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Description of the Magnetic Tape Version of the Bulletin of Thermodynamics and Thermochemistry, No. 14 (1971)

U.S.
DEPARTMENT
OF
COMMERCE
National
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Standards

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Robert McClenon

Office of Standard Reference Data
National Bureau of Standards
Washington, D.C. 20234

William H. Evans and David Garvin

Physical Chemistry Division
Institute for Materials Research
National Bureau of Standards
Washington, D.C. 20234

and

Blanton C. Duncan

Computer Services Division
Institute for Computer Sciences and Technology
National Bureau of Standards
Washington, D.C. 20234



U.S. DEPARTMENT OF COMMERCE, Frederick B. Dent, *Secretary*

NATIONAL BUREAU OF STANDARDS, Richard W. Roberts, *Director*

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CONTENTS

1. Introduction	1
2. General Summary of the Work	3
3. Description of an Entry	5
4. Sequence of Files and Structure	10
5. Technical Description of the Record	12

Appendices

A. Codes for Properties Used on B.T. and T. Tapes	18
B. Glossary of Symbols for the Substance-Property Index	19
C. Codes for States Used on B.T. and T. Tapes	21
D. Organic Compound Main and Group Classes	22
E. Finding Number Sequence for the Elements Used on B.T. and T. Tapes	31
F. Flags (Used on B.T. and T. Tapes)	33
G. Display of Data Recording ("Dump")	34

Description of the
Magnetic Tape Version of the
Bulletin of Thermodynamics and
Thermochemistry, No. 14 (1971)

Robert C. McClenon, William H. Evans
David Carvin and Blanton C. Duncan

Abstract

The substance-property index and bibliography sections of the Bulletin of Thermodynamics and Thermochemistry, No. 14 (May 1971) have been converted to a magnetic tape version designed for computerized searching written in an extended form of the American National Standard Code for Information Interchange (X 3.4-1968). In this version each substance-property entry has been supplemented by a searching key. This report describes the magnetic tape version.

Key words: Bibliography; chemical thermodynamics; extended character codes; information retrieval; magnetic tape.

1. Introduction

The Bulletin of Thermodynamics and Thermochemistry (B. T. and T.) is an annual publication prepared under the auspices of the Commission of Thermodynamics and Thermochemistry of the Division of Physical Chemistry of the International Union of Pure and Applied Chemistry. It is edited by Professor Edgar F. Westrum, Jr., University of Michigan, Ann Arbor, Michigan.

The Bulletin contains (a) abstracts of work in progress during a calendar year, (b) a substance-property index to these abstracts and to papers published during the same period, and, (c) a bibliography to which the index is keyed.

The final stages of preparing the substance-property index and the bibliography are carried out at the National Bureau of Standards by the Chemical Thermodynamics Data Group, Physical Chemistry Division, Institute for Materials Research. At this stage the entire contents of the index and bibliography are stored on magnetic tape and are manipulated using the General Purpose Scientific Document Code System.

The tapes for Bulletin of Thermodynamics and Thermochemistry, No. 14 (May 1971), covering 1970, have been used to prepare a machine-readable record that can be used in computerized information retrieval systems. This report explains the structure of the records, the chemical symbolism used and the technical characteristics of the machine record. It should be a sufficient starting point for the transcription of the record at a computer center and use of the material by chemists.

2. General Summary of the Work

Chemistry requires a complex symbolism, even for a compound-oriented index. Figure 1, a page from the Bulletin shows this. There are upper and lower case letters, subscripts and superscripts and occasional Greek letters. Underscoring is used to indicate type-face changes.

All of these features are present on the machine-readable record. The index sections of the record are line-by-line copies of each column in the index supplemented by a searching key that summarizes the entry in a rigidly prescribed manner (See Section 3). The bibliography sections of the record are line-by-line copies of the bibliography in the Bulletin.

The substance-property index in the Bulletin is in three parts: organic substances, organic mixtures and inorganic substances. The machine record also is in several parts corresponding to the division in the Bulletin. This overall structure is described in Section 4.

The machine record is written in the American National Standard Code for Information Interchange (ASCII-1968) which is a variant of the International Standardization Organization Code (ISO/IS 646). In order to obtain special features (subscripts, Greek etc.) the ASCII-1968 code has been supplemented with an additional set of characters and several specially defined escape code sequences. The technical details of the machine record are described in Section 5.

The potential user of the tape will face two major tasks which are not discussed further in this report. First, he must obtain a program that will read and transcribe the ASCII records into a form usable on his computer system. Second, he must develop or obtain a program that can search the records.

The first task is one which should preferably be done by the computer service center rather than by the individual user, since the result will be a utility program applicable to any ISO or ASCII tape. The second task may be either simple or complex. This depends upon whether a simple character by character comparison of chemical formulae is to be used or whether the detailed information in the searching key is to be used to make the search more efficient.

3. Description of an Entry

Each of the index files in the Bulletin of Thermodynamics and Thermochemistry is divided into basic logical groups of information known as entries. Each entry contains a reference number, correlating it to an entry in the corresponding bibliographic file, and additional information intended to permit mechanized searching of the Bulletin.

The entry consists of:

- (a) Two lines of coded information followed by one line per compound in the entry.
- (b) The text as printed in the Bulletin. This is often one line, but may be several lines long.

A typical entry is shown in figure 2.

3.1 First Line:

The first character in the first line of an entry is an ASCII Group Separator. This denotes the start of an entry. Columns 2 through 6 contain a sequence number which is assigned to the entry by the program generating the tape. The entry appearing first on the tape is assigned the number 1; the second number is assigned the number 2; the thousandth entry is assigned the number 1000, and so on. This number (like every number in the first two lines of an entry) is right justified in its field: the units digit is in column 6. In the example shown in figure 2, the sequence number is 141.

Columns 8 and 9 (or, if the number is one digit, column 9 only) contain the number of lines in the entry. In the example shown, there are five lines, therefore this number is 5.

Column 11 contains the number of substances for which chemical formulas are given, one per line. The maximum number of substances indexed in this way is 3. If more than three substances are present in an alloy or a mixture, only the first three are indexed, and the entry is permuted "end-around" so that all substances are indexed. In the example shown, two substances (water and hydrogen chloride) are indexed.

