NBS TECHNICAL NOTE 1122

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Summary of On-Line or Interactive Physico-Chemical Numerical Data Systems

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A brief description is given of 53 interactive physico-chemical numerical data systems, most of which are on-line on international computer networks. The systems are listed under five headings: those useful for identification of substances from spectroscopic data; those providing thermodynamic and transport properties of pure components and mixtures; those which perform metallurgical calculations and draw phase diagrams; systems producing complete tables of thermodynamic properties of individual substances; and those for chemical process simulation, optimization, and design. References to published descriptions of the systems, where they exist, are also given.

Key words: Chemical data; data banks; data bases; data networks; interactive systems; numerical data bases; on-line data; physical data; spectroscopic data systems.

1. Introduction

The development of multi-user computer hardware and operating systems and associated national and international communications networks has made it technically and economically possible to provide users with on-line access to a wide variety of data systems.

Aside from bibliographic information, the data bases that are now on stream practically around-the-clock include: marketing, economic, actuarial, financial, and regulatory data; demographic and other census statistics; and weather, ecological, geological, geographical, and other Earth data.

Two of the leading U.S. value-added networks—GTE Telenet and Tymnet—offer more than 250 data bases. Nearly half of these are available on both networks.

These data bases have been cataloged by a number of organizations, and most recently by the American Society for Information Science (ref. 1). There is a growing demand for a convenient listing of on-line physical and chemical numerical data systems. This summary has been prepared in response to this interest.

2. Physico-Chemical Numerical Data Systems

The 53 computerized numerical data systems included in this summary have been grouped into 6 largely mutually exclusive categories. They are listed in tables A through F as follows:

Table A lists 17 systems useful for identification of unknown compounds via IR, UV, NMR, and mass spectra as well as crystallographic data.

Table B lists 14 systems to retrieve, compute, or estimate thermodynamic and transport properties of pure compounds or mixtures.

Table C lists five systems for metallurgical calculations and generation of these diagrams.

Table D lists four systems to compute complete tables of thermodynamic properties of technically important fluids.

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Table E lists two systems for physical properties of plastics including interaction of polymers with propellants and other energetic materials.

Table F lists 11 systems for chemical process simulation, optimization, and design. See Appendix A for a discussion of the ASPEN survey of computer programs for chemists.

The systems in group A are based on relatively large data bases with 10,000 to 150,000 compounds. They are usually restricted to a single type of data, although three of the systems listed (A5, A13, A16) combine a number of types of data in the same system. The systems in groups B, C, and E contain data or parameters for estimating hundreds rather than thousands of compounds. Those in group D provide detailed tables of thermal properties as a function of temperature and pressure for a single substance, such as ammonia (D2); for a small group of substances, such as cryogenic fluids (D1); or for atmospheric gases (D4).

A number of references are to proceedings of CODATA conferences. The Committee on Data for Science and Technology (CODATA) was organized in 1967 by the International Council of Scientific Unions (ICSU) to "work on an inter-disciplinary basis to improve the quality, reliability, and accessibility of data of importance to science and technology." The activities of CODATA and its Task Groups were discussed in a paper by N. Kurti (ref. 2).

The National Bureau of Standards and a number of other Government agencies including NASA, DOE, NIH, and EPA collect, evaluate, and disseminate compendia of physico-chemical data. Many of these were computer produced, and are often available on magnetic tape as well as in published form. They are prime candidates for inclusion in on-line or batch mode retrieval systems. It is beyond the scope of this report to list the data collections available in computer-readable form. A useful, though incomplete, list of numerical data bases now under development can be found in an article by F. U. Wetzler (ref. 3), "Data Banks for R and D." The NBS Office of Standard Reference Data sells or leases a number of data tapes listed in Appendix C reprinted from the current list of publications (ref. 4) of the National Standard Reference Data System.

3. International Access to Numerical Data Systems

In the United States most networks can be reached by local telephone call in 200 or more cities. Such "toll-free," actually, distance-independent network, access is now also possible in a dozen or so countries. A listing of available networks and associated communications charges in European countries can be found in a report (ref. 5) by A. Tomberg of the European Association of Scientific Information Dissemination Centres (EUSIDIC).

Table 1 shows countries able to access the numerical data systems, listed here as well as five of the major U.S. networks. Of the 39 countries listed, all but 4 can access one or more of these networks. Both of the U.S. value-added networks —GTE Telenet and Tymnet—can be accessed in 25 of the countries listed. Twelve of these countries are served by at least four U.S. networks, and in some cases by one or more local networks as well.

4. Comments on Tables A Through F

Six of the systems listed in Table A are part of the NIH-EPA Chemical Information System (CIS). These are available from the same vendor on an international network (TELENET) and are integrated via the chemical registry number with eight other CIS systems (SANSS, OHM-TADS, RTECS, MLAB, CAMSEQ II, CTCP, GINA, and the Federal Register Notices). A brief description of these systems is contained in Appendix B. Fuller accounts are to be found in a series of papers by S. R. Heller and associates (refs. 6-8, A8.1-A8.3, A10.1, A10.2).

The ELIZA program listed as A13 differs from the others in that it combines information on IR, UV, NMR, and mass spectra with a number of chemical properties in a single system for identifying organic compounds. It was designed for use in teaching analytical chemistry, and the data base includes compounds normally found in college and university laboratories.

Zupan and colleagues at the Boris Kidric Chemical Institute in Yugoslavia have also implemented a system (A16) which combines IR, NMR, and mass spectra. A similar system (A5) has been in operation for a decade or so at the Siberian Institute of Organic Chemistry in Novosibirsk.

The x-ray crystallographic search system (A11) merits special notice. The data base upon which it depends originated with and is kept current by the Crystallographic Data Centre at Cambridge University. The Cambridge crystallographic data base contains atomic coordinates, bond angle, etc., as well as cell parameters and references for 25,000 organic compounds. This system has been leased to accredited information centers and research laboratories in 18 countries, though few yet have them on-line. Table 1 shows which countries operate accredited crystallographic data centers.

The systems B1, B2, and B7 have a common characteristic. Each was developed with joint industrial and governmental cooperation and support under the supervision of the local engineering society which is actively engaged in its promotion and marketing.

In the area of metallurgy there is an even more interesting cooperative program which crosses national borders. Systems C2, C4, and C5 are national implementations of the fruits of an international collaboration between English, French, German, and Swedish metallurgists working together under a semi-formal group called Scientific Group Thermodata Europe (SGTE). The secretariat for the group is located at the National Physical Laboratory at Teddington, England.

