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IAEA CONSULTANTS' MEETING ON
"ATOMIC DATA BASE AND FUSION APPLICATIONS INTERFACE"

Vienna, 9-13 May 1988

SUMMARY REPORT

Prepared by R.K. Janev

September 1988

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

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Abstract

The Summary Report of the IAEA Consultants' Meeting on the "Atomic Data Base and Fusion Applications Interface" held at the IAEA Headquarters in Vienna on May 9-13, 1988, is provided. The Report contains a brief review of the meeting proceedings, and the reports of the Working Groups on the A+M dictionary (labelling/indexing system) and on the data storage and exchange system. The conclusions and recommendations of the meeting are also summarized.

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Table of Contents

1. <u>Summary of the Meeting</u>	1
1.1. Introduction	1
1.2. Meeting Proceedings	1
1.3. Results of the Meeting	2
2. <u>Reports of the Working Groups</u>	3
2.1. Report of the Working Group on the Atomic and Molecular Data Base and Data Exchange Dictionary ..	3
2.2. Report of the Working Group on the Atomic and Molecular Data Exchange Format and Interactive System	10
3. <u>Meeting Conclusions and Recommendations</u>	14

Appendices

Appendix A: List of Participants	15
Appendix B: Meeting Agenda	17
Appendix C: ALADDIN	20
Appendix D: Labelling for ALADDIN Data Entries	52

1. SUMMARY OF THE MEETING

1.1. Introduction

The principal role of the IAEA Atomic and Molecular (A+M) Data Unit in the Agency's Fusion Programme is to create, in close collaboration with national Atomic Data Centres for Fusion and fusion laboratories, an international base of recommended A+M data for use in fusion research. This data base should be structured and formatted in such a way that data exchange between the IAEA A+M data bank, national data centres and fusion laboratories can be effectuated in a straightforward, computer-readable and format-compatible manner. While the body of existing A+M recommended data for fusion stored at the IAEA and national data centres is already considerably large and is growing rapidly, the lack of an adequate, internationally agreed upon data exchange system continues to prevent the easy incorporation of these data into fusion application codes and the over-all interaction between the evaluated data producers and users.

The main goal of the Consultants' Meeting on "Atomic Data Base and Fusion Applications Interface", organized by the IAEA Atomic and Molecular Data Unit (IAEA-AMDU), was to establish and accept such a data storage, exchange and interface system. About twenty experts from the major fusion laboratories in the world, all national A+M data centres and from the IAEA Nuclear Data Section attended the meeting (see Appendix A, List of participants). A brief account of the discussions during the Meeting and its main results are given in the rest of this section.

1.2. Meeting Proceedings

The work of the meeting proceeded in four plenary sessions and in two working groups. The sessions of the meeting were (see Appendix B: Meeting Agenda)

- 1) Atomic and molecular data requirements and uses in current fusion research,
- 2) Current data centre A+M data evaluation activities and data formatting practices,
- 3) Data exchange files and interactive systems (in fusion laboratories),
- 4) The structure and format of the IAEA A+M data base and exchange system.

The A+M data requirements in current fusion research associated with the large-tokamak experiments and the design of next-step fusion reactors were reviewed by H.W. Drawin, K. Behringer and D. Reiter. These requirements were contrasted with the existing A+M data bases and was found that a significant amount of important A+M data is still lacking to meet the needs in plasma modelling and diagnostics. In the discussions of K. Behringer and D. Reiter the question of the most appropriate data formats for interfacing large modelling and diagnostic codes was also addressed. The data bases and formatting practices in the national data centres were described by W.L. Wiese, H. Tawara, J.G. Hughes, K. Katsonis, Y. Nakai, E. Menapace, at JET by H.P. Summers, and at the IAEA AMDU by R.K. Janev and J.J. Smith. A number of these data bases have already been interfaced with some fusion application codes (at JET, Bologna, JAERI), or include subroutines for further data processing (Belfast, Nagoya).

The data storage, exchange and interactive systems, existing in major fusion laboratories, and their interfaces to fusion application codes were described in a series of presentations by R. Hulse (Princeton PPL), H.P. Summers (JET) and T. Hirayama (JT-60, JAERI). It was found that the levels of generality, exchangeability and completeness of these systems differ considerably from each other, as well as the amount, quality and formats of the incorporated atomic data. In the general discussion following these presentations an attempt was made to define the structure and the features of a general, multipurpose A+M data base and data exchange system which would be relatively easily interfaced to different fusion application codes, conformal with a broad range of computer facilities, and with the atomic data centre evaluation, storage and exchange possibilities. The existing commercial systems were found to be an unsatisfactory option in this respect.

It was found that the Princeton PPL system ALADDIN, developed by R. Hulse, basically satisfies all the above mentioned criteria and represents a good base, both from a conceptual and practical point of view, for the IAEA A+M data storage and exchange system.

The meeting participants then split into two working groups to discuss in more detail the data exchange format and interactive system, and the associated labelling/indexing system (data dictionaries), and to formulate recommendations along these lines. The Working Group Reports are given in the next Section of this Summary Report.

1.3. Results of the Meeting

The main result of the Meeting is the adoption of a unique A+M data storage and exchange system to be used in future by the atomic data producers (atomic data centres) and atomic data users in fusion applications. This system is ALADDIN, the structure and features of which are described in detail in Appendix C. Although the system is open to further developments, the consensus of the Meeting was to start its implementation into the A+M data storage and exchange practices immediately. The Meeting participants made commitments to introduce ALADDIN into their A+M data bases and to include ALADDIN interfaces to their fusion application codes.

Another important result of the Meeting is the adoption of a standard labelling/indexing system for the A+M data and processes. This system, together with a number of other conventions is given in the Report of the Working Group on A+M Data Base and Data Exchange Dictionary (see the next Section).

The implementation of ALADDIN into a A+M data base by using the adopted Reaction Dictionary and standardized conventions is illustrated in Appendix D. This Appendix has been prepared by R.A. Phaneuf.

2. REPORTS OF THE WORKING GROUPS

2.1. REPORT OF THE WORKING GROUP ON ATOMIC AND MOLECULAR DATA BASE AND DATA EXCHANGE DICTIONARY

H. Tawara (Chairman), H.B. Gilbody, H.-W. Drawin, K. Katsonis,
R.K. Janev, Y. Nakai, and W.L. Wiese

1. Introduction

The task of this Working Group was to propose a classification scheme of A+M collision processes of relevance to magnetic fusion research, suggest a labelling (indexing) system for identification of different types of collision processes, individual reactions and types of data, and to define a set of conventions for the reactants and reaction products involved in a particular reaction. In performing this task, the Working Group was guided by the idea of practical functionality of the classification and labelling system (e.g., fusion relevance, data availability, minimum required labels for unique identification of a reaction), but also tended to retain a certain degree of generality and completeness in view of the anticipated future developments of the A+M data storage and exchange system. An effort was made to separate these two aspects in the report.

2. Process Labels

The process labels serve to identify a particular reaction and describe the physical content of the data. They followed a logically organized process/reaction classification scheme and their number should be sufficient to uniquely identify any reaction data set stored in the A+M data base. For purpose of a computer data search, they should appear in an ordered sequence. The recommended set of process labels is given in Table 1.

Table 1. Categorization and labelling of collision processes

-
1. Class of collision (see Table 2)
 - (*)2. Type of collision (collision process) (see Table 3)
 - (*)3a. Chemical symbol of projectile
 - (*)3b. Charge state of projectile
 - (#*)3c. Quantum state of projectile
 - (*)4a. Chemical symbol of target
 - (*)4b. Charge state of target
 - (**)4c. Quantum state of target
 - (collision)
 - (#*)5a. Chemical symbol of projectile product
 - (#*)5b. Charge state of projectile product
 - (#*)5c. Quantum state of projectile product
 - (**)6a. Chemical symbol of target product
 - (**)6b. Charge state of target product
 - (**)6c. Quantum state of target product
 7. Other reaction product (if any), specified by their chemical symbol, charge state, and quantum state, when necessary.
-

- Notes: (1) The labels marked by (*) are mandatory. Other labels should be added when necessary to specify a particular reaction channel, e.g., (**) for particle impact excitation, (#*) for state selective electron capture, and/or two-electron rearrangement processes.
- (2) In the initial and final channel, the electron is specified only by its symbol e.
- (3) The label "class of collision" is redundant from the point of view of data exchange (e.g., for computer data searching), but can be useful as an index in the data storage system (Data Library).

3. Classes of Collisions

The following classes of collisions are considered (Table 2). Here collisions with photons are not taken into account, though some photon collision processes might come to play a role in the divertor region where particle densities are high.

Table 2. Classes of collisions

Collision	Explanation
1. e + Atom	Electron collision with atom or atomic ion
2. e + Molecule	Electron collision with molecule or molecular ions
3. e + Two Particles	Three-body collisions involving at least one electron
4. Atom + Atom	Collision of atom or atomic ion with atom or atomic ion
5. Atom + Molecule	Collision of atom or atomic ion with molecule or molecular ion
6. Molecule + Molecule	Collision of molecule or molecular ion with molecule or molecular ion
7. Three-body Atom/ Molecule	Three-body collision among heavy particles

In this notation, Atom (molecule) represents atom (molecule) or atomic (molecular) ion.

4. Types of Collisions (Collision Processes)

In Table 3, the collision processes relevant to fusion are listed, together with their abbreviations and symbolic notation (for clarity). They are divided into groups, according to their importance in fusion plasma research. This division is only conditional and reflects the present A+M data needs in fusion applications, as well as the data availability.

Table 3. Dictionary of collision processes

No.	Process	Abbreviation	Symbolic Notation*
<u>Group A: Processes of primary interest</u>			
A.1	Elastic scattering	ES	$A + B \rightarrow A + B$
A.2	Electronic excitation (of target)	EXC	$A + B \rightarrow A + B^*$
A.3	Collisional de-excitation (of target)	DEXC	$A + B^* \rightarrow A + B$
A.4	Ionization (of target), single	ION	$A + B \rightarrow A + B^+ + e$
A.5	Ionization (of target), multiple	IONk	$A + B \rightarrow A + B^{k+} + ke \quad (k \geq 2)$
A.6	Radiative electron-ion recombination	RREC	$e + B^{q+} \rightarrow B^{(q-1)+} + h\nu$
A.7	Dielectronic recombination	DREC	$e + B^{q+} \rightarrow \dots \rightarrow B^{(q-1)+} + h\nu$
A.8	Dissociative recombination	DISREC	$e + AB^{q+} \rightarrow A + B^{(q-1)+}$ $\rightarrow A^{(q-1)+} + B$

A.9	Bremsstrahlung	BREMS	$e + A^{q+} \rightarrow e + A^{q+} + h\nu$
A.10	Rotational excitation of molecules	ROEXC	$A + BC(j) \rightarrow A + BC(j')$
A.11	Vibrational excitation of molecules	VIBEXC	$A + BC(v) \rightarrow A + BC(v')$
A.12	Rotational-vibrational excitation of molecules	ROVIBEXC	$A + BC(v;j) \rightarrow A + BC(v';j')$
A.13	Direct (impact) dissociation	DIS	$A + BC \rightarrow A + B + C$
A.14	Dissociative excitation of molecules	DISEXC	$A + BC \rightarrow A + BC^* \rightarrow A + B + C$
A.15	Dissociative ionization of molecules	DISION	$A + BC \rightarrow A + B + C^+ + e$ $\rightarrow A + B^+ + C + e$
A.16	Multiple dissociative ionization of molecules	DISIONk	$A + BC \rightarrow A + B^{k_1+} + C^{k_2+} + ke$ ($k_1 + k_2 = k$)
A.17	Charge exchange (single), total	CX	$A^{q+} + B \rightarrow A^{(q-1)+} + B^+$
A.18	Multiple charge exchange, total	CXk	$A^{q+} + B \rightarrow A^{(q-k)+} + B^{k+}$
A.19	State selective electron capture, single	CXSS	$A^{q+} + B \rightarrow A^{(q-1)+} (\gamma) + B^+$
A.20	Excitation transfer	EXCTR	$A + B^* \rightarrow A^* + B$
A.21	Heavy particle exchange	PX	$A + BC \rightarrow AB + C$
<u>Group B: Other relevant binary collision processes</u>			
B.1	Electron attachment (radiative)	ELATT	$e + A \rightarrow A^- + h\nu$
B.2	Electron detachment	ELDET	$A + B^- \rightarrow A + B + e$
B.3	Dissociative electron attachment	DISATT	$e + BC \rightarrow B + C^-$
B.4	Associative detachment	ASDET	$A + B^- \rightarrow AB + e$

