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Automation of the Ion Energetics Data Center

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U.S. DEPARTMENT OF COMMERCE, Juanita M. Kreps, *Secretary*

Dr. Sidney Harman, *Under Secretary*

Jordan J. Baruch, *Assistant Secretary for Science and Technology*

NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Acting Director*

Abstract

The Ion Energetics Data Center is engaged in the compilation, evaluation and dissemination of experimental information on gaseous ion energetics. Outputs include bibliographic and tabular information on ionization potentials, appearance potentials, electron affinities and heats of formation of gaseous positive and negative ions. The operation of the data center is discussed. This operation has recently been automated by the development of a set of computer programs, called IONPACK, which minimize the manual effort required for the numerous file manipulations and editing steps necessary to produce the data center output. The functions of the programs are outlined and the associated operating procedures are described in detail. Full documentation of the programs is presented in a separate report.

CONTENTS

1. THE ION ENERGETICS DATA CENTER

1.1 Introduction

The Ion Energetics Data Center has recently carried out a major automation of its scientific data processing activities. The present report is a detailed description of the newly automated data center activity, prepared in order to provide:

a. an acccurate record of the objectives, mechanics, and procedures of the data center for its own staff.

b. a well defined point of departure for future additions and modifications of the automated system.

c. a detailed example of data center automation which may be of use to other data centers.

The report is divided into three parts describing the technical subject matter and objectives of the data center (Section 1), the structure and function of the automated information processing system (Sections 2 to 5), and, lastly, a detailed operating manual for the technical information specialist responsible for the effective implementation of the various automated information processing steps comprising the system.

1.2 The Subject Matter - Ion Energetics

For purposes of the present report the term ion energetics includes most experimental data which can be interpreted or extrapolated to yield standard heats of formation of gaseous positive ions. Examples of such data include measurements of ionization and appearance potentials by a variety of techniques including vacuum ultraviolet spectroscopy,

photoionization, electron spectroscopy, electron impact, surface ionization, empirical relationships between charge transfer spectra and ionization potentials. These techniques differ greatly in their accuracy depending both on the degree of care and refinement of their experimental realization and, frequently, also on the molecular structure and complexity of the system studied. Details of the various techniques, their accuracies and associated problems of data interpretation are described in a recent critical review.[1]

In 1969 and 1977 the Data Center compiled, evaluated, organized and disseminated this type of ion energetics data in the form of published data compilations[2,3]. A typical page of the 1977 compilation is shown in figure 1. All measurement information pertinent to one ion is organized in a form showing the nature of the ionic species, its electronic state where known, the molecular system studied (reactant), other products formed in the ionization process (where known), the experimental datum and its quoted accuracy or precision, an acronym describing the experimental technique (see Table 4, page 31), the heat of formation derived from the measurement datum for those measurements which are judged most reliable, and the reference number or numbers. The latter are random access ion numbers of the individual articles in the data center document files. The last line of the figure shows a name for the compound $(CH_2)_2O$ for which a one-line formula representation is not sufficient to uniquely indicate its chemical composition, namely the ring compound 1,2-epoxyethane.

In addition to this main table, the compilation also contains an ion index bibliography, author index, and diverse auxiliary information.

Ion	Reactant	Other products	Ionization or appearance potential (eV)	Method	Heat of formation (kJ mol^{-1})	Ref.
			CD_3^+			
CD_3^+	CD_3		9.832±0.002	S		349
CD_3^+	CD_4	D	14.38±0.03	PI		1128
CD_3^+	CH_3CD_3	CH_3	15.10±0.10	EI		2421
CD_3^+	C_2D_6	CD_3	15.54±0.10	EI		2421
CD_3^+	CD_3COOH		15.56	EI		171
CD_3^+	CD_3Cl	Cl	13.8	PI		2637
		$CH_4^+(^2B_2)$	**$\Delta H_{f0}^\circ \leq 1150$ kJ mol^{-1} (275 kcal mol^{-1})**			
		$CH_4^+(^2A_1)$	**$\Delta H_{f0}^\circ = 2094$ kJ mol^{-1} (500 kcal mol^{-1})**			
$CH_4^+(^2B_2)$	CH_4		≤12.615±0.010	PI	≤1150	3415
$CH_4^+(^2B_2)$	CH_4		12.704±0.008	PI		1253
$CH_4^+(^2B_2)$	CH_4		12.71±0.02	PI		1128
$CH_4^+(^2B_2)$	CH_4		12.55±0.05	PI		2013
$CH_4^+(^2B_2)$	CH_4		12.75±0.05	RPI		2857, 2858, 3293
$CH_4^+(^2B_2)$	CH_4		12.70	PE		2803
$CH_4^+(^2B_2)$	CH_4		12.75	PE		3092
$CH_4^+(^2B_2)$	CH_4		12.78	PE		3116
$CH_4^+(^2B_2)$	CH_4		12.9	PEN		2430
$CH_4^+(^2B_2)$	CH_4		≤12.70	EM		2798
$CH_4^+(^2B_2)$	CH_4		13.00±0.02	RPD		224
$CH_4^+(^2B_2)$	CH_4		12.99±0.05	RPD		2776

The ion ground state has a large Jahn–Teller distortion, see for example R. N. Dixon, Mol. Phys. **20**, 113 (1971), F. A. Grimm and J. Godoy, Chem. Phys. Letters **6**, 336 (1970) and refs. 3092, 3116, 3119. Consequently the onset is not sharp and the adiabatic value may be lower. Several PE studies (refs. 2803, 3092, 3119) have resolved vibrational structure near onset with a separation of ~1200 cm^{-1} (0.15 eV). This is just the difference between the PI threshold value given by Brehm, ref. 2013, and those determined by Nicholson, ref. 1253, and Dibeler *et al.*, ref. 1128.

See also – S: 138
PI: 182, 230, 331, 416, 2605, 3115, 3132
PE: 1130, 2801, 2829, 2843, 3072, 3119, 3132
PEN: 2467
EI: 289, 1072, 1129, 2136, 2154, 2414, 2535, 2575, 3435

$CH_4^+(^2A_1)$	CH_4		22.39	PE	2094	3092
$CH_4^+(^2A_1)$	CH_4		22.4	PE		3119
$CH_4^+(^2A_1)$	CH_4		23.1 (V)	PE		3072
$CH_4^+(^2A_1)$	CH_4		24	RPD		2414
$CH_4^+(^2A_1)$	CH_4		23.5–24	D		2846

Earlier electron impact work (refs. 289, 1072) gave values around 19.4 eV. These are due to autoionization or collision processes, see refs. 2414, 2575, 2846.

CH_4^+	C_3H_6		14.7±0.5	EI		2542
CH_4^+	$(CH_2)_2O$ (1,2-Epoxyethane)	CO	12.3±0.2	EI		50

Figure 1. A typical page of the 1977 compilation.

1.3 Objectives of the Automation Effort

The purpose of the automation effort is to automate to the maximum feasible extent the many routine data management activities associated with the creation, updating, and editing of the many ordered files, all of which are ultimately derivable from the abstracted document. The automated data management system described here is designed to provide a set of computer files which are suited for computer typesetting via the Government Printing Office Linatron machine. Finally, the system is designed to allow the extraction of chemically meaningful subsets of information such as topical bibliographies and information on specific ions or classes of ions. Ultimately, it is hoped to develop a data base that can be interrogated and output via a remote terminal and at the same time to provide ordered, edited material suitable for typesetting. At present, the latter objective has dominated our planning.

It is planned to issue from time to time supplements to the existing compilation which lists the more recent unevaluated measurements and associated references in ordered form. Then, when the unevaluated data file is brought up-to-date, it is planned to combine the material with the 1977 data compilation and to produce a revised, updated compilation.

1.4 Activities

The activities leading to these objectives can be divided into three categories.

a. Searching, abstracting and encoding the abstracted information.

b. Processing of the encoded information to yield various desired files and outputs. We note here explicitly that part of the

processing involves, stripping, sorting and ordering the information on the abstracts.

c. Merging the information with the existing compilation, evaluating and editing the new body of information and producing a new typeset hard copy.

Needless to say, the objective of producing a new compilation which is merged with the existing one imposes the necessity of generating information files which are as similar as possible in format and ordering philosophy to the existing compilation.

2. THE INFORMATION

2.1 The Abstract

The abstract consists of all ion data from a given document with associated citation information. The data are discussed in detail below. This is the fundamental document from which all subsequent files and outputs are derived. Thus it is extremely important to check the accuracy of abstracting and encoding.

A form as filled out by the abstractor is shown in figure 2. The ID number or accession number of the reprint is added to the form and the reprint by the scientific data clerk at the time for encoding. The computer program will associate it with each ion datum.

The author, title and reference are checked and modified by the scientific data clerk for consistency of format and abbreviation.

Since almost all papers employ only one method, the abstractor circles the appropriate method, and the scientific data clerk will associate it with each ion datum as it is encoded. If a paper cites

ID #

AUTHOR: Benezra, S. A. and Bursey, M. M

INT. DATE

ABSTR. OHS "/E

REF. CK. ____ ____

NOM. CK. ____ ____

KEYED IN ____ ____

PROOFED ____ ____

SHEET # 1 of 8

TITLE: ortho- Effects on ordering factors in mass spectral rearrangements. Loss of ketene from halogenated phenyl acetates and acetanilides.

REFERENCE: J. Chem. Soc. B, 1516 (1971).

CODE	ION + STATE	MOLECULE	OTHER PRODUCT	APPEARANCE POT.	OTHER MEAS.
	$C_8H_6O_2F_2^+$	$C_6H_3F_2OCOCH_3$ (2,4-Difluorophenyl acetate) (RN 36914-77-9)		8.60±0.03	
	$C_6H_4OF_2^+$		$CH_2=CO$	9.63±0.03	
		SAME			
	$C_6H_5NF_2^+$	$C_6H_3F_2NHCOCH_3$ (N-(2,4-Difluorophenyl)acetamide) (RN 399-36-0)	$CH_2=CO$	9.93±0.03	
	(MIT) (TR)				
	$C_8H_7NOF^+$			8.76±0.03	
	(CD 0.08)	SAME			
	$C_2H_3O^+$			8.92±0.03	
		SAME			

COMMENTS:

Figure 2. The abstractor's form.

METH. D S PI

EM RPD EDD SRF

NRE FD SD

(EI) PE AUG RFI

two or more methods, provision is made in the other method column for entering the other method acronym.

At the left hand margin of the form, five columns are set aside for flagging symbols which are entered by the scientific data clerk at the time of encoding. The nature and purpose of the flagging is described in a later section.

After encoding, the written abstract form is attached to the reprint and filed. The encoded form of the abstract is shown in figure 3.

Detailed guidelines for abstracting are given in a separate document.[4]

2.2 The Basic Unit of Information

The basic unit of information of the data base is the numerical value of a measurement relating to a particular ionic species and its associated detail and documentation. We will call this an ion datum. It consists in all cases of the following items of information arranged horizontally

ION	REACTANT	OTHER PRODUCT	AP or IP (eV)	METHOD	REF

and a number of parenthetical comments.

2.2.1 Ion - The ion is always represented by an empirical molecular formula and a charge. In addition, where pertinent, the electronic state of the ion is also given in parentheses.

Examples: CH_3^+, Ar^{+4}, $Ne^+(^2P_{3/2})$, $N_2O^+(X^2\Pi_{1/2})$, N_2^{+3}, $C_3H_6^+$

2.2.2 Reactant - This is the species on which the measurement is made. It consists in most, but not all, instances of stable gas phase molecules in their ground electronic state. Occasionally this species may consist

2.2.3 Other Product - In some processes leading to ion energetic information, the ion of interest is formed by fragmentation of the subject molecule, and is thus accompanied by another atomic, ionic or polyatomic fragment species. Such processes include

$$C_2H_6 + e \rightarrow C_2H_5^+ + H + 2e$$

$$CH_3Cl + h\nu \rightarrow CH_3^+ + Cl^-$$

$$C_6H_5C_2H_5 + e \rightarrow C_7H_7^+ + CH_3 + 2e$$

(Ethylbenzene)

$$N_2O + h\nu \rightarrow NO^+ + N(^4S_o) + e$$

All products except electrons are tabulated under other products. In some instances the other product may consist of more than one fragment.

$$B_5H_{11} + e \rightarrow B_5H_7^+ + 2H_2 + 2e$$

2.2.4 AP or IP - This is the measured quantity, the appearance potential (AP) or ionization potential (IP). It is always given in electron volts. The probable error of the quantity is always the one given in the source paper, where stated. Occasionally the AP or IP is given as an upper bound, $\leq$ 10.2 eV or a range 15.4225 - 15.4255 eV or an approximation $\sim$ 10.72 eV.

2.2.5 Method - The ion energetics measurements are carried out by a variety of techniques. They are denoted by two-or three-letter acronyms. The acronyms and names of the methods are given in the accompanying list. The methods are ordered according to generally decreasing reliability, although in some particular instances a

measurement by a "high ranking" method may give a less precise answer than a measurement on the same system by a "lower ranking" method. In general a given paper may give information on one or more ions based on measurements of one or more molecules. But almost always a given paper reports on measurements using only one method. Some of the "methods" are rather indirect, such as use of the Born-Haber cycle or application of semi-empirical relations between charge transfer spectra in solution and gas phase ionization potentials. The methods are described and discussed in detail in reference 1.

