of compounds related to the one under investigation (finger-printing approach). There may also be a need for re-analysing the raw/reduced data using more sophisticated analysis procedures.

It was proposed [2] and generally accepted by the EXAFS community that Daresbury Laboratory provides an international service for contribution and exchange of data files. It is hoped that the assistance of other international SR sites will provide national collection and distribution points for the databank. It is proposed that each of these centres receives a machine readable copy of the databank and associated reference listings on a regular basis in return for which they act as a collecting point for datasets to be forwarded to Daresbury. Local access to the databank will then be controlled by the individual sites.

The database system that has been implemented on the Daresbury AS/7000 computer uses the RAPPORT database management system purchased from Logica Ltd. It is used in Daresbury to manage other databases as well, such as the SRS raw data database [3] and the Computer Grant Monitoring system [4]. RAPPORT provides a set of FORTRAN callable data management routines, used in the cataloguing program, and an Interactive Query Language which has been used to set up on-line search commands for the databank. Examples are given in Appendix II.

The FAMULUS suite of programs [5] has been used to provide facilities for producing reference listings and indices to these reference listings. In particular author indices, keyword in context and keyword out of context indices are available. Examples are given in Appendix III.

The Database Management System allows selected information from the datasets to be stored in a manner which allows efficient on-line or off-line retrieval, report generation, and searches on key fields identifying the data such as atom type and edge, experiment type, author etc. Searching more than a very few datasets for this information would be a costly excercise on the computer if a sophisticated storage and retrieval system had not been used. Utilities are provided for inserting new entries or dispatching data in machine readable form on request.

3. Atomic wavefunctions, Crystal structures and Phaseshifts

Clementi wavefunctions [6-7] for neutral and excited atoms are available in machine readable form for all elements from Lithium to Uranium. The excited atom wavefunctions are modelled using the wavefunction of the neutral atom one place higher in the periodic table but with a hole in the 1s electron shell.

Crystal structure datasets for all metals and many other elements and compounds are also available. These datasets assign closed-packed structures to metals, diamond/zincblende to covalent element compounds and NaCl and CaF2 structures to most others. All structures use classical metallic, covalent or ionic radii as the muffin-tin radii.

The atomic wavefunction and crystal structure datasets have been used to compute the phaseshifts of several systems using MUFPOT [1]. The naming convention is described in detail in Appendix IV. On-line access by Daresbury users is described by SRSPL command EXDBS [1]. Magnetic tape copies of these files are available on request.

Acknowledgments

The atomic wavefunction, crystal structure and phaseshift datasets were prepared by J.Weir and K.Caskell under the supervision of Dr G.N.Greaves. We would also like to thank Dr S.S.Hasnain for his cooperation in designing the reduced data Database.

References

[1] E.PANTOS "The SRS Program Library", Int.Conf. X-ray & VUV Instr., Hamburg, Aug. 1982. Daresbury Preprint DL/SCI/P346E.

[2] E.PANTOS and G.D.FIRTH "Exafs Database and Program Library", Int.Conf. on EXAFS and Near Edge Structure, Frascati, Sept. 1982.

[3] J.SEGAR and M.GOUGH, "The SRS raw data Database", Daresbury Internal Report, in preparation.

[4] E.A.BAILEY, G.D.FIRTH and C.M.JEFFCOCK, "Grant Monitoring System - User's Guide", Daresbury Internal Report DL/CSE/TM 19, (May 1982).

[5] G.D.FIRTH, "FAMULUS User Guide", Daresbury Internal Report DL/CSE/TM 20, (May 1982).

[6] E.CLEMENTI and C.ROETTI, "Atomic Data and Nuclear Data Tables", 14 (1974) 177.

[7] A.D.McLEAN and R.S.McLEAN, "Atomic Data and Nuclear Data Tables", 26 (1981) 197.

Appendix 1 - The EXAFS Database. Dataset Format.

It is proposed that each dataset contributed to the databank should have the format outlined below. EXAFS users are requested to submit their suggestions for additions/enhancements as soon as possible so that they can be considered before publication of the finalised version of the format definition (Daresbury Technical Memorandum, currently in preparation.)