Table 3. (continued)

No.	Process	Abbreviation	Symbolic Notation*
B.5	Ion-pair production	IPP	$A + B \rightarrow A^- + B^+$
B.6	Mutual ion-ion neutralization	MNREC	$A^+ + B^- \rightarrow A + B$
B.7	Associative ion-ion recombination	ASREC	$A^+ + B^- \rightarrow AB$
B.8	Dissociative charge exchange	DISCX	$A^{q+} + BC \rightarrow A^{(q-1)+} + B + C^+$
B.9	Multiple dissociative charge exchange	DISCXk	$A^{q+} + BC \rightarrow A^{(q-k)+} B^{k_1+} + C^{k_2+}$ ($k_1 + k_2 = k$)
B.10	Transfer ionization	TIk l	$A^{q+} + B \rightarrow A^{(q-k)+} B^{l+} + (l-k)e$
B.11	Transfer excitation (of target)	TEXT	$A^{q+} + B \rightarrow A^{(q-1)+} + B^{+*}(\gamma)$
B.12	Transfer excitation (of projectile)	TEXP	$A^{q+} + B \rightarrow A^{(q-1)+**}(\gamma; \gamma') + B^+$
B.13	Stripping (of projectile)	STRIP	$A^{q+} + B \rightarrow A^{(q+1)+} + B + e$
B.14	Multiple stripping	STRIPk	$A^{q+} + B \rightarrow A^{(q+k)+} + B + ke$
B.15	Stripping-ionization	SIONk l	$A^{q+} + B \rightarrow A^{(q+k)+} + B^{l+} + (k+l)e$
B.16	Spin exchange	SPX	$A(\uparrow) + B(\downarrow) \rightarrow A(\downarrow) + B(\uparrow)$
B.17	Dissociative particle exchange	DISPX	$A + BCD \rightarrow AB + C + D$
B.18	Particle exchange with excitation	PXEXC	$A + BC \rightarrow AB + C^*$
B.19	Particle exchange with ionization	PXION	$A + BC \rightarrow AB + C^+ + e$ $\rightarrow AB^+ + C + e$

Group C: Three-body reactions

C.1	Three-body electron attachment (3rd-body = electron)	3-ELATT-EL	$e + A + e \rightarrow A^- + e$
C.2	Three-body electron attachment (3rd body = heavy particle)	3-ELATT-HP	$e + A + B \rightarrow A^- + B$
C.3	Three-body electron-ion recombination (3rd body = EL)	3-REC-EL	$e + A^+ + e \rightarrow A + e$
C.4	Three-body electron-ion recombination (3rd body = HP)	3-REC-HP	$e + A^+ + B \rightarrow A + B$
C.5	Three-body mutual neutralization	3-MNREC	$A^+ + B^- + C \rightarrow A + B + C$
C.6	Three-body associative recombination	3-ASREC	$A^+ + B^- + C \rightarrow AB + C$
C.7	Three-body association	3-AS	$A^{(+)} + B + C \rightarrow AB^{(+)} + C$

Group D: Composite processes

D.1	Spectral line emission	LEM	$A + B \rightarrow \lambda$
D.2	Spectral band emission	BEM	$A + BC \rightarrow \lambda, \lambda'$

Table 3. (continued)

No.	Process	Abbreviation	Symbolic Notation*
D.3	Total electron-ion recombination	TREC	RREC + DREC
D.4	Total ion-ion recombination	IIREC	MNREC + ASREC
D.5	Electron removal (from target)	ELREM	CX + ION
D.6	Electron production	ELP	$A + B \rightarrow \text{total } e$
D.7	Ion production	IP	$A + B \rightarrow \text{total ions}$
D.8	Neutral production	NP	e.g., $A + BC_n \rightarrow \text{total } C$
D.9	Three-body electron attachment (total)	3-ELATT-T	3-ELATT-EL + 3-ELATT-HP
D.10	Three-body electron-ion recombination (total)	3-REC-T	3-REC-EL + 3-REC-HP
D.11	Three-body ion-ion recombination (total)	3-IIREC	3-MNREC + 3-ASREC

*The symbols A, B, and C may stand for any atomic particle (electron, ion, atom, molecule, molecular ion), if otherwise explicitly not indicated. The first (second) symbol indicates the projectile (target). γ designates a set of quantum numbers.

Note: For the three-body reactions the labelling system in Table 1 can be used. If the identification of the third particle is necessary, it can be contained in the process label, such as shown in reactions C.1 and C.2 above, replacing HP with its specific chemical symbol (e.g., 3-ELATT-He).

5. Conventions about the order of reactants and products

The following conventions are suggested for distinguishing between the projectile and target, and the reaction products.

A. Initial reaction channel: reactants

1. The first chemical symbol appearing in the set of reaction labels designates the "projectile"; the second one designates the "target".
2. In electron-heavy particle collisions (including ions), the electron is always projectile.
3. In direct excitation (EXC) or ionization (ION) reactions, the particle being excited or ionized is always the target, and in stripping reactions (STRIP), the projectile is always ionized.
4. In other heavy-particle collisions, the particle having higher charge state is the projectile (e.g., $AP^+ + BQ^+, p > q$). This holds also for neutral particles (charge 0) and negatively charged particles.
- 4a. If the heavy-particles have the same charge state ($p=q$), the projectile is the particle with lighter mass ($m_A < m_B$, in the above example).

5. In collisions of atoms with neutral molecules, the atom is always the projectile.
6. In molecule-molecule collisions, the molecule with smaller number of nuclei is the projectile.
7. In collisions of neutrals with excited neutrals, the excited particle is always the target.
8. In three-body reactions, the third "non-reacting" particle does not appear as a separate reactant label, but (when necessary) is indicated within the reaction label (e.g., 3-ELATT-He).

B. Final reaction channel: products

1. When the reaction is uniquely specified by the process label and the reactants (together with their charge state and, when necessary, quantum state), the indication of the reaction products is not necessary and may be omitted.
2. If inclusion of the reaction products is needed to specify the reaction channel, their chemical symbols appear in the same order as in the initial channel. This order is preserved also in the case of dissociative processes (e.g., the dissociated target products appear after the projectile-product, and vice versa).

6. Quantities of data

Two quantities, namely, cross sections and rate coefficients averaged over particle energy distributions, are most relevant in plasmas (see Table 4).

Table 4. Quantities of data

No.	Resolved Processes	Comments	Abbreviation
1	Cross section	Integrated	XS
2	Differential cross section	Single and double in angle or energy, and both	DXS1 DXS2
3	Rate coefficient for Maxwellian distribution		RC
4	Rate coefficient for beam-Maxwellian distribution		RCB

7. Standard data reference labels

The data reference labels serve to describe the character of the data. For uniformity, it is suggested that they appear in the following order:

1. Type of data (for instance XS, RC, RCB, DXS1, etc).
2. Form of data presentation (tabular: TAB, analytic fit: FIT).
3. Data status (recommended: REC, critically evaluated: EVAL, compilation: COMP, original source: ORIG).
4. Accuracy: ACC = A⁺, A, B, C, D, E, with A, B, ... denoting an agreed range of uncertainty.*

5. Data source (e.g., IAEA, A+M Data Center compendium, etc).
6. Reference (DOC = abbreviation pointing to documentation in the dictionary file)
7. Data of the last data entry or latest revision, if changed (day/month/year).

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- *A⁺ - accuracy better than 3%
 - A - accuracy better than 10%
 - B - accuracy better than 10%-25%
 - C - accuracy better than 25%-50%
 - D - accuracy better than 50%-100%
 - E - uncertainty larger than 100%

2.2. REPORT OF THE WORKING GROUP ON THE ATOMIC AND MOLECULAR
DATA EXCHANGE FORMAT AND INTERACTIVE SYSTEM

R.A. Hulse (Chairman), K. Behringer, T. Hirayama, J.G. Hughes, R.A. Phaneuf,
D. Reiter, L. Roszman, M. Seits, J.J. Smith and H.P. Summers

1. Introduction

The papers presented by the meeting participants represented a range of perspectives on the atomic data - fusion applications interface. An illustrative example of an extensive code system developed to support the generation and display of results from a large atomic physics calculation effort was provided by J. Hughes of the Queens University, Belfast. For the rather different needs of bibliographic and spectral line data bases, commercial database software is often used. As one example, W. Wiese described the databases at the U.S. National Bureau of Standards.

Several participants described their methods for incorporating atomic data into their fusion modeling codes. The atomic physics codes developed by H. Summers (JET) and their close interface with K. Behringer's modeling code represented a notable "close coupling" of atomic data with a fusion modeling code. D. Reiter (KFA Julich) described the special atomic data requirements of large Monte-Carlo neutral gas modeling codes. These codes rely on large quantities of data, including special moments of the cross-sections taken over the plasma distributions, stored in tabular form for rapid access.

These presentations clearly indicated the variety of existing atomic physics data bases used by the meeting participants. While these ranged widely in the level of detail accommodated, and their primary application, these systems were all primarily designed for local, internal use by their developers. The ALADDIN atomic data system, presented by R. Hulse (PPPL, Princeton), differed in this regard in having been designed specifically to address the data exchange and interface requirements of an international database system.

In addition to consideration of the systems described in the presentations, the applicability of commercial database software to the development of a fusion atomic database system was discussed in more general terms. However, critical shortcomings were found in this approach (cf ALADDIN presentation, Appendix C). Chief among these were the lack of universal transportability and availability on all types of computer hardware, along with the related issues of expense. The efficient interface of such systems to modeling codes also provided a serious problem. In the end, commercial systems were found to be inappropriate for the comprehensive data base under discussion, despite their utility for certain individual applications.

Following the presentations and initial discussions of the range of possible data storage and exchange systems, the ALADDIN system emerged as the focal point for detailed consideration. Appendix C provides the complete text of the ALADDIN presentation given by R. Hulse.

2. Basic Features of ALADDIN

The ALADDIN system consists of several related components. Most fundamental is the definition of the required characteristics of such a database, from which a specific data structure and other organizational precepts are derived. The specific software supporting this database structure consists of the ALADDIN interactive database search code, and the associated ALPACK subroutine package, which provides an interface for user codes to ALADDIN data.

ALADDIN is intended to be a medium for communication, exchange and manipulation of atomic data amongst a wide range of users. This leads to the requirement for multiple levels of access to an arbitrary variety of data types, with data entries that can be modified, edited, created, and otherwise manipulated by data users as well as data providers.

The basic ALADDIN data structure consists of an ASCII data file, with concatenated entries. Such files can be almost universally transmitted, edited, and read, and can even be directly printed out and published. An important concept is that most information should be kept in such data files, rather than coded into subroutines, as information is much more easily manipulated in files than in computer code. However, some information must inevitably be incorporated in the computer code. First, there are the data access and search procedures; these are kept as general as possible, independent of the data types being read. Also, the mathematical forms for the fitted data must appear in coded form. This is handled by using a basic set of mathematical representations of the stored data, with a uniform procedure for selecting the correct procedure to call, based on a pointer incorporated within the data entry itself.

Each ALADDIN data entry consists of a header containing searchable attribute labels, followed by the data itself. Two types of searchable labels provide flexibility in searching for and identifying the data. Hierarchical labels are labels in an ordered sequence, and are typically used to represent the physics description of the data. Such a sequence of labels might be of the form: process-type element charge-state initial-quantum-state final-quantum-state. Boolean labels are sequence-independent attributes, such as the data source, version date, etc. The Boolean labels can be searched using logical operators such as 'AND' and 'NOT'. Among the Boolean labels is one which points to the correct subroutine to call in order to interpret the data representation used in each entry.