Column 13 contains the number of property codes for which the substance described has been indexed. The maximum value of this number is 3. The property codes are given in columns 14 and 15; columns 16 and 17; and columns 18 and 19. The document described by the entry in figure 2 discusses two properties, having the codes 17 and 28. The zero in column 19 occurs because there is no third property. If more than three property codes are present in the entry, only the three lowest are given. Appendices A and B give the meanings of the property codes.

Note that there are two sets of property codes. One is for compounds for which a formula is given. The other is for miscellaneous subjects. The numerical values in the two sets overlap.

Columns 21 and 22 contain a numerical state code. Meanings of the state codes are given in Appendix C. The 45 in figure 2 indicates a liquid-gas transition.

Columns 24 through 27 give the class code for an organic compound. Columns 28 through 30 give the subclass code. These are explained in Appendix D. In figure 2 they are zeroes because the entry is from the inorganic file. Values of 1023 for the class code and 255 for the subclass may also occur for inorganic entries.

Columns 32 through 34 contain a "finding number" for the substances described on the first substance line. The finding number is based on the standard order of arrangement of the elements (see NBS Technical Note 270). It indicates the element in the first substance that occurs last in the standard order. Appendix E lists the element to which each finding number corresponds. For example, in figure 2, the substance listed first is water. Since hydrogen follows oxygen in the standard order, the finding number is that of hydrogen, which is 2. Certain entries may have anomalously large finding numbers, such as 117. Such a number indicates that the item was filed in the "General and Miscellaneous" section of the index, e.g. starting at p. 252 of the Bulletin, number 14. The subheadings in this section are the property codes for miscellaneous items.

Columns 41 through 48 contain the reference number. This specifies the bibliographic entry to which this index entry refers. In the example shown, the reference number is 5157-70. Note that this number appears twice in each index entry.

This line is always present. It is 47 or 48 characters long, not including control codes.

3.2 Second Line:

The second line contains numerical "flags" alerting a searcher to special characteristics of an indexed substance. Column 1 contains the number of flags for the first substance, column 2, for the second substance, column 3, for the third substance. There may be from 0 to 5 flags for a substance. Each flag consists of two digits. Since there may be up to 15 flags, 30 columns are reserved for the flags (10 columns

for each substance). The flags for the first substance are in columns 4 through 13. Those for the second substance are in columns 14 through 23. Those for the third substance are in columns 24 through 33. The information in columns 1 through 3 indicates that there is a single flag for the first substance. This flag, a 3, is found in column 5 (actually columns 4 and 5). Appendix F makes it clear that this flag identifies the first compound, water, as a component of a mixture, to be followed by (at least) one more component. The flags 2, indicating a hydrate, 11, indicating positive charge, and 12, indicating negative charge, are each followed by a number which is not actually another flag but a count. For a hydrate it is the number of molecules of water of hydration. For an ion it represents the number of charges.

This line is always present; it may be 3 to 33 characters long, not including control codes.

3.3 Formula Lines:

An empirical formula for each substance is part of each entry. Each formula appears on a separate line. The example given in Figure 2 illustrates two significant features of the formula. First, the elements in a formula are arranged in reverse standard order of arrangement. Thus hydrogen chloride is written Cl_1H_1 . Second, a subscript "1" follows the symbol for an element of which the compound contains one atom. This permits the formula to be converted into a 6-bit code (e.g., BCD) in which no distinction is made between upper and lower case, without ambiguity. The formula may be followed by a slash, which indicates that it is one of the components of an alloy or a system, in which case the next component is on the next line.

3.4 Text:

Following the substance lines, the text of the index as printed in the Bulletin appears on the tape. One may note the correspondence between the substance lines and the formula in the text; between the state abbreviation following the formula in the text, and the state code in columns 21 and 22 of the first line; and between the property symbols beginning in column 31 of the first line of text, and the property codes in columns 14 through 19.

4. Sequence of Files and Structure

The Bulletin tape consists of six files. The first record on the tape is a standard volume header label as described in ANSI X3.27-1969. It is followed immediately by the file header labels for the first file. Each file is preceded by two standard file header labels (followed by a tape mark). The file itself is followed by a tape mark; and the file and its tape mark are followed by a standard end-of-file label and a tape mark. Two tape marks follow the final end-of-file label. This structure is shown in figure 3.

The first file contains the substance-property index to the inorganic section of the Bulletin. Its format is described in Chapter 3. The second file contains the index for organic compounds. The third file contains the index for organic mixtures. The maximum length of a line in an index file is 48 characters.

The fourth through sixth files contain the bibliographic portion of the Bulletin for the inorganic, organic compound, and organic mixture sections respectively. * These files are images of the bibliographic parts of the printed Bulletin. The first line of a bibliographic entry begins in column 1 with a digit. Each continuation line of an entry begins in column 4. The maximum length of a line is 110 characters. Note that group separators do not precede entries in the bibliography.

The following table gives the number of 1008-character blocks and of lines in each file. (A "line" consists of a line feed followed by at

*Note that the inorganic reference numbers start 3001, organic substances at 0001 and organic mixtures at 1001.

least one graphic character and possibly other characters, followed by a carriage return).

<u>File</u>	<u># Blocks</u>	<u># Lines</u>
1	1526	40470
2	347	8917
3	980	26301
4	493	5224
5	101	1097
6	249	2441

5. Technical Description of the Record

5.1 The tape is a standard 0.5 in. (1.27 cm) wide magnetic tape.

5.2 The recording is in 9 tracks at a density of 800 characters per inch (\sim 315 per cm). There are 1008 characters per physical record. Each record is followed by an 0.6 in. (1.52 cm) record gap.

5.3 The information is recorded using the American National Standard Code for Information Interchange, ASCII-1968, Document X 3.4-1968, with certain extensions described in section 5.5, below. This is a 7 bit code. The eighth bit available for recording information on a 9 track tape is always zero. That means that the information itself has been recorded without the parity bit usually included on paper tape records.

5.4 Standards. The recording has been prepared in conformance with the pertinent standards. The American National Standard Code is a recognized variant of the International Standard Code for Information Processing Interchange, ISO/IS 646. Recipients not familiar with the developing body of formal standards for information interchange will find it useful to study some of the basic standards. Within the U.S.A. the essential set of standards (one still in draft) is:

- (1) X 3.4-1968, American National Standard Code for Information Interchange (FIPS Publication 1)
- (2) X 3.22-1967, American National Standard Recorded Magnetic Tape for Information Interchange (800 CPI, NRZI) (FIPS Publication 3)
- (3) X 3.26-1970, American National Standard Hollerith Punched Card Code (FIPS Publication 14)
- (4) X 3.27-1969, American National Standard Magnetic Tape Labels for Information Interchange
- (5) X3L2/1199, American National Standard Code Extension Techniques for Use with the 7-Bit Coded Character Set of ASCII.