All data should be in card image format with the first records of the dataset being header records describing the dataset. The header record section will be followed by the actual data. The following header records are currently envisaged and they should be entered in the order given below. The TEMPERATURE and COMMENT records are optional but all other information should be supplied.

```
SAMPLE
AUTHORS
REFERENCE
MACHINE
MONOCHROMATOR
ATOM
EDGE
MODE
TEMPERATURE
COMMENTS
DATA
```

Header records will be separated from data records by a DATA card (mandatory). The above header keywords will be separated from the text associated with them by a colon (:). Text for any keyword may be continued over more than one line by leaving the first character of the continuation line blank, a maximum of three lines being permitted for each keyword.

The following conventions should be adopted when entering data

1) The SAMPLE card should be filled in such a way that the first 40 characters form a brief description of the system, separated from any fuller description by a slash (/) character. This is to aid on-line information retrieval.

e.g.

```
SAMPLE : CA3(PO4)2 / BETA-TRICALCIUM PHOSPHATE
```

2) The AUTHORS card should be entered in the format

```
AUTHORS : SURNAME,INITIALS ; SURNAME,INITIALS ; ....
```

e.g.

```
AUTHORS : SMITH, RS ; JONES, AP ; BROWN, O
```

3) The REFERENCE card should be given in the format

REFERENCE : JOURNAL ABBREVIATION, VXX NOXX PART/DATE (YEAR) PX-X

e.g.

REFERENCE : PROC ROY SOC, V369 NO8 (1973) P58-59

Journal abbreviations should be taken from a list which will be given in the Daresbury technical memorandum currently in preparation.

In cases of unpublished data the contributing author's affiliation should be given instead.

4) The MACHINE card should have the format

MACHINE : MMMMM E : EEE I : III

Where MMMMM is the machine name (i.e., ACO, ADONE, DORIS, NSLS, SRS, SSRL, etc) , EEE is the machine energy in GEV and III is the machine current in milliamps. The E and I fields are optional. A list of acceptable machine name abbreviations will be published.

e.g.

MACHINE : SRS E : 1.7 GEV I : 90 MA

5) ATOM type and EDGE type are indicated by atomic symbol (capitals).

e.g.

ATOM : FE
EDGE : K

6) MODE may be one of the following

TRAN : transmission
FLOU : flourescence
ELEC : electron yield

when entering the mode only the first 4 characters will be placed in the RAPPORT database, so it is essential that the entry starts with one of the above.

e.g.

MODE : TRANSMISSION

EXAFS related data, e.g., interferometric measurements of f' and f'', may also be contributed. The MODE classification will be decided by the database administrator if it does not correspond to one of the above mentioned three mode types.

7) The DATA card may contain descriptive text of the coordinate type.

e.g.

DATA : ENERGY VS ABSORPTION

8) The coordinate values follow in columns of numbers in integer, F or E format separated by at least one space.

The following example shows the header records and some data records for a sample dataset.

```
SAMPLE : HUMAN DEOXYHAEMOGLOBIN / 15MMOL SOLN PREPARED FROM RED
 CELL LYSATE BY PRESSURE DIALYSIS FOLLOWED BY DEOXYGENATION AND
 ADDITION OF NEUTRAL NA2S2O4.
AUTHORS : PERUTZ,MF ; HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
REFERENCE : NATURE, V295 (1982) P535
ATOM : FE
EDGE : K
MODE : FLUORESCENCE LIF ANALYSER
MACHINE: SPEAR  E: 3.4    I: 50MA
MONOCHROMATOR : SI 220
COMMENT : AVERAGE OF FIVE SPECTRA 3 AT 10K ONE EACH AT 44K AND 110K
DATA : COLUMN 1 ENERGY, COLUMN 2 AVERAGED FLUORESCENCE
  0.7053480E+04  0.2013828E+05
  0.7055309E+04  0.2040415E+05
  0.7057148E+04  0.2041654E+05
  0.7058988E+04  0.2073329E+05
  0.7060828E+04  0.2069356E+05
  0.7062672E+04  0.2090060E+05
  0.7064512E+04  0.2098775E+05
  0.7066352E+04  0.2118981E+05
  ..............  ..............
  ..............  ..............
```

These datasets will be distibuted on magnetic tape as card image files in the same format as submitted datasets. Tapes will be written in EBCDIC or ASCII as requested at 800 bpi, 1600 bpi or 6250 bpi.