2.2.6 Reference - This ties the ion datum to the journal reference and document (reprint) file. It is simply a four-digit accession number.

2.2.7 Associated Comments - There are several purposes for the comments on an ion datum as indicated above. For cyclic compounds a one-line formula representation is inadequate to identify the compound. Therefore it has been decided to provide the name for all such compounds. We have arbitrarily chosen to adopt the Chemical Abstract nomenclature system. However, this nomenclature system is not static, new names are added and old names are ocasionally changed. Thus we have decided to give the CAS Registry Number as well, both for cyclic and acyclic compounds. The Registry Number, although arbitrary, is not subject to change and offers the possibility of entering into other nomenclature and structure representation systems such as the Wisswesser system and schemes for generating formulas and structures by computer techniques. Thus, for acyclic systems we always have the CAS Registry Number and for cyclic systems the CA Name and CAS Registry Number as comments. Besides these two, there are eighteen other comments which given additional information

Table 1. List of Comments and Coding Acronyms (continued)

RC	Mean value of Renner components
NA	Name used by author:
OP	The other product(s) is (are) ____
MT, NI, TR	are used principally as an aid in establishing the validity of other product statement. They may be discarded (or not) in the final revised edition. Use as many as appropriate.
*	One cannot simply give sum of kinetic energies of two successive metastables.
**	The reason is simply that one looks for evidence that one reaction step occurred.
***	Used where limits are impossible to assign to spin-orbit components.
****	Used where there are several CTS values.
*****	Used for transient species produced in ion source by electron impact.
******	Used for ion pair processes.

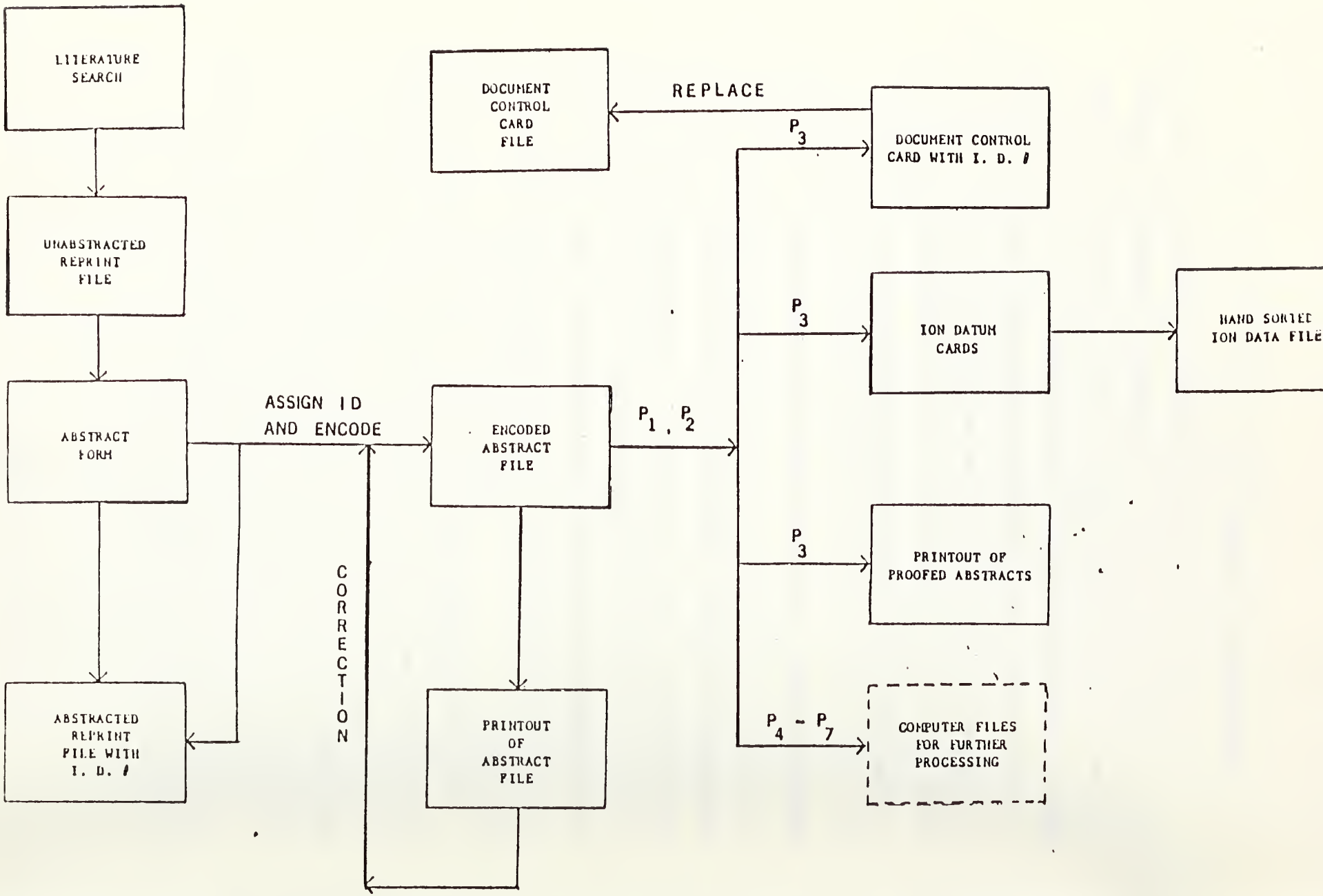
3. DOCUMENT CONTROL AND STATUS FILES

In this section we discuss the logistics and file structure associated with the production of a correct archival tape of abstracted information. The general scheme is shown in figure 4. P_1, P_2, P_3, P_4, P_5, P_6, and P_7 refer to computer programs described in section 5.

The literature search identifies articles which may contain information of interest. As the reprints are processed they are stored in an unabstracted reprint file and a document control card is typed and filed alphabetically by first author. This is an accessible reference file for documents on hand. After a batch of reprints have been abstracted, the abstracts are encoded on a Model 37 TTY, a printout of the encoded material is produced, proofed and, if necessary, corrected. The processed reprints and associated abstracts are stored in a separate file ordered by accession number. The corrected abstract tape is now processed to produce the following printed outputs: a printout of the abstracts in serial order of accession number, a printed document control card with ID number and a series of separate cards, one for each ion datum. Additional outputs are discussed in the next section.

The printed document control card then is used to replace the typed card in the document control file, thus indicating which of the documents have been processed. Also if it is needed to refer to a document by conventional author and journal reference it and/or its abstract can be located in the ID ordered file or the printout of abstracts.

The ion datum cards are further sorted by hand according to molecule composition of the ion and generate a card file useful in locating processed information on a particular ion.


LITERATURE SEARCH
UNABSTRACTED REPRINT FILE
ABSTRACT FORM
ABSTRACTED REPRINT FILE WITH I. D. #
ASSIGN I D AND ENCODE
CORRECTION
ENCODED ABSTRACT FILE
PRINTOUT OF ABSTRACT FILE
DOCUMENT CONTROL CARD FILE
REPLACE
P3
DOCUMENT CONTROL CARD WITH I. D. #
P1 , P2
P3
ION DATUM CARDS
HAND SORTED ION DATA FILE
P3
PRINTOUT OF PROOFED ABSTRACTS
P4 - P7
COMPUTER FILES FOR FURTHER PROCESSING

4. INTERIM OUTPUT FILES AND ORDERED INFORMATION

4.1 Output Files

It was mentioned above that it is intended to prepare during the course of the work a series of raw data supplements for interim use by the user community prior to issuance of the revised compilation. The supplements will list in ordered form all measurements abstracted for the later calendar years, 1972, 1973 etc. as the work progresses. They would be similar in format to the compilation, and will include bibliographies and author indexes. As these are issued it is intended to establish and maintain a set of cumulative files of this type which will ultimately be merged with the existing compilation.

In order to accomplish this it is necessary to separate the abstract information into certain component parts, generate a means of sorting the required parts, i.e. develop and attach a sort key, cumulate the processed batched into files holding the information for a year, sort the files into ordered files, format them and print them. This is shown schematically in figure 5.

4.2 Ordering Principles

4.2.1 Bibliography and Author Index - The ordering principle for the bibliography is, of course, simply the accession number and the author index is alphabetical with the proviso that composite letters such as Å, Č, Û, ü, etc are treated as the corresponding ordinary letters, and hyphens and apostrophes are ignored in the alphabetical ordering process.

4.2.2 Ion Data - The ordering of the ion data is considerably more complex and is based on a hierarchy of four considerations:

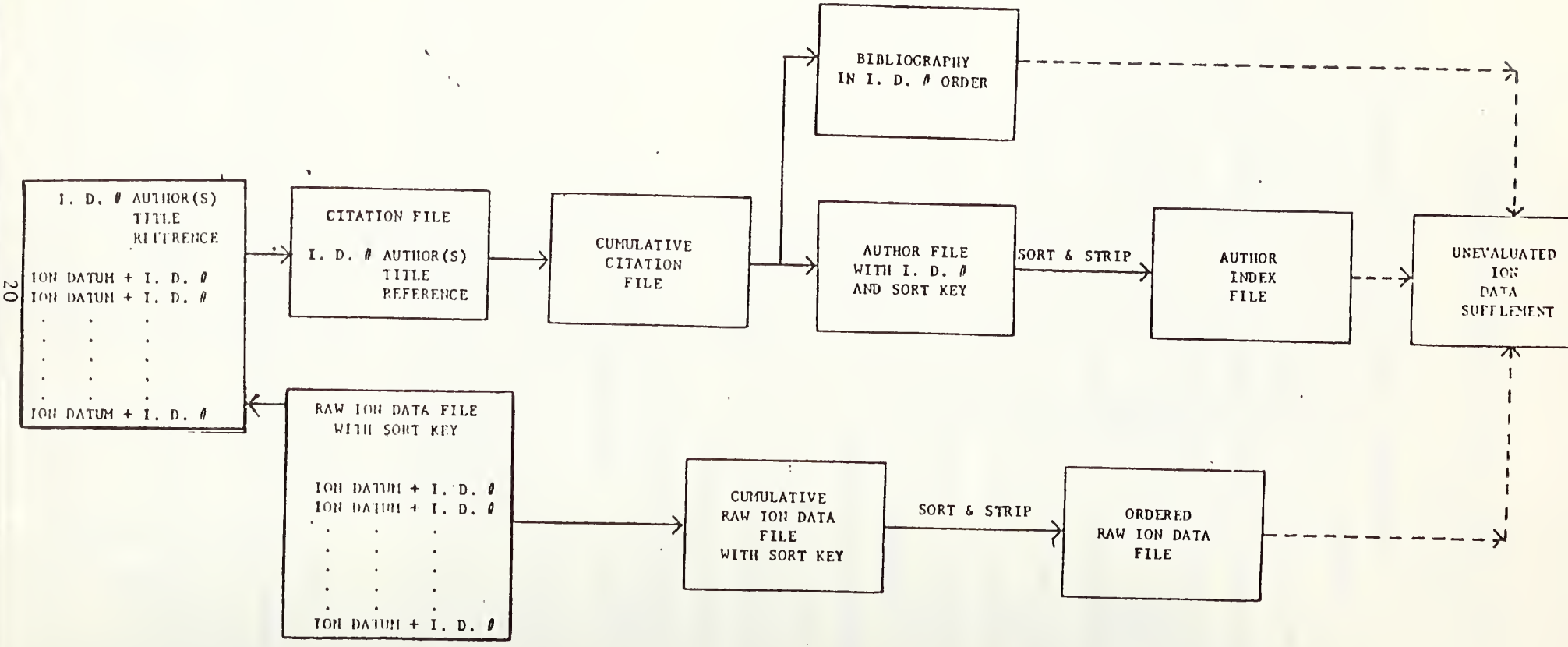


Figure 5. Separating the abstract into various files.

a. Atomic composition, complexity and charge of the ion and reactant species.

b. Chemical nature of the reactant species.

c. The measurement method.

d. The numerical value of the measurement.

A. Atomic Composition, Complexity and Charge

The ordering principle for atomic composition and complexity is expressed in the following way:

Species are grouped in increasing order according to the element of highest atomic number which they contain.

Within each group they are separated into subgroups consisting of species containing one chemical element, two chemical elements, three ... etc.

Within each subgroup those that contain the additional element(s) of lowest atomic number come first and are ordered by increasing number of atoms starting with the element of lowest atomic number.

All isotopes are ignored except for deuterium and tritium which are ordered according to increasing extent to which they substitute for hydrogen. Thus CH_4, CH_3D, CH_2D_2, ... CH_3T and then C_2H_6, C_2H_5D, $C_2H_4D_2$...

For a species of given atomic composition, the species are listed according to increasing positive charge.

B. Reactant Species

For a given ion the reactant species are again ordered according to the same principle of atomic composition, complexity and charge.