All these standards can be considered as derivatives of corresponding ISO standards. They may be obtained from the American National Standards Institute. Recipients in other countries can expect to be able to obtain copies of their own corresponding national standards from their national standards agencies.

5.5 Special features on this tape. The tape is designated as being a "GPDW03" tape (General Purpose Document Writer-03). This means that we have (a) defined the meaning of six Escape sequences and (b) defined an alternative set of graphics to supplement the basic ASCII set.

(a) The escape sequences and their uses here are:

Sequence	Meaning at a Teletypewriter	Use in GPDW03
<u>ESC 3</u>	Shift to Red Ribbon	(alternative graphic set)
<u>ESC 4</u>	Shift to Black Ribbon	(basic graphic set)
<u>ESC 7</u>	Reverse Line Feed	(up one line)
<u>ESC 8</u>	Reverse One-half Line Feed	(up 1/2 line)
<u>ESC 9</u>	Forward One-half Line Feed	(down 1/2 line)
<u>ESC % 3</u>	Standard Designator for GPDW03 as a Code Requiring Special Interpretation	

The first five Escape sequences occur in the body of the text. ESC 3 and ESC 4 signal changes of graphic character sets. "Shift Out" (SO) is not used on this tape to signal changes of graphic sets because it has been assigned a specific meaning in some national standards. On the other hand, Shift In (SI) does occur at the beginning of each page of text.

ESC 7, ESC 8 and ESC 9 are used to signal the motion of a printing device to and from positions needed for superscripts and subscripts.

The final sequence, ESC % 3 appears at the start of each physical record. It warns that the GPDW03 conventions are being used.

(b) The graphic character sets and their numerical codes are defined in figure 4.

5.6 Examples of recordings. A computer programmer who must arrange to read a magnetic tape that has been prepared outside his installation needs a printed example of the record on the tape. This will be used to check the performance of the hardware tape-reading facility when reading the foreign tape. Appendix G contains such a printed record, a "dump" of part of this tape. It is a representation in limited symbolism, character by character, of several lines of text. The actual numerical codes can be obtained by interpreting this dump using figure 4.

It may also help the recipient who plans to transcribe this tape to be aware of the following conventions:

(1) The text is broken into lines. A carriage return (CR), line feed (LF) sequence signals the end of the line. This sequence has several delete (DEL) codes in it.

(2) The only other use of carriage return is in a sequence at the start of a page. A page start is indicated by form feed (FF) and carriage return together with several (DEL) codes.

(3) Delete codes (DEL) have been inserted whenever it is desirable to provide for a time delay during the mechanical motion of a printing device.

(4) Lines of text may start in one physical record and end in the next. Even in this case, the sequence ESC % 3 is placed at the start of the second physical record.

(5) Line feed (LF) controls may occur within the recording for a line of text. This can happen when movement from a superscript level to a subscript level is required.

(6) Lines are always separated by at least one blank half-line interval.

(7) Backspace (BSP) is used, often to achieve overstriking of characters. Backspace does not carry the meaning "backspace and delete the previous character."

(8) Shift In (SI) occurs regularly in the pagination sequence (see 2, above). This is done in order to reestablish periodically a standard default condition in case of error.

5.7. Discussion. Although the statements above are definitive, they do not make it clear that we have exploited almost all of the features of the ASCII (or ISO) code system in this recording. This subsection attempts to explain the matter.

The record on the tape is a teletypewriter driver record, that is, a sequence of control and graphic codes that could cause a typewriter-like device that responds to ASCII to produce a clean copy, line by line, of the information. The features that this idealized teletypewriter (the target device) must have are described below.

(1) The target device is a character sequential page printer, i.e. a "typewriter-like reference transducer." This assumption reflects an attempt to invoke a broadly acceptable lowest common denominator for data interchange and dissemination.

(2) The target printer can print only the 94 graphic characters of ASCII, e.g. in the columns labeled "Std", figure 4.

(3) The target printer provides two color printing, e.g. black and red, subject to being invoked under code control. Symbols printed in red are to be interpreted as symbols from the alternative set of 94 graphic characters.

(4) The target printer provides forward and reverse half line feed under code control. By this means all symbols are subject to being placed in the positions of superscripts or overscores and subscripts or underscores.

(5) The target printer provides backspace under code control so that the effective graphic repertory includes composite symbols formed by overstriking.

(6) The target printer provides separate "carriage return" and "line feed" functions, i.e. carriage return implies no vertical motion. In addition, the device provides a reverse line feed function under code control. It may be noted that two-half line feed intervals are taken to equal one line feed interval, exactly.

(7) The target printer provides a "form feed" or "page eject" function under code control.

Teletypewriters with these capabilities are available as off-the-shelf items. One of them was used to keyboard the copy from which figure 4 was printed.

Typewriter-like devices with more limited characteristics can still produce interpretable, but slightly less readable records from GPDW03 tapes. In addition, such a tape can be "dumped" on a line printer. Such a dump is shown in Appendix G.

Appendix A

Codes for Properties used on BT of T tapes

Property Class	Tape Code	Property Class	Tape Code
none(blank)	0	8	30
0	1	8c	31
1	3	8h	33
2	4	8s	35
2p	7		
2q	9	9	37
		9c	41
3	10	9r	39
3d	11		
3e	13		
3k	15		
3s	17		
4	19		
4e	21		
4f	19 (=4)		
5	23		
6	25		
7	26		
7c	27		
7g	28		
7t	29		