The preferred medium for input is EBCDIC coded, no labels, 1600 bpi magnetic tape. However tapes in any of the formats mentioned above or punched paper tape, cards and RT-11 formatted single-sided single-density 8" floppy disks will also be accepted.

It is suggested that once national collecting and distribution centres have been established, correspondence and requests are forwarded to Daresbury by them rather than from user-to-Daresbury and vice-versa. The Daresbury database administrator is Dr S.S.Hasnain.

Appendix II - Examples of Online Retrievals.

RAPPORT provides a set of FORTRAN callable data management routines, used in the cataloguing program, and an Interactive Query Language (IQL) which has been used to set up online search commands for the databank. Examples of RAPPORT data management commands are : SEARCH to search for records meeting given criteria, ORDER to sort records which match SEARCH conditions to a required order, INSERT to add new records to the database, UPDATE to allow modification of existing entries and DELETE to remove records from the database.

The fields stored in the RAPPORT database are :

CATALOG NUMBER
SAMPLE
AUTHOR
ATOM
EDGE
NODE
DATE OF ENTRY

Only the above fields may be used in specifying interactive search conditions. However, full header details for records meeting these conditions may be displayed.

The following commands are available at present

ASSIST - Online help information

AFIND - Give summary details of entries associated with an author

ASHOW - Give full details of entries associated with an author

ESHOW - List full details of a dataset

CFIND - Give summary details of records meeting a selection criteria

CSHOW - Give full details of records meeting a selection criteria

More commands will be added at a later stage.