In addition, now, there is further ordering according to chemical structure. First, straight chain and branched chain compounds are

placed before ring compounds, using the fact that all ring compounds have a name associated with them.

The straight-chain compounds of a given isomer are further ordered according to whether in the semi-structural formula representation there are any italicized prefixes indicative of different isomer structure. A complete list of these prefixes is given in Table 2 together with the decimal and octal equivalent numbers which represent them in the sort key (some are only applicable to ring substitution, see below). The applicable ones include n-, sec-, iso-, tert-, cis- and trans-.

Those molecules with no prefixes at all will precede all molecules with prefixes. Finally, if necessary, the CA Registry Number is used for further sorting.

As for the ring compound isomers, they are ordered according to the compound name. Since the nomenclature is quite complex, containing isomer prefixes, numbers locating double bonds or atom connections, as well as italicized or greek letters, the following scheme is employed.

a. Form the "proper name" by scanning the name and extracting the first upper case latin letter and all subsequent lower case latin letters.

b. Add to this string all isomer prefix symbols or phrases, numbers or greek letters in the order that they appear in the entire name. These symbols or phrases are identified by the fact that they are lower case italic followed by a dash (see Table 2, page 23).

c. Substitute for each of the letters phrases, or numbers of the string, an associated numerical value and sort the resulting string of numbers. The decimal equivalent numerical values associated with each letter, phrase or number are given in Table 3.

Table 2. List of Isomer Prefixes
in order of sort preference

	Decimal Equivalent	Octal		Decimal Equivalent	Octal
o-	17	021	cyclo-	55	067
m-	18	022	bicyclo-& dicyclo-	60	074
p-	19	023	tricyclo-	65	101
n-	20	024	spiro-	70	106
sec-	25	031	syn-	75	113
iso-	30	036	anti-	80	118
tert-	35	043	endo-	85	125
neo-	40	050	exo-	90	132
cis-	45	055	qra-	95	137
trans-	50	062	opqra-	100	144

Table 3. Numerical Equivalents of GPSDC Symbols, Isomer Prefixes, Methods and Chemical Element Symbols

DECIMAL	GPSDC CHAR.	PREFIX or ELEMENT	METHOD
1	!		
2	"		
3	#		
4	$		
5	%		
6	&		
7	'		
8	(		
9	)		
10	*		S
11	+		
12	,		
13	-		
14	.		
15	/		PI
16	0		
17	1	*o*	
18	2	*m*	
19	3	*p*	
20	4	*n*	TPE
21	5		
22	6		
23	7		
24	8		
25	9	*sec*	PE
26	;		
27	:		
28	<		
29	=		
30	>	*iso*	AUG
31	?		
32	@		
33	A		
34	B		
35	C	*tert*	PEN
36	D		
37	E		
38	F		
39	G		
40	H	*neo*	EM
41	I		
42	J		
43	K		
44	L		
45	M	*cis*	RPD

Table 3. Numerical Equivalents of GPSDC Symbols, Isomer Prefixes, Methods and Chemical Element Symbols (continued)

DECIMAL	GPSDC CHAR.	PREFIX or ELEMENT	METHOD
46	N		
47	O		
48	P		
49	Q		
50	R	*trans*	EDD
51	S		
52	T		
53	U		
54	V		
55	W	*cyclo*	NRE
56	X		
57	Y		
58	Z		
59	[		
60		*bicyclo*	SRP
61	]		
62	^		
63	—		
64	`		
65	a	*tricyclo*	FD
66	b		
67	c		
68	d		
69	e		
70	f	*spiro*	SD
71	g		
72	h		
73	i		
74	j		
75	k	*syn*	SEQ
76	l		
77	m		
78	n		
79	o		
80	p	*anti*	EI
81	q		
82	r		
83	s		
84	t		
85	u	*endo*	SI
86	v		
87	w		
88	x		
89	y		
90	z	*exo*	CTS

Table 3. Numerical Equivalents of GPSDC Symbols, Isomer Prefixes, Methods and Chemical Element Symbols (continued)

DECIMAL	GPSDC CHAR.	PREFIX or ELEMENT	METHOD
91	{		
92			
93	}		
94	~		
95		*qra*	BH
96			
97			
98			
99			
100		*opqra*	DM
101		H	
102		He	
103		Li	
104		Be	
105		B	
106		C	
107		N	
108		O	
109		F	
110		Ne	
111		Na	
112		Mg	
113		Al	
114		Si	
115		P	
116	Π	S	
117	Σ	Cl	
118	∇	Ar	
119	×	k	
120	§	Ca	
121	∞	Sc	
122	•	Ti	
123	†	V	
124		Cr	
125	∝	Mn	
126	↑	Fe	
127	→	Co	
128	↓	Ni	
129	←	Cu	
130		Zn	
131		Ga	
132		Ge	
133	∫	As	
134	∂	Se	
135	√	Br	

Table 3. Numerical Equivalents of GPSDC Symbols, Isomer Prefixes, Methods and Chemical Element Symbols (continued)

DECIMAL	GPSDC CHAR.	PREFIX or ELEMENT	METHOD
136	Γ	Kr	
137	Δ	Rb	
138	Θ	Sr	
139	Λ	Y	
140	Ξ	Zr	
141	Π	Nb	
142	Σ	Mo	
143	Τ	Tc	
144	Φ	Ru	
145	Ψ	Rh	
146	Ω	Pd	
147	α	Ag	
148	β	Cd	
149	γ	In	
150	δ	Sn	
151	ε	Sb	
152	ζ	Te	
153	η	I	
154	θ	Xe	
155	κ	Cs	
156	λ	Ba	
157	μ	La	
158	υ	Ce	
159	ξ	Pr	
160	π	Nd	
161	ρ	Pm	
162	σ	Sm	
163	τ	Eu	
164	φ	Gd	
165	χ	Tb	
166	ψ	Dy	
167	ω	Ho	
168		Er	
169		Tm	
170	~	Yb	
171		Lu	
172		Hf	
173	≈	Ta	
174		W	
175		Re	
176		Os	
177		Ir	
178		Pt	
179		Au	
180	••	Hg	

Table 3. Numerical Equivalents of GPSDC Symbols, Isomer Prefixes, Methods and Chemical Element Symbols (continued)

DECIMAL	GPSDC CHAR.	PREFIX or ELEMENT	METHOD
181		Tl	
182		Pb	
183		Bi	
184		Po	
185		At	
186		Rn	
187		Fr	
188		Ra	
189		Ac	
190		Th	
191		Pa	
192		U	
193	O	Np	
194		Pu	
195	~	Am	
196		Cm	
197		Bk	
198		Cf	
199		Es	
200		Fm	
201		Md	
202		No	
203		Lr	
204			
205			
206			
207			
208			
209			
210			
211			
212			
213			
214			
215			
216			
217			
218			
219			
220			
221			
222			
223			

Table 3. Numerical Equivalents of GPSDC Symbols, Isomer Prefixes, Methods and Chemical Element Symbols (continued)

DECIMAL	GPSDC CHAR.	PREFIX or ELEMENT	METHOD
224			
225			
226			
227			
228			
229			
230			
231			
232			
233			
234			
235			
236			
237			
238			
239			
240			

The procedure is illustrated with two examples below with the number string generated from the decimal equivalent endo-5-Chlorobicyclo [2.2.1] hept-2-ene

C h l o r o b i c y c l o h e p t e n e endo 5 2 2
= 35 72 76 79 82 79 66 73 67 89 67 76 79 72 69 80 84 69 78 69 85 21 18 18 1

and

anti-Tricyclo [4.2.0.02, 5] octa-3,7-diene

T r i c y c l o o c t a d i e n e anti 4 2 0 0 2 5
= 52 82 73 67 89 67 76 79 79 67 84 65 68 73 69 78 69 80 20 18 16 16 18 21 1

In the computer these numbers are represented by their octal equivalent.

The above procedure provides a crude but systematic way of ordering different isomer names. It was be useful for deciding unambiguously on the ordering if, as is typically the case, one has only a dozen or so isomers in a typical case. If on the other hand one had to derive an ordering principle applicable to several hundred isomers a totally different approach may be necessary, such as the use of the Wisswesser line notation.

C. Method

The next level of ordering the information, which is by now categorized by ion and specific reactant molecule, is to order according to measurement technique. The different methods are given in Table 4, and are shown in order of generally decreasing accuracy. This order is not universally valid but is a good first approximation. This ordering is adopted here.

D. Measured Value

Lastly, within these categories the information is ordered according to increasing numerical value of the measurement. The principal purpose of this ordering is to group together the information

Table 3. Numerical Equivalents of GPSDC Symbols, Isomer Prefixes, Methods and Chemical Element Symbols (continued)

DECIMAL	GPSDC CHAR.	PREFIX or ELEMENT	METHOD
224			
225			
226			
227			
228			
229			
230			
231			
232			
233			
234			
235			
236			
237			
238			
239			
240			

The procedure is illustrated with two examples below with the number string generated from the decimal equivalent endo-5-Chlorobicyclo [2.2.1] hept-2-ene

C h l o r o b i c y c l o h e p t e n e endo 5 2 2
= 35 72 76 79 82 79 66 73 67 89 67 76 79 72 69 80 84 69 78 69 85 21 18 18 1

and

anti-Tricyclo [4.2.0.02, 5] octa-3,7-diene

T r i c y c l o o c t a d i e n e anti 4 2 0 0 2 5
= 52 82 73 67 89 67 76 79 79 67 84 65 68 73 69 78 69 80 20 18 16 16 18 21 1

In the computer these numbers are represented by their octal equivalent.

The above procedure provides a crude but systematic way of ordering different isomer names. It was be useful for deciding unambiguously on the ordering if, as is typically the case, one has only a dozen or so isomers in a typical case. If on the other hand one had to derive an ordering principle applicable to several hundred isomers a totally different approach may be necessary, such as the use of the Wisswesser line notation.

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D. Measured Value

Lastly, within these categories the information is ordered according to increasing numerical value of the measurement. The principal purpose of this ordering is to group together the information

Table 4. Techniques for Ion Energetics Measurements in Order of Sort Preference

		Numerical Equivalent Decimal	Octal
S	Spectroscopic	10	012
PI	Photoionization	15	017
TPE	Threshold Photoelectron Spectroscopy	20	024
PE	Photoelectron Spectroscopy	25	031
AUG	Auger Electron Spectroscopy	30	036
PEN	Penning Ionization	35	044
EM	Electron Monochromator Studies	40	050
RPD	Retarding Potential Difference	45	055
EDD	Energy Distribution Difference	50	062
NRE	N^{th} Root Extrapolation	55	067
SRP	Square Root Plot	60	074
FD	First Derivative	65	101
SD	Second Derivative	70	106
SEQ	Sequential Ionization	75	113
EI	Other Electron Impact	80	118
SI	Surface Ionization	85	125
CTS	Charge Transfer Spectrum	90	132
BH	Born-Haber Cycle	95	137
D	Derived Value	100	144

on the various ionization potentials of a given molecule which is obtained by the photoelectron spectroscopy technique. Although the various electronic states of the ions have each a different spectroscopic designation, there is no ordering criterion based on the electronic state which is of wide enough validity for use here.

Comparing the more detailed ordering of ring compound isomers by compound name with the less detailed ordering of chain compound isomers, it is evident that the latter will not be totally ordered in some instances where there are no isomer prefixes and the isomers are distinguished by the one line structural formula alone.

Example: CH_3COCH_3 vs. CH_3CH_2CHO.

Here the ordering according to numerical value alone will be of some help if, as is often the case, the isomers have different IP or AP values.

In any event, the ordering will not always be perfect, and in the future it will be extremely useful to have a means of permitting the ordering of a group of ion datum lines.

E. Output

The interim output is obtained from the ordered raw ion data, bibliography and author index files in the form of computer printout which will be xeroxed or photocopied. In order to do this it will be necessary to strip the sort key from the material prior to printing out. The printout will be carried out on the NBS IBM 360 printer, using the extended character chain printer. This extended character chain comprises a set of characters appropriate to the presentation of scientific information (See Appendix A and table 3).

5. PRESENT STATUS OF THE AUTOMATED SYSTEM

The dashed lines illustrated earlier in figure 5 indicate procedures and programs that remain to be written. A list of the programs and their function is given in Table 5. The programs specially written or adapted for this system are underlined. They are grouped into a package called IONPACK. The system is developed to the point that intermediate control and output files can be prepared. Information subsets and final compilation merging and editing remain to be developed.

When the typist is satisfied, a copy is made to be proofread by the abstractor. When all corrections have been made, an archival tape is requested and GPSDC programs are used to convert the archival tape to a GPSDC file and print the file using the extended character printer. If any mistakes are found in the printout, corrections are made in ATS and a new archival tape is requested.