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TABLE 1. AVAILABILITY BY COUNTRIES OF NETWORKS AND DATA BASES

COUNTRY	NETWORKS: GTN	NETWORKS: TYMNET	NETWORKS: EURONET	NETWORKS: GENISCO	NETWORKS: HERMES	NETWORKS: INFONET	NETWORKS: SCITOR	NETWORKS: UNINET	DATA BASES: CHEMICAL ABSTRACTS	PHYSICO-CHEMICAL NUMERICAL DATA SYSTEMS
ARGENTINA		X	X							A2,A3,A6,A7-A12,A17
AUSTRALIA		X	X	X	X				X	A2,A3,A6,A7-A12,A17,F6
AUSTRIA		X	X	X	X					A2,A3,A6,A7-A12,A17,F6
BAHARAIN		X	X							A2,A3,A6,A7-A12,A17
BELGIUM		X	X	X	X				X	A2,A3,A6,A7-A12,A17,B2,F6
BERMUDA		X	X							A2,A3,A6,A7-A12,A17
BRAZIL		X	X						X	A2,A3,A6,F6
CANADA		X	X	X	X				X	A2,A3,A4,A6-A12,A17 B13,C3,F1,F6
DENMARK		X	X	X	X					A2,A3,A6,A7-A12,A17,F6
FINLAND		X	X	X	X				X	A2,A3,A6,A7-A12,A17,F6
FRANCE		X	X	X	X				X	A2,A3,A6,A7-A12,A15,A17 B2,C4,C5,F1,F6
GREECE			X							F6
GERMANY (WEST)		X	X	X	X	X			X	A2,A3,A6-A12,A17,B4,B7,F6,F8
HUNGARY									X	
HONG KONG		X	X	X						A2,A3,A6-A12,A17,F6
INDIA									X	
IRELAND		X	X	X						F6
ISRAEL		X	X	X					X	A2,A3,A6-A12,A17,F6
ITALY		X	X	X	X	X			X	A2,A3,A6-A12,A17
JAPAN				X					X	A2,A3,A6,A14 B1,B5,F6,F7

TABLE 1. AVAILABILITY BY COUNTRIES OF NETWORKS AND DATA BASES

COUNTRY	NETWORKS: GTE GLOBENET	NETWORKS: GTE TELENET	NETWORKS: CompuServe	NETWORKS: DIALOG	NETWORKS: ADP NETWORK SERVICES	NETWORKS: CAN/SCAN	NETWORKS: TYMNET	PHYSICO-CHEMICAL NUMERICAL DATA SYSTEMS
MEXICO	X	X	X	X				A2,A3,A6-A12,A17,F6
NETHERLANDS	X	X	X	X		X		A2,A3,A6-A12,A17 B2,B3,F6,F10
NEW ZEALAND	X	X				X		A2,A3,A6-A12,A17
NORWAY	X	X	X	X		X		A2,A3,A6-A12,A17,F6
PHILIPPINES	X	X						A2,A3,A6-A12,A17
PORTUGAL	X	X	X					A2,A3,A6,F6
PUERTO RICO	X	X	X					A2,A3,A6-A12,A17,F6
SAUDI ARABIA			X					F6
SINGAPORE	X	X	X					A2,A3,A6-A12,A17,F6
SOUTH AFRICA			X					F6
SPAIN	X	X	X	X				A2,A3,A6-A12,A17,F6
SWEDEN	X	X	X	X		X		A2,A3,A6-A12,A17,F6
SWITZERLAND	X	X	X	X	X			A2,A3,A6-A12,A17,F6
TAIWAN	X							F6
UNITED KINGDOM	X	X	X	X	X	X		A2,A3,A6-A12,A17 B2,B9,B10,C2,D3,F1,F6,F8,F9
UNITED STATES	X	X	X	X	X	X		A2,A3,A6-A12,A17 B2,B8,B11,B13,B14,C1,C2, D1,D2,F1 - F6,F9,F11
U.S.S.R.								A5,B6,B12,D4
VENEZUELA			X	X				
YUGOSLAVIA								A16

ACTIVE COMPUTERIZED PHYSICO-CHEMICAL NUMERICAL DATA SYSTEMS

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
TABLE A. SYSTEMS FOR IDENTIFICATION OF UNKNOWN SUBSTANCES						
A1 ---- FIRST-1 INFRARED DATA RETRIEVAL PRDGRAM	SEARCHES AN INFRARED SPECTRA DATA FILE FOR A MATCH AGAINST THE SPECTRUM OF AN UNKNDWN SUBSTANCE	143,000 IN ASTM INDEX	SEE SPIR	IBM 1130 IBM 1800 IBM 360/370 UNIVAC 1108 DSC-META 4	MR. BUD BLACKNEY DNA SYSTEMS, INC. 1258 S. WASHINGTON ST. P.O. BOX 1424 SAGINAW, MICH. 48605 TEL (517) 793-0185	API NRC-NBS DMS-BUTTERWORTHS COBLENTZ SOCIETY MCA RES. PROJ. INFRARED DATA COM. OF JAPAN SADTLER FILES
A2 ---- IRGD INFRARED DATA RETRIEVAL PROGRAMS	SEE FIRST-1 RETRIEVAL ALSO BASED ON CHEMICAL CLASSES AND ELEMENTAL COMPONENTS	150,000	VIA TYMNET FROM TYMSHARE	?	DR. CLARA D. CRAVER CHEMIR LABORATORIES 761 WEST KIRKHAM ST. LOUIS, MO 63122 TEL. (314) 962-5752	SEE FIRST-1 FOR A LIST OF FILES PRIVATE FILES CAN BE ADDED
A3 --- IRIS INFRARED INFORMATION SYSTEM	SEE FIRST-1	110,000	VIA TYMNET FROM UNIVERSITY COMPUTING CORP. (UCC)	UNIVAC 1108	MARIE SCANDONE SADTLER RESEARCH LAB 3316 SPRING GARDEN ST PHILADELPHIA, PA. 19104 TEL (215) 382-7800	SEE FIRST-1 FOR A LIST OF FILES --- PRIVATE FILES CAN BE ADDED
A4 ---- SPIR SEARCH PRDGRAM FOR INFRARED SPECTRA	SEE FIRST-1	SEE FIRST-1	ONLY IN CANADA VIA DATAPAC		DR. G. H. WOOD CANADIAN INSTITUTE FOR SCIENTIFIC AND TECHNICAL INFORMATION MONTREAL RDAD OTTAWA KIAOR6 ONTARIO, CANADA TEL (613) 993-3294	RUNS ON THE COMPUTER AT THE CANADIAN NATIONAL RESEARCH COUNCIL
A5 --- SPECTRUM	SEARCHES IR AND UV SPECTRAL DATA FILES FOR A MATCH AGAINST SPECTRA OF UNKNOWN SUBSTANCES	50,000+	IN DEVELOPMENT STAGE	BESM6	PROF. V.A. KOPTYUG INSTITUTE OF ORGANIC CHEMISTRY SIBERIAN DIVISION USSR ACADEMY OF SCIENCE NOVOSIBIRSK, USSR	SPECTRUM ALSO PROVIDES RETRIEVAL ON MELTING AND BOILING TEMPERATURES MOLECULAR WEIGHT AND CHROMOPHORIC CODES
A6 ---- 2DTS DIFFRACTION DATA TELE-SEARCH	SEARCHES THE POWDER DIFFRACTION DATA FILE OF THE JOINT COMMITTEE ON POWDER DIFFRACTION STANDARDS (JCPDS) TO IDENTIFY UNKNOWN COMPOUNDS	33,000 PHASES	UNIVERSITY COMPUTING CORP. (UCC)	IBM 360/370 ---- UNIVAC 1100 SERIES ---- CDC 6000/7000+ CYBER	MR. MARK A. HOLOMANY JOINT COMMITTEE ON POWDER DIFFRACTION STANDARDS 1601 PARK LANE SWARTHMORE, PA 19081 TEL (215) 328-9400 OR UCC AT 1930 HIGH LINE DRIVE DALLAS TX 75207 TEL. (214) 655-8795	SOFTWARE WAS WRITTEN AND IS MAINTAINED BY PROF. G.G. JOHNSON, JR., PENN. STATE UNIV.,