A set of examples is given below based on a test database of 8 files .

```
+exquery
-
-RAPPORT 1.01 COPYRIGHT LOGICA LTD; RELEASED    MARCH-1980
-* IS BACKUP REQUIRED (Y/N)
+n
-
-
-*************************************************************************
-*                                                                       *
-*                              THE                                      *
-*                                                                       *
-*                        ======================                         *
-*                        "      RAPPORT       "                         *
-*                        ======================                         *
-*                        " INTERACTIVE  QUERY "                         *
-*                        ======================                         *
-*                        "      FACILITY      "                         *
-*                        ======================                         *
-*                                                                       *
-*                                                                       *
-*************************************************************************
-
-* PLEASE SUBMIT YOUR COMMANDS.
-:
+assist
-
-
-------------------------------------------------------------------------
-
-
-     THE FOLLOWING COMMANDS ARE AVAILABLE -
-
-     1. AFIND NAME - DISPLAYS SUMMARY OF AUTHORS ENTRIES
-
-     2. ASHOW NAME - DISPLAYS DETAILS OF AUTHORS ENTRIES
-
-     3. ESHOW CATNO - DISPLAY DETAILS OF CATALOG ENTRY
-
-     4. CFIND FIELD,VALUE - DISPLAY SUMMARY OF SELECTED ENTRIES
-
-     5. CSHOW FIELD,VALUE - DISPLAY DETAILS OF SELECTED ENTRIES
-
-
-     EXAMPLES
-
-     AFIND JONES
-
-     ASHOW SMITH
-
-     ESHOW 75
-
-     CFIND ATOM,"FE"
-
-     CSHOW EDGE,"K"
-
-
------------------------- END OF EXECUTION ------------------------
```

```
-:
+afind hasnain
-
------------------------------------------------------------------------
-
-AUTHOR HASNAIN IS ASSOCIATED WITH THE ENTRIES BELOW
-   ENTRY NO  ATOM  EDGE  MODE  SYSTEM
-          8  CA    K     TRAN  HORATITE
-          7  CA    K     TRAN  BRUSHITE CAHPO4.2H2O
-          6  CA    K     TRAN  HYDROXY APATITE CA5OH(PO4)3
-          5  CA    K     TRAN  MILK CA PHOSPHATE GEL
-          4  CA    K     TRAN  CALCIUM TETRAHYDROGEN DIORTHOPHOSPATE
-          3  CA    K     TRAN  CA3(PO4)2
-          2  FE    K     TRAN  FE(2+)(T PIV PP)-(2-MEIM).ETOH
-          1  FE    K     FLUO  HUMAN DEOXYHAEMOGLOBIN
-
---------------------------- END OF EXECUTION ----------------------------
-
-:
+eshow duke
-
------------------------------------------------------------------------
-
- SEARCH FOR ENTRIES BELONGING TO AUTHOR DUKE
-
-ENTRY           2
-
-SAMPLE : FE(2+)(T PIV PP)-(2-MEIM).ETOH / 2 METHYLIMIDAZOLE-MESO-
-        TETRA O-PIVALAMIDO PHENYL PORPHI-NATOIRON(II) ETHANOL
-AUTHORS : PERUTZ,MF ; HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
-REFERENCE : NATURE, V295 (1982) P535
-MACHINE : SPEAR  E : 3.4  I : 40 MA
-MONOCHROMATOR : SI 220
-ATOM : FE
-EDGE : K
-MODE : TRANSMISSION
-TEMPERATURE : 100K
-COMMENT : PICKET FENCE COMPLEX
-     ------------------------------------------------
-
-ENTRY           1
-
-SAMPLE : HUMAN DEOXYHAEMOGLOBIN / 15MMOL SOLN PREPARED FROM RED
-  CELL LYSATE BY PRESSURE DIALYSIS FOLLOWED BY DEOXYGENATION AND
-  ADDITION OF NEUTRAL NA2S2O4.
-AUTHORS : PERUTZ,MF ; HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
-REFERENCE : NATURE, V295 (1982) P535
-MACHINE : SPEAR  E : 3.4  I : 40 MA
-MONOCHROMATOR : SI 220
-ATOM : FE
-EDGE : K
-MODE : FLOURESCENCE LIF ANALYSER
-COMMENT : AVERAGE OF FIVE SPECTRA 3 AT 10K ONE EACH AT 44K AND 110K
-     ------------------------------------------------
-
---------------------------- END OF EXECUTION ----------------------------
-
-:
+eshow 4
-
-
------------------------------------------------------------------------
-
-ENTRY 4
-SAMPLE : CALCIUM TETRAHYDROGEN DIORTHOPHOSPHATE / CA(H2PO4)2 H2O
-AUTHORS : HOLT,C ; HASNAIN,SS ; HUKINS,DWL
-MACHINE : SRS 1.7 GEV 90 MA
-MONOCHROMATOR : SI 111 CHANNEL CUT
-ATOM : CA
-EDGE : K
-MODE : TRANSMISSION
-TEMPERATURE : 300K
-
--------------------------- END OF EXECUTION ----------------------------
-
-:
+eshow atom,'fe'
-
------------------------------------------------------------------------
-
-SEARCH FOR ENTRIES WHERE ATOM='FE'
-
-ENTRY           2
-
-SAMPLE : FE(2+)(T PIV PP)-(2-MEIM).ETOH / 2 METHYLIMIDAZOLE-MESO-
-        TETRA O-PIVALAMIDO PHENYL PORPHI-NATOIRON(II) ETHANOL
-AUTHORS : PERUTZ,MF ; HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
-REFERENCE : NATURE, V295 (1982) P535
-MACHINE : SPEAR  E : 3.4  I : 40 MA
-MONOCHROMATOR : SI 220
-ATOM : FE
-EDGE : K
-MODE : TRANSMISSION
-TEMPERATURE : 100K
-COMMENT : PICKET FENCE COMPLEX
-
-ENTRY           1
-
-SAMPLE : HUMAN DEOXYHAEMOGLOBIN / 15MMOL SOLN PREPARED FROM RED
-  CELL LYSATE BY PRESSURE DIALYSIS FOLLOWED BY DEOXYGENATION AND
-  ADDITION OF NEUTRAL NA2S2O4.
-AUTHORS : PERUTZ,MF ; HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
-REFERENCE : NATURE, V295 (1982) P535
-MACHINE: SPEAR  E: 3.4    I: 50MA
-MONOCHROMATOR : SI 220
-ATOM : FE
-EDGE : K
-: FLUORESCENCE MODE  LIF ANALYSER
-COMMENT : AVERAGE OF FIVE SPECTRA 3 AT 10K ONE EACH AT 44K AND 110K
-
--------------------------- END OF EXECUTION ----------------------------
-
-:
+abandon
-
---------------- INTERACTIVE QUERY SESSION TERMINATED.----------------
```