IPABS1 is used to read this file and generate the files required by the data center. These files are: The abstract print file, the card image file, the reference file and the raw ion data file. DGMDMP is used to print the abstract print file and the card image file. The abstract printout is used as an archival record of the abstracts that have been processed. The card images are printed on 5 x 8 cards. The cards containing the citations are used as document control care replacements. They indicate which papers have been processed. The ion data cards are sorted manually by ion and provide a manual alternative to the machine readable ion data file. (At a later date these cards may be

Table 5. List of Programs Used

P_1 - ATSIN:	Program used to convert an ATS archival tape to a GPSDC file containing abstract information to be used as input for P_2.
P_2 - IPABS1:	Reads GPSDC file containing abstract information and generates, working files (abstract print file, card image file, bibliographic data file, raw ion data file with sort key) necessary to produce the required output files.
P_3 - DGMDMP:	Prints card image file generated by P_2 (ion data + DOC, control replacements) to produce 5 x 8 document control replacement.
P_4 - WREF:	Inputs bibliographic data file and outputs an unsorted author file with sort key and a reference file.
P_5 - IPSORT:	Sorts the raw ion data file generated by P_2.
P_6 - ISTRIP:	Inputs the sorted raw ion data file, strips the sort key from the entries and write them out as a GPSDC file.
P_7 - IPASRT:	Sorts the unsorted author file generated by P_4.
P_8 - MERGE:	To be developed later.

dispensed with). The raw ion data file is added to the year's cumulative raw ion data file. The cumulative files for each year are combined to form a master cumulative file.

IPSORT is used to sort a raw ion data file when the evaluator wishes to see the material ordered by ion. ISTRIP is used to remove the sort key from a sorted ion data file and generate a GPSDC file. DGMDMP is used to print the file on the extended character printer.

The GPSDC file from ISTRIP can be edited using EDBOSS or it can be converted to an ATS archival tape and loaded into ATS for editing. The next sections contain detailed instructions for each computerized step of the procedure, and form an operating manual for the present data center.

6. KEYBOARDING THE ABSTRACT

6.1 Format of the abstract

The abstract is to be keyboarded into the Department of Commerce ATS system using a model 37 teletype or an equivalent terminal. The standard GPSDC method of keyboarding should be used to get the characters that are not in the 96 character ASCII set. Appendix A contains all characters that are defined in GPSDC.[5]

The previous example in figure 3 shows a sample abstract as it would be keyboarded. The document control number is on the first line beginning in position 1. The bibliographic information is next. The first author's surname begins in position 7 followed by his initials. The authors are separated by semicolons. The title is separated from the authors and the journal by double daggers. The Chemical Abstracts abbreviation is used for the journal. The volume number is to be bold

face (put red hats over the number). The bibliographic information ends with the year in parentheses. The lines of bibliographic information shall not extend past position 60. While the first line begins in position 7, continuation lines shall begin in position 9.

The ion data line is flagged by a section mark (a red Z) in position 1. The ion formula begins in position 6. Only the document control number and flags are allowed in positions 1 thru 6. Flags shall always be in position 1. The reactant formula begins in position 27. The other products formula begins in position 47 unless the reactant formula runs over the space allotted, in which case it starts two spaces after the reactant formula. The measured value shall be in positions 57 to 76 the decimal point shall be in position 62. The method shall be in positions 77 to 79. If there is a heat of formation it shall be in positions 85 to 93. The decimal point shall be in position 92. This field will normally be blank.

The name of the reactant follows. It shall begin with an open parenthesis in position 27. If the name is so long that it would extend past position 115, it may be continued on the next line. The name may be followed by up to three comment lines. If the comment is a parenthetical comment, the open parenthesis shall be in position 9. Regular comments shall begin in position 6. Do an extra carriage return before the next ion data line.

An abstract shall be terminated by a dagger (red V) in position 1. It is important that the abstracts be in increasing order of ID number. If they are out of order the abstract and reference files will be out of order.

7. CONVERTING ATS KEYBOARDING TO GPSDC FILE

7.1 Requesting an ATS Archival Tape

The procedure for requesting an archival tape is to first put the document or documents in the archival queue. The command used is x; archive; document name.

The AQR form must then be filled out and sent to operator 0 (zero) and operator 20. A sample form is shown in figure 6. The form must request that the archival tape be sent to NBS via the NBS shuttle.

7.2 Converting the Archival Tape to GPSDC

The program ATSIN is used to convert the ATS Archival tape to a GPSDC file for processing by the programs in IONPACK. The tape must be labeled for use on the NBS computer. The first three letters of the label shall be ION. This may be followed by the last three numbers of the Department of Commerce tape number for the reel. Make a 5 x 8 card with the new tape label and the Department of Commerce tape number. The card will contain the date the material was archived, a description of the material archived, and the date the tape was received. The card shall then be filed in the tape file box. Record all movement of the tape of the 5 x 8 card. Figure 7 shows a sample card.

The job request card, a listing of the run, and a 360 printout of the GPSDC input file are shown in figures 8, 9, and 10 respectively.

The first card is the standard run card. The job is run under N priority. This means it is run overnight for cheaper computer costs. The second card assigns the GPSDC program file. The third card invokes the collector to gather the routines required for this run. The fourth card assigns the ATS archival tape as file 8. The U9V means the tape is 9

A: ATS//ATS ARCHIVE QUEUE REQUEST FORM (AQR) ATS/ATS/ATS

1. User Name and Operator Number: candy schmidt 070

2. Bureau/Account No.: nbs 2501

3. Telephone Number: 921 2732

4. Building and room number: 222 A145

5. Tape Release Date: 6 30 80

6. Total number of Documents to be archived: 1

7. Type of Documents: abstracts

8. Date of Request: july 11, 1977

9. Queue Name(archive, archive2, archive3):archive

10. Tape Reel number:
Please ship to me via the NBS shuttle the above tape. Thank you very much. candy

ADVANCED PREPARATION MUST BE MADE WITH THE COMPUTER CENTER PRIOR TO THIS REQUEST. CONTACT YOUR ATS REPRESENTATIVE 9o7-5526) TO CO-ORDINATE YOUR ARCHIVE REQUEST WITH THE COMPUTER CENTER. PLEASE REPORT ANY PROBLEMS WITH THE USE ARCHIVE QUEUE AT ONCE. DO NOT DELETE YOUR DOCUMENTS FROM PERMANENT STORAGE UNTIL YOU HAVE BEEN NOTIFIED OF YOUR REEL NUMBER.

Figure 6. AQR form

009523

CS003 9 Track ATS labeled tape

@ ASG,TJ 8., U9V, CS003

contains abstract entries 3476-3484 6-29-77

Figure 7. GPSDC tape description to be recorded on 5 x 8 card and kept in the tape file box.

PR.	RUN ID	ACCOUNT NO.	TIME	PAGES	CARDS	NAME	PHONE	BIN
N	CANDY 3	34061-SCHMID	8	1000		C SCHMIDT	2792	

REEL NO.	WRITE ENABLE
C5003	NO

PERIPHERAL OPERATIONS
- [ ] KEYPUNCH
- [ ] VERIFY
- [ ] INTERPRET
- [ ] LIST CARDS ____ TIMES
- [ ] DUPE CARDS ____ TIMES
- [ ] DIGIDATA
- [ ] OTHER _____ (Specify)

- [ ] MAIL TO:
- [X] WILL PICK UP
- [ ] SEND TO 2ND FLOOR
- [ ] SEND TO 3RD FLOOR

SC 4020		CALCOMP	
[ ] PRINT MODE	[ ] 16 MM	INK COLOR	PEN
[ ] PLOT MODE	[ ] 35 MM	PAPER	FRAME COUNT
[ ] DUPE FILM	[ ] HARD COPY		

BRKPTED REEL NO.	PGS. EST.	CDS. EST.	NOR	EXT	PART PAPER	SPECIAL FORMS

FRAME COUNT	TAPE(S)	TAPE(S)

SPECIAL INSTRUCTIONS
Please return reel.C5003

- [ ] CONT. ON REVERSE

JOB LOADED	JOB PICKED UP	
AT ____ BY ____	BY _____	[X] OK TO RELOAD

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JOB REQUEST CARD

DATE: 6/29/77

Figure 8. Job request card for ATSIN run.

```
@:ELT,L,ID    FILE.ATS
ELT007 R72-16 10/21/77 17:47:54 (,0)
000001        000    @RUN,N/NR    SCHMAR,34060-SCHMID,IPOT,5,200
000002        000    @ASG,A    GPSDC*DICX8.
000003        000    @MAP,NX    GPSDC*DICX8.ATSIN,ATSIN
000004        000    @ASG,TJ    8.,U9V,ION123
000005        000    @REWIND    8.
000006        000    @DELETE,C    IPOT*ION3476.
000007        000    @ASG,UP    IPOT*ION3476.,F2
000008        000    @USE    2.,IPOT*ION3476.
000009        000    @XQT    ATSIN
000010        000    OTFILE = 2
000011        000    FILE 2 NEW                    ION FILE 3476 TO 3484 4JUN77
000012        000    PGWDTH2 = 160
000013        000    LF2 = 2
000014        000    LM = 1
000015        000    RM = 116
000016        000    TABS 6 7 27 47 60 77 88 102 108
000017        000    DMPOPT = 0
000018        000    RUN
000019        000    @ASG,A    TEXTPROCESS*LIB.
000020        000    @MAP,NX    GPSDC*DICX8.DGMDMP,DGMDMP
000021        000    @MSG,W    34060-SCHMID     WRITE ENABLE REEL 1534
000022        000    @ASG,TJ    11.,8C,1534W
000023        000    @MARK    11.
000024        000    @CLOSE    11.
000025        000    @XQT    DGMDMP
000026        000    INFILE = 2
000027        000    RUN
000028        000    @EOF
```

Figure 9. Listing of ATSIN run.

```
Hook    1  Page   1    *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100..105..110..115..120- y   Ln mode

3476                                                                                                                     -   3  1
     Hedaya, E.; Kent, M. E.; McNeil, D. W.; Lossing, F. P.;                                                             -   6  2
       and McAllister, T. $The thermal rearrangement of                                                                  -   9  3?
       phenylnitrene to cyanocyclopentadiene, $Tetra-                                                                    -  12  4?
       hedron Letters 30, 3415 (1968).                                                                                   -  15  5
$    C6H5N*               C5H5CN              **           9.7              E1                                           -  19  6
                          (Cyclopentadienecarbonitrile)                                                                  -  22  7
                          (RN-CAS Registry Number 27659-36-5)                                                            -  25  8
$    C5H6*                C5H6                **           9.0              E1                                           -  28  9
                          (1,3-Cyclopentadiene)                                                                          -  31 10
                          (RN-CAS Registry Number 542-92-7)                                                              -  34 11
*                                                                                                                        -  37 12
3477                                                                                                                     -  40 13
     Harris, M. M.; Loudon, A. G.; and Mazengo, R. Z. $Ring                                                              -  43 14?
       expansion reactions in aromatic systems. A study                                                                  -  46 15
       of steric strain in some n,n'-dimethyl-1,1'-bi-                                                                   -  49 16
       naphthyls. $Org. Mass Spectrom. 5, 1121 (1971).                                                                   -  52 17?
$    C22H18*              C10H6(CH3)C10H6CH3  **           8.20             E1                                           -  56 18
                          (1,1'-Binaphthyl, 2,2'-dimethyl-)                                                              -  59 19
                          (RN-CAS Registry Number 32834-84-7)                                                            -  62 20
$    C21H15*              C10H6(CH3)C10H6CH3  CH3          13.25            E1                                           -  65 21
                          (1,1'-Binaphthyl, 2,2'-dimethyl-)                                                              -  68 22
                          (RN-CAS Registry Number 32834-84-7)                                                            -  71 23
$    C22H18*              C10H6(CH3)C10H6CH3  **           8.00             E1                                           -  74 24
                          (1,1'-Binaphthyl, 3,3'-dimethyl-)                                                              -  77 25
                          (RN-CAS Registry Number 34042-82-5)                                                            -  80 26
$    C21H15*              C10H6(CH3)C10H6CH3  CH3          12.25            E1                                           -  83 27
                          (1,1'-Binaphthyl, 3,3'-dimethyl-)                                                              -  86 28
                          (RN-CAS Registry Number 34042-82-5)                                                            -  89 29
$    C22H18*              C10H6(CH3)C10H6CH3  **           8.15             E1                                           -  92 30
                          (1,1'-Binaphthyl, 7,7'-dimethyl-)                                                              -  95 31
                          (RN-CAS Registry Number 34003-80-0)                                                            -  98 32
$    C21H15*              C10H6(CH3)C10H6CH3  CH3          12.75            E1                                           - 101 33
                          (1,1'-Binaphthyl, 7,7'-dimethyl-)                                                              - 104 34
                          (RN-CAS Registry Number 34003-80-0)                                                            - 107 35
$    C22H18*              C10H6(CH3)C10H6CH3  **           8.00             E1                                           - 110 36
                          (1,1'-Binaphthyl, 8,8'-dimethyl-)                                                              - 113 37
                          (RN-CAS Registry Number 32693-05-3)                                                            - 116 38
$    C21H15*              C10H6(CH3)C10H6CH3  CH3          11.50            E1                                           - 119 39
                          (1,1'-Binaphthyl, 8,8'-dimethyl-)                                                              - 122 40
                          (RN-CAS Registry Number 32693-05-3)                                                            - 125 41
*                                                                                                                        - 128 42
```

Figure 10. 360 printout of the GPSDC input file using ASTIN.

tracks, 1600 bpi. The 6th, 7th, and 8th cards assign a file called IPOT*ION3476 as file 2. This name was used because the tape contains abstracts for papers 3476 thru 3484. The 9th card starts execution of the program ATSIN. Cards 10 and 11 tell the program the output file is file 2 and it is to have GPSDC label ION FILE 3476 to 3484. These cards are the beginning of the random order data which is described in more detail in the GPSDC users manual.