This system of searchable labels provides a minimum number of restrictions as to the type and form of data that can be stored in the database, along with easy access and modification in response to changing needs. Standard labels can be defined by the IAEA for consistency, while other users are free to create labeling schemes as needed for special applications.

An additional aspect of information storage in the ALADDIN system is the dictionary file. This file supports a simple label-based search structure for accessing documentation associated with the data entries.

All ALADDIN database supporting software is written in FORTRAN 77 for maximum portability between computer systems. The ALADDIN interactive code allows users to read ALADDIN format files and search for entries containing the required data. These entries can then be displayed to the computer terminal, compiled into new ALADDIN files, or data values can be calculated at any number of specified points. The ALADDIN dictionary files can be queried on line at any time to access documentation for the data entries.

The ALPACK subroutine package provides 'black box' code routines which can be called from a user's FORTRAN 77 program to search for and read in data from ALADDIN files. It provides user's codes with search capabilities identical to those in the ALADDIN interactive code.

3. Conclusions and Recommendations

This working group was charged with detailed consideration of the data base formats to be adopted. An organizing focus was to develop specific ALADDIN labeling sequences for those principal atomic processes for which important sets of atomic data were already available. This approach, beginning from existing data, was complementary to the more global considerations of the other working group.

This focus on present data and immediate needs proved important in helping define various issues. In particular, a balance was struck between the conflicting desires for sparse efficiency versus complete generality in labeling schemes. The resulting labeling schemes encompassed immediately definable data search needs, leaving for the future questions of how to best represent some examples of extremely complex data, and more hypothetical search requirements. The specific atomic processes considered, and their corresponding labeling schemes, are given in Appendix D.

These discussions also helped build confidence in the basic soundness of the ALADDIN system, particularly the advantages in carefully keeping the data labeling flexible. Since labeling schemes can be readily modified, or new ones added, as experience dictates change, there is no need to worry in paralyzing detail about labeling decisions, out of fear that they will be irrevocable.

The setting up of these practical labeling schemes also provided useful feedback for further ALADDIN development. For example, while ALADDIN presently allows "wild card" search matches to entire labels, it was seen to be very helpful to add the ability to do character-by-character wild card matches within individual labels. This would minimize the need for decisions about grouping some specifications (such as spectroscopic level designations) into single or multiple labels. It was also seen as useful to be able to do search matches on labels treated as real numbers, in addition to the standard character string match criteria.

After consideration and discussion of these issues, the decision of the working group was to adopt the ALADDIN system as the IAEA standard database system for exchange of atomic data for fusion applications. This decision included commitments by those present to provide appropriate ALADDIN interfaces to their existing atomic physics and modeling codes.

After the adoption of ALADDIN by the working group, Hulse volunteered to continue development work on ALADDIN. This will include addition of new functionality, such as the extended search protocols described above. Hulse will also finalize the code and associated documentation into a paper to be submitted to a journal such as "Computer Physics Communications", in order to both encourage its dissemination and establish a standard reference for the ALADDIN system and supporting software. There was agreement that further development of ALADDIN software beyond this standard published version could be done by Hulse and/or users as needs developed. However, it was considered to be very important to keep straightforward, standard codes available, and to avoid having these essential tools overburdened and unnecessarily complicated by uncoordinated code development.

The IAEA Atomic and Molecular Data Unit was seen as playing a vital continuing role in coordinating fusion atomic data activities, especially with respect to developing the role of the ALADDIN database system. This will include the standardization of ALADDIN labeling conventions, as well as establishing standard sets of evaluated atomic and molecular data in ALADDIN form. The IAEA will also provide a needed center for the distribution of ALADDIN software and these ALADDIN database files. There is also a clear IAEA role in continuing to help organize appropriate meetings as required to provide a forum for future development and assessment of all aspects of the ALADDIN data storage and exchange system.

3. MEETING CONCLUSIONS AND RECOMMENDATIONS

The Meeting conclusions and recommendations can be summarized as follows:

- 1) The necessity of creating a unique data storage and exchange system for communication of recommended A+M data for fusion between atomic data centres, the IAEA Atomic and Molecular Data Unit and the fusion laboratories was recognized as an urgent problem. In order to satisfy these needs, the PPPL ALADDIN system was adopted as presently the most adequate one.
- 2) Although ready for an immediate use, ALADDIN has to undergo further developments to enhance its functionality, extend its supporting software, and capabilities for interfacing. R. Hulse volunteered to collaborate with the IAEA A+M Data Unit staff in implementing these developments. The national data centres and fusion A+M data users will use the ALADDIN for data formatting, exchange and interfacing.
- 3) The labelling/indexing system contained in the Report of the Working Group on A+M data base and reaction dictionary (Sect. 2.1) is at present adopted as a standard one. As needs develop, this system may also be subject of agreed extensions (for instance to include plasma-wall interaction processes, a "template" label to classify the reactions with the same labelling structure, etc).
- 4) All further developments and extensions of the ALADDIN data base and exchange system should be effectuated in a co-ordinated manner, through the IAEA A+M Data Unit. This Unit should be responsible for maintaining and distribution of the standard and up-dated versions of ALADDIN, and organize forums for its regular assessment.

Consultants' Meeting on the "Atomic Data Base and Fusion
Applications Interface"

9-11 May 1988

at

IAEA Headquarters in Vienna, Austria

(in Meeting Room: A-19-72)

LIST OF PARTICIPANTS

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- 16:30 - 16:45 E. Menapace (ENEA, Bologna)
Activities in the A+M Data at ENEA-Bologna
- 16:45 - 17:00 Y. Nakai (JAERI, Tokai)
Atomic collision and structure data base at JAERI
- 17:00 - 17:15 K. Katsonis (GAPHYOR, Orsay):
The GAPHYOR bibliographic base and format
- 17:15 - 18:00 Discussion of Data Centres formating practices

Tuesday, 10 May 1988

Session III: Data exchange files and interactive systems

Chairman: K. Behringer

- 9:00 - 9:40 R. Hulse (PPPL, Princeton)
ALADDIN - A labeled atomic data interface for fusion applications
- 9:40 - 10:20 H.P. Summers (JET, Culham)
An interactive atomic data and application structure at JET
- 10:20 - 10:40 Coffee Break
- 10:40 - 11:20 T. Hirayama (JAERI)
Activities of diagnostic and modelling for fusion plasma and comments on interface between atomic data and simulation codes
- 11:20 - 12:00 J.J. Smith (IAEA, Vienna)
Components and a structure for exchange of A+M collision data
- 12:00 - 14:00 Lunch Break

Session IV: The structure and format of A+M data base and exchange files

Chairman: R.K. Janev

- 14:00 - 15:15 Discussion of the elements, structure, functions and formats of the A+M numerical data system, exchange file, interactive files, supporting software etc.
Formation of working groups*

* At least two working groups are envisaged:

- 1) Working group for the A+M Dictionary (data labelling/indexing system)
- 2) Working group for the exchange file and interactive system(s)

15:15 - 15:30 Coffee Break

15:30 - 18:00 Discussions within working groups
Preparation of working group reports (Meeting Rooms: A-19-72
and C07-55)

Wednesday, 11 May 1988

9:00 - 10:45 Preparation of working group reports (Meeting Rooms: A-19-72
and C07-55)

10:45 - 12:10 Discussion of working group reports

Chairman: R.K. Janev

12:10 - 14:00 Lunch Break

14:00 - 17:00 Integration of working group proposals into one data exchange
-interface system
Meeting conclusions.

ALADDIN

**A LABELED ATOMIC DATA INTERFACE
FOR FUSION APPLICATIONS**

**Russell A. Hulse
Princeton University
Plasma Physics Laboratory**

**Presented at the IAEA Consultants Meeting on
The Atomic Physics Data Base and Fusion Applications Interface
May 9-13, 1988
Vienna, Austria**

* Supported by U.S. Department of Energy contract DE-AC02-76-CHO-3073

A wide range of atomic and molecular data
is required for fusion research

- Much valuable work has been done in order to provide this data; however:
 - Data must be efficiently accessible to large computer modeling codes, and
 - Data must be efficiently accessible by interactive computer searching
-
- ALADDIN addresses the need for such a fusion atomic physics database, providing multiple levels of access to an arbitrary variety of data types

Outline

- begin by considering the nature of the required data, the range of users and modes of access required
- examine in detail the required information in each data entry and how it can best be organized, drawing in part on experience using atomic data in the MIST impurity transport code
- describe the resulting ALADDIN database structure
- describe the ALADDIN code for interactive database searching and access
- describe ALPACK routines for interfacing user applications to ALADDIN data

General Database Considerations

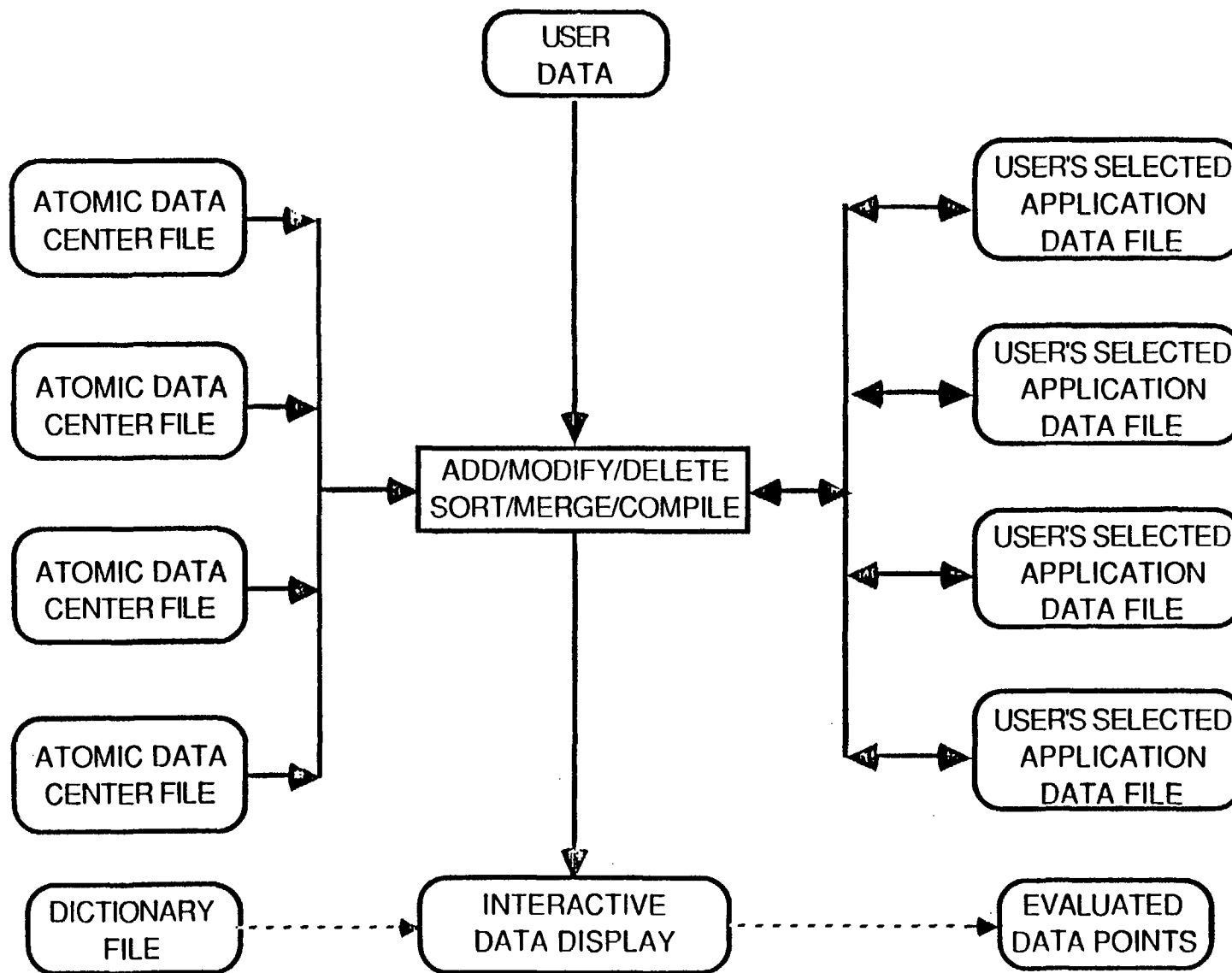
- we need a medium for broadly based exchange and manipulation of data
- atomic physicists must be readily able to compile a wide variety of data
- data must be readily transmitted to, and used by, a wide variety of users
- the database medium and format must be readily edited by users
 - cannot be just a rigid data compiler-to-user information path
 - fusion atomic data needs are diverse and continuously evolving
 - needs typically must be met by combining data from various sources
 - transform data into more computationally efficient/compact forms
 - mix, match, modify and add data to create a personal database
- interactive access to the atomic data base is a fundamental requirement
 - main access for users who do not need extensive data for code use
 - large scale users still need to manually access and verify data
 - suitable hardcopy still best for many users and should be supported
- straightforward, efficient interface to user's codes is also critical
 - need logical structure and supplied 'black box' access routines
 - cannot be a significant computational burden to large codes
 - data points must often be evaluated repetitively in inner loops

A prime factor - we must keep the database structure **straightforward**, as well as **flexible**, in order to be broadly accepted and used.