Appendix B

TABLE I. GLOSSARY OF SYMBOLS FOR THE SUBSTANCE-PROPERTY INDEX

Property Symbol		<u>Description of Properties</u>
Category	Subgroup	
0		<u>Calorimetric heats of reaction</u>
1		<u>Calorimetric heats of solution, mixing and dilution</u>
2		<u>Phase change equilibria</u>
	2p	Physical properties for pure substances, melting point, transition temperature, boiling point, vapor pressure, and derived data
	2q	Calorimetric heats and entropies of transition, fusion and vaporization
3		<u>Equilibrium data and derived properties</u>
	3d	Dissociation pressures
	3e	Electrochemical data
	3k	Equilibrium constants
	3s	Solubilities, vapor pressures of solutions, activities, and related data
4		<u>Thermodynamic functions from molecular properties</u>
	4a	Molecular and spectroscopic data
	4f	Thermodynamic functions of gases
5		<u>Physical properties of single phases. Density, refractive index, and viscosity</u>
6		<u>Spectroscopic studies of molecular bonding</u>
7		<u>P-V-T data</u>
	7c	Effect of pressure on condensed phases: compressibility, Mollier diagrams
	7g	Effect of pressure on gases, PVT data, critical state, Joule-Thomson coefficient
	7t	Tables and charts
8		<u>Calorimetric enthalpy:</u>
	8c	Low temperature heat capacity and enthalpy
	8h	High temperature heat content (enthalpy) and capacity
	8s	Third Law entropy
9		<u>Reviews and compilations:</u>
	9c	Correlation reviews
	9r	Reviews and compilations

Papers on apparatus, theoretical topics, etc., are contained in the section headed Miscellaneous (below)

Physical States: (c)rystal, solid (aq)ueous
 (amorp)hous (nonaq)ueous, includes fused salts
 (liq)uid (ads)orbed
 (g)as (sol)ution
 (gls) glass

MISCELLANEOUS PROPERTIES AND TECHNIQUES

Subject

1. Properties of real materials
2. Calorimetric apparatus - Reaction calorimetry
3. Calorimetric apparatus - Heat capacity and heat content
4. Solutions and solution theory
5. Properties of real fluids
6. Temperature measurement and scales
7. Pressure measurement and scales
8. Correlations, bond energies, and estimates
9. Thermodynamic theory

Appendix C

Codes for States used on BT and T Tapes

c	11								
amorph	12	22							
glass	13	23	33						
liquid	14	24	34	44					
gas	15	25	35	45	55				
aq	16	26	36	46	56	66			
soln	17	27	37	47	57	67	77		
nonaq	18	28	38	48	58	68	78	88	
adsorbed	19	29	39	49	59	69	79	89	99

Examples: 12 = c/amorph or amorph/c [process]

22 = amorph (single state) or amorph/amorph

00 = no state given

Appendix D

National Bureau of Standards
Chemical Thermodynamics Data Group
Tentative List (1972) of

Organic Compound Main Classes

a	01	Organic (general, used with subclasses)
	02	Aliphatic
	03	Alicyclic
	04	Aromatic
b	05	Aliphatic-Alicyclic
c	06	Aliphatic-Aromatic
c	07	Alicyclic-Aromatic
c	08	Aliphatic-Alicyclic-Aromatic
	09	Spiro
	10	Terpene
	11	Heterocyclic-Oxygen Compounds, Monocyclic Ring, <5 atoms
d	12	Heterocyclic-Oxygen Compounds, Monocyclic Ring, 5 atoms
d	13	Heterocyclic-Oxygen Compounds, Monocyclic Ring, 6 atoms
d	14	Heterocyclic-Oxygen Compounds, Monocyclic Ring, >6 atoms
	15	Heterocyclic-Oxygen Compounds, Fused Ring <9 atoms
e	16	Heterocyclic-Oxygen Compounds, Fused Ring 9 atoms
e	17	Heterocyclic-Oxygen Compounds, Fused Ring 10 atoms
e	18	Heterocyclic-Oxygen Compounds, Fused Ring >10 atoms
	19	Inter-Linked Heterocyclic-Oxygen Compounds
	20	Heterocyclic-Sulfur Compounds, Monocyclic Ring, <5 atoms
f	21	Heterocyclic-Sulfur Compounds, Monocyclic Ring, 5 atoms
f	22	Heterocyclic-Sulfur Compounds, Monocyclic Ring, >5 atoms
	23	Heterocyclic-Sulfur Compounds, Fused Ring
	24	Inter-Linked Heterocyclic-Sulfur Compounds
	25	Heterocyclic Sulfur-Oxygen Compounds, Monocyclic Ring
	26	Heterocyclic S-O Compounds, Fused Ring, S,O in same ring
	27	Heterocyclic S-O Compounds, Fused Ring, S,O in different ring
	28	Heterocyclic S-O Compounds, Non-Fused Ring, S,O in same ring
	29	Heterocyclic S-O Compounds, Non-Fused Ring, S,O in different ring
	30	Heterocyclic Selenium Compounds
	31	Heterocyclic Se-O Compounds
	32	Heterocyclic Tellurium Compounds
	33	Heterocyclic Te-O Compounds
	34	Heterocyclic Nitrogen Compounds, Monocyclic Ring, <5 atoms
g	35	Heterocyclic Nitrogen Compounds, Monocyclic Ring, 5 atoms
g	36	Heterocyclic Nitrogen Compounds, Monocyclic Ring, 6 atoms
g	37	Heterocyclic Nitrogen Compounds, Monocyclic Ring, >6 atoms
	38	Heterocyclic Nitrogen Compounds, Fused Ring, >9 atoms
h	39	Heterocyclic Nitrogen Compounds, Fused Ring, 9 atoms
h	40	Heterocyclic Nitrogen Compounds, Fused Ring, 10 atoms

- a used only in Bull. Thermodynamics and Thermochem.
- b merged with 3 for Bull T. T.
- c merged with 4 for Bull T. T.
- d merged with 11 for Bull T. T.
- e merged with 15 for Bull T. T.
- f merged with 20 for Bull T. T.
- g merged with 34 for Bull T. T.
- h merged with 38 for Bull T. T.