The next map card invokes the collector to gather the routines required to print the GPSDC file created by ATSIN. The next two cards assign a tape for DGMDMP to write which is printed on the IBM 1403 printer using the GPSDC train. The label and description is put on a 5 x 8 card and stored in the tape file box (figure 11). The mark and close cards put end of files at the beginning of the tape so that a lot of useless printout is not received if the run does not write on the tape. Combining smaller input files into larger ones is done using EDCARD or EDBOSS.

8. GENERATING THE REQUIRED OUTPUTS

The production of the various required outputs necessitates several steps. The program IPABS1 reads the GPSDC file and writes three new GPSDC files and a binary file. The file input which was generated as file 2 in the previous run is assigned file 1. The file of abstracts to be printed is output on file 2. The file of card images to be printed on 5 x 8 cards is output on file 3. The reference file is written on file 4 and the raw ion data file is written on tape on unit 7. The program DGMDMP is used to generate the tapes used to drive the 360 printer to print the abstracts, the document control card replacements and the ion data cards.

```
NBS
0409
@ ASG,TJ 11., 8C, 0409 assigned to 30062-WEBBWI
To be used as DGMDMP tape
Printed abstract entries 3476-3484                    29 Jun 77
```

Figure 11. Description of tape that is assigned to print the GPSDC file created by ATSIN.

The job request card, a listing of the run, a 360 printout of the abstract file, and the 5 x 8 card describing the tape are illustrated in figures 12 through 15 respectively.

Note in the run deck, that the next three cards beginning after the FILE 1 OLD card should have the words ABSTRACT, CARD, and REF beginning in column 26. The dump option card (DMPOPT) will produce a one line dump if DMPOPT = 1, and no dump if DMPOPT = 0. The miscellaneous card (MISC) provides the option of diagnostic printout if desired (e.g. printing the sort key).

The raw ion data file produced by this run will be kept for some time and will be merged with the yearly cumulative raw ion data file which in turn will be merged with a total cumulative file. Therefore the file should be put on a labeled tape that has been purchased. A description of the file and the date of the run will be written on the 5 x 8 card for the tape that is kept in the tape file box.

The raw ion data file consists of a 55 word sort key followed by the ion data line, name, and comments in GPSDC characters packed two characters per word. There is an octal 777777777777 word separating each line. The file is written on tape using NTRAN and cannot be read as a GPSDC file.

8.1 Printing the 5 x 8 Cards

The DGMDMP program is used to generate the tape for printing the 5 x 8 cards. It is necessary to supply the 5 x 8 card stock to the computer room. Examples of the job request card, a listing of the run, and a 360 printout on 5 x 8 cards are shown in figures 16, 17, and 18 respectively.

8.2 Sorting the Raw Ion Data File

When IPABS1 generates the raw ion data file it puts a sort key at the beginning of each ion data line. The program IPSORT is used to order the data by increasing atomic number of the elements in the

PR.	RUN ID	ACCOUNT NO.	TIME	PAGES	CARDS	NAME	PHONE	BIN
N	IPABS1	30062-WEBB WJ	15	1000		W J WEBB		

REEL NO.	WRITE ENABLE
0409	YES
ION01	

PERIPHERAL OPERATIONS
- [ ] KEYPUNCH
- [ ] VERIFY
- [ ] INTERPRET
- [ ] LIST CARDS ____ TIMES
- [ ] DUPE CARDS ____ TIMES
- [ ] DIGIDATA
- [ ] OTHER ____ (Specify)

[ ] MAIL TO:

[X] WILL PICK UP
[ ] SEND TO 2ND FLOOR
[ ] SEND TO 3RD FLOOR

BRKPTED REEL NO.	PGS. EST.	CDS. EST.	NOR	EXT	PART PAPER	SPECIAL FORMS
0409	10			*	1	PLAIN

SC 4020		CALCOMP	
[ ] PRINT MODE	[ ] 16 MM	INK COLOR	PEN
[ ] PLOT MODE	[ ] 35 MM	PAPER	FRAME COUNT
[ ] DUPE FILM	[ ] HARD COPY		

FRAME COUNT	TAPE(S)	TAPE(S)

SPECIAL INSTRUCTIONS
SYMSDF, 7-track, 800 bpi tape, reel 0409, using GPSDC train and 16 lines/inch.

[ ] CONT. ON REVERSE

JOB LOADED	JOB PICKED UP		DATE
AT ____ BY ____	BY ____	[X] OK TO RELOAD	

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JOB REQUEST CARD

Figure 12. Job request card for IPABS1 run.

```
@:ELT,LID   FILE.ABS
ELT007 R72-16 10/19/77 18:01:27 (,0)
000001       000   @RUN,N/NR  IPABS1,34030-SCHMID,IPOT,15,1000
000002       000   @ASG,A    GPSDC*DICX8.
000003       000   @ASG,A    IPOT*IONPACK.
000004       000   @ASG,A    TEXTPROCESS*LIB.
000005       000   @ASG,A    GPSDC*3476-3484.
000006       000   @USE      1.,GPSDC*3476-3484.
000007       000   @DELETE,C  IPOT*ABS3476-3484.
000008       000   @ASG,UP  IPOT*ABS3476-3484.,F2
000009       000   @USE      2.,IPOT*ABS3476-3484.
000010       000   @DELETE,C  IPOT*CRD3476-3484.
000011       000   @ASG,UP  IPOT*CRD3476-3484.,F2
000012       000   @USE      3.,IPOT*CRD3476-3484.
000013       000   @DELETE,C   IPOT*REF3476-3484.
000014       000   @ASG,UP  IPOT*REF3476-3484.,F2
000015       000   @USE      4.,IPOT*REF3476-3484.
000016       000   @ASG,T    IPOT*RAWION3476.,8C9,ION01W,4000
000017       000   @MSG,W    34060-ROSENS WRITE ENABLE TAPE ION01
000018       000   @USE      7.,IPOT*RAWION3476.
000019       000   @MAP,INX IPABS
000020       000     LIB  IPOT*IONPACK
000021       000     LIB  GPSDC*DICX8
000022       000     LIB  TEXTPROCESS*LIB
000023       000      IN  IPABS1
000024       000   @XQT     IPABS
000025       000   FILE 1 OLD
000026       000   FILE 2 NEW                ABSTRACTS 3476-3484 28JUN77
000027       000   FILE 3 NEW                CARD FILE TEST 28JUN77
000028       000   FILE 4 NEW                REF FILE TEST 28JUN77
000029       000   DMPOPT = 0
000030       000   MISC  00
000031       000   RUN
000032       000   @MARK  7.
000033       000   @CLOSE  7.
000034       000   @MAP,NX  GPSDC*DICX8.DGMDMP,DGMDMP
000035       000   @MSG,W   30062-WEBBWI WRITE ENABLE REEL 0409
000036       000   @ASG,TJ   11.,8C,0409W
000037       000   @MARK  11.
000038       000   @CLOSE  11.
000039       000   @XQT   DGMDMP
000040       000   INFILE=2
000041       000   RUN
000042       000   @EOF
```

Figure 13. Listing of IPABS1 run.

```
Book   1  Page  1    *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100..105..110..115- y  Ln edit

3476                                                                                                       -  3  1
Helaya, F., Kent, M. F., McNeil, D. W., Lossing, F. P., and McAllister, T.                                 -  6  2
The thermal rearrangement of phenylnitrene to cyanocyclopentadiene,                                        -  9  3
Tetra- hedron Letters 39, 3415 (1968).                                                                     - 12  4
C6H5N*          C5H5CN              **         9.7          EI                      3476                   - 16  5
                (Cyclopentadienecarbonitrile)                                                              - 19  6
               (RN-CAS Registry Number 27659-36-5)                                                         - 22  7

C5H6*           C5H6                **         9.0          EI                      3476                   - 27  8
                (1,3-Cyclopentadiene)                                                                      - 30  9
               (RN-CAS Registry Number 542-92-7)                                                           - 33 10

Book   1  Page  2    *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100..105..110..115- y  Ln edit

3477                                                                                                       -  3  1
Harris, M. M., Loudon, A. G., and Mazengo, R. Z.                                                           -  6  2
Ring expansion reactions in aromatic systems. A study of steric strain in some n,n'-dimethyl-1,1'-binaphthyls,  -  9  3
$                                                                                                          - 12  4?
Org. Mass Spectrom. 5, 1123 (1971).                                                                        - 15  5
C22H19*         C10H6(CH3)C10H6CH3  **         8.20         EI                      3477                   - 19  5
                (1,1'-Binaphthyl, 2,2'-dimethyl-)                                                          - 22  7
               (RN-CAS Registry Number 32834-84-7)                                                         - 25  8

C21H15*         C10H6(CH3)C10H6CH3  CH3       13.25         EI                      3477                   - 30  9
                (1,1'-Binaphthyl, 2,2'-dimethyl-)                                                          - 33 10
               (RN-CAS Registry Number 32834-84-7)                                                         - 36 11

C22H18*         C10H6(CH3)C10H6CH3  **         8.00         EI                      3477                   - 41 12
                (1,1'-Binaphthyl, 3,3'-dimethyl-)                                                          - 44 13
               (RN-CAS Registry Number 34042-82-5)                                                         - 47 14

C21H15*         C10H6(CH3)C10H6CH3  CH3       12.25         EI                      3477                   - 52 15
                (1,1'-Binaphthyl, 3,3'-dimethyl-)                                                          - 55 16
               (RN-CAS Registry Number 34042-82-5)                                                         - 58 17

C22H18*         C10H5(CH3)C10H6CH3  **         8.15         EI                      3477                   - 63 18
                (1,1'-Binaphthyl, 7,7'-dimethyl-)                                                          - 66 19
               (RN-CAS Registry Number 34003-80-0)                                                         - 69 20

C21H15*         C10H6(CH3)C10H6CH3  CH3       12.75         EI                      3477                   - 74 21
                (1,1'-Binaphthyl, 7,7'-dimethyl-)                                                          - 77 22
               (PN-CAS Registry Number 34003-80-0)                                                         - 80 23

C22H18*         C10H6(CH3)C10H6CH3  **         8.00         EI                      3477                   - 85 24
                (1,1'-Binaphthyl, 8,8'-dimethyl-)                                                          - 88 25
               (RN-CAS Registry Number 32693-05-3)                                                         - 91 25

C21H15*         C10H6(CH3)C10H6CH3  CH3       11.50         EI                      3477                   - 96 27
                (1,1'-Binaphthyl, 8,8'-dimethyl-)                                                          - 99 28
               (RN-CAS Registry Number 32693-05-3)                                                         -102 29
```

Figure 14. 360 printout of the abstract file created by IPABS1.

IONO1, 9 track, labeled tape 3-10-76

@ ASG,T RAWION 3476., 8C9, IONO1, 4000

From output file 2, printed abstracts 3476-3486 29 Jun 77

Figure 15. Description of tape containing raw ion data file is. recorded on 5 x 8 card and stored in the tape file box.

PR.	RUN ID	ACCOUNT NO.	TIME	PAGES	CARDS	NAME	PHONE	BIN
N	CDIMGS	34030-SCHMID	10	2000		W J WEBB	2173	

REEL NO.	WRITE ENABLE
0409	YES

PERIPHERAL OPERATIONS

- [ ] KEYPUNCH
- [ ] VERIFY
- [ ] INTERPRET
- [ ] LIST CARDS ____ TIMES
- [ ] DUPE CARDS ____ TIMES
- [ ] DIGIDATA
- [ ] OTHER ____ (Specify)

- [ ] MAIL TO:
- [X] WILL PICK UP
- [ ] SEND TO 2ND FLOOR
- [ ] SEND TO 3RD FLOOR

SC 4020		CALCOMP	
[ ] PRINT MODE	[ ] 16 MM	INK COLOR	PEN
[ ] PLOT MODE	[ ] 35 MM	PAPER	FRAME COUNT
[ ] DUPE FILM	[ ] HARD COPY		

FRAME COUNT	TAPE(S)	TAPE(S)

BRKPTED REEL NO.	PGS. EST.	CDS. EST.	NOR	EXT	PART PAPER	SPECIAL FORMS
0409	600			X		5x8 cards

SPECIAL INSTRUCTIONS

SYMSDF, 7-track, 800 bpi tape, reel 0409, using GPSDC train, 16 lines/inch. 5x8 cards attached.