Appendix III - Examples of reference listings and reports.

FAMULUS is an information storage and retrieval system which was originally developed at the Pacific South West Forest and Range Experimental Station (California) of the U.S. Department of Agriculture in 1969. It was adapted and further developed at University College, London, and then implemented on the Rutherford Laboratory IBM 360/195 computers from where the version mounted on the NAS AS/7000 at Daresbury was obtained.

FAMULUS offers various information retrieval facilities, such as sorting, indexing, searching and catalogue production.

The following commands are available to produce reference listings and indices, and to generate reports.

EXINDX - produce an index.
EXKWIC - keyword in context index.
EXKWOC - keyword out of context index.
EXREF - print a reference listing.
EXSORA - sorted print of selected fields.
EXSRCH - search for records meeting condition(s).

Examples of output produced by the commands are given below :

EXINDX submits a batch job in which the FAMULUS INDEX program produces an index to the database. The sample output below is an author index to database entry number.

EXAFS DBS 10/08/82

DUKE,PJ 1, 2

HAHN,JE 1, 2

HASNAIN,SS 1, 2, 3, 4, 5, 6, 7, 8

HOLT,C 3, 4, 5, 6, 7, 8

HUKINS,DWL 3, 4, 5, 6, 7, 8

PERUTZ,MF 1, 2

SESSLER,JL 1, 2

F I N I S H E D

EXKWIC submits a batch job which uses the FAMULUS KWIC program to produce a KWIC (Key Word In Context) index to the database. EXKWIC has been used to produce a KWIC index to the words APATITE, BRUSHITE, CA, MILK, MONATITE and PHOSPHATE from the SAMPLE card in the example below.

EXAFS DBS 10/08/82

6 HYDROXY APATITE CA5OH(PO4)3

7 BRUSHITE CAHPO4.2H2O

5 MILK CA PHOSPHATE GEL

5 MILK CA PHOSPHATE GEL

8 MONATITE

3 CA3(PO4)2 / BETA-TRICALCIUM PHOSPHATE

5 MILK CA PHOSPHATE GEL

EXKWOC submits a batch job to produce a KWOC (Key Word Out of Context) index to the database. A KWOC may be produced from any field or combination of fields in the database. The EXKWOC command uses two of the FAMULUS programs, KEY and INDEX and in the example below has been used to produce a KWOC index for all significant words in the SAMPLE card i.e. words like OF, THE, etc have been specifically omitted.

```
EXAFS DBS                                10/08/82


APATITE              6
BETA-TRICALCIUM      3
BRUSHITE             7
CA                   5
CAHPO4               7
CALCIUM              4
CA5OH                6
CELL                 1
DEOXYHAEMOGLOBIN     1
DIALYSIS             1
DIORTHOPHOSPHATE     4
ETHANOL              2
HUMAN                1
HYDROXY              6
H2PO4                4
LYSATE               1
MILK                 5
MONATITE             8
NATOIRON             2
NEUTRAL              1
O-PIVALAMIDO         2
PHENYL               2
PHOSPHATE            3, 5
PORPHI-              2
```