- h 41 Heterocyclic Nitrogen Compounds, Fused Ring, >10 atoms
- 42 Inter-Linked Heterocyclic Nitrogen Compounds
- 43 Heterocyclic N-O Compounds, Fused Ring, N,O in same ring
- 44 Heterocyclic N-O Compounds, Fused Ring, N,O in different ring
- 45 Heterocyclic N-O Compounds, Non-Fused Ring, N,O in same ring
- 46 Heterocyclic N-O Compounds, Non-Fused Ring, N,O in different ring
- 47 Inter-Linked Heterocyclic Nitrogen-Oxygen Compounds
- 48 Heterocyclic N-S Compounds, Fused Ring, N,S in same ring
- 49 Heterocyclic N-S Compounds, Fused Ring, N,S in different ring
- 50 Heterocyclic N-S Compounds, Non-Fused Ring, N,S in same ring
- 51 Heterocyclic N-S Compounds, Non-Fused Ring, N,S in different ring
- 52 Heterocyclic N-S-O Compounds, Monocyclic Ring
- 53 Heterocyclic N-S-O Compounds, Fused Ring

- 54 Heterocyclic Phosphorus Compounds

- 55 Heterocyclic Phosphorus-Oxygen Compounds

- 56 Heterocyclic P-S Compounds

- 57 Heterocyclic P-N Compounds

- 58 Heterocyclic P-O-S Compounds

- 59 Heterocyclic P-N-S Compounds

- 60 Heterocyclic P-N-O Compounds

- 61 Heterocyclic P-N-O-S Compounds

- 62 Heterocyclic As Compounds
- 63 Heterocyclic As-O Compounds

- 64 Heterocyclic Sb Compounds
- 65 Heterocyclic Sb-O Compounds

- 66 Heterocyclic Bi Compounds
- 67 Heterocyclic Bi-O Compounds

70	Dyes
71	Natural and Synthetic Rubber
72	Natural and Synthetic Plastics and Resins
73	Natural and Synthetic Fibers
74	Alkaloids
75	Vitamins and Vitamin Related Compounds
76	Steroids
77	Monosaccharides
78	Disaccharides and Other Oligosaccharides
79	Polysaccharides
80	Miscellaneous I
81	Miscellaneous II
82	Miscellaneous III
83	Miscellaneous IV
84	Miscellaneous V
85	Miscellaneous VI
a 99	General (unclassified)

National Bureau of Standards
Chemical Thermodynamics Data Group
Tentative List (1972) of

Organic Compound Group Classes

- 040 Hydrocarbons (general)
050 Saturated Hydrocarbons (alkanes or cycloalkanes)
052 Saturated Hydrocarbons (Bicycloalkanes)
054 Saturated Hydrocarbons (polycycloalkanes)
056 Saturated Hydrocarbons (alkyl subst. cycloalkanes <5 C atoms)
058 Saturated Hydrocarbons (alkyl subst. cycloalkanes 5 C atoms)
060 Saturated Hydrocarbons (alkyl subst. cycloalkanes 6 C atoms)
062 Saturated Hydrocarbons (alkyl subst. cycloalkanes >6 C atoms)
068 Miscellaneous Saturated Hydrocarbons
- 070 Unsaturated Hydrocarbons (alkenes or cycloalkenes)
072 Unsaturated Hydrocarbons (alkyl subst. cycloalkenes)
074 Unsaturated Hydrocarbons (bicycloalkenes)
076 Unsaturated Hydrocarbons (polycycloalkenes)
078 Unsaturated Hydrocarbons (dialkenes or cycloalkenes)
080 Unsaturated Hydrocarbons (polyalkenes or cyclopolyalkenes)
082 Unsaturated Hydrocarbons (alkynes or cycloalkynes)
084 Unsaturated Hydrocarbons (dialkynes)
086 Unsaturated Hydrocarbons (polyalkynes)
088 Unsaturated Hydrocarbons (cyclo(alkene-alkynes))
090 Unsaturated Hydrocarbons (di(alkene-alkynes))
092 Unsaturated Hydrocarbons (poly(alkene-alkynes))
094 Miscellaneous Unsaturated Hydrocarbons
- 096 Inter-Linked (Catenated) alicyclic ring systems (saturated)-(chains)
098 Inter-Linked (Catenated) alicyclic ring systems (unsaturated)-(chains)
100 Inter-Linked (Catenated) alicyclic ring systems (miscellaneous)-(chains)
- 102 Intra-Linked alicyclic ring systems (saturated)
104 Intra-Linked alicyclic ring systems (unsaturated)
106 Intra-Linked alicyclic ring systems (miscellaneous)
- 110 Benzene, Naphthalene and Polynuclear Parent Hydrocarbons
112 Alkane substituted aromatic hydrocarbons
114 Alkene substituted aromatic hydrocarbons
116 Alkyne substituted aromatic hydrocarbons
118 Alicyclic substituted aromatic hydrocarbons
- 120 Catenated aromatic ring systems (chains)
- 124 Partially Hydrogenated aromatic hydrocarbons
- 128 Miscellaneous aromatic hydrocarbons

Note: polyfunctional compounds are classed under the highest applicable number.

130	Saturated primary alcohols*
132	Saturated secondary alcohols
134	Saturated tertiary alcohols
136	Saturated diols alcohols
138	Saturated polyols alcohols
140	Unsaturated alcohols
142	Phenolic Compounds
144	Miscellaneous alcohols
148	Saturated Ethers or Sulfides
150	Unsaturated Ethers or Sulfides
152	Hydroxy Ethers or Sulfides
158	Miscellaneous Ethers or Sulfides
162	Peroxides or Polysulfides
164	Ozonides
166	Hemiacetals
168	Acetals
170	Orthoesters
174	Saturated Aldehydes
176	Unsaturated Aldehydes
178	Miscellaneous Aldehydes
180	Saturated Ketones
182	Unsaturated Ketones
184	Quinones
186	Miscellaneous Ketones
190	Monobasic Saturated Acids
192	Monobasic Unsaturated Acids
194	Monobasic Hydroxy and Keto Acids
196	Polybasic Saturated Acids
198	Polybasic Unsaturated Acids
200	Polybasic Hydroxy and Keto Acids
202	Miscellaneous Acids
204	Carbonic Acid Derivatives
206	Peroxy Acids
208	Acid Anhydrides
210	Lactones
212	Lactides
215	Acid Halides
220	Saturated Methyl Esters
221	Unsaturated Methyl Esters
222	Hydroxy and Keto Methyl Esters

*Note: Functional S, Se, Te is put in the same subclass as the corresponding oxygen function throughout the scheme.