[ ] CONT. ON REVERSE

JOB LOADED	JOB PICKED UP		NBS-777 (Rev. 9-73)	U.S. DEPARTMENT OF COMMERCE NATIONAL BUREAU OF STANDARDS	DATE
AT ____ BY ____	BY ____	[ ] OK TO RELOAD		JOB REQUEST CARD	

Figure 16. Job request card for printing card images on 5 x 8 card stock.

```
@:ELT,LID    FILE.CRD
ELT007 R72-16 10/19/77 18:54:22 (.0)
000001       000    @RUN,N/NR  CDIMGS.34030-SCHMID.IPOT.10.3000
000002       000    @ASG,A  GPSDC*DICX8.
000003       000    @ASG,A  TEXTPROCESS*LIB.
000004       000    @MSG,W  30062-WEBB%I  WRITE ENABLE REEL 0409
000005       000    @ASG,TJ  11..EC.C409W
000006       000    @MARK   11.
000007       000    @CLOSE  11.
000008       000    @ASG,A   IPOT*CRD3476-3484.
000009       000    @USE     3..IPOT*CRD3476-3484.
000010       000    @MAP,NX  GPSDC*DICX8.DGMDMP,DGMDMP
000011       000    @XQT DGMDMP
000012       000    INFILE=3
000013       000    PARAM 2=1
000014       000    RUN
000015       000    @EOF
```

Figure 17. Listing of run using DGMDMP to print the card image file.

				3476
Tedeya, E., Kent, M. E., McNeil, D. W., Lossing, F. P., and McAllister, T. The thermal rearrangement of phenylnitrene to cyanocyclopentadiene, Tetrahedron Letters 10, 3415 (1968).				
$C_6H_5N^+$	C_5H_5CN ** (Cyclopentadienecarbonitrile) (RN-CAS Registry Number 27659-36-5)	9.7	EI	3476
$C_5H_6^+$	C_5H_6 ** (1,3-Cyclopentadiene) (RN-CAS Registry Number 542-92-7)	9.0	EI	3476
				3477
Harris, M. M., Loudon, A. G., and Mazengo, R. Z. Ring expansion reactions in aromatic systems. A study of steric strain in some n,n'-dimethyl-1,1'-binaphthyls, Org. Mass Spectrom. 5, 1123 (1971).				
$C_{22}H_{18}^+$	$C_{10}H_6(CH_3)C_{10}H_6CH_3$ ** (1,1'-Binaphthyl, 2,2'-dimethyl-) (RN-CAS Registry Number 12534-44-7)	8.20	EI	3477
$C_{22}H_{18}^+$	$C_{10}H_6(CH_3)C_{10}H_6CH_3$ ** (1,1'-Binaphthyl, 3,3'-dimethyl-) (RN-CAS Registry Number 34042-82-5)	8.00	EI	3477
$C_{21}H_{15}^+$	$C_{10}H_6(CH_3)C_{10}H_6CH_3$ CH_3 (1,1'-Binaphthyl, 3,3'-dimethyl-) (RN-CAS Registry Number 34042-82-5)	12.25	EI	3477
$C_{22}H_{18}^+$	$C_{10}H_6(CH_3)C_{10}H_6CH_3$ ** (1,1'-Binaphthyl, 7,7'-dimethyl-) (RN-CAS Registry Number 34003-80-0)	8.15	EI	3477
$C_{21}H_{15}^+$	$C_{10}H_6(CH_3)C_{10}H_6CH_3$ CH_3 (1,1'-Binaphthyl, 7,7'-dimethyl-) (RN-CAS Registry Number 34003-80-0)	12.75	EI	3477
$C_{22}H_{18}^+$	$C_{10}H_6(CH_3)C_{10}H_6CH_3$ ** (1,1'-Binaphthyl, 8,8'-dimethyl-) (RN-CAS Registry Number 32693-05-3)	8.00	EI	3477
$C_{21}H_{15}^+$	$C_{10}H_6(CH_3)C_{10}H_6CH_3$ CH_3 (1,1'-Binaphthyl, 8,8'-dimethyl-) (RN-CAS Registry Number 32693-05-3)	11.50	EI	3477
$C_{21}H_{15}^+$	$C_{10}H_6(CH_3)C_{10}H_6CH_3$ CH_3 (1,1'-Binaphthyl, 2,2'-dimethyl-) (RN-CAS Registry Number [illegible])	13.25	EI	3477

Figure 18. 360 printout of card images on 5 x 8 card stock using DGMDMP.

ion. The program can be used on the original raw ion data file, the cumulative raw ion data file, or to combine and sort serveral raw ion data files on the same input tape. The sorted raw ion data file produced by this run will be kept for some time. It may be merged with other files to produce cumulative sorted raw ion data files. Therefore the sorted file should be written on a labeled tape that has been purchased. A description of the file and the date of the run shall be written on the 5 x 8 card for the tape that is kept in the tape file box.

Examples of the job request card, a listing of the run, and the 5 x 8 card describing the tape follow in figures 19 - 21.

In this run the input file is assigned as file 7 and is the labeled tape generated by the earlier IPABS run. The output file is a labeled tape and assigned as file 8. The card following the @XQT card is the parameter card for IPSORT in 315 format. The first number is the number of the input file, the second is the number of the output file. The third number is the number of files to be read off the input tape and sorted together.

8.3 Printing the Raw Ion Data File

The program ISTRIP removes the sort keys from the records and writes a GPSDC file. The GPSDC file can then be printed using DGMDMP. This is the method used to print the contents of the sorted files. The program starts each ion on a new page.

The job request card, a listing of the ISTRIP run, and a 360 printout of the sorted ion data are illustrated in figures 22, 23, and 24 respectively.

PR.	RUN ID	ACCOUNT NO.	TIME	PAGES	CARDS	NAME	PHONE	BIN
N	IPSORT	34030-SCHMID	10	1000		W J WEBB	2173	

REEL NO.	WRITE ENABLE
ION02	YES

PERIPHERAL OPERATIONS
- [ ] KEYPUNCH
- [ ] VERIFY
- [ ] INTERPRET
- [ ] LIST CARDS ____ TIMES
- [ ] DUPE CARDS ____ TIMES
- [ ] DIGIDATA
- [ ] OTHER ____ (Specify)

[ ] MAIL TO:

[X] WILL PICK UP
[ ] SEND TO 2ND FLOOR
[ ] SEND TO 3RD FLOOR

SC 4020		CALCOMP	
[ ] PRINT MODE	[ ] 16 MM	INK COLOR	PEN
[ ] PLOT MODE	[ ] 35 MM	PAPER	FRAME COUNT
[ ] DUPE FILM	[ ] HARD COPY		
FRAME COUNT	TAPE(S)	TAPE(S)	

BRKPTED REEL NO.	PGS. EST.	CDS. EST.	NOR	EXT	PART PAPER	SPECIAL FORMS

SPECIAL INSTRUCTIONS

[ ] CONT. ON REVERSE

JOB LOADED	JOB PICKED UP		NBS-777 (Rev. 9-73)	U.S. DEPARTMENT OF COMMERCE NATIONAL BUREAU OF STANDARDS	DATE
AT ____ BY ____	BY ____	[X] OK TO RELOAD		JOB REQUEST CARD	7/6/77

Figure 19. Job request card for IPSORT run.

```
@:ELT.LID    FILE.SOR
ELT007 R72-16 11/03/77 13:39:22 (.0)
000001       000    @RUN.N/NR  IPSORT.34030-SCHMID.IPOT.10.1000
000002       000    @ASG.T    IPOT*RAWION3476..8C9.ION01
000003       000    @ASG.A  NBS*SORTIT.
000004       000    @ASG.A  IPOT*IONPACK.
000005       000    @ASG.T  IPOT*RAWION2..8C9.ION02W.4000
000006       000    @MSG.W  34060-ROSENS WRITE ENABLE TAPE ION02
000007       000    @USE  7..IPOT*RAWION3476.
000008       000    @USE  8..IPOT*RAWION2.
000009       000    @MAP.INX SORT
000010       000      LIB IPOT*IONPACK
000011       000      LIB NBS*SORTIT
000012       000      LIB IPOT*IONPACK
000013       000      IN IPSORT
000014       000    @XQT  SORT
000015       000        7    8    1
000016       000    @EOF
```

Figure 20. Listing of IPSORT run.

IONO2, 9 track, prelabeled tape 3-10-76

@ ASG,T IPOT*RAWION2., 8C9, IONO2 W, 4000

contains sorted raw ion data 3476-3484 13 Jul 77

Figure 21. Description of the sorted raw ion data file should be recorded on a 5 x 8 card and kept in the tape file box.

PR.	RUN ID	ACCOUNT NO.	TIME	PAGES	CARDS	NAME	PHONE	BIN
N	ISTRIP	34030-SCHMID	10	2000		W J WEBB	2173	

REEL NO.	WRITE ENABLE
0409	YES
IONO2	

PERIPHERAL OPERATIONS
- [ ] KEYPUNCH
- [ ] VERIFY
- [ ] INTERPRET
- [ ] LIST CARDS ____ TIMES
- [ ] DUPE CARDS ____ TIMES
- [ ] DIGIDATA
- [ ] OTHER ____ (Specify)

[ ] MAIL TO:

[X] WILL PICK UP
[ ] SEND TO 2ND FLOOR
[ ] SEND TO 3RD FLOOR

SC 4020		CALCOMP	
[ ] PRINT MODE	[ ] 16 MM	INK COLOR	PEN
[ ] PLOT MODE	[ ] 35 MM	PAPER	FRAME COUNT
[ ] DUPE FILM	[ ] HARD COPY		

FRAME COUNT	TAPE(S)	TAPE(S)

BRKPTED REEL NO.	PGS. EST.	CDS. EST.	NOR	EXT	PART PAPER	SPECIAL FORMS
0409	600			*	1	PLAIN

SPECIAL INSTRUCTIONS
SYMSDF, 7-track, 800 bpi tape, reel 0409 using GPSDC train and 16 lines/inch.

[ ] CONT. ON REVERSE

JOB LOADED AT ____ BY ____

JOB PICKED UP BY ____

[X] OK TO RELOAD

NBS-777 (Rev. 9-73) U.S. DEPARTMENT OF COMMERCE NATIONAL BUREAU OF STANDARDS

JOB REQUEST CARD

DATE 7/13/77

Figure 22. Job request card for ISTRIP run.

```
@:ELT,LID    FILE.STR
ELTC07 R72-16 10/18/77 19:53:17 (.0)
000001       000    @RUN,N/NR  ISTRIP,34060-SCHMID,IPOT,10,2000
000002       000    @ASG,A  IPOT*IONPACK.
000003       000    @ASG,A  GPSDC*DICX8.
000004       000    @ASG,A  TEXTPROCESS*LIB.
000005       000    @ASG,T    IPOT*RAWION2..8C9,ION02
000006       000    @USE    7..IPOT*RAWION2.
000007       000    @DELETE,C  IPOT*STRIP3476.
000008       000    @ASG,UP  IPOT*STRIP3476.
000009       000    @USE      4..IPOT*STRIP3476.
000010       000    @MAP,INX  STRIP
000011       000      LIB  IPOT*IONPACK
000012       000      LIB  GPSDC*DICX8
000013       000      LIB  TEXTPROCESS*LIB
000014       000      IN ISTRIP
000015       000    @XQT  STRIP
000016       000    FILE 4 NEW                    SORTED ION DATA 13JUL77
000017       000    RUN
000018       000    @MSG,W    30062-WEBBWI      WRITE ENABLE REEL 0409
000019       000    @ASG,TJ     11..8C,0409W
000020       000    @MARK 11.
000021       000    @CLOSE 11.
000022       000    @MAP,NX     GPSDC*DICX8.DGMDMP,DGMDMP
000023       000    @XQT  DGMDMP
000024       000    INFILE=4
000025       000    RUN
000026       000    @EOF
```

Figure 23. Listing of ISTRIP run.