EXREF submits a batch job which produces a print of all or part of the database using the FAMULUS GALLEY program. The main use of the command is to produce a reference listing of all entries in the database. The entries are printed out in dataset reference number order. In the example below the database fields for entry numbers 6-8 are printed.

```
EXAFS DBS                                10/08/82

 6 AUTH  HOLT,C ; HASNAIN,SS ; HUKINS,DWL
   REFE  BIOCHEM. BIOPHYS. ACTA (1982). IN PRESS.
   SAMP  HYDROXY APATITE CA5OH(PO4)3
   MACH  SRS  E : 1.7 GEV  I : 90 MA
   MONO  SI 111 CHANNEL CUT
   MODE  TRANSMISSION
   EDGE  K
   ATOM  CA
   TEMP  300K

 7 AUTH  HOLT,C ; HASNAIN,SS ; HUKINS,DWL
   REFE  BIOCHEM. BIOPHYS. ACTA (1982). IN PRESS.
   SAMP  BRUSHITE CAHPO4.2H2O
   MACH  SRS  E : 1.7 GEV  I : 90 MA
   MONO  SI 111 CHANNEL CUT
   MODE  TRANSMISSION
   EDGE  K
   ATOM  CA
   TEMP  300K

 8 AUTH  HOLT,C ; HASNAIN,SS ; HUKINS,DWL
   REFE  BIOCHEM. BIOPHYS. ACTA (1982). IN PRESS.
   SAMP  MONATITE
   MACH  SRS  E : 1.7 GEV  I : 90 MA
   MONO  SI 111 CHANNEL CUT
   MODE  TRANSMISSION
   EDGE  K
   ATOM  CA
   TEMP  300K
```

EXSOCA submits a batch job which produces a sorted print of the database. In the example below the output has been ordered on the ATOM field and AUTHOR and SAMPLE information has been printed.

```
EXAFS DBS                                10/08/82

CA

    HOLT,C ; HASNAIN,SS ; HUKINS,DWL
            BRUSHITE CAHPO4.2H2O

    HOLT,C ; HASNAIN,SS ; HUKINS,DWL
            CALCIUM TETRAHYDROGEN DIORTHOPHOSPHATE / CA(H2PO4)2 H2O

    HOLT,C ; HASNAIN,SS ; HUKINS,DWL
            CA3(PO4)2 / BETA-TRICALCIUM PHOSPHATE

    HOLT,C ; HASNAIN,SS ; HUKINS,DWL
            HYDROXY APATITE CA5OH(PO4)3

    HOLT,C ; HASNAIN,SS ; HUKINS,DWL
            MONATITE

    HOLT,C ; HASNAIN,SS ; HUKINS,DWL
            MILK CA PHOSPHATE GEL

FE

    PERUTZ,MF ; HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
            HUMAN DEOXYHAEMOGLOBIN / 15MMOL SOLN PREPARED FROM RED
            CELL LYSATE BY PRESSURE DIALYSIS FOLLOWED BY DEOXYGENATION AND
            ADDITION OF NEUTRAL NA2S2O4.

    PERUTZ,MF  ;  HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
            FE(2+)(T PIV PP)-(2-MEIM).ETOH / 2 METHYLIMIDAZOLE-MESO-
            TETRA O-PIVALAMIDO PHENYL PORPHI-NATOIRON(II) ETHANOL
```

EXSRCH submits a batch job which will cause the database to be searched for any entries which meet the criteria specified. In the example given the AUTHOR field has been searched for those entries associated with the name PERUTZ.

```
INPUT CARD.../FIELDS/(AUTH)
INPUT CARD.../SEARCH/PERUTZ

EXAFS DBS                        10/08/82

1.  PERUTZ,MF ; HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
    NATURE, V295 (1982) P535
    HUMAN DEOXYHAEMOGLOBIN / 15MMOL SOLN PREPARED FROM RED
    CELL LYSATE BY PRESSURE DIALYSIS FOLLOWED BY DEOXYGENATION AND
    ADDITION OF NEUTRAL NA2S2O4.
    AVERAGE OF FIVE SPECTRA 3 AT 10K ONE EACH AT 44K AND 110K
    SPEAR E: 3.4 I: 50MA   SI 220
    FLUORESCENCE LIF ANALYSER

2.  PERUTZ,MF ; HASNAIN,SS ; DUKE,PJ ; SESSLER,JL ; HAHN,JE
    NATURE, V295 (1982) P535
    FE(2+)(T PIV PP)-(2-MEIM).ETOH / 2 METHYLIMIDAZOLE-MESO-
    TETRA O-PIVALAMIDO PHENYL PORPHI-NATOIRON(II) ETHANOL
    SPEAR E : 3.4 I : 40 MA   SI 220
    TRANSMISSION   K   FE   100K


2 CITATIONS SATISFY THE SEARCH REQUEST.

8 CITATIONS WERE SEARCHED.
```