224	Saturated Ethyl Esters
225	Unsaturated Ethyl Esters
226	Hydroxy and Keto Ethyl Esters
228	Saturated Aliphatic Esters
229	Unsaturated Aliphatic Esters
230	Hydroxy and Keto Aliphatic Esters
232	Saturated Alicyclic Esters
233	Unsaturated Alicyclic Esters
234	Hydroxy and Keto Alicyclic Esters
236	Aromatic Esters
238	Miscellaneous Esters
240	Carbonates
242	Salts of Aliphatic Acids
243	Salts of Alicyclic Acids
244	Salts of Aromatic Acids
245	Miscellaneous Salts
250	Sulfoxides
258	Sulfones
266	Sulfinic Acids RSO_2H
268	Sulfonic Acids RSO_3H
270	Sulfenyl Halides RSX
272	Sulfinyl Halides RSOX
274	Sulfonyl Halides RSO_2X
276	Thionic Acids RCSOH
278	Thiolic Acids RCOSH
280	Esters of Sulfenic Acids RSOR'
282	Esters of Sulfinic Acids $\text{RSO}_2\text{R}'$
284	Esters of Sulfonic Acids $\text{RSO}_3\text{R}'$
286	Esters of Thionic Acids RCSOR'
288	Esters of Thiolic Acids RCOSR'
290	Esters of Sulfuric Acids $\text{RHSO}_4, \text{R}_2\text{SO}_4$
292	Esters of Sulfurous Acids $\text{RHSO}_3, \text{R}_2\text{SO}_3$
294	Miscellaneous C-H-S- Compounds
296	Miscellaneous C-H-S-O Compounds

300	Primary Amines
302	Secondary Amines
304	Tertiary Amines
306	Quaternary Amines
308	Amine Salts
310	Diamines
312	Triamines
314	Tetraamines and Higher Amines
316	Amine-Acid Complexes (EDTA)
340	Miscellaneous Amines
342	Nitriles
344	Miscellaneous Nitriles
346	Carbylamines
348	Miscellaneous Carbylamines
350	Azides
352	Imines
354	Cyanamides
356	Amidines
358	Substituted Hydrazines or Hydrazo Compounds
360	Hydrazones
362	Guanidine and its Derivatives
364	Diazonium Compounds
366	Purine and its Derivatives
368	Quinoline and its Derivatives
370	Azo Compounds
380	Miscellaneous C-H-N Compounds
382	Amino Acids
384	Amino Acids Containing a Phenyl Group
386	Dipeptides
388	Tripeptides
390	Polypeptides
392	Proteins
394	Miscellaneous Amino Acids.

400	Amides
404	Miscellaneous Amides
410	Urea Derivatives
420	Miscellaneous Urea Derivatives
430	Nitro Compounds
432	Nitro Aldehydes
433	Nitro Alcohols
434	Nitro Ethers
436	Nitro Acids
438	Nitro Amides
440	Nitro Amines
442	Nitro Ketones
444	Nitro Esters
446	Nitro Phenols
448	Miscellaneous Nitro Compounds
450	Hydroxylamines
452	Aldoximes
454	Ketoximes
456	Imides
458	Lactams
460	Nitramines
462	Nitroso Compounds
464	Nitrosamines
466	Cyanates
468	Isocyanates
470	Nitrites RNO_2
472	Nitrates RNO_3
474	Semicarbazides
476	Osazones
478	Amine Oxides
482	Carbamates and Their Derivatives
490	Nitro Dyes
492	Nitroso Dyes
494	Azo Dyes
496	Triphenylmethane Dyes
498	Phthalein Dyes
500	Anthraquinone Dyes
502	Indigo Dyes
504	Sulfur Dyes
506	Auramine Dyes
508	Azine, Thiazine and Oxazine Dyes
510	Anthocyanins and Flavones
512	Phthalocyanine Dyes
514	Miscellaneous Dyes

- 520 Miscellaneous C-H-N-O Compounds
- 530 Diaminosulfides and Their Derivatives, $H_2N-S-NH_2$
 532 Sulfenamides $R-S-NH_2$
 534 Miscellaneous C-H-N-S Compounds
- 540 Sulfinamides $RSONH_2$
 542 Sulfonamides RSO_2NH_2
 544 Sulfamide and its Derivatives $H_2N-SO_2-NH_2$
 546 Sulfamates RSO_3NH_2
 548 Aminosulfinates
 550 Aminosulfonates
 554 Nitrosulfonates
 556 Amine Disulfinic Acids and Their Derivatives
 558 Amine Trisulfinic Acids and Their Derivatives
 560 Amine Disulfonic Acids and Their Derivatives
 562 Amine Trisulfonic Acids and Their Derivatives
- 568 Miscellaneous C-H-N-O-S Compounds
- 580 Phosphines
 582 Phosphine Oxides
 590 Miscellaneous C-H-P Compounds
- 600 Substituted Phosphinic Acids $R_2PO(OH)$
 602 Substituted Phosphonic Acids $R^1PO(OH)_2$
 604 Phosphites
 606 Phosphates
 608 Esters of Phosphinic Acids
 610 Esters of Phosphonic Acids
- 616 Miscellaneous C-H-P-O Compounds
- 620 Miscellaneous C-H-P-S Compounds
- 630 Miscellaneous CHPN Compounds
 640 Miscellaneous CHPSO Compounds
 650 Miscellaneous CHPNO Compounds
 660 Miscellaneous CHPSN Compounds
 670 Miscellaneous CHPOSN Compounds
- 700 Arsines
 702 Arsenites
 704 Arsenates
 706 Miscellaneous CHAs Compounds
 708 Miscellaneous CHAsO Compounds

710	Stibines
712	Stibnites
714	Stibnates
716	Miscellaneous CHSb Compounds
718	Miscellaneous CHSbO Compounds
720	Bismuthines
722	Bismuthates
724	Miscellaneous CHBi Compounds
726	Miscellaneous CHBiO Compounds

APPENDIX E

This sequence, in which the elements have the same order as in the Standard Order of Arrangement (see NBS TN 270-3), is used on Bulletin Tapes. The numbers are different because deuterium and tritium are assigned their own numbers, there is a generalized halogen (16) and a generalized lanthanide (83), and allowance has been made for elements 105 and 106. A compound is filed (or appears on the tape) under its constituent element having the highest finding number.