Book 1 Page 3 *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100..105..110..115..120- y Ln sedd

$C_{21}H_{15}^{+}$ $C_{10}H_6(CH_3)C_{10}H_6CH_3$ CH_3 13.25 EI 3477 - 3 1
(1,1'-Binaphthyl, 2,2'-dimethyl-) - 6 2
(RN-CAS Registry Number 32834-84-7) - 9 3

$C_{21}H_{15}^{+}$ $C_{10}H_6(CH_3)C_{10}H_6CH_3$ CH_3 12.25 EI 3477 - 12 4
(1,1'-Binaphthyl, 3,3'-dimethyl-) - 15 5
(RN-CAS Registry Number 34042-82-5) - 18 6

$C_{21}H_{15}^{+}$ $C_{10}H_6(CH_3)C_{10}H_6CH_3$ CH_3 12.75 EI 3477 - 21 7
(1,1'-Binaphthyl, 7,7'-dimethyl-) - 24 8
(RN-CAS Registry Number 34003-80-0) - 27 9

$C_{21}H_{15}^{+}$ $C_{10}H_6(CH_3)C_{10}H_6CH_3$ CH_3 11.50 EI 3477 - 30 10
(1,1'-Binaphthyl, 8,8'-dimethyl-) - 33 11
(RN-CAS Registry Number 32693-05-3) - 36 12

Book 1 Page 4 *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100..105..110..115..120- y Ln sedd

$C_{22}H_{18}^{+}$ $C_{10}H_6(CH_3)C_{10}H_6CH_3$ ** 8.20 EI 3477 - 3 1
(1,1'-Binaphthyl, 2,2'-dimethyl-) - 6 2
(RN-CAS Registry Number 32834-84-7) - 9 3

$C_{22}H_{18}^{+}$ $C_{10}H_6(CH_3)C_{10}H_6CH_3$ ** 8.00 EI 3477 - 12 4
(1,1'-Binaphthyl, 3,3'-dimethyl-) - 15 5
(RN-CAS Registry Number 34042-82-5) - 18 6

$C_{22}H_{18}^{+}$ $C_{10}H_6(CH_3)C_{10}H_6CH_3$ ** 8.15 EI 3477 - 21 7
(1,1'-Binaphthyl, 7,7'-dimethyl-) - 24 8
(RN-CAS Registry Number 34003-80-0) - 27 9

$C_{22}H_{18}^{+}$ $C_{10}H_6(CH_3)C_{10}H_6CH_3$ ** 8.00 EI 3477 - 30 10
(1,1'-Binaphthyl, 8,8'-dimethyl-) - 33 11
(RN-CAS Registry Number 32693-05-3) - 36 12

Book 1 Page 5 *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100..105..110..115..120- y Ln sedd

$C_4H_5N^{+}$ C_4H_5N ** 8.40±0.05 EI 3482 - 3 1
(1H-Pyrrole) - 6 2
(RN-CAS Registry Number 109-97-7) - 9 3

Book 1 Page 6 *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100..105..110..115..120- y Ln sedd

$C_5H_7N^{+}$ $C_4H_4NCH_3$ ** 8.01±0.05 EI 3482 - 3 1
(Pyrrole, 2-methyl-) - 6 2
(RN-CAS Registry Number 636-41-9) - 9 3

Book 1 Page 7 *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100..105..110..115..120- y Ln sedd

$C_6H_5N^{+}$ C_5H_5CN ** 9.7 EI 3476 - 3 1
(Cyclopentadienecarbonitrile) - 6 2
(RN-CAS Registry Number 27669-30-5) - 9 3

Figure 24. 360 printout of a sorted ion data file using ISTRIP.

8.4 Program WREFS

This program is designed to input the bibliographic data file and output a reference file and an unsorted author file. The bibliographic data file is a GPSDC file.

Each entry begins with the identification number enclosed in brackets in columns 1-6 of the first line. The authors begin in column 8. They are separated by semicolons and terminated by a double dagger. The authors are followed by the title which is terminated by a double dagger. This is followed by the citation. The output reference file is identical to the input file except the semicolons between authors are replaced by commas and the double daggers are replaced by blanks. The unsorted author file is generated by writing out each author followed by the idiot number. This file is later sorted and entries for a given author merges to generate the author index.

DGMDMP may be used to print the reference file. A sample test run of WREFS is shown in figure 25.

8.5 Sorting the Author Index Entries

IASORT is designed to sort the author index entries. The Exec 8 version of SORTIT is used to interface with the SORT/MERGE package. IASORT is a main program used to call SORTIT. SORTIT calls two routines IASRDS and IASWRT to read and write files or tapes.

IASTRP is designed to input an author file with sort key, strip off the sort key and output an author index as a GPSDC file. The GPSDC file can then be printed using DGMDMP. A listing of the IASORT run, IASTRP, and a 360 printout of the sorted author file are shown in figures 26, 27, and 28 respectively.

```
@:ELT.LID    FILE.WRF
ELT007 972-16 11/23/77 18:21:09 (,0)
000001       000    @RUN.N/NR    WREFS.34030-WEBBWI.IPOT.10.100
000002       000    @ASG.A  IPOT*IONPACK.
000003       000    @ASG.A   TEXTPROCESS*LIB.
000004       000    @ASG.A  GPSDC*DICX8.
000005       000    @MAP.IS  REFILE
000006       000       LIB  IPOT*IONPACK.,GPSDC*DICX8.,TEXTPROCESS*LIB.
000007       000       LIB  IPOT*IONPACK.,GPSDC*DICX8.,TEXTPROCESS*LIB.
000008       000       LIB  GPSDC*DICX8
000009       000        IN WREFS
000010       000    @ASG.A    IPOT*REF3476-3484.
000011       000    @USE      1.,IPOT*REF3476-3484.
000012       000    @DELETE.C  IPOT*BIB3476-3484.
000013       000    @ASG.PU  IPOT*BIB3476-3484.
000014       000    @USE      2.,IPOT*BIB3476-3484.
000015       000    @DELETE.C  IPOT*AU3476-3484.
000016       000    @ASG.PU  IPOT*AU3476-3484.
000017       000    @USE      3.,IPOT*AU3476-3484.
000018       000    @XQT REFILE
000019       000    FILE 1 OLD
000020       000    FILE 2 NEW                    BIBLIO. BATCH 3476-3484 27JUL77
000021       000    FILE 3 NEW                    AUTHOR BATCH 3476-3484 27JUL77
000022       000    RUN
000023       000    @EOF
```

Figure 25. Listing of WREFS run.

```
@:ELT,LID    FILE.ASR
ELT007 R72-16 01/18/78 20:19:03 (,0)
000001       000    @RUN,N/NR    IASORT,34030-WEBBWI,IPOT,10,300
000002       000    @ASG,A  NBS*SORTIT.
000003       000    @ASG,A  IPOT*IONPACK.
000004       000    @ASG,A   GPSDC*DICX8.
000005       000    @ASG,A  TEXTPROCESS*LIB.
000006       000    @ASG,A  IPOT*AU3476-3484.
000007       000    @USE    1.,IPOT*AU3476-3484.
000008       000    @DELETE,C  IPOT*ASR3476-3484.
000009       000    @ASG,UP  IPOT*ASR3476-3484.
000010       000    @USE    4.,IPOT*ASR3476-3484.
000011       000    @MAP,IX    ASRT
000012       000      LIB IPOT*IONPACK
000013       000      LIB NBS*SORTIT
000014       000      LIB GPSDC*DICX8
000015       000      LIB TEXTPROCESS*LIB
000016       000      IN IASORT
000017       000    @XQT  ASRT
000018       000    FILE 1 OLD
000019       000    FILE 4 NEW                    SORTED AUTHORS 3476-3484 06JAN
000020       000    PGWDTH 4 = 110
000021       000    PGLENG 4 = 160
000022       000    DMPOPT = 1
000023       000    INFILE = 1
000024       000    OTFILE = 4
000025       000    RUN
000026       000    @EOF
```

Figure 26. Listing of IASORT run.

```
)ELT,LID    FILE.AST
ELT007 R72-16 01/18/78 20:19:03 (,0)
000001       000    @RUN,N/NR   IASTRP,34030-WEBBWI,IPOT,10,2000
000002       000    @ASG,A   IPOT*ICNPACK.
000003       000    @ASG,A   GPSDC*DICX8.
000004       000    @ASG,A   TEXTPROCESS*LIB.
000005       000    @ASG,A   TEXTPROCESS*LIB.
000006       000    @ASG,A   IPOT*ASR3476-3484.
000007       000    @USE   1.,IPOT*ASR3476-3484.
000008       000    @DELETE,C    IPOT*AUTHR3476.
000009       000    @ASG,UP    IPOT*AUTHR3476.
000010       000    @USE     2.,IPOT*AUTHR3476.
000011       000    @MAP,IX    ASTRP
000012       000      LIB   IPOT*ICNPACK
000013       000      LIB   GPSDC*DICX8
000014       000      LIB   TEXTPROCESS*LIB
000015       000      IN IASTRP
000016       000    @XQT   ASTRP
000017       000    FILE 1 OLD                    AUTHORS WITH SORT KEY ATTACHED 04OCT77
000018       000    FILE 2 NEW                    STRIPPED UNSORTED AUTHORS 04OCT77
000019       000    *INFILE 1
000020       000    *OTFILE 2
000021       000    DMPOPT=1
000022       000    *RUN
000023       000    @MSG,W    34030-WEBBWI     WRITE ENABLE REEL 0409
000024       000    @ASG,TJ     11.,8C,0409W
000025       000    @MARK 11.
000026       000    @CLOSE 11.
000027       000    @MAP,NX     GPSDC*DICX8.DGMDMP,DGMDMP
000028       000    @XQT    DGMDMP
000029       000    FILE 2 OLD
000030       000    INFILE=2
000031       000    RUN
000032       000    @EOF
```

Figure 27. Listing of IASTRP run.

```
Book     1  Page   1     *...30...35...40...45...50...55...60...65...70...75...80...85...90...95..100- y  Ln eedd

Benezra, S. A., 3480                                                                                  -  3  1
Benezra, S. A., 3483                                                                                  -  6  2
Bursey, M. M., 3480                                                                                   -  9  3
Bursey, M. M., 3483                                                                                   - 12  4
Cooks, R. G., 3476                                                                                    - 15  5
Gamble, A. A., 3486                                                                                   - 16  6
Gilbert, J. K., 3484                                                                                  - 21  7
Harris, M. M., 3477                                                                                   - 24  8
Hedaya, E., 3476                                                                                      - 27  9
Howe, I., 3476                                                                                        - 30 10
Jalonen, J., 3481                                                                                     - 33 11
Kent, M. E., 3476                                                                                     - 36 12
Linda, P., 3482                                                                                         39 13
Lossing, F. P., 3476                                                                                    42 14
Loudon, A. G., 3477                                                                                     45 15
Marino, G., 3482                                                                                      - 48 16
Mazengo, K. Z., 3477                                                                                    51 17
McAllister, T., 3476                                                                                    54 18
McNeil, D. W., 3476                                                                                     57 19
Pignataro, S., 3482                                                                                   - 60 20
Pihlaja, K., 3481                                                                                     - 63 21
Simmie, J. M., 3476                                                                                     66 22
Tillett, J. G., 3484                                                                                    69 23
Tschulkow-Roux, E., 3476                                                                                72 24
Williams, D. H., 3479                                                                                   75 25
```

Figure 28. 360 printout of sorted author file.

9. ACKNOWLEDGMENTS

We are indebted to Mr. Keith Draxl and Mrs. Candyce Schmidt for their numerous helpful suggestions and assistance in the preparation of this publication. Special appreciation goes to Mrs. Carla Messina, and Dr. William H. Evans for programming contributions. We also thank Mrs. Janice L. Jones for her valuable secretarial assistance.

10. LIST OF FIGURES

11. LIST OF TABLES

12. REFERENCES

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13. APENDIX A

NBS Composite and Red Shift Symbols Table - August 1976 Version.

Symbol	Type	Components		Name	NBS No.
A	A			A	33
Å	Å	A	°	Angstrom	257
Á	Á	A	´	A acute	318
Ă	Ă	A	˘	A circumflex	258
À	À	A	`	A grave	259
Ä	Ä	A	"	A umlaut	260
Ã	Ã	A	~	A tilde	314
Ą	Ą	A	,	A cedilla	465
a	a			a	65
å	à	a	°	angstrom	261
á	á	a	´	a acute	319
ă	á	a	˘	a breve	366
ā	ā	a	¯	a macron	368
â	â	a	^	a circumflex	262
à	à	a	`	a grave	263
ä	ä	a	"	a umlaut	264
ã	ã	a	~	a tilde	315
ą	ą	a	,	a hook	375
B	B			B	34
b	b			b	66
C	C			C	35
Ć	Ć	C	´	C acute	466
Č	Ć	C	˘	C breve	320
C̄	C	C	¯	C macron	390
©	©	C	#	copyright	428
Ç	Ç	C	,	C cedilla	287
c	c			c	67
ć	ć	c	´	c acute	347
č	ć	c	˘	c breve	356
¢	¢	c	/	cent	294
ç	ç	c	,	c cedilla	288
D	D			D	36
d	d			d	68
E	E			E	37
È	È	E	`	E grave	267
Ê	Ê	E	^	E circumflex	266
É	É	E	´	E acute	265
Ē	E	E	¯	E macron	394
Ë	Ë	E	"	E umlaut	268
Ẽ	Ẽ	E	~	E tilde	467
Ę	Ę	E	,	E cedilla	468
e	e			e	69
é	é	e	´	e acute	269
ĕ	é	e	˘	e breve	367
ē	ē	e	¯	e macron	369
ê	ë	e	^	e circumflex	270
è	è	e	`	e grave	271

NBS Composite and Red Shift Symbols Table - August 1976 Versi

Symbol	Type	Components		Name	NBS No
ë	ë	e	"	e umlaut	272
ẽ	ẽ	e	~	e tilde	469
ę	ę	e	,	e hook	378
F	F			F	38
F̄	F̄	F	~	F macron	397
f	f			f	70
G	G			G	39
Ğ	Ğ	G	˘	G breve	470
Ḡ	Ḡ	G	~	G macron	387
g	g			g	71
g̃	g̃	g	~	g tilde	348
ğ	ğ	g	˘	g breve	357
g̀	g̀	g	`	g grave	358
H	H			H	40
H̄	H̄	H	~	H macron	388
h	h			h	72
I	I			I	41
Í	Í	I	´	I acute	331
Î	Î	I	^	I circumflex	273
Ì	Ì	I	`	I grave	333
Ï	Ï	I	"	I umlaut	274
I°	I°	I	°	I degree	384
Ĩ	Ĩ	I	~	I tilde	471
i	i			i	72
í	í	i	´	i acute	332
ĭ	ĭ	i	˘	i breve	381
ĩ	ĩ	i	~	i tilde	472
ī	ī	i	¯	i macron	370
î	î	i	^	i circumflex	275
ì	ì	i	`	i grave	334
ï	ï	i	"	i umlaut	276
i̯	i̯	i	,	i hook	376
J	J			J	42
j	j			j	74
K	K			K	43
Ķ	Ķ	K	,	K cedilla	341
k	k			k	75
ķ	ķ	k	,	k cedilla	342
L	L			L	44
Ł	Ł	L	/	Polish L	345
£	£	L	=	pound	441
L̄	L̄	L	~	L macron	396
l	l			l	76
ĺ	ĺ	l	´	l acute	343
ĭ	ĭ	l	˘	l breve	344
ł	ł	l	/	Polish l	346
!	!			!	45

* * NBS Composite and Red Shift Symbols Table - August 1976 Version.