TABLE A. SYSTEMS FOR IDENTIFICATION OF UNKNOWN SUBSTANCES (CONT.)

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
A7 ---- PDSM POWDER DIFFRACTION SEARCH MATCH	SEE 2DTS	33,000 PHASES	VIA GTE TELENET FROM INTERACTIVE SCIENCES CORP.	DEC-10	SEE MSSS	A PART OF THE NIH-EPA-CIS CHEMICAL INFORMATION SYSTEM BASED ON JCPDS POWDER DIFFRACTION FILE
A8 ---- MSSS MASS SPECTRAL SEARCH SYSTEM	SEARCHES THE MASS SPECTRA FILE FOR A MATCH AGAINST THE MASS SPECTRUM OF AN UNKNOWN COMPOUND ---- SEE PROTON DATA (A17)	33,000	VIA GTE TELENET FROM INTERACTIVE SCIENCES CORP.	DEC-10	KAY POOL INTERACTIVE SCIENCES CORP. 918-16TH ST. ,SUITE 500 WASHINGTON, DC 20006 TEL. (800) 424-9600 DR. C. CITROEN CID - TNO P.O.BOX 36 2600 AA DELFT THE NETHERLANDS TEL. 015-56-93-30 DR.J.C. VEAL UKCIS THE UNIVERSITY NOTTINGHAM NG7 2RD ENGLAND TEL. (0602)57411	THIS IS A JOINT EFFORT BETWEEN MSDC-NOTTINGHAM, ENGLAND, THE NATIONAL INSTITUTE OF HEALTH, AND THE ENVIRONMENTAL PROTECTION AGENCY IN THE U.S. EPA CONTACT IS DR. STEPHEN R. HELLER, TEL (202) 755-4938 -------- A PART OF THE NIH-EPA-CIS CHEMICAL INFORMATION SYSTEM
A9 ---- PBM/STIRS PROBABILITY BASED MATCHING AND SELF-TRAINING INTERPRETIVE AND RETRIEVAL SYSTEMS	PBM COMPARES UNKNOWN SPECTRUM AGAINST A REFERENCE FILE --- STIRS INTERPRETS UNKNOWN SPECTRUM TO IDENTIFY STRUCTURAL FEATURES OF THE MOLECULE	41,429 SPECTRA OF 32,860 COMPOUNDS	VIA TYMNET OR GTE TELENET FROM CORNELL UNIV OFFICE OF COMPUTER SERVICES ON IBM 370/168	PDP11/45	PROF. F.W. MCLAFFERTY DEPT. OF CHEM. OR DR. ALEC GRIMISON OFFICE OF COMP. SERVICES CORNELL UNIV. ITHACA, N.Y. 14853 TEL (607) 256-5100	FOR A COMPARISON OF THE SEARCH STRATEGIES OF PBM AND MSSS SEE REFERENCE A9.3
A10 ---- C-13 NMR	SEARCHES THE CARBON-13 NUCLAR MAGNETIC RESONANCE SPECTRA DATA FILE	8800 SPECTRA	VIA GTE TELENET FROM INTERACTIVE SCIENCES CORP.	DEC-10	SEE MSSS	A PART OF THE NIH-EPA-CIS CHEMICAL INFORMATION SYSTEM
A11 ---- CRYST --- X-RAY CRYSTALLOGRAPHY SEARCH SYSTEM	SEARCHES FOR ATOMIC COORDINATES CRYSTAL CELL PARAMETERS AND BIBLIOG. ITEMS	25,000 COMPOUNDS	VIA GTE TELENET FROM INTERACTIVE SCIENCES CORP.	?	SEE MSSS	A PART OF THE NIH-EPA-CIS CHEMICAL INFORMATION SYSTEM BASED ON STRUCTURAL FILES OF THE CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE

TABLE A. SYSTEMS FOR IDENTIFICATION OF UNKNOWN SUBSTANCES (CONC.)