Appendix IV - The MUFPOT databank.

1) Atomic Wavefunctions used by MUFPOT.

The neutral atom wavefunction datasets are labelled AWxx.DATA, where xx is the usual chemical symbol of the element. For example, the wavefunctions for Sulphur will be AWS.DATA and those for Scandium will be AWSC.DATA .

The excited atom wavefunction datasets are labelled AWxxH.data, where xx is the chemical symbol of the element with the electron vacancy. For example, the excited form of Oxygen will be represented by Fluorine with a hole which is in AWFH.DATA The excited form of Niobium will be in AWNBH.DATA

Users wishing to adapt these files for L edges should change the occupancy of the 1s shell from 0.5 to 1.0,and change the 2p occupancy from 1.0 to 0.833333.

However experience has shown that in most cases this makes little difference to the calculated phaseshifts for the excited atom.

All wavefunction data are titled, and in the format used by the MUFPOT program.

2) Crystal structures used by MUFPOT.

These exist for all the structures listed in the table of phaseshifts (TABLE I).

The data files are named XTxx.DATA, where xx is the usual chemical symbol for the element or compound.

For example, the Magnesium metal structure is in the dataset XTMG.DATA and Magnesium Fluorite structure as XTMGF2.DATA

Most compounds are listed in two forms as, AB and BA.

For instance, XTNACL has Na as the excited atom whilst XTCLNA has Cl as the excited atom.

The only exceptions to the naming conventions are:
a) Niobium metal which is in XTNB.METAL.DATA
b) Nitrogen Boron structure which is in XTNB.NITRIDE.DATA

3) Phaseshift files used by EXAFS and EXINT:

Many sets of phaseshifts have been computed (see Table I). They are stored as partioned datasets with one section for each set of phaseshifts.

They are named PHPDS.xxl.DATA, where xx is the usual chemical symbol for the element or compound. The chemical symbol is the identifier for the structure and bonding. For example:
The phaseshifts for Strontium metal are in the dataset PHPDS.SR1.DATA

The phaseshifts for Germanium are in the dataset PHPDS.GE1.DATA

These datasets are partitioned with separate members for the phaseshifts for an excited atom and one or more near neighbour atoms. The partitions in the phaseshift files are named in accordance with the wavefunctions used to produce them. In the case of Germanium the wave functions used were for Germanium (AWGE), and Arsenic with a hole (AWASH). Hence the dataset PHPDS.GE1.DATA will be partioned into:
PHPDS.GE1.DATA(PHASH) and PHPDS.GE1.DATA(PHGE).

The phaseshifts for Germanium Dioxide will be found in the dataset PHPDS.GEO21.DATA and this will have three partitions:

PHPDS.GEO21.DATA(PHASH)
PHPDS.GEO21.DATA(PHGE)
PHPDS.GEO21.DATA(PHO)

The dataset PHPDS.GEO21.DATA gives phaseshifts for this structure with Germanium as the excited atom. For many of the structures on the databank there is a companion dataset which gives phaseshifts for the same structure but with the second atom as the excited atom. Thus there is a dataset PHPDS.O2GE1.DATA which contains phaseshifts with Oxygen as the excited atom. This is partitioned into three sections:

PHPDS.O2GE1.DATA(PHNH)
PHPDS.O2GE1.DATA(PHO)
PHPDS.O2GE1.DATA(PHGE)

There are only two exceptions to these naming conventions:
a) The phaseshifts for Niobium metal are in PHPDS.NB1.METAL.DATA
b) The phaseshifts for Nitrogen Boron structure are in PHPDS.NB1.NITRIDE.DATA

No systematical attempt has been made to check the phaseshifts against experiment. However previous experience has shown that they are suitable for EXAFS analysis, and that they can be transferred to structures other than those for which they were calculated, provided that the local chemistry is similar.