Symbol	Type	Components		Name	NBS No.
m	m			m	77
m̃	m̃	m	~	m tilde	379
N	N			N	46
Ñ	Ñ	N	~	N tilde	289
Ń	Ń	N	´	N acute	349
n	n			n	78
ñ	ñ	n	~	n tilde	290
ń	ń	n	´	n acute	350
n̆	n̆	n	˘	n breve	360
n̄	n̄	n	¯	n macron	392
ņ	ņ	n	,	n cedilla	359
O	O			O	47
Ó	Ó	O	´	O acute	335
Ô	Ô	O	^	O circumflex	277
Ò	Ò	O	`	O grave	337
Ö	Ö	O	"	O umlaut	278
Õ	Õ	O	~	O tilde	316
Ø	Ø	O	/	Danish O	292
o	o			o	79
ó	ó	o	´	o acute	336
ò	ó	o	˘	o breve	371
õ	õ	o	¯	o macron	380
ô	ô	o	^	o circumflex	279
ò	ò	o	`	o grave	338
ö	ö	o	"	o umlaut	280
õ	õ	o	~	o tilde	317
ø	ø	o	/	Danish o	293
P	P			P	48
p	p			p	80
Q	Q			Q	49
q	q			q	81
R	R			R	50
®	®	R	#	registered	427
r	r			r	82
ŕ	ŕ	r	´	r acute	385
r̆	ŕ	r	˘	r breve	362
ŗ	ŗ	r	,	r cedilla	361
S	S			S	51
S̄	S̄	S	¯	S macron	389
Ś	Ś	S	´	S acute	473
Ş	Ş	S	,	S cedilla	474
s	s			s	83
ś	ś	s	´	s acute	386
s̆	ś	s	˘	s breve	363
ş	ş	s	,	s cedilla	353
T	T			T	52
t	t			t	84

* * NBS Composite and Red Shift Symbols Table - August 1976 Versi

Symbol	Type	Components		Name	NBS No
ţ	ţ	t	,	t cedilla	364
U	U			U	53
Ũ	Ũ	U	~	U tilde	475
Ú	Ú	U	´	U acute	339
Û	Û	U	^	U circumflex	281
Ù	Ù	U	`	U grave	282
Ü	Ü	U	"	U umlaut	283
u	u			u	85
ũ	ũ	u	~	u tilde	476
ú	ú	u	´	u acute	340
ū	ū	u	¯	u macron	372
ů	ů	u	°	u degree	373
û	û	u	^	u circumflex	284
ù	ù	u	`	u grave	285
ü	ü	u	"	u umlaut	286
ų	ų	u	,	u hook	377
V	V			V	54
v	v			v	86
W	W			W	55
w	w			w	87
X	X			X	56
X̄	X̄	X	¯	X macron	391
x	x			x	88
x̄	x̄	x	¯	x macron	395
Y	Y			Y	57
y	y			y	89
ý	ý	y	´	y acute	374
Z	Z			Z	58
Ź	Ź	Z	´	Z acute	477
Ż	Ż	Z	`	Z grave	478
z	z			z	90
ż	ż	z	°	degree over z or z dot	354
ź	ź	z	´	z acute	355
ž	ž	z	ˇ	z breve	365

* * NBS Composite and Red Shift Symbols Table - August 1976 Version.

Symbol	Type	Components	Name	NB. .o.
α a	a		alpha	147
β	b		beta	148
γ	g		gamma	149
Γ	G		Gamma	136
δ	d		delta	150
Δ	D		Delta	137
ε	e		epsilon	151
é	é	e '	epsilon acute	383
ζ	z		zeta	152
η	h		eta	153
Θ	Θ	O -	Theta	138
θ	q		theta	154
ι	i		iota	151
κ	k		kappa	155
Λ	L		Lambda	139
λ	l		lambda	156
μ	m		mu	157
ν	n		nu	158
o	o		ellipse or omicron	194
ξ	j		xi	159
Ξ	J		Xi	140
π	p		pi	160
Π	P		Pi	141
Π	B		product	116
ρ	r		rho	161
σ	s		sigma	162
Σ	S		Sigma	142
∑	C		sum	117
τ	t		tau	163
υ	u		upsilon	182
Υ	U		Upsilon	143
φ	φ	o ¦	phi	164
Φ	Φ	O ¦	Phi	144
χ	x		Chi	165
ψ	y		psi	166
Ψ	Y		Psi	145
ω	w		omega	167
Ω	W		Omega	146

* * NBS Composite and Red Shift Symbols Table - August 1976 Version

Symbol	Type	Components	Name	NBS No.
!	!		Exclamation	1
"	"		double prime	2
'	'		prime, accent acute, or apostrophe	7
`	`		accent grave	32
#	#		number or scratch	3
$	$		dollar sign	4
%	%		percent	5
&	&		ampersand	6
@	@		commercial at	64
(	(		left parenthesis	8
)	)		right parenthesis	9
[	[		left bracket	59
]	]		right bracket	61
{	{		left brace	91
}	}		right brace	93
*	*		asterisk	10
.	.		period	14
:	:		colon	26
,	,		comma	12
;	;		semicolon	27
/	/		slant/slash	15
\	\		reverse slash	60
|	|		vertical bar	92
?	?		question mark	31
+	+		plus	11
−	-		minus	13
–	-		hyphen	106
—	?		thick dash	100
=	=		equal	29
<	<		less than	28
>	>		greater than	30
~	~		tilda	94
^	^		circumflex	62
_	_		underline	63
×	X		multiplied by	119
∇	H		del	118
∂	P		differential	134
◇	A		diamond	171
⌑	H		lozenge	130
Π	B		product	116
Σ	C		sum	117
°	o		ellipse	194
∫	I		integral	133
∮	&	I	contour integral	401
√	*		square root	135
÷	+	- :	divided by	297
+	+		plus	11
±	±	+ ,	plus or minus	291
∓	∓	+	minus or plus	292

* * NBS Composite and Red Shift Symbols Table - August 1976 Version. *

Symbol	Type	Components		Name	NBS No.
<	<			less than	28
>	>			greater than	30
≥	≥	>	=	greater than or equal	299
≤	≤	<	=	less than or equal	298
≮	≮	<	¦	not less than	311
≯	≯	>	¦	not greater than	312
⟨	⟨	<	.	average brace	109
⟩	⟩	>	.	average brace	110
∝	R			varies directly as	125
∞	c			infinity	121
≈	v			equivalent; similar	195
	=			nearly equal	173
≡	≡	=	~	is congruent	301
≠	≠	=	/	not equal	295
≠	≠	=	¦	not equal	313
≢	≢	=,	,	is identical	300
≢	≠	=	/	not identically equal	443
¬	¦			logical not	131
∀	∀	V	-	logical for all	406
⊂	⊂			is a subset	112
∩	∩			intersection of two sets	107
⊃	⊃			contained as a subset	111
∪	∪			union of two sets	108
⊄	⊄	⊂	\	is not a subset of	402
⊅	⊅	⊃	/	is not contained as a subset	403
∃	E			there exists	113
∈	∈	⊂	-	is an element of	404
∋	∋	⊃	-	such that	405
⇌	K			reversible reaction	188
·	2			center dot	175
¶	Q			paragraph	189
†	V			dagger	123
†	†	¦	M	dagger	123
‡	‡	¦	=	double dagger	124
..	+			two dot leader	180
...	5	.	5	three dot leader	393
¤	¤	X	o	currency	442
¢	¢	C	/	cent	294
£	£	L	=	pound	441
®	®	R	#	registered	427
©	©	C	#	copyright	426
§	§			section	120

* * NBS Composite and Red Shift Symbols Table - August 1976 Version

Symbol	Type	Components		Name	NBS No.
´	´			accent aigu	7
`	`			accent grave	32
¨	¨			accent umlaut	2
‘	‘	`		open quote	450
’	’	'		close quote	451
¸	¸			accent cedilla	12
°	°			degree	122
¯	¯			macron	190
˘	˘			breve	174
˜	˜			tilde	94
^	^			circumflex	62
_	_			underline	63
$\bar{0}$	0	0	¯	zero macron	330
$\bar{1}$	1	1	¯	one macron	321
$\bar{2}$	2	2	¯	two macron	322
$\bar{3}$	3	3	¯	three macron	323
$\bar{4}$	4	4	¯	four macron	324
$\bar{5}$	5	5	¯	five macron	325
$\bar{6}$	6	6	¯	six macron	326
$\bar{7}$	7	7	¯	seven macron	327
$\bar{8}$	8	8	¯	eight macron	328
$\bar{9}$	9	9	¯	nine macron	329
1/2	½	1	⁄	one half	453
$\overline{1\backslash 2}$	½	2	-	bar one half	452
1/3	⅓	1	⁄	one third	456
2/3	⅔	2	⁄	two thirds	457
1/4	¼	1	⁄	one fourth	454
3/4	¾	3	⁄	three fourths	455
1/6	⅙	1	⁄	one sixth	462
5/6	⅚	5	⁄	five sixths	463
1/8	⅛	1	⁄	one eighth	458
3/8	⅜	3	⁄	three eighths	459
5/8	⅝	5	⁄	five eighths	460
7/8	⅞	7	⁄	seven eighths	461

* * NBS Composite and Red Shift Symbols Table - August 1976 Version. *

Symbol	Type	Components		Name	NBS No.
⇄	K			reversible reaction	188
↔	B	6	7	left-right arrow	416
⇇	<	<	-	3 bonds right	308
←	6			left arrow	129
↘	>	>	-	right bond corner	307
→	7			right arrow	127
↑	8			up arrow	126
↓	9			down arrow	123
↕	B	8	9	double head arrow	413
↖	S	\	3	N.W. arrow	409
↘	S	\	5	S.E. arrow	410
↗	H	/	4	N.E. arrow	411
↙	/	/	.	S.W. arrow	412
'	"			left high vertical bar	98
-	0			right horizontal bar	183
-	:			left horizontal bar	184
'	;			right high vertical bar	185
-	-			hyphen	106
▬	$			thick dash	100
⟋	!			single bond left	97
⟋	/			long slant	15
⟍	#			single bond right	99
⟍	\			reverse slash	60
'	%		'	left vertical bar	101
⫽	&			double bond left	103
⫽	'			double bond right	104
‖	1			vertical double bond	172
⫼	)	¦	1	vertical triple bond	417
:	.			S.W. dot	178
·	3			N.W. dot	176
·	4			N.E. dot	177
·	5			S.E. dot	179
·	2			centered dot	175
•	?-			big centered dot	132
O	,			box with round corners	193
□	—			open box	168
(	<	<	.	left corner	109
)	>	>	.	right corner	110
^	^	^	.	top corner	166
v	v	v	.	bottom corner	167

* * NBS Composite and Red Shift Symbols Table - August 1976 Version.

Symbol	Type	Components		Name	NBS No.
	1	1	?	mystery no. 1	481
	2	2	?	mystery no. 2	482
	3	3	?	mystery no. 3	483
	4	4	?	mystery no. 4	484
	5	5	?	mystery no. 5	485
	6	6	?	mystery no. 6	486
	7	7	?	mystery no. 7	487
	8	8	?	mystery no. 8	488
	?.	9	?	mystery no. 9	489

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14. Sponsoring Agency Code

15. SUPPLEMENTARY NOTES

16. ABSTRACT (*A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.*)

The Ion Energetics Data Center is engaged in the compilation, evaluation and dissemination of experimental information on gaseous ion energetics. Outputs include bibliographic and tabular information on ionization potentials, appearance potentials, electron affinities and heats of formation of gaseous positive and negative ions. The operation of the data center is discussed. This operation has recently been automated by the development of a set of computer programs, called IONPACK, which minimize the manual effort required for the numerous file manipulations and editing steps necessary to produce the data center output. The functions of the programs are outlined and the associated operating procedures are described in detail. Full documentation of the programs is presented in a separate report.

17. KEY WORDS (*six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons*)

Abstract; appearance potential; archival tape; computer program; data base; data base management; empirical molecular formula; GPSDC; ion energetics; ionization potential

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