1	O	31	B	61	[106]	91	Am
2	H	32	Al	62	Ti	92	Pu
3	D	33	Ga	63	Zr	93	Np
4	T	34	In	64	Hf	94	U
5	He	35	Tl	65	Ku [104]	95	Pa
6	Ne	36	Zn	66	Sc	96	Th
7	Ar	37	Cd	67	Y	97	Ac
8	Kr	38	Hg	68	Lu	98	Be
9	Xe	39	Cu	69	Yb	99	Mg
10	Rn	40	Ag	70	Tm	100	Ca
11	F	41	Au	71	Er	101	Sr
12	Cl	42	Ni	72	Ho	102	Ba
13	Br	43	Co	73	Dy	103	Ra
14	I	44	Fe	74	Tb	104	Li
15	At	45	Pd	75	Gd	105	Na
16	X (halogen)	46	Rh	76	Eu	106	K
17	S	47	Ru	77	Sm	107	Rb
18	Se	48	Pt	78	Pm	108	Cs
19	Te	49	Ir	79	Nd	109	Fr
20	Po	50	Os	80	Pr	110	
21	N	51	Mn	81	Ce		
22	P	52	Tc	82	La		
23	As	53	Re	83	Ln (lanthanides)		
24	Sb	54	Cr	84	No		
25	Bi	55	Mo	85	Md		
26	C	56	W	86	Fm		
27	Si	57	[105]	87	Es		
28	Ge	58	V	88	Cf		
29	Sn	59	Nb	89	Bk		
30	Pb	60	Ta	90	Cu		

Flags

Codes used to indicate variable composition compounds, alloys, mixtures, entities in equations, hydrates and ions.

These flags follow the number of atoms of the last element in the compound, e.g. in words 7-12 for the first component. That a flag code is stored can be determined by examining the element symbol storage field, e.g. words 1-6, where the corresponding region is set to zero.

- 000 compound (normal)
- 001 compound is a hydrate. The next byte stores the no. of molecules of water
- 002 compound occurs in a chemical equation
- 003 "dash" indicates a component of a mixture
- 004 compound is of variable composition, e.g. Fe^{3+} : Cl^- indicates the group of compounds Fe_nCl_m
- 005 "slash" indicates an alloy, e.g. Al/Sn
- 010 "*" excitation or activated state
- 011 "+" formal positive charge or oxidation state
the next byte stores the number of charges
- 012 "-" formal negative charge
the next byte stores the number of charges

Note: When more than one flag appears, they are stored in descending numerical order.

Display of Data Recording ("Dump")

The first few physical records from two of the files on the Bulletin No. 14 (1971) tape are displayed here in a printer dump. These show every character recorded, both controls and graphics. The explanation of the conventions used in the dump follows the examples.

Example 1. Header Labels - the first three physical records on the tape.

Example 2. File # 1 - first two physical records. The valid data start at the mark in the ninth line of Block 1. The first valid entry corresponds to the first entry in figure 1b - Substance-property index.

Example 3. Header labels for File 4.

Example 4. File # 4 - first physical record. The data correspond exactly to the start of figure 1a - Bibliography.

This character by character "dump" was prepared on a printer that has a limited character repertory. This consists of space and 60 of the characters in columns 2 through 4 of the ASCII table plus two special graphics. One of these, Greek capital Δ, is used in the dump to show double quotes, circumflex and underscore.

The dump has messages showing the number and size of each physical block. Then the text of each block is shown, in groups of ten characters. This is a "three level dump". ASCII controls are indicated by their mnemonics written vertically:

E	B	D	S	S	C
S	S	E	:	:	:
C	P	L	P	I	R

Note that a colon is inserted in two letter mnemonics.

Letters, numerals and special characters are written in clear text. A comma above an ASCII character means that it should be read as the corresponding character from columns 6 and 7, e.g. lowercase for letters. This usage and that for Δ is shown below

,
 A means a (used for all letters)

)
 Δ means " (quote)

*
 Δ means (circumflex)

+
 Δ means underscore

,
 Δ means ~ (tilde)

Each line is recorded from left to right in a three level line (superscript, main line, and subscript). The lines are of variable length and are closed by carriage returns.

Figure Captions

1. Samples of Printed Text of the Bulletin.
 - a. Bibliography. Top of page 320, Bull. Thermodyn. Thermochem. 14 1971.
 - b. Substance-Property Index. Top of page 184, Bull. Thermodyn. Thermochem. 14 1971.
2. Example of a Substance-Property Index Entry as it, appears on the Bulletin Tapes. See Section 3 for an explanation.
3. File Structure on the Bulletin Tapes, showing Labels (VOL 1, HDR 1, HDR 2, EOF 1, EOF 2), Tape marks (TM) and positions of files. See Section 4 for explanation.
4. Character Set (ASCII plus an alternative graphic set) used on GPDW03 tapes. The numerical value for a character is an eight bit number based on the position of the character in the table: $value = 16 * Column + Row$ (Space, 2/0 = 32; N, 4/14 = 78). Printout from a teletypewriter equipped with red-ribbon shift but not with the alternative graphic set would show (in red) the corresponding character from the standard set.

Figure 1a

- 3001-70. Lynworth, L. C., and Benes, J. J., Design guide: measuring temperature, Mach. Des. 41, No. 26, 189-204 (1969): CA 72-14128.
- 3002-70. Makranko, Y. G., A. V., and Filippov, I. F., Apparatus for measuring the thermal characteristics of metals at high temperatures, Zavod. Lab. 35, 129-132 (1969): CA 72-14170.
- 3003-70. Benedict, P. B., International practical temperature scale of 1968, Instrum. Contr. Syst. 42, No. 16, 85-86 (1969): CA 72-14131.
- 3004-70. Zaharia, M. A., Marinescu, O., and Sandulescu, D., Differential thermal analysis, Rev. Chim. (Bucharest) 20, 433-441 (1969): CA 72-14132.
- 3005-70. Farzane, N. G., and Ilyasov, I. V., Laboratory calorimeter for measuring the volume heat of combustion of gases, Zavod. Lab. 35, 1132-1134 (1969): CA 72-14133.
- 3006-70. Giles, M., and Terry, C., Small reproducible carbon resistance thermometers for the helium-3 temperature range, Cryogenics 9, 390-391 (1969): CA 72-14134.
- 3007-70. Grail, E., ISO standard for precision glass thermometers, GIT Fachz. Lab. 13, 1059-1060 (1969): CA 72-14135.
- 3008-70. Maim, I. H., Thermocouples tell it like it is, Iron Age 204, No. 9, 67-71 (1969): CA 72-14137.
- 3009-70. Poille, W., New types of sheathed thermocouples, Neue Huette 14, 627-628 (1969): CA 72-14138.
- 3010-70. Pokrovskaya, G. N., and Tyuvin, Yu. D., Alloys for thermocouples, Tsvet. Metal. 42, No. 9, 93 (1969): CA 72-14139.
- 3011-70. Nedelko, B. P., and Krestov, G. A., Apparatus for determining the solubility of inert gases in liquids at high temperatures, Izv. Vyssh. Ucheb. Zaved., Khim. Khim. Tekhnol. 12, 998-999 (1969): CA 72-14140.
- 3012-70. Hottel, H. C., and Williams, G. N., Differential vaporization curves for complex mixtures, Chem. Eng. Sci. 24, 1734-1738 (1969): CA 72-14234.
- 3013-70. Chappell, M. S., and Cookshutt, E. P., Gas-turbine cycle calculations: thermodynamic data tables for air and combustion products, Nat. Res. Council, Canada, Rep. NCR-ER-27, 114 pp. (1969): CA 72-14250.
- 3014-70. Sagesse, G. J., [enthalpy]-log p [pressure] diagram application to thermo-electric power plants, Termotecnica 23, 347-350 (1969): CA 72-14263.