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
A12 XTAL CRYSTAL DATA DETERMINATIVE TABLES	RETRIEVAL AND ANALYSIS OF THE FOLLOWING DATA ---- DETERM. RATIO R1 ANGLES: ALPHA,BETA,GAMMA CELL CONST:A,B,C SPACE GROUPS DENS: DM AND DX ELEMENTAL CONST. STRUCT. FORM. FORMULA FRAG. COMPOUND NAME	50,000 CRYSTALS	VIA GTE TELENET FROM INTERACTIVE SCIENCES CORP.	DEC-10	SEE MSSS	CAN BE USED TO IDENTIFY SINGLE CRYSTALS FOR WHICH: THE UNIT CELL, OR DENSITY, OR OTHER PARAMETERS IN COLUMN 2 ARE KNOWN
A13 ELIZA	A SYSTEM FOR IDENTIFYING COMPOUNDS FROM THEIR PHYSICAL PROPERTIES AND SPECTRA. SEE REMARKS	2000 ORGANIC COMPOUNDS FOUND IN COLLEGE CHEM LABS		DEC 10	JAMES HAMILTON 1 HACIENDA WAY ANDOVER MASS. 01810 TEL.(617) 687-2718	THE DATA BASE INCLUDES IR,UV,NMR AND MASS SPECTRA SYSTEM NAME,CAS REG.#,TRANS.POINTS, FUNCTIONAL GROUPS AND REF.TO SPECTRA
A14 MXDS MOLECULAR AND CRYSTALLINE DATA SYSTEM	SEE CRYST (A11)	10,000 COMPOUNDS	ON-LINE UNDER TOOL-IR AT UNIV. OF TOKYO	HITACH 8800/8700	Y.TITAKA OR T.YAMAMOTO AT TOKYO UNIV. BUNKYO-KU TOKYO JAPAN	PART OF A COMPREHENSIVE DATA DISSEMINATION SYSTEM UNDER DEVELOPMENT
A15 DPDS DARC PLURIDATA SYSTEM	SEARCHES FOR MASS,C13 NMR SPECTRA,AND ATOMIC COORDINATES IN CRYSTAL CELLS COUPLED WITH STRUCTURE AND SUBSTRUCTURE SEARCHES	13295 C 13 NMR ---- 31502 MASS ---- 22267 CRYSTALS	TRANSPAC AND EURONET	PDP 11/35 VAX 11/780	PROF. J.E.DUBOIS CENTRE D'INFORMATIQUE ET DE DOCUMENTATION AUTOMATIQUE(CIDA) 1,RUE GUY DE LA BROSSE, 75005 PARIS, FRANCE	DPDS USES CIDA DATA FOR C-13 NMR, THE CAMBRIDGE CRYSTALLOGRPHIC DATA FILES, AND THE NIH/EPA MASS SPECTRAL DATA BASE, AS WELL AS OTHER DATA
A16 KISIK	COMBINED RET. SYST. FOR IR, MASS, AND NMR SPECTRA SEE REMARKS	CONTAINS 1000 SPECTRA OF EACH TYPE	PDP 11/34		DR. J. ZUPAN CHEMICAL INSTITUTE BORIS KIDRIC HAJDRIHOVA, 19 61000 LJUBLJANA YUGOSLAVIA	SEARCHES POSSIBLE ON WLN, CONNECTIVITY, SUB-STRUCTURE, ETC.
A17 PROTON DATA	PROVIDES RETRIEVAL ON GAS-PHASE BASICITY AND PROTON AFFINITY	450	VIA GTE TELENET FROM INTERACTIVE SCIENCES CORP.		SEE MSSS	THESE DATA FROM THE NBS ION ENERGETICS DATA CENTER ARE INCORPORATED IN THE NIH-EPA MASS SPECTRA SEARCH SYSTEM

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
TABLE B. SYSTEMS FOR PROPERTIES OF PURE SUBSTANCES AND MIXTURES						
B1 JUSE-AESOPP AN ESTIMATOR FOR PHYSICAL PROPERTIES	RETRIEVAL OF STORED DATA AND ESTIMATION OF THERMODYNAMIC AND TRANSPORT PROPERTIES VIA CORRELATING EQUATIONS FOR PURE COMPONENTS AND MIXTURES		ON-LINE ACCESS UNDER IN-HOUSE TEST	IBM 360/370 CDC 6600 UNIVAC 1100 GE635 TOSBAC 3400, 5600 HITACH 8400 FACOM 230-45/65 MELCOM	DR. KEIJI YAJIMA MANAGING DIRECTOR INSTITUTE OF THE UNION OF JAPANESE SCIENTISTS AND ENGINEERS 5-10-11 SENDAGAYA SHIBUYA-KU TOKYO, JAPAN	16 SYSTEMS INSTALLED IN JAPAN AS OF JUNE 1980 SEE ALSO F7
B2 PPDS PHYSICAL PROPERTY DATA SYSTEMS	CALCULATION OF PROPERTIES OF PURE COMPOUNDS AND MIXTURES AS REQUIRED FOR CHEMICAL PROCESS DESIGN	400 LARGELY HYDROCARBONS	G.E.MARK III GAMMA UNIVERSITY COMPUTING CO.(UK)LTD. ALSO FROM SERVICE BUREAUS IN FRANCE, NETHERLANDS		DR. BERYL EDMONDS THE INSTITUTION OF CHEMICAL ENGINEERS 165/171 RAILWAY TERRACE RUGBY CV21 3HQ ENGLAND	FOR A SINGLE COMPOUND THE PROGRAM GIVES 17 CONSTANTS AND 14 STREAM VARIABLES F(T,P) FOR BOTH SINGLE AND MULTICOMPONENT STREAMS
B3 TISDATA TECHNOLOGICAL INFORMATION SYSTEM	COMPUTES PHYSICAL PROPERTIES FOR CHEMICAL PROCESS CALCULATIONS	480	NETHERLANDS COMPUTER CENTRE AT HEERLEN	UNIVAC 1108 CDC6600	J.A. DE LEEUW DEN BOUTER DSM REASEARCH AND PATENTS P.O.BOX 18, 6160MD GELEEN,HOLLAND	INTERFACES WITH USER PROGRAMS AND TISFLO AND TISUNOP SEE F4
B4 THERMO-PHYSICAL PROPERTIES PROGRAM PACKAGE	COMPUTER PROGRAMS FOR ESTIMATING THERMODYNAMIC AND TRANSPORT PROPERTIES OF PURE SUBSTANCES AND MIXTURES	350			DR. KLAUS KURT NEUMANN FRIEDRICH UHDE GMBH 46 DORTMUND DEGGINSTRASSE 10-12 P.O. BOX 262 FEDERAL REPUBLIC OF GERMANY	THE DATA FILE CONSISTS OF APPROXIMATELY 400 DATA ITEMS COMPRISING CRITICAL CONSTANTS, PROPERTIES AT SPECIFIC TEMPERATURES AND PRESSURES, AND PARAMETERS FOR ESTIMATING METHODS.
B5 EROICA	ESTIMATION AND RETRIEVAL OF PROPERTIES OF ORGANIC COMPOUNDS	5000 COMPOUNDS	THE UNIVERSITY OF TOKYO COMPUTER CENTER	HITACH 8800 IBM 370	DR. YUKIO YONEDA DEPT. OF SYNTHETIC CHEMISTRY UNIVERSITY OF TOKYO HONGO, BUNKYO-KU, TOKYO, JAPAN	ESTIMATIONS, WHEN REQUIRED, EMPLOY GROUP CONTRIBUTION METHODS
B6 AVESTA ABECTA	THERMOPHYSICAL PROPERTIES OF PURE SUBSTANCE MIXTURES AND PETROLEUM PRODUCTS				GOSSTANDART (GSSSD) DATA CENTER FOR HYDROCARBONS AND OIL PRODUCTS VNII PKNEFTEKIM 252068,KIEV-68 PALLADIN AV., 46 USSR	THIS IS A SERVICE OF GSSSD THE USSR STATE SERVICE OF STANDARD REFERENCE DATA
B7 DETHERM DECHEMA THERMO-PHYSICAL PROPERTY DATA BANK	ON-LINE SYSTEM FOR DATA RETRIEVAL(SRD) AND CALCULATION (SDC)	SDR:3000 SDC:500	EURONET ODIN	IBM 370 SIEMANS 4004, 7.760	DR. REINER ECKERMAN DECHEMA DEUTSCHE GESELLSCHAFT FUR CHEMISCHES APPARATEWESEN E.V. FRANKFURT GERMANY POSTFACH 971046 FRANKFURT 97 WEST GERMANY	A COOPERATIVE PROGRAM OF THE CHEMICAL INDUSTRY, UNIVERSITIES, AND THE FRG, UNDER DECHEMA ADMINISTRATION.