The basic data storage format:

ASCII data files consisting of concatenated, independent entries

- readily transmitted and read across all computer systems
- text editor can serve as the most basic and familiar way of searching, accessing and editing data entries
- files can simply be sorted by entry type and hardcopy created, which can be published and used even by those without computers
- basic data entry in a database file will contain:
 - searchable attributes
 - the data itself, typically in the form of fitting coefficients
- Figure 1 shows a schematic representation of the data flow involved in the first level of user interaction with the database.
- For large codes, efficiency of data access can be very important (Fig 2)
 - data files typically be read only once at the beginning of each run
 - custom data files minimize searching through unneeded data
 - efficient fitting formulas are evaluated to yield the data points



COMPILATION OF REQUIRED DATA FOR USER'S APPLICATIONS

Fig. 1

USER'S CODE

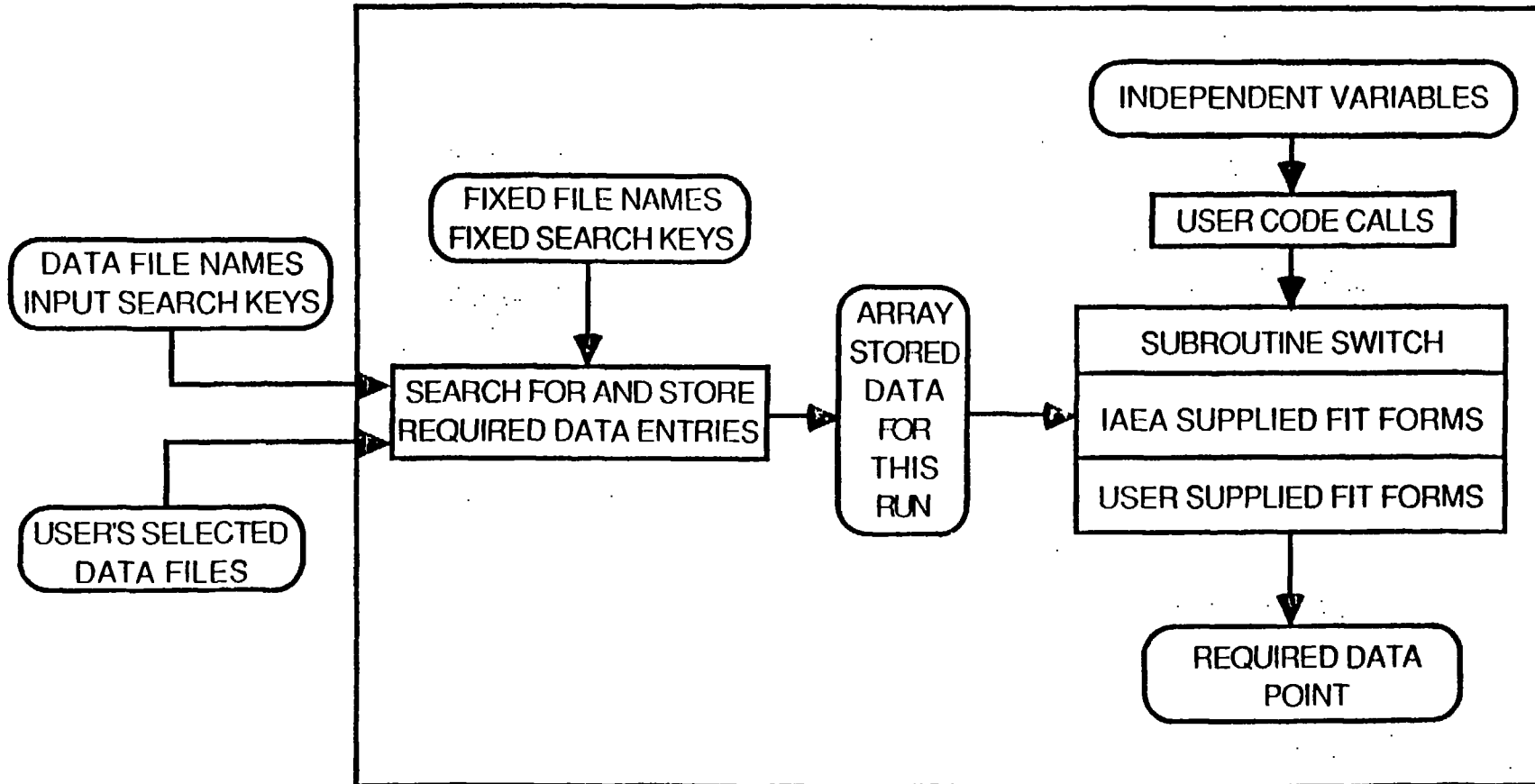


Fig. 2

Supporting software in FORTRAN 77

- principal programming language for scientific applications
- widely available, on full range of systems from PC's to Crays
- supports character string manipulation
- can be used as a guide for ALADDIN routines in other languages
- commercial database software is not suitable for our purposes
 - relatively simple structure and relational searching requirements
 - need transportability across many user systems
 - need to directly and efficiently interface data to applications codes

Data files vs. Subroutines

To what extent should the information be conveyed in data files or, alternatively, coded into subroutines?

- data files as the main information-carrying entity is supported by MIST impurity transport code experience
- MIST ionization and recombination rates from a subroutine package
 - data is hard to modify (large code must be edited and recompiled)
 - new data requires new data structure and decision paths
- MIST spectral line excitation rates from fitting coefficients in data file
 - a few simple subroutines used to evaluate the fitted forms
 - fitted forms are computationally quick to evaluate
 - new or modified data quickly added to data file with a text editor
 - separate files with spectral data for special applications
 - editing and re-compilation of the code only if a new fit is needed
 - made easy by using a uniform array structure and pointers
 - typically only a few lines of code must be added
- In essence, information in data files is more easily manipulated than in coding, so keep most information in data files

However, structure of languages such as FORTRAN require that some of the required information be compiled into each program as lines of code:

- data file read/search/store procedure must be compiled into code
 - should be kept as general as possible, insensitive to data types
 - receives only key searching information from the calling program
 - passes back to calling program data type information from entry
 - returns data from desired entries into generalized buffer arrays
- the mathematical equations for the fitted forms must also be compiled
 - use a basic set of fitting forms for various different data types
 - setup uniform procedure for data types to call correct subroutines

Further Considerations in Accessing the Data

Atomic data to be stored can be looked at as a function of the form

$$F_{ijk\dots}(x, y \dots | a, b, c \dots)$$

- (i, j, k ...) are a set of (discrete) selection variables describing the data (atomic process type, element, charge state, etc.) and the functional form
- the mathematical form uses one or more fitting coefficients (a, b, c ...)
- the independent variables (x, y ...) of the function are typically continuous
- searchable attributes (i,j,k...), represented by various labels in the entry
 - physics identifiers
 - where the entry came from, etc.
 - the routine to use to access (process) the entry
 - the routine to use to mathematically evaluate the data function F
- non-searchable information, or coefficients (a, b, c...)
 - input for the evaluation function referenced by the labels

Searchable labels: Hierarchical and Boolean types

Hierarchical labels

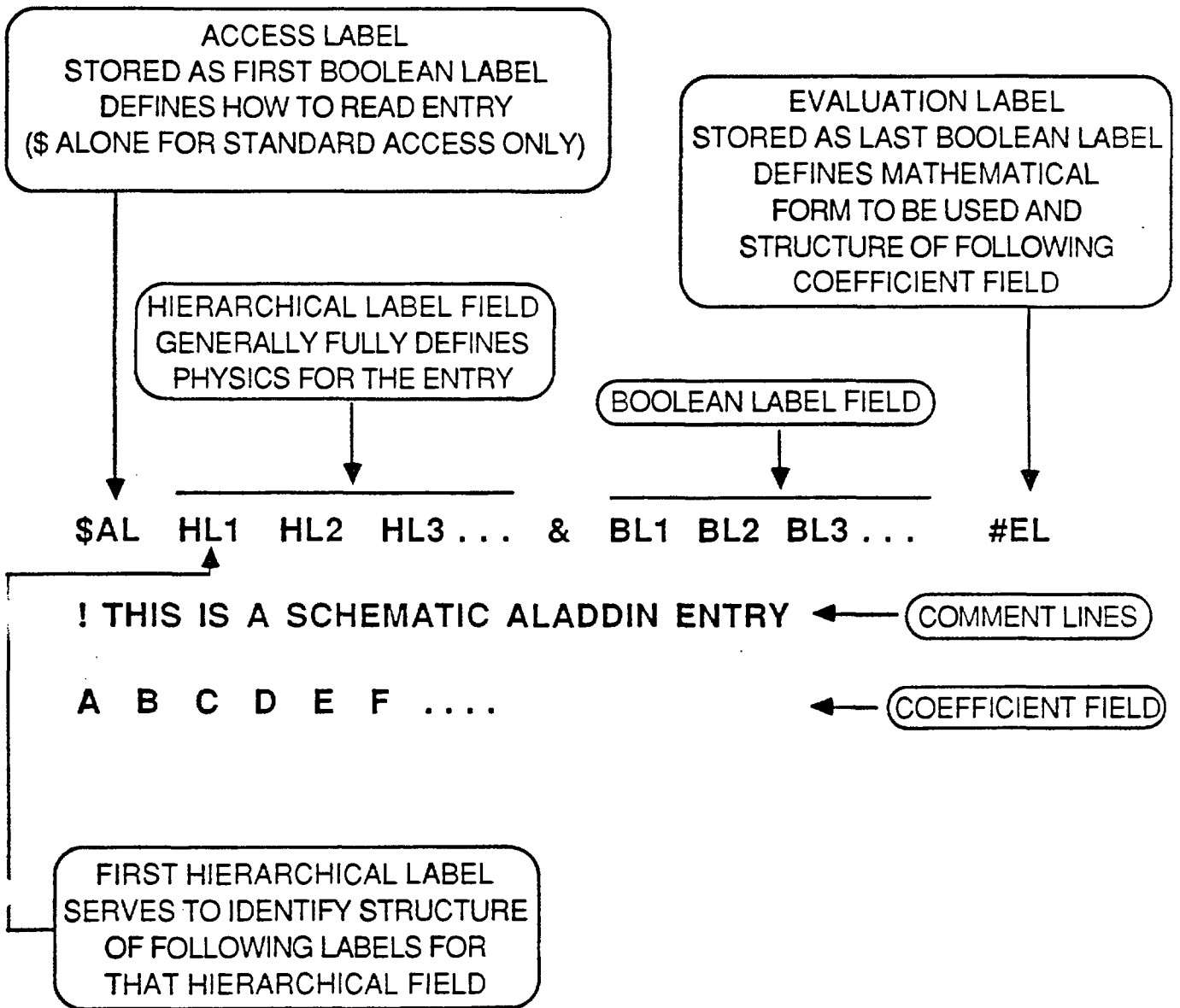
- a sequence of labels where the order of appearance is important
- much information (esp. physics labelling) naturally has this form
- for example, a hierarchical label sequence for spectral line excitation:

SLEXR	26	24	255.2
(DATA TYPE)	(ELEMENT)	(CHARGE STATE)	(WAVELENGTH)

Boolean labels

- independent attributes whose entry order is unimportant
- searched using Boolean logical operators such as .AND., .NOT., etc.
- examples: data source, version, documentation, fit accuracy, etc.
- special Boolean "access label" provides for optional special entry formats
 - can direct code to re-read entry after standard top-level processing
 - example: non-numeric data in the coefficient field
 - example: searches acting on a labels as real numbers
- special Boolean "evaluation label" specifies functional form to use

Combination of hierarchical and Boolean attribute labels allows great flexibility and open-ended development of the database structure



ALADDIN Data File Entry Structure

- entry begins with access label "\$" symbol in column 1
 - "\$" (with suffix) access label is treated as the first Boolean label
 - blank access label suffix means standard ALADDIN access routines
- hierarchical label field follows the "\$" label string
 - blank-delimited hierarchical labels read in sequence
- Boolean label field follows "&" symbol
 - blank-delimited
 - if there are no Boolean labels, "&" character can be omitted
- "#" evaluation label denotes the end of the header labels field
 - "#" (with suffix) evaluation function label is the last Boolean label
- note that there are always two Boolean labels for any entry
 - the "\$" prefix access label as the first
 - the "#" prefix evaluation label as the last
- the header label field may extend across one or more lines
 - but "#" label is followed by a new line w/ comments or coefficients
- Optional free-form comment lines follow the header field and must begin with a "!" character in the first column. The first line not beginning with a "!" character after the header label field is taken as the first line of the coefficient field.
- The coefficient field extends from the first non-comment line after the header labels to the beginning of the next entry, or end of file. These lines will typically be read as single-precision real numbers into data arrays in the code, unless there is a special access label for the entry.

AL.DAT

THIS IS A TEST DATA FILE FOR ALADDIN, WITH #MEWE AND #TAB1D DATA

\$ SLEXR 8 3 703.36 & RAH/PPPL #MEWE

703.36 0.0 0.18 1.0 0.6 0.0 0.0 0.28

\$ SLEXR 8 4 790.36 & RAH/PPPL #MEWE

790.36 0.0 0.15 1.0 0.6 0.0 0.0 0.28

\$ SLEXR 8 8 18.97 & RAH/PPPL #MEWE

18.97 0.0 0.4162 1.0 0.04 0.21 -0.04 0.28

\$ SLEXR 8 8 102.5 & RAH/PPPL #MEWE

! THIS IS A COMMENT LINE IN THE FOURTH ENTRY

0.0 774.37 0.0791 0.1100 0.27 0.08 0.0 0.28

\$ SLEXR 26 24 192.1 & FEXXIV RAH/PPPL #MEWE

192.1 0.0 0.0478 1.0 0.6848 0.9652 -0.4783 0.28

\$ SLEXR 26 24 255.2 & FEXXIV RAH/PPPL #MEWE

255.2 0.0 0.0177 1.0 0.6648 0.9652 -0.4783 0.28

\$ TEST #TAB1D

0.0 0.0 100.0 100.0 200.0 100.0

Assignment of Labels and Effective Use of the ALADDIN Data Structure

- The assignment of standard labels for ALADDIN databases is largely to be left for consideration by the atomic physics and fusion communities as the database is developed. ALADDIN labels are treated as character strings, so that they can be freely chosen as useful mnemonics for readability. An important feature is that the basic ALADDIN search and access procedures need not need to know the number or meaning of the labels in an entry in order to read it in or to do a search comparison. However, since the basic search procedure is a strict character by character comparison, consistency of form is essential for successful data searching.
- The first hierarchical label should define the number and meaning of the following hierarchical labels. The searching procedure includes "wild card" constructs as well as seeking perfect matches to the hierarchical labels. Usually, the hierarchical label field is the most natural place to describe the full physical specification for an entry (e.g., process type, element, charge state, etc.).
- A consideration for the hierarchical field is that, often, one will want to search for and read in a whole class of related data, for example, ionization rates for all charge states of iron.
- Another circumstance which is important to deal with is that where there is some overlap between two different sources of the same data. This can be resolved beforehand by either the atomic data center or the user setting up input data files which contain only ordered, complete sets of data, with priorities thus sorted out in the compilation process. Another possibility is to use a special Boolean flag, such as "vpr=" ("version priority ="), which will communicate to the accessing code the relative priorities of entries with identical hierarchical search fields.

- An interesting possibility in the label structure would be to give some labels formats within themselves, interpretable at a deeper level by the accessing codes. For example, by using namelist-style forms: `date=1/20/88`, `doc=12345`, `wvl=235.4`, or the `vpr=2` form mentioned above.
- While use of comment lines within the entry is encouraged, more extensive documentation (such as literature references, physical units, valid range of the data, etc.) is most appropriately referenced by an appropriate Boolean label in order to allow computerized searching and access using the dictionary file.
- An important feature of the ALADDIN system is that user modification and augmentation is supported. This must extend to the ability to define labels for the user's own data formats, etc. These will be distinguished from IAEA standard labels by a "@" prefix, but are otherwise treated identically by the system.

ALADDIN STARTUP AND DATA SEARCH

USC\$ RU ALADDIN

INPUT FILE NAME ? AL.DAT

QUERY DICTIONARY FILE NAME (C/R FOR NONE)? AL.QDC

ALADDIN>> SL

USE ".*" AFTER LAST SEARCH LABEL IS ENTERED

HIERARCHICAL SEARCH LABELS (* AND ** ARE WILDCARDS) ?

SLEXR 26 ** .

BOOLEAN .AND. SEARCH LABELS ?

#MEWE .

BOOLEAN .NOT. SEARCH LABELS ?

ALADDIN>> S

STARTING SEARCH AT ENTRY SEQUENCE NUMBER 1

MATCH FOUND AT ENTRY SEQUENCE NUMBER 5

"D" DISPLAY COMMAND

ALADDIN>> D*

INPUT DATA FILE: AL.DAT
OUTPUT DATA FILE: **NONE**
QUERY DICTIONARY FILE: AL.QDC
EV OUTPUT DATA FILE: **NONE**

HSL: 1[SLEXR] 2[26] 3[**]

BASL: #MEWE

BNSL:

ENTRY SEQUENCE NUMBER = 5

1[\$ SLEXR 26 24 192.1 & FEXXIV RAH/PPPL #MEWE]
2[192.1 0.0 0.0478 1.0 0.6848 0.9652 -0.4783 0.28]

HL: 1[SLEXR] 2[26] 3[24]
HL: 4[192.1]

BL: \$ FEXXIV RAH/PPPL
BL: #MEWE

NO COMMENT LINES IN THIS ENTRY

CF: 1[1.921000E+02] 2[0.000000E+00] 3[4.780000E-02] 4[1.000000E+00]
CF: 5[6.848000E-01] 6[9.652000E-01] 7[-4.783000E-01] 8[2.800000E-01]

USE OF THE DICTIONARY

ALADDIN>> #MEWE?

GENERALIZED GAUNT FACTOR LINE EXCITATION CALCULATION
REFERENCE: R. MEWE, ASTRON. AND ASTROPHYS. 20, 215 (1972)

INPUT: ELECTRON TEMPERATURE (keV)
RETURNS: SPECTRAL LINE EXCITATION RATE COEFFICIENT (CM³/S)

#MEWE DATA TYPE COEFFICIENTS ARE (IN ORDER):

- 1) EXCITATION WAVELENGTH (ANGSTROMS)
- 2) EXCITATION ENERGY (EV)
(IF PEIJ=0, ASSUME A RESONANCE LINE AND CALCULATE EIJ FROM PWVL)
- 3) OSCILLATOR STRENGTH
- 4) BRANCHING RATIO
- 5-8) A, B, C, D COEFFICIENTS FOR MEWE GAUNT FACTOR FORMULA

ALADDIN>>

ALADDIN>>

H, {C/R}	HELP (SHOW THIS COMMAND SUMMARY)
{LABEL}?	QUERY THE ALADDIN DICTIONARY ABOUT {LABEL}
SL, L	SEARCH LABELS (DEFINE NEW SEARCH LABELS)
S	SEARCH FOR NEXT MATCHING ENTRY
G##	GO TO ENTRY AT SPECIFIED SEQUENCE NUMBER
N	NEXT (GO TO NEXT SEQUENTIAL ENTRY NUMBER)
D{FEL!CS*}	DISPLAY TO TERMINAL ITEM(S) SPECIFIED BY SUFFIX CHARACTER(S): Files, Entry, Labels, !comments, Coefficients, Search labels, *all display fields
WR	WRITE CURRENT ENTRY TO OUTPUT ALADDIN FILE
EV	EVALUATE FITTED DATA POINTS FOR CURRENT ENTRY
R	REWIND INPUT ALADDIN DATA FILE
F	FILE (SELECT INPUT ALADDIN DATA FILE)
OF	OUTPUT FILE (SELECT WR COMMAND OUTPUT FILE)
EF	EV FILE (SELECT EV COMMAND OUTPUT DATA FILE)
QF	QUERY FILE (SELECT QUERY DICTIONARY FILE)
EX, EN	EXIT OR END ALADDIN

"EV" EVALUATE DATA COMMAND

ALADDIN>> EV

EVALUATE DATA TYPE: #MEWE

MEWE SPECTRAL LINE EXCITATION RATE COEFFICIENT (cm³/s),
AS FUNCTION OF ELECTRON TEMPERATURE (keV)

EV OUTPUT DATA CURRENTLY DIRECTED TO FILE: **NONE**
(TO CHANGE OUTPUT FILE, USE EF COMMAND AFTER EXITING AT NEXT PROMPT)

LOG OR LINEAR DATA POINT SERIES (C/R TO EXIT) ? LOG

NUMBER OF POINTS, FIRST, LAST VALUE (,, TO EXIT) ? 10 0.1 10.

INPUT	DATA VALUE
1.000000E-01	7.639596E-10
1.668101E-01	7.843433E-10
2.782559E-01	7.335799E-10
4.641589E-01	6.514873E-10
7.742637E-01	5.625643E-10
1.291550E+00	4.784145E-10
2.154435E+00	4.032642E-10
3.593814E+00	3.379251E-10
5.994843E+00	2.818762E-10
1.000000E+01	2.341796E-10

EV OUTPUT DATA CURRENTLY DIRECTED TO FILE: **NONE**
(TO CHANGE OUTPUT FILE, USE EF COMMAND AFTER EXITING AT NEXT PROMPT)

LOG OR LINEAR DATA POINT SERIES (C/R TO EXIT) ?

ALADDIN>>

USING THE "EV" COMMAND TO WRITE DATA POINTS TO A FILE

ALADDIN>> EF

EV DATA OUTPUT FILE NAME (C/R=OUTPUT TO TERMINAL) ? TESTEV.DAT
NEW (N) OR APPEND (A) ? N

ALADDIN>> EV

EVALUATE DATA TYPE: #MEWE

MEWE SPECTRAL LINE EXCITATION RATE COEFFICIENT (cm³/s),
AS FUNCTION OF ELECTRON TEMPERATURE (keV)

EV OUTPUT DATA CURRENTLY DIRECTED TO FILE: TESTEV.DAT
(TO CHANGE OUTPUT FILE, USE EF COMMAND AFTER EXITING AT NEXT PROMPT)

LOG OR LINEAR DATA POINT SERIES (C/R TO EXIT) ? LIN

NUMBER OF POINTS, FIRST, LAST VALUE (,, TO EXIT) ? 10 1. 10.