TABLE I. Computed phaseshifts on databank showing structure used.

INamel	Element	FCC	BCC	NaCl	ZnS	IDiamond	SiO2	CaF2
Ac	Actinium	ACI						
Ag	Silver	AGI						
Al	Aluminium	ALI			ALPI			
Ar	Argon	ARI						
As	Arsenic				aSGAI			
Au	Gold	AUI						
B	Boron				BNI			
Ba	Barium	BAI						
Be	Beryllium	BEI			BEOI			BEF2I
Bi	Bismuth		BII					
Br	Bromine			BRKI				
C	Carbon					CI		
Ca	Calcium	CAI		CASI	CASEI			CABR2I
								CACL2I
								CAF2I
Ce	Cerium	CEI						
Cl	Chlorine			CLNAI				
Cr	Chromium		CRI					
Cs	Cesium	CSI						
Co	Cobalt	COI						
Cu	Copper	CUI						
Dy	Dysprosium	DYI						
Er	Erbium	ERI						
Eu	Europium		EUI					
F	Fluorine			FLII				
Fe	Iron		FEI					
Ga	Gallium				GAASI			
Gd	Gadolinium	GDI						
Ge	Germanium					CEI	GEO2I	
							GESE2I	
							GES2I	
							GETE2I	
Hf	Hafnium	HFI						
Hg	Mercury		HGI					
Ho	Holmium	HOI						
I	Iodine			IRBI				
In	Indium						INSBI	
Ir	Irridium	IRI						
K	Potassium		KI	KBRI				
Kr	Krypton	KRI						
La	Lanthanum	LAI						
Li	Lithium		LII	LIFI				
Lu	Lutecium	LUI						
Mg	Magnesium	MGI		MGSI				
Mn	Manganese	MNI		MNSEI				
				MNSI				
Mo	Molybdenum		MOI					
N	Nitrogen						INBI.NITRIDE	
Na	Sodium		NAI	NACLI				
Nb	Niobium		INDI.METAL					
Nd	Neodymium	NDI						
Ne	Neon	NEI						
Ni	Nickel	NII						
O	Oxygen			OCAI		OBEI		O2CEI
Os	Osmium	OSI						
P	Phosphorous						PALI	
Pa	Protoactinium		Pal					
Pb	Lead	PBI						
Pd	Palladium	PDI						
Pm	Promethium	PMI						
Po	Polonium		POI					
Pr	Praseodymium	PRI						
Pt	Platinum	PTI						

Ra	Radium		RA						
Rb	Rubidium		RB	RBI					
Re	Rhenium	RE							
Rh	Rhodium	RH							
Ru	Ruthenium	RU							
S	Sulphur			SCA				SZGB	
				SIG					
Sb	Antimony					SBIN			
Sc	Scandium	SC							
Se	Selenium			SECA				SE2GE	
				SEHN					
Si	Silicon						SI	SIO2	
Sm	Samarium	SM							
Sn	Tin						SN		
Sr	Strontium	SR		SRTE				SRCL2	
				SRS				SRF2	
Ta	Tantalum	TA							
Tc	Technecium	TC							
Te	Tellurium			TECA				TE2GE	
				TESR					
Th	Thorium	TH							
Ti	Titanium	TI							
Tl	Thallium	TL							
Tm	Thulium	TM							
V	Vanadium		V						
W	Tungsten		W						
Xe	Xenon	XE							
Y	Yttrium	Y							
Yb	Ytterbium	YB							
Zn	Zinc	ZN				ZNS			
Zr	Zirconium	ZR		ZRS					