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
TABLE B. SYSTEMS FOR PROPERTIES OF PURE SUBSTANCES AND MIXTURES (CONC.)						
B7 DETHERM DECHEMA THERMO-PHYSICAL PROPERTY DATA BANK	ON-LINE SYSTEM FOR DATA RETRIEVAL(SRD) AND CALCULATION (SDC)	SDR:3000 SDC:500	EURONET ODIN	IBM 370 SIEMANS 4004, 7.760	DR. REINER ECKERMAN DECHEMA DEUTSCHE GESELLSCHAFT FUR CHEMISCHES APPARATEWESEN E.V. FRANKFURT GERMANY POSTFACH 971046 FRANKFURT 97 WEST GERMANY	A COOPERATIVE PROGRAM OF THE CHEMICAL INDUSTRY, UNIVERSITIES, AND THE FRG, UNDER DECHEMA ADMINISTRATION.
BB TRL CORRELATION PACKAGE	ACCESSES EVALUATED DATA BANK FOR THERMODYNAMIC DATA FROM A DATA BASE FOR PURE COMPOUNDS	350+	DESIGNED FOR IN-HOUSE USE	IBM 360	DR. BUFORD D. SMITH THERMODYNAMICS RESEARCH LABORATORY BOX 1144 WASHINGTON UNIVERSITY ST.LOUIS MO. 63130	AVAILABLE TO TRL SPONSORS GROUP
B9 NEL-APPES	A PHYSICAL PROPERTIES DATA SYSTEM	200	ON THE NEL UNIVAC 1100/21		DR.J.T.R.WATSON NATIONAL ENGINEERING LABORATORY EAST KILBRIDE GLASGOW G750QU SCOTLAND	A REPROGRAMMED AND REVISED INTERACTIVE VERSION OF THE (CIRCA 1970) AICHE APPES
B10 KEYDATA	DATA RETRIEVAL AND CALC FOR PROCESS SIMULATION	500+ INCLUDING PPDS DATA BASE	SCICON(UK), CSC, UCS CDC	UNIVAC 1100 SERIES --- PRIME CDC ICL 2900 SERIES	DR.P. WINTER PROCESS INDUSTRIES GROUP COMPUTER AIDED DESIGN CENTRE MADINGLY RD. CAMBRIDGE CB3 OHB ENGLAND	INTERFACES WITH DESIGN PROGRAMS CONCEPT AND MULTICOL SEE F9
B11 CHETAH	ASTM CHEMICAL THERMODYNAMIC AND ENERGY RELEASE EVALUATION PROGRAM			UNIVAC 1108 IBM 360	ROBERT MELTZER AMERICAN SOCIETY FOR TESTING AND MATERIALS 1916 RACE ST. PHILADELPHIA,PA 19103	PROGRAM ESTIMATES PROPERTIES FROM SECOND-ORDER CONTRIBUTIONS ACCORDING TO BENSON ET. AL CHEM. REVS. 69, 279-324 (1969)
B12 THERMOCHEM-ICAL DATA SYSTEM	COMPUTES THERMODYNAMIC PROPERTIES OF INORGANIC AND SIMPLE ORGANIC COMPOUNDS	1200	UNDER DEVELOPMENT	HP 3000	PROF. L.V. GURVICH DEPT. OF CHEMICAL THERMODYNAMICS INST. OF HIGH TEMPERATURE MOSCOW U.S.S.R. I27412	THE SYSTEM COMPUTES THERMODYNAMIC PROPERTIES FROM SPECTROSCOPIC, MOLECULAR, AND CHEMICAL EQUILIBRIUM DATA
B13 TBANK	COMPUTES THERMOCHEMICAL FUNCTIONS FOR INDIVIDUAL SUBSTANCES AND CHEMICAL REACTIONS	1500	VIA GTE TELENET AND I.P. SHARP ASSOC. ALSO VIA TELEX	IBM 360/370 UNDER APL ----	PROF. C.B. ALCOCK DEPT. OF METALLURGY AND MATERIAL SCIENCE UNIV. OF TORONTO TORONTO, CANADA M5S1A4 TEL. 416-978-6808	SYSTEM ALLOWS 2ND AND 3RD LAW ANALYSIS OF EXPERIMENTAL DATA
B14 CPPDMS CELANESE PHYSICAL PROPERTIES DATA MANAGEMENT SYSTEM	AN INTERACTIVE DATA RETRIEVAL SYSTEM FOR PROPERTIES OF CHEMICAL COMPOUNDS IN FUNCTIONAL, TABULAR, AND GRAPHIC FORM IN SI AND OTHER UNITS	200	UNIVERSITY COMPUTING CO. OFFERS ONLY THE DATA BASE MANAGEMENT SYSTEM BUT NOT THE DATA BASE	UNIVAC 1100/81	J.DAVID CHASE CELANESE CHEMICAL CO. P.O.BOX 9077 CORPUS CHRISTI,TX 78408 TEL.(512)241-2343 XT4267	CONTACT UCC TEL.(214)655-8627 FOR ACCESS TO THE SOFTWARE AND THE CELANESE CHEMICAL CO. FOR THE DATA BASE