ENTER HEADER LINE FOR THIS DATA

THIS DEMONSTRATES THE EV COMMAND WRITING TO A DATA FILE

INPUT	DATA VALUE
1.000000E+00	8.158804E-09
2.000000E+00	6.498793E-09
3.000000E+00	5.650057E-09
4.000000E+00	5.103018E-09
5.000000E+00	4.709366E-09
6.000000E+00	4.406985E-09
7.000000E+00	4.164411E-09
8.000000E+00	3.963691E-09
9.000000E+00	3.793690E-09
1.000000E+01	3.647072E-09

EV OUTPUT DATA CURRENTLY DIRECTED TO FILE: TESTEV.DAT
(TO CHANGE OUTPUT FILE, USE EF COMMAND AFTER EXITING AT NEXT PROMPT)

LOG OR LINEAR DATA POINT SERIES (C/R TO EXIT) ?

"WR" COMMAND TO WRITE AN ENTRY TO A NEW ALADDIN FILE

ALADDIN>> DE

ENTRY SEQUENCE NUMBER = 1

```
1[$ SLEXR 8 3 703.36 & RAH/PPPL #MEWE ]
2[703.36 0.0 0.18 1.0 0.6 0.0 0.0 0.28 ]
```

ALADDIN>> OF

NEW OUTPUT FILE NAME (C/R=NONE) ? ALTEST.DAT
NEW (N) OR APPEND (A) ? N

ALADDIN>> WR

2 LINE ENTRY WRITTEN TO FILE: ALTEST.DAT

ALADDIN>> N

NOW AT ENTRY SEQUENCE NUMBER 2

ALADDIN>> DE

ENTRY SEQUENCE NUMBER = 2

```
1[$ SLEXR 8 4 790.36 & RAH/PPPL #MEWE ]
2[790.36 0.0 0.15 1.0 0.6 0.0 0.0 0.28 ]
```

ALADDIN>> WR

2 LINE ENTRY WRITTEN TO FILE: ALTEST.DAT

ALADDIN>> OF

CLOSING OUTPUT FILE ALTEST.DAT

NEW OUTPUT FILE NAME (C/R=NONE) ?

ALADDIN>> EX

FORTRAN STOP

ALPACK PROVIDES A SIMPLE INTERFACE TO ALADDIN DATA
FOR USER'S APPLICATION CODES

C

C READ IN NEXT ENTRY FROM ALADDIN DATA FILE

C

CALL ALREAD(LUDF, LESEQN, EOF, ERRMSG)

C

C COMPARE THIS ENTRY'S LABELS WITH DESIRED LABELS

C

CALL ALCOMP(HSL, NHSL, BASL, NBASL, BNSL, NBNSL, MATCH)

C

IF(MATCH) THEN

C

C CONVERT COEFFICIENT FIELD TO REAL NUMBERS

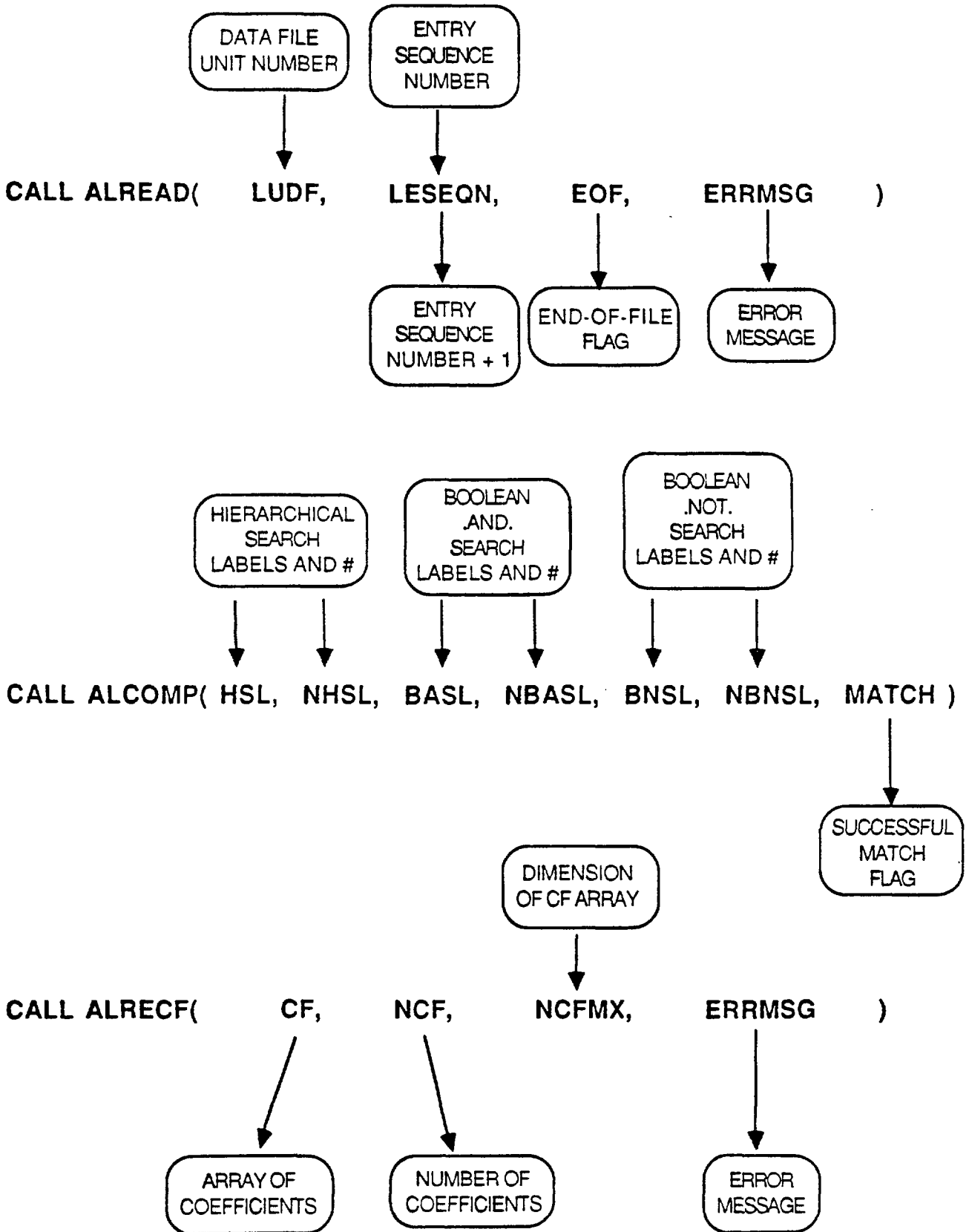
C

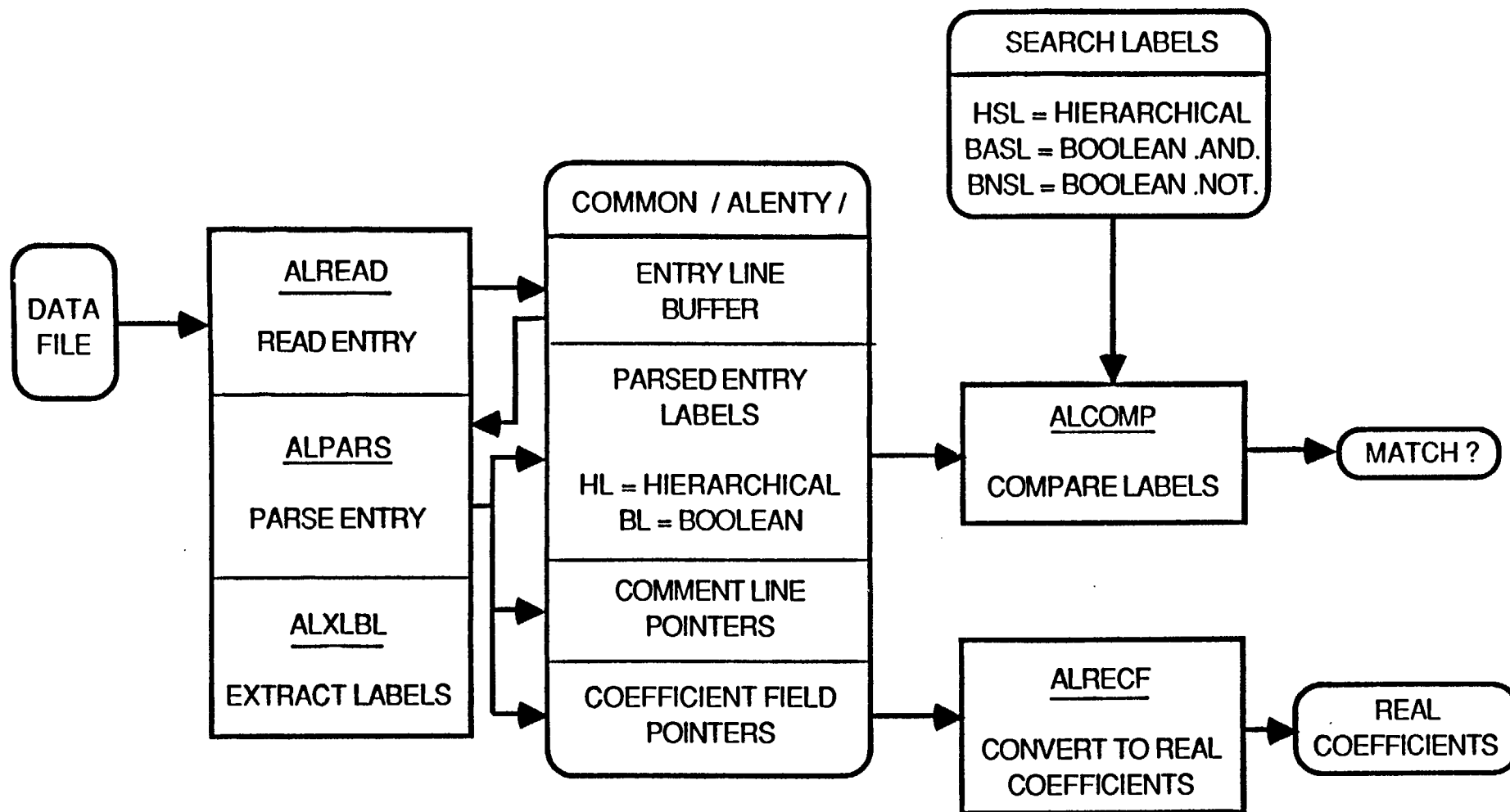
CALL ALRECF(CF, NCF, NCFMX, ERRMSG)

C

C CALL APPROPRIATE EVALUATION ROUTINE WITH COEFFICIENTS

C





- 45 -

ALADDIN DATA FLOW
STANDARD "TOOLBOX" ROUTINES

Fig. 8

Summary

- The ALADDIN data structure allows a wide variety of data types to be accommodated within a common interface. Maximum flexibility is provided to handle complex data, while retaining simplicity for simple data.
- The data can be efficiently searched and accessed at a variety of levels, thereby providing a broadly based medium for data manipulation and exchange. Basic access begins with text editors and hardcopy output, while the ALADDIN interactive code provides higher level searching and manipulation capabilities. The associated ALPACK subroutine package provides straightforward access to ALADDIN data files for plasma modeling codes.
- Careful thought must be given to choosing a set of standard data representations, in order to avoid creating awkward labeling constructs or fitted forms which might blunt the usefulness of the ALADDIN database.
- Finally, of course, we have the important task of providing comprehensive sets of evaluated atomic and molecular data in ALADDIN form.