Figure 1b

1 - <u>CXYGEN</u>						
O	- Cu - Sn (liq)	3e3s	A-39-70	H ₂ (g)	7g	4725-70.
O	- Cu - Pb (liq)	3e3s	A-39-70	H ₂ (g)	7g	4412-70.
O	- Cu - Ag (liq)	3e3s	A-39-70	H ₂ (g)	7g/t	4853-70.
O	- Cu - Co (liq)	3e3s	A-39-70	H ₂ (g)		
O	- Cu - Fe (liq)	2m	D-39-70	parahydrogen		
O	- U - Pu - C - N	2e3s	A-39-70	H ₂ (g)	7t	3690-70.
O	- U - Th (c)	2g	B-55-70	H ₂ (g/nonag)	3s	4343-70.
O ₂ (liq)		5	D-60-70	H ₂ (g/nonag)	3s	4044-70.
O ₂ (liq/g)		5	F-12-70	H ₂ (g/nonag)	3s	3961-70.
O ₂ (g)		3s	D-75-70	H ₂ (g/nonag)	3s	3078-70.
O ₂ (g)		7c	4625-70.	H ₂ (g/nonag)	3s	3300-70.
O ₂ (g)		7g	4725-70.	H ₂ (g/nonag)	3s	3094-70.
O ₂ (g)		7t	4793-70.	H ₂ (g/nonag)	3s	3077-70.
O ₂ (g/nonag)		3s	4837-70.	H ₂ - Steel (c/g)	3s	3747-70.
O ₂ (g/nonag)		3s	5070-70.	H ₂ - F ₂ (g)	7t	4253-70.
O ₂ (g/nonag)		3s	5126-70.	H ₂ (g) - N ₂ (g)	1	A-19-70
O ₂ (g/nonag)		3s	5139-70.	H ₂ - N ₂ (g)	2m	D-42-70
O ₂ (g/nonag)		3s	4472-70.	H ₂ - N ₂ (g)	7g	4412-70.
O ₂ (g/nonag)		3s	4783-70.	H ₂ - NH ₃ - N ₂ (g)	7g	4065-70.
O ₂ (g/nonag)		9c	5132-70.	H ₂ - CH ₄ (g)	7g	4412-70.
O ₂ (sg)		3k6	4994-70.	methane	7g	4412-70.
O ₂ - O ₂ ⁺ (g)		3k6	4994-70.	H ₂ - C ₂ H ₆ (g)	3s	3788-70.
O ₂ - O ₄ ⁺ (g)		3k6	4994-70.	H ₂ - ethane	1	D-21-70
O ₂ - O ₆ ⁺ (g)				H ₂ - Al (c/liq)		
				H ₂ (g) - Pd (c)		

Figure 2. Example of a substance-property index entry as it appears on the bulletin Tape. See Chapter 3 for an explanation.

Line 1.	G S	141	5	2	21728	0	45	0	0	2	5157-70.
Line 2.		100	3								
Line 3.	H ₂ O										
Line 4.	Cl ₁ H ₁										
Line 5.	H ₂ O - HCl				(liq/g)					3s7g	5157-70.
		0		10		20		30		40	50

FIGURE 3. STRUCTURE OF THE TAPE SHOWING POSITIONS
OF LABELS, TAPE MARKS AND FILES

VOL 1 81 characters
HDR 1 "
HDR 2 "
(TM)
File 1 Blocks of 1008 char.
(TM)
EOF 1 81 characters
EOF 2 "
(TM)
HDR 1
HDR 2
(TM)
File 2
(TM)
.
.
.
HDR 1
HDR 2
(TM)
File 6 (Last)
(TM)
EOF 1
EOF 2
(TM)
(TM)

Figure 4

Row\Col.	2	3	4	5	6	7
	Std.	Alt.	Std.	Alt.	Std.	Alt.
0		0	@	P	`	p
1	!	1	A	Q	a	q
2	"	2	B	R	b	r
3	#	3	C	S	c	s
4	\$	4	D	T	d	t
5	%	5	E	U	e	u
6	&	6	F	V	f	v
7	'	7	G	W	g	w
8	(8	H	X	h	x
9)	9	I	Y	i	y
10	*	:	J	Z	j	z
11	+	;	K	[k	{
12	,	<	L	\	l	
13	-	=	M	>	m	}
14	.	>	N	^	n	~
15	/	?	0	_	o	-

The symbol [] indicates that an alternate graphic character is undefined.

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4. TITLE AND SUBTITLE Description of the Magnetic Tape Version of the Bulletin of Thermodynamics and Thermochemistry, No. 14 (1971)		5. Publication Date March 1973	
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		11. Contract/Grant No.	
12. Sponsoring Organization Name and Address Same as above		13. Type of Report & Period Covered Final	
		14. Sponsoring Agency Code	
15. SUPPLEMENTARY NOTES			
<p>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.)</p> <p>The substance-property index and bibliography sections of the Bulletin of Thermodynamics and Thermochemistry, No. 14 (May 1971) have been converted to a magnetic tape version designed for computerized searching written in an extended form of the American National Standard Code for Information Interchange (X 3.4-1968). In this version each substance-property entry has been supplemented by a searching key. This report describes the magnetic tape version.</p>			
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