ACTIVE COMPUTERIZED PHYSICO-CHEMICAL NUMERICAL DATA SYSTEMS

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
TABLE C. SYSTEMS FOR METALLURGICAL CALCULATIONS						
C1 ---- DATABANK SYSTEM FOR BINARY AND TERNARY PHASE DIAGRAMS	COMPUTES AND DISPLAYS ISOTHERMAL SECTIONS OF BINARY AND TERNARY PHASE DIAGRAMS	DATA FOR 10 METALS AND 45 BINARY SYSTEMS ALLOW FOR 120 TERNARY SYSTEMS	MANLABS	IBM 1130 360/370	DR. LARRY KAUFMAN MANLABS, INC. 21 ERIE STREET CAMBRIDGE,MASS 02139 TEL (617) 491-2900	THE SYSTEM HANDLES SOLUTIONS INVOLVING ALUMINUM, CARBON, TITANIUM, CHROMIUM, IRON, COBALT, NICKEL, NIOBIUM, MOLYBDINUM , AND TUNGSTEN
C2 ---- MTDATA METAL-LURGICAL THERMO-DYNAMIC DATA BANK MEMBER OF SGTE++	METALLURGICAL CALCULATIONS: FOR PURE COMPOUNDS, FOR MIXTURES, FOR REACTIONS INVOLVING GASES,SOLIDS OR LIQUIDS, FOR DILUTE SOLUTIONS OF GASES AND METALS IN METALS	2000 INOR-GANIC	UK-NPL		DR. THOMAS I BARRY NATIONAL PHYSICAL LABORATORY TEDDINGTON, ENGLAND TEL.01-977-3222	GIBBS ENERGY MINIMIZATION CHEM. REACTION CALCULATIONS GIVING DELTAH, DELTAG, DELTACP, DELTAS, AND LOGKP FOR CHEMICAL REACTIONS ALSO DELTAH(298), S(298), AND CSUBP FOR EACH REACANT OVER A SPECIFIED TEMPERATURE RANGE SEE C4
C3 ---- F A C T FACILITY FOR THE ANALYSIS OF CHEMICAL THERMODYNAMICS	INTERACTIVE SYSTEM FOR COMPUTING REACION EQUILIBRIA AND DISPLAY OF PHASE DIAGRAMS OF VARIOUS TOPOLOGIES	1905 MAINLY SEE REMARKS	VIA TELENET AND DATAPAC FROM MC GILL COMP. CENTRE		DR.W.T.THOMPSON DEPT. OF MINING AND METALLURGICAL ENGINEERING MCGILL UNIV. MONTREAL, CANADA	A JOINT METALLURGICAL PROJECT OF THE ECOLE POLYTECHNIQUE AND MCGILL UNIV. --- USES STORED FREE ENERGY DATA TO GENERATE 50+ BINARY AND TERNARY PHASE DIAGRAMS
C4 ---- THERMODATA DATA BANK MEMBER OF SGTE++	METALLURGICAL CALCULATIONS PURE CMPDS, MIXTURES, AND REACTIONS INVOLVING GASES, SOLIDS, OR LIQUIDS	2500 INORGANI C	EURONET TRANSPAC	HB-68 (DPS3) MULTICS	DR. YVES DENEIL BIBLIOTHEQUE UNIVERSITAIRE DES SCIENCES B.P.22-38402 SAINT-MARTIN-D'HERES FRANCE (76)42.76.90	SEE MTDATA (C2) PART OF A COOPERATIVE PROGRAM BETWEEN METALLURGISTS IN BRITAIN, FRANCE, GERMANY, AND SWEDEN ----- BASED LARGELY ON JANAF, HULTGREN, AND KUBASCHEWSKI ET AL
C5 ---- DATA BANK FOR MULTI-COMPONENT SYSYSTEMS MEMBER OF SGTE++	METALLURGICAL CALCULATIONS OF MULTICOMPONENT PHASE DIAGRAMS	100 BINARY SYSTEMS	EURONET CONNECTION PLANNED	HB-68 (DPS3) MULTICS	DR. I. ANSARA OR DR. C. BERNARD LABORATOIRE DE THERMODYNAMIQUE ET PHYSICO-CHIMIE METALLURGIQUES E.N.S.E.E.G.-BP 44 38401- SAINT MARTIN D'HERES FRANCE TEL. (76) 54.41.27	SEE C2 SEE C4

++ SCIENTIFIC GROUP THERMODATA EUROPE

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
TABLE D. SYSTEMS FOR TABLES OF THERMODYNAMIC AND THERMOCHEMICAL PROPERTIES OF INDIVIDUAL SUBSTANCES						
D1 ---- FLUIDS PACK	AN INTERACTIVE FORTRAN IV SYSTEM FOR THERMODYNAMIC AND TRANSPORT PROPERTIES OF SELECTED CRYOGENS SEE REMARKS	7	CAN BE MADE AVAILABLE ON TYMNET ON REQUEST TO OSRD	CDC 6400 UNIVAC 1108	MRS. BETTIJOYCE MOLINO OFFICE OF STANDARD REFERENCE DATA WASHINGTON D.C. 20234 TEL.(301) 921-2050	PROVIDES TABLES FOR HYDROGEN, HELIUM, NITROGEN, OXYGEN, NEON, ARGON, AND METHANE SEE BELOW
D2 ---- AMMONIA TABLES	AN INTERACTIVE FORTRAN PROGRAM FOR THERMODYNAMIC PROPERTIES OF AMMONIA	1	CAN BE MADE AVAILABLE ON TYMNET ON REQUEST TO OSRD	UNIVAC 1108	SEE FLUIDS PACK	THIS PROGRAM AND FLUIDS PACK ARE AVAILABLE ON MAG TAPE FROM THE OFFICE OF STANDARD REFERENCE DATA
D3 ---- COMPUTER ANALYZED THERMOCHEM- ICAL DATA	PROVIDES STD. ENTHALPY OF FORMATION AND OF COMBUSTION FOR ORGANIC AND ORGANOMETALLIC COMPOUNDS ALSO STD. ENTH. CHANGES FOR 1133 REACTIONS				DR.J.B.PEDLEY SCHOOL OF MOLECULAR SCIENCES UNIV. OF SUSSEX BRIGHTON BN 9QJ ENGLAND	A MAG TAPE VERSION OF THE CITED PEDLEY AND RYLANCE BOOK IS AVAILABLE
D4 ---- VNIIS-GSSSD	THERMODYNAMIC PROPERTIES OF TECHNICALLY IMPORTANT GASES AND LIQUIDS TO 1500 K AND 100 MPA	8		?	DR. A. D. KOZLOV AUTOMATED SYSTEM SERVICE VNIIS-GSSSD EZDAKOV PER.1, 117334 MOSCOW B-334 USSR TEL. 250-0190	INCLUDES:AIR, METHANE, ETHYLENE, WATER, CARBON DIOXIDE OXYGEN, AND AMMONIA
TABLE E. PROPERTIES OF PLASTICS ETC.						
E1 ---- COMPAT COMPATABILITY OF MATERIALS WITH PROPELLANTS AND EXPLOSIVES	DELIVERS TEST DATA ON THE INTERACTION OF POLYMERS AND METALS WITH PROPELLANTS,EXPL OSIVES, AND PYROTECHNICS	SEVERAL THOUSAND MATERIAL COMBIN- ATIONS	DIAL-UP TO THE CDC 6600		HARRY PEBLY PLASTICS TECHNICAL INFORMATION CENTER U.S. ARMY ARMAMENT R AND D COMMAND DOVER,N.J. 07801 TEL.(201) 328-4222	ALSO INCLUDES A COMPILATION OF OBSERVED MATERIAL DEFICIENCIES CALLED HAZARD-FAILURE
E2 ---- PLASTEC DATA SYSTEM	PROVIDES MECHANICAL,ELECTRICAL,THERMAL, OPTICAL,PHYSICAL,AND PERMANENCE PROPERTIES OF PLASTICS		LATE IN 1980	CDC 6600	JOHN NARDONE PLASTICS TECHNICAL INFORMATION CENTER U.S. ARMY ARMAMENT R AND D COMMAND DOVER,N.J. 07801 TEL.(201) 328-5859	MECH. PROPERTIES INCLUDE: CREEP, STRESS RELAXATION, POISSON RATIO, STRESS FATIGUE, HARDNESS, FRICTION, AND ABRASION