ALADDIN Interactive Program

ALADDIN.FOR

ALADDIN ALADDIN driver program
ALL "L" and "SL" commands
ALS "S" command
ALG "G" and "N" commands
ALD "D" command
ALR "R" command
ALF "F" command
ALOF "OF" command
ALEF "EF" command
ALWR "WR" command
ALH "H" command
ALQMRK commands containing "?"
ALQF "QF" command
ALEX "EX" and "EN" commands

ALEV.FOR

ALEV "EV" command; user accessible to add new data types
ALEV1D handles interactive generation of data series for ALEV

ALCOM.FOR contains common blocks for ALADDIN program

ALPACK Interface Package for User's Codes

ALPACK.FOR

ALREAD read next entry from ALADDIN data file
ALPARS standard parser for ALADDIN entries
ALXLBL extracts blank-delimited labels from character string
ALCOMP ALADDIN standard label comparator
ALCIEQ case-insensitive character string .EQ. function
ALRECF converts coefficient field to real numbers

ALPCOM.FOR contains common blocks for ALPACK routines

ALFLIB.FOR

ALMEWE calculate #MEWE type fits
ALTAB1 calculate #TAB1D type tabular data
ALCHEB calculate #CHEB Chebyshev polynomial fits

Sample Data and Dictionary Files

AL.DAT sample ALADDIN data file (from 2/26/88 preprint)

ORNL.DAT sample ALADDIN data file (from R. Phaneuf, ORNL)

AL.QDC sample query dictionary file

CALLING STANDARD-FORM 1-D EVALUATION ROUTINES
IN SUBROUTINE ALEV

```
IF(BL(NBL) .EQ. '#MEWE') THEN
  WRITE(LUTOUT,
    & '(/" MEWE SPECTRAL LINE EXCITATION RATE COEFFICIENT (cm3/s),"',
    & /" AS FUNCTION OF ELECTRON TEMPERATURE (keV)")')
  CALL ALEV1D(ALMEWE)
C
C-----
C
  ELSE IF(BL(NBL) .EQ. '#TAB1D') THEN
    WRITE(LUTOUT,
      & '(/" GENERAL ONE-DIMENSIONAL TABULAR DATA")')
    CALL ALEV1D(ALTAB1)
C
C-----
C
  ELSE IF(BL(NBL) .EQ. '#CHEB') THEN
    WRITE(LUTOUT,
      & '(/" ORNL:CFADC CHEBYSHEV POLYNOMIAL FIT")')
    CALL ALRECF(CF, NCF, NCFMX, ERRMSG)
    IF(NCF .NE. 11 .AND. ERRMSG .EQ. '')
      & ERRMSG = 'INCORRECT NUMBER OF COEFFICIENTS'
    IF(ERRMSG .EQ. '') THEN
      WRITE(LUTOUT, '(/" (INPUT VALID RANGE FROM",
        & 1PE10.2, " TO", 1PE10.2, ")")') CF(10), CF(11)
    ELSE
      WRITE(LUTOUT, '(/1X,A)' ERRMSG
      RETURN
    ENDIF
    CALL ALEV1D(ALCHEB)
```

STANDARD 1-D EVALUATION SUBROUTINE ARGUMENT LIST

SUBROUTINE EVSUB(PX, PCF, PNCF, PY, KERMSG)

AL.QDC

HELP?

TO QUERY THE ALADDIN DICTIONARY ABOUT AN ALADDIN LABEL, TYPE THE LABEL FOLLOWED BY A QUESTION MARK

FOR A SUMMARY OF ALADDIN INTERACTIVE COMMANDS USE THE COMMAND "H"

SLEXR ?

SPECTRAL LINE EXCITATION RATE
(PRESENT FORM PPPL:RAH)

CEX?

CHARGE EXCHANGE
(PRESENT FORM FROM ORNL:CFADC)

#MEWE ?

GENERALIZED GAUNT FACTOR LINE EXCITATION CALCULATION
REFERENCE: R. MEWE, ASTRON. AND ASTROPHYS. 20, 215 (1972)

INPUT: ELECTRON TEMPERATURE (keV)
RETURNS: SPECTRAL LINE EXCITATION RATE COEFFICIENT (CM³/S)

#MEWE DATA TYPE COEFFICIENTS ARE (IN ORDER):

- 1) EXCITATION WAVELENGTH (ANGSTROMS)
- 2) EXCITATION ENERGY (EV)
(IF PEIJ=0, ASSUME A RESONANCE LINE AND CALCULATE EIJ FROM PWVL)
- 3) OSCILLATOR STRENGTH
- 4) BRANCHING RATIO
- 5-8) A, B, C, D COEFFICIENTS FOR MEWE GAUNT FACTOR FORMULA

#TAB1D ?

GENERAL ONE-DIMENSIONAL TABULAR DATA TYPE

ARBITRARY NUMBER OF (X,Y) DATA PAIRS ARE SUPPLIED AS COEFFICIENTS:

X1, Y1, X2, Y2, ...

THESE (X,Y) DATA PAIRS MUST BE ENTERED IN ORDER WITH X STRICTLY INCREASING.

EVALUATION OF #TAB1D DATA USES LINEAR INTERPOLATION BETWEEN THESE (X,Y) DATA PAIRS TO RETURN A Y VALUE FOR A SPECIFIED X. IF THE GIVEN X IS BELOW THE FIRST X DATA VALUE OR LARGER THAN THE LAST X DATA VALUE, AN ERROR RETURN OCCURS.

#CHEB?

CHEBYSHEV POLYNOMIAL FITTING FROM ORNL:CFADC

Reference:

Electron Impact Ionization Data for the Iron Isoelectronic Sequence
Pindzola, Griffin, Bottcher, Younger, and Hunter
Nuclear Fusion Special Supplement p.21 (1988)

USED TO FIT CROSS SECTIONS (CM**2) VERSUS ENERGY (EV/AMU)
AND RATE COEFFICIENTS (CM**3/S) VERSUS MAXWELLIAN TEMPERATURE (EV)

THE POLYNOMIAL COEFFICIENTS ARE THE FIRST 9 ENTRIES IN THE COEFFICIENT FIELD. THESE FITS ARE VALID ONLY BETWEEN THE ENERGY OR TEMPERATURE LIMITS WHICH ARE GIVEN AS COEFFICIENT FIELD ENTRIES 10 AND 11.

ORNL:CFADC?

OAK RIDGE NATIONAL LABORATORY: CONTROLLED FUSION ATOMIC DATA CENTER

CONTACT: DR. R. PHANEUF

PPPL:RAH?

PRINCETON PLASMA PHYSICS LABORATORY: RUSSELL A. HULSE

LABELING FOR ALADDIN DATA ENTRIES

The structure and format of ADADDIN allows considerable flexibility in defining labels for atomic and molecular data. The major initial application will be for collision data, although spectroscopic data may be accommodated with equal facility. The working group for the A & M dictionary has established guidelines for labelling and indexing collision processes, and has produced a dictionary of fusion-relevant processes. Based on these guidelines, specific labelling conventions are proposed, and examples are presented of suggested ALADDIN formats for a number of fusion-relevant collision processes.

I. HIERARCHICAL SEARCH LABELS.

In establishing conventions for the hierarchical search labels, an attempt has been made to strike a compromise between generality and completeness in specification of a reaction, and ease of search and retrieval. In each case, the nature of the particular process, the type of data available for it, and its application in fusion have been considered.

While it will be desirable to have uniform label formats for all processes and data sources, it is not essential for data exchange using ALADDIN. In a particular data file, the label format used for a given process can easily be examined by the ALADDIN user by searching the data file for that process (using the dictionary abbreviation which will always be the first hierarchical label) and using wild-card defaults for the reactant string. One may also sequentially "read through" the data file using the "next entry" (N) and the "display entry" (DE) or "display labels" (DL) commands. A user constructing his own ALADDIN data file from a number of different source files can also modify the format using a text editor.

To simplify searching, labels representing quantum states should be included only where they are needed to define the process being represented, and where included, they should be concatenated into a single hierarchical label (i.e. should contain no blank spaces). Similarly, labels for reaction products should be included only when they are needed to define a particular reaction. Plans call for future versions of ALADDIN to permit "wildcard" specifications within a label (either character-by-character or on the remainder of that label), and thus search capabilities will be both augmented and simplified.

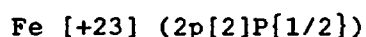
The suggested ordering of hierarchical labels for two-body collisions is as follows:

Process label from dictionary:	PROCESS
First reactant/projectile:	SYMBOL [CHARGE] (quantum state)
Second reactant/target:	SYMBOL [CHARGE] (quantum state)
First product/projectile after collision:	SYMBOL [CHARGE] (quantum state)
Second product/target after collision:	SYMBOL [CHARGE] (quantum state)
Other reaction products:	SYMBOL [CHARGE] (quantum state)

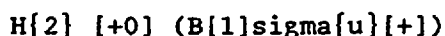
Conventions and Special Cases:

1. The chemical symbols defining reactant species and charge-state designation [+q] are mandatory for heavy particles.
2. Electrons are always designated by the symbol e and have no charge or quantum-state designation.
3. Electrons are always the first reactant.
4. In ion-neutral collisions, the ion is always the first reactant.
5. In ion-ion collisions, the ion with the higher charge is the first reactant, or the ion with the smaller mass if the charges are equal.
6. In atom-atom collisions, the lighter species is always the first reactant. In atom-molecule collisions, the atom is always the first reactant; in molecule-molecule collisions, the molecule with the smaller number of atoms is the first reactant.
7. Reaction products are optional except when required to specify a particular reaction channel.
8. Quantum states are included only where needed to specify the reaction, and are enclosed in regular parentheses. The ground state of an atom or atomic ion is denoted by (G). Filled core electron shells or subshells are omitted.
9. The ground electronic state of a molecule or molecular ion is denoted by (X).
10. Other electronic states are labelled according to the normal spectroscopic conventions. Superscripts are enclosed in square brackets, e.g. (2p[5]), and subscripts are enclosed in braces, e.g., H{2} for molecular hydrogen, H{2} [+1] for the molecular hydrogen ion. The quantum state designation $n l^i 2s+1 L_j^p$ is written: (nl[i][2s+1]L[j][p]). Greek symbols are spelled out as sigma, pi, delta, phi, omega, epsilon, lambda. Subscripts precede superscripts if there is an ambiguity.

An example of hierarchical labels for the first excited state of Li-like iron would be:



The $B^1\Sigma_u^+$ 2p σ electronic state of molecular hydrogen would be:



II. BOOLEAN SEARCH LABELS.

It was agreed that certain Boolean search labels should be mandatory. While the order of these labels is irrelevant to ALADDIN, some uniformity is desirable for ease of identification of the content of data files. The required labels are, in recommended order:

1. Data type: XS for cross section, RC for rate coefficient, WL for wavelength, EN for energy, TP for transition probability, LT for lifetime.
2. Data class: REC, recommended by IAEA; EVAL, critically evaluated or recommended data; COMP, data compilation; FORM, analytic formula; ORIG, original source.
3. Estimated accuracy: ACC=C.
4. Data Source: abbreviation for Data Center, University, etc.

5. Reference: DOC=abbreviation pointing to documentation in dictionary file (e.g. reference to publication).
6. Date entered into file or last revised: day/month/year.
7. Other optional labels.
8. The last Boolean label, which begins with # (e.g. #CHEB) points to the subroutine which is used to recover the data from the fitting parameters, or to interpolate between tabular x,y data (e.g. #TAB1D). This subroutine must be incorporated into ALADDIN in order to retrieve that particular data.

An ultimate objective will be for the IAEA to produce, in collaboration with the A+M Data Center Network, one recommended data set for each reaction, which will be assigned the Boolean label REC as noted above. The estimated accuracy scale is based on criteria established at the IAEA Specialists' Meeting on Carbon and Oxygen Collision Data for Fusion Plasma Research (May 12-13, 1988). This scale is as follows:

3% or better	A+
between 3% and 10%	A
between 10% and 25%	B
between 25% and 50%	C
between 50% and 100%	D
worse than a factor of 2	E

The recommended (default) units for the various physical parameters are as follows:

Collision cross section	cm[2]
Collision rate coefficient	cm[3]/s
Three-body rate coefficient	cm[6]/s
Electron Energy	eV
Heavy-particle energy	eV/u (or eV/amu)
Temperature (kT)	eV
Level energy	eV
Wavelength	nm
Lifetime (or decay rate)	s (or /s)

Use of any other units should be stated clearly in a comment line in the ALADDIN data file.