TABLE F. SYSTEMS FOR CHEMICAL PROCESS SIMULATION AND DESIGN

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
F1 CHEMTRAN	A PHYSICAL PROPERTIES GENERATION AND CORRELATION SYSTEM FOR PURE COMPOUNDS AND MIXTURES	856	GENERAL ELECTRIC MARK III SERVICES CONTROL DATA CORP. TYMSHARE UNITED COMPUTING SYSTEMS UNITED COMPUTING CO.	UNIVAC 1100 SERIES CDC 6600 AND CYBER SERIES IBM 370 AND 360 DOS PRIME ICL	JOHN ADAMS CHEMSHARE CORP. SUITE 1900 3000 POST OAK HOUSTON, TX 77056 TEL (713) 627-8945	CHEMTRAN INTERFACES WITH PROGRAMS DISTIL,REFINE,AND DESIGN TO SOLVE PROBLEMS IN THE PROCESSING OF PETRO-CHEMICALS
F2 CHESS CHEMICAL ENGINEERING SIMULATION SYSTEM	PROCESS SIMULATION DATA RETRIEVAL CALCULATION DATA ESTIMATION	98		IBM 360 XDS SIGMA 7 CDC 6400 U1108 RCA SPECTRA 70/45	PROF R.L. MOTARD DEPT OF CHEM ENG WASHINGTON UNIV ST. LOUIS MO 63130 TEL (314) 889-6072	THIS SYSTEM IS AVAILABLE ONLY TO UNIVERSITIES AND U.S.GOVT AGENCIES
F3 FLOWTRAN SIMULATION	PROCESS SIMULATION DATA RETRIEVAL DATA CALCULATION DATA ESTIMATION	180	UNITED COMPUTING SYSTEMS FOR EDUCATIONAL USE ONLY	IBM 360/50 370/135 CDC 6400 H 6080 UNIVAC 1108	DR. ALVIN H. LARSEN MONSANTO CO. - F4EE 800 N. LINDBERGH BLVD ST. LOUIS, MO 63166 TEL (314) 694-6311	THIS PACKAGE HAS BEEN MADE AVAILABLE FOR EDUCATIONAL USE THROUGH THE INITIATIVE OF THE CACHE CORP.
F4 TISFLO TISUNOP	FLOWSHEET SIMULATION AND UNIT OPERATIONS CALCULATIONS	99	NETHERLANDS COMPUTER CENTRE AT HEERLEN	UNIVAC 1100 SERIES	SEE TISDATA (B3)	INTERFACES WITH TISDATA AND USER PROGRAMS
F5 PDA PROCESS DESIGN ANALYSIS GPS GENERAL PROCESS SIMULATION	CHEMICAL PROCESS SIMULATION PHYSICAL PROPERTIES RETRIEVAL AND GENERATION	200	MCDONNELL DOUGLAS AUTOMATION		FRANCIS MUNCASTER MC DONNELL DOUGLAS AUTOMATION CO. BOX516 ST LOUIS MO 63166 TEL.(314)232-2585	DATA BASE DEVELOPED AND MAINTAINED BY PHILLIPS PETROLEUM CO. BARTLESVILLE,OK 74004
F6 PROCESS SIMULATION PROGRAM VLE/REGRESS	PERFORMS RIGOROUS DISTILLATION SIMULATION INVOLVING STEADY-STATE ENERGY AND MASS BALANCE	650 INCLUDING PPDS DATA BASE	CONTROL DATA CORP. UNITED COMP. SYSTEMS UNIV. COMP. CO. MC DONNELL DOUGLAS AUTOM. CO. G. E. MARK III SERVICE	IBM 360/370 CDC 6600 AND CYBER 172,174 UNIVAC 1100 SERIES	DR. N.F. BRANNOCK SIMULATION SCIENCE INC. 1400 N. HARBOR BLVD FULLERTON, CA 92635 TEL (714) 879-9180	ALSO AVAILABLE FROM ------ SIA LTD. IN THE UK AND THE NETHERLANDS ------ BOC DATASOLVE IN THE UK ------ AQUATAINE SYSTEM IN FRANCE CENTURY RESEARCH CENTER, TOKYO

TABLE F. SYSTEMS FOR CHEMICAL PROCESS SIMULATION AND DESIGN (CONC.)

NAME	FUNCTION	CMPDS IN DATA BASE	NETWORK OR DIAL-UP	BATCH VERSION RUNS ON	CONTACT	REMARKS
F7 DPS JUSE-L-GIFS JUSE-MIDIST-1	DYNAMIC PROCESS SIMULATION MASS AND HEAT BALANCE OPTIMIZATION NON-IDEAL MULTICOMP. SIMULATION		UNDER DEVELOPMENT	SEE B1	SEE B1	INSTALLATIONS DPS (7) JUSE-L-GIFS (24) JUSE-MIDIST (17)
F8 FLOWPACK II	A THIRD GENERATION PROCESS SIMULATION SYSTEM	800 INCLUDING PPDS DATA BASE		IBM 370 3033 DEC 10	D.J. SAWERS IMPERIAL CHEMICAL INDUSTRIES LTD. P.O. BOX NO. 11 THE HEATH RUNCORN CHESHIRE WA7 4QE ENGLAND TEL (092 85) 73456	CURRENT VERSION IS A JOINT EFFORT OF ICI AND LINDE AG (MUNICH, FRG)
F9 CONCEPT MULTICOL	PROCESS DESIGN AND SIMULATION	USES KEYDATA SEE B10	SCICON (UK)CSC UCS CDC	UNIVAC 1100 SERIES ---- PRIME CDC ICL 2900 SERIES	DR. P. WINTER PROCESS INDUSTRIES GROUP COMPUTER AIDED DESIGN CENTRE MADINGLEY ROAD CAMBRIDGE CB3 0HB ENGLAND	U.S. REP IS AAA TECHNOLOGY AND SPEC. CO. INC. P.O. BOX 37189 HOUSTON, TX 77036 TEL (713) 789-6200
F10 FLASH	MULTI-PURPOSE FLASH RECOMBINATION AND PLANT RECOVERY PROGRAMS		UCS G.E. MARK III		GARRETT COMPUTING SYSTEMS INC. 1111 REPUBLIC BANK TOWERS DALLAS TX 75201 TEL (214) 741-1026	
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Appendix A

The ASPEN Computer Program Survey

The earlier version of this summary, dated June 1976, contained information on a number of programs for chemical process simulation and design. Since then the staff of the ASPEN project at MIT has completed an extensive survey of computer programs for chemical engineers. The results of that survey, published in a series of five papers in Chemical Engineering (ref. 9–13), contains information on 437 listings—a number of which describe entire suites of programs. The table shows how these programs are distributed among 11 technical areas.