Since labels are de-limited by spaces, and since the total number of adjacent spaces is unimportant to ALADDIN, creative use of multiple spaces can facilitate the visual identification of data entries. Sample ALADDIN data entries for a number of common fusion-relevant processes follow.

III. EXAMPLES OF ALADDIN DATA FORMATTING

A. COMPLETE SAMPLE DATA FILE ENTRIES

1. Charge Exchange Cross Section (to all product quantum states):

```
$ CX O [+5] H [+0]
& XS EVAL ACC=C ORNL-CFADC DOC=ORNL-6090 6/7/88 #CHEB
-68.588100000 -2.676120000 -1.815780000 -1.077430000 -0.743688000
-0.413203000 0.173738000 -0.019629000 0.071981800 1.000 420000.0
```

2. Charge Exchange into a Specific Quantum State (Cross Section):

```
$ CXSS O [+6] H[2] [+0] O [+5] (4s) H[2] [+1]
& XS COMP ACC=C RIC-NAGOYA DOC=IPPJ-AM-56 6/7/88 #TAB1D
!eV/u, cm[2]
1.0E3 1.2E-15 1.2E3 1.2E-15 1.9E3 1.0E-15 3.0E3 8.4E-16 4.0E3 6.0E-16
5.8E3 3.0E-16 7.5E3 2.6E-16
```

3. Double Charge Exchange Cross Section:

```
$ CX2 C [+4] He [+0]
& XS EVAL ACC=C ORNL-CFADC DOC=ORNL-6090 14/7/88 #CHEB
-76.288500000 -3.236860000 -2.381690000 -0.343270000 -0.173548000
0.185487000 0.081984400 -0.069984100 -0.067464800 30.000 600000.0
```

4. Electron-Impact (Single) Ionization Cross Section:

```
$ ION e He [+1]
& XS EVAL ACC=A BELFAST DOC=JPCRD-1 7/7/88 #BELFI
54.42 .1845 .089 .131 .388 -1.091 1.354
```

5. Electron-Impact (Single) Ionization Rate Coefficient:

```
$ ION e Fe [+10] (G)
& RC EVAL ACC=B ORNL-CFADC DOC=NUC-FUS-SUPP/87 27/7/88 #CHEB
-47.6203 5.69424 -3.96549 1.64309 -0.582510 0.196176 -.0645722 0.0
0.0 20. 2.E4
```

```
$ ION e Fe [+10] (3p[3]3d)
& RC EVAL ACC=C ORNL-CFADC DOC=NUC-FUS-SUPP/87 27/7/88 #CHEB
! Ionization from metastable states
-46.1026 4.66058 -3.30853 1.31704 -0.451134 0.150961 -0.0518364
0.0 0.0 20. 2.E4
```

6. Heavy-Particle (Single) Ionization Cross Section:

```
$ ION C [+6] He [+0]
& XS EVAL ACC=C ORNL-CFADC DOC=ORNL-6090 6/7/88 #CHEB
-71.415800000 -0.433084000 -0.787646000 0.287762000 -0.061766300
-0.015559100 0.023577300 -0.005561580 -0.010240800 7.0E4 1.0E6
```

```
$ ION H [+1] H[2] [+0] H[+1] H[2] [+1] (v<10) e
& XS EVAL ACC=C PPPL DOC=H-HE-PLASMA 26/7/88 #JANKS
1.681920096116E1 -8.751084517093E1 5.024534132103E1 -1.560982391827E1
2.931478842554E0 -3.421137108600E-1 2.429148918124E-2 -9.612735627840E-4
1.625014598463E-5
```

7. Electron-Impact Excitation Rate Coefficient:

```
$ EXC e Fe [+23] (G) e Fe [+23] (2p[2]P[o])
& RC EVAL ACC=C BELFAST DOC=NUC-FUS-SUPP/87 7/7/88 #KINGEX
4.695E1 -.15188198E5 .17109807E5 -.84276377E4 .23662952E4 -.41379184E3
.46106556E2 -.31945927E1 .12577721 -.21536872E-2
```

8. Heavy-Particle Excitation Cross Section:

\$ EXC He [+2] H [+0] (G) He [+2] H [+0] (n=5)
& XS FORM ACC=D PPPL DOC=H-HE-PLASMA 26/7/88 #FORM1
! Accuracy varies over energy range from C to E
5 1.394E-2

B. OTHER SAMPLE PROCESS (HIERARCHICAL) LABELS

1. Dielectronic Recombination (Total):

\$ DREC e O [+5] O [+4]

2. Dielectronic Recombination (For Specific Excitation):

\$ DREC e O [+5] (G) O [+4] (1s2s2pnl)

3. Radiative Recombination (Total):

\$ RREC e O [+6] O [+5]

4. Dissociative Ionization:

\$ DISION e H{2} [+1] e H [+1] H [+1] e
\$ DISION He [+2] H{2} [+0] He [+2] H [+0] H [+1] e

5. Particle Exchange:

\$ PX H [+1] D{2} [+0] HD [+1] D [+0]
\$ PX H{2} [+1] H{2} [+0] H{3} [+1] H [+0]

6. Dissociative Charge Exchange:

\$ DISCX H [+1] D{2} [+0] H [+0] D [+1] D [+0]

7. Electronic Excitation of a Molecule:

\$ EXC H [+1] H{2} [+0] (X) H [+1] H{2} [+0] (C[1]pi{u})

8. Double Ionization:

\$ ION2 He [+2] He [+0]

9. Vibrational Excitation (v):

\$ VIBEXC e H{2} [+0] (1) e H{2} [+0] (2)

10. Rotational Excitation (j):

\$ ROEXC H [+1] CH{4} [+0] (4) H [+1] CH{4} [+0] (6)

11. Rotational-vibrational Excitation (v,j):

\$ ROVIBEXC e CO [+0] (0,3) e CO [+0] (1,5)

12. Three-body Electron-Ion Recombination:

\$ 3-REC-HP e H [+1] H{2} [+0]
\$ 3-REC-EL e H [+1] e

13. Electron Removal (from Target):

\$ ELREM C [+6] H [+0]

14. Spectral Line Emission:

\$ LEM H [+1] H{2} [+0] 486

15. Spectral Band Emission:

\$ BEM e H{2} [+0] 122 145

16. Ion Production:

\$ IP H [+1] He [+0]

IV. SAMPLE ALADDIN DICTIONARY FILES

A. GENERAL ALADDIN GLOSSARY (incomplete)

CX ?

Single Charge exchange (summed over product ion quantum states). This is also frequently referred to as single electron capture or charge transfer. Reactant quantum states need not be specified.

CX2 ?

Double charge exchange (electron capture, charge transfer) summed over product quantum states.

CXSS ?

Single charge exchange (electron capture, charge transfer) into a particular product ion quantum state (state-selective).

ION ?

Single ionization of the target (second reactant) by electron or heavy particle impact. ION2 refers to double ionization, ION3 to triple ionization, etc.

ION2 ?

Double ionization of the target by electron or heavy particle impact.

EXC ?

Excitation of the target (second reactant) by electron or heavy particle impact. Quantum states of the second reactant and second product are specified.

REC ?

Data recommended by IAEA Atomic and Molecular Data Unit

EVAL ?
Data evaluated and/or recommended by a source other than the IAEA
Atomic and Molecular Data Unit

COMP ?
Data compilation

FORM ?
Analytical formula

ORIG ?
Taken from original data source

XS ?
Cross section in cm²

RC ?
Rate Coefficient in cm³/s

DOC ?
Reference source for data

{ } ?
Subscript

[] ?
Superscript

() ?
Quantum state (where needed to specify reactant or product)

B. DICTIONARY TO ACCOMPANY DATA FILE

BELFAST ?
Belfast Data Base on Atomic and Molecular Physics
Department of Computer Science
The Queen's University of Belfast
Belfast BT7 1NN, U.K.

ORNL-CFADC ?
Controlled Fusion Atomic Data Center
Oak Ridge National Laboratory
P. O. Box 2008
Oak Ridge, TN 38731-6372
USA
Telephone: (615)-574-4707 [FTS: 624-4707]
COMPUTER NETWORK COMMUNICATIONS ADDRESS: PHANEUF@ORN.MFENET

PPPL ?
Princeton Plasma Physics Laboratory
P.O. Box 451
Princeton, NJ 08544 USA

RIC-NAGOYA ?

Research Information Center
Institute of Plasma Physics
Nagoya University
Chikusa-ku, Nagoya 464, Japan

#CHEB ?

ORNL Chebyshev polynomial fitting subroutine. The parameter list consists of nine polynomial coefficients followed by two additional parameters which define the lower and upper limits for the independent variable over which the fit is valid. For a reference, see page 40 of the document DOC=NUC-FUS-SUPP/87.

#FORM1 ?

Analytic formula for cross section. Coefficients are, in order:
n = principal quantum number of final state
f[ln] = oscillator strength for 1s-np transition
See DOC=H-HE-PLASMA (subroutine yet to be written!)

#JANXS ?

PPPL subroutine (yet to be written!) to calculate cross section in cm² versus projectile energy in eV from 9-term polynomial fit. See DOC=H-HE-PLASMA.

#KINGEX ?

Belfast subroutine (yet to be written!) for electron-impact excitation rate coefficient calculation from fitting parameters. See DOC=JPCRD-1.

#TAB1D ?

GENERAL ONE-DIMENSIONAL TABULAR DATA TYPE
ARBITRARY NUMBER OF (X,Y) DATA PAIRS ARE SUPPLIED AS COEFFICIENTS
X1, Y1, X2, Y2, ...
THESE (X,Y) DATA PAIRS MUST BE ENTERED IN ORDER WITH X INCREASING.
EVALUATION OF #TAB1D DATA USES LINEAR INTERPOLATION BETWEEN THESE (X,Y) DATA PAIRS TO RETURN A Y VALUE FOR A SPECIFIED X. IF THE GIVEN X IS BELOW THE FIRST X DATA VALUE OR LARGER THAN THE LAST X DATA VALUE, AN ERROR RETURN OCCURS.

DOC=H-HE-PLASMA ?

"Elementary Processes in Hydrogen-Helium Plasmas," R.K. Janev, W.D. Langer, K. Evans and D.E. Post, Jr., Springer Series on Atoms and Plasmas, Springer-Verlag (Berlin, Heidelberg, New York) 1987.

DOC=IPPJ-AM-56 ?

"Total and Partial Cross Sections for Electron Capture for C[q+] (q=6-2) and O[q+] (q=8-2) Ions in Collisions with H, H[2] and He Atoms," H. Tawara, Report IPPJ-AM-56, Institute of Plasma Physics, Nagoya University, October, 1987.

DOC=JPCRD-1 ?

"Recommended Cross Sections and Rates for Electron Ionisation of Light Atoms and Ions," K.L. Bell, H.B. Gilbody, J.G. Hughes, A.E. Kingston and F.J. Smith, J. Phys. Chem. Ref. Data 12, 891-916 (1983).

DOC=NUC-FUS-SUPP/87 ?

"Recommended Data on Atomic Collision Processes Involving Iron and its Ions," C. Bottcher, D.C. Griffin, H.T. Hunter, R.K. Janev, A.E. Kingston, M.A. Lennon, R.A. Phaneuf, M.S. Pindzola and S.M. Younger
Special Supplement to Nuclear Fusion, 1987.

DOC=ORNL-6090 ?

Atomic Data for Fusion, Volume 5

"Collisions of Carbon and Oxygen Ions with Electrons, H, H[2] and He"

R.A. Phaneuf, R.K. Janev and M.S. Pindzola

Oak Ridge National Laboratory Report ORNL-6090, February, 1987