An examination of the sources of the 437 computer systems shows the following interesting distribution:

- North American Universities 39%
- Other Universities 10%
- Consult. & Eng. Firms (U.S.) 33%
- Consulting & Engineering (other) 8%
- U.S. Government 5%
- Chemical Industry 5%

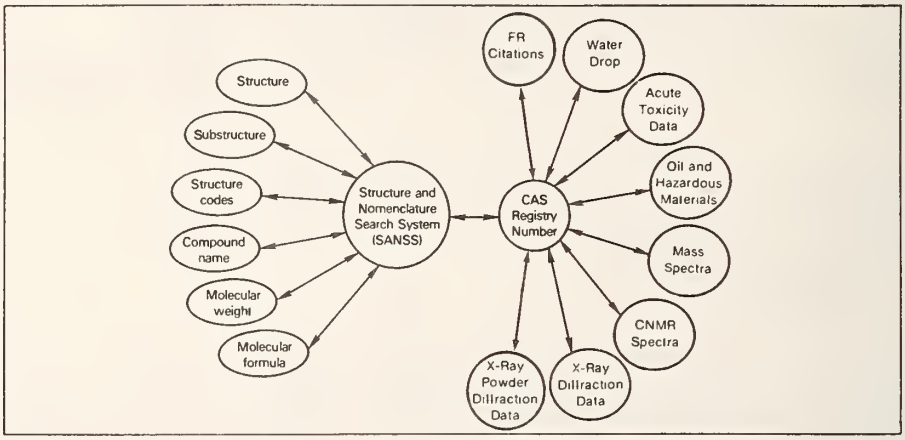
Programs developed in departments of chemical engineering make up the largest source, while those from consulting and engineering firms represent a close second.

In view of the availability of the ASPEN survey, we have included here only those chemical process and design systems which we know to be available on-line, or soon to be so available, or those batch systems which utilize one of the more current physical properties data bases, listed in Table B. We have included references to published descriptions of the listed systems, wherever they were available.

Application Areas for 437 Computer Programs
Covered by the ASPEN Survey (Chem.Eng. vol.85,86)

NUMBER	FUNCTION
9	Thermodynamics of chemical equilibrium
18	Vapor-liquid equilibrium
31	Thermal properties
45	Steady state flowsheet and dynamic simulation
42	Special processes
147	Unit Operations
23	Cost estimation and related economics
45	Mathematical techniques
40	Vessels, tanks, and piping technology
16	Dynamic process control
21	Miscellanious
---	---
437	TOTAL

NIH-EPA
Chemical Information System



Research chemists, environmental scientists, and librarians—in private industry, universities or government—can now retrieve chemical information quickly and inexpensively without sophisticated knowledge of computers.

The NIH/EPA Chemical Information System (CIS) is a collection of scientific data bases available through an interactive computer program. No other publicly available information system can provide such diverse numeric, as opposed to bibliographic, data on so many (over 192,000) chemical substances. CIS has a unique linking system, the heart of which is the Structure and Nomenclature Search System (SANSS). SANSS allows the user, in a single operation, to search 66 different files including the TSCA inventory. The CIS data bases can be searched by:

1. **Chemical Structure**: a two-dimensional representation that can be generated by the user.
2. **CAS Index Name, Trade Names, Common Names and Synonyms**: over 450,000 names which can be searched in complete or truncated form.
3. **CAS Registry Number**: the key to unlock the doors of the CIS file and link the CIS to Chemical Abstracts.

The Chemical Information System has been developed by agencies of the United States Government in cooperation with other governments and organizations. It is available only in the private sector (via Telenet) for use by the government, industry, and the public through an annual subscription fee of $300.00 and either $36.00 or $60.00 per connect hour, depending on which component is used. The annual subscription fee has been waived for academic institutions.

For further information contact —.

U.S.A.	**Kay Pool**, CIS Project, 2135 Wisconsin Ave., NW, Washington, D.C. 20007 Phone: (202) 298-6200 or (800) 424-2722
The Netherlands	**Dr. Charles Citroen**, CID-TNO, PO Box 36, 2600 AA, Delft, Phone: (015) 56-93-30
Switzerland	**Dr. T. Clerc**, Pharmacy Department, University of Bern, 3012 Bern, Phone: (031) 65-41-71
Finland	**Dr. S. Laitinen**, Technical Research Center of Finland, Technical Information Center, Vuorimiehentic 5, 02150 Espoo 15, Phone: (0) 456-4370
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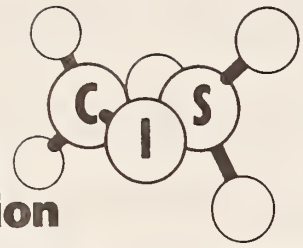

NIH/EPA

Chemical Information System

CIS includes the following components:

Structure and Nomenclature Search System (SANSS)—provides a data base of over 192,000 compounds collected from over 66 different sources. All of the CIS data bases are searchable through SANSS by structure, substructure, chemical code, or full, partial or left- or right-truncated name. The data obtained from SANSS includes the CAS registry number, other data bases associated to the substances, structural diagram, and systematic names as well as synonyms. ($60.00 per connect hour)*

Mass Spectral Search System (MSSS)—contains mass spectra of over 33,000 compounds which can be searched on the basis of normal peak and intensity requirements, as well as by Biemann and probability based-matched (PBM) techniques. ($36.00 per connect hour)*

Carbon-13 Nuclear Magnetic Resonance Spectral Search System (CNMR)—contains CNMR spectra of over 8,500 compounds. Searches by chemical shift requirements are permitted; analysis and display of this information for compounds of interest may also be obtained. ($36.00 per connect hour)*

Nuclear Magnetic Resonance Literature Search System (NMRLIT)—retrieves bibliographic information for over 34,000 literature references in the field of NMR. Searches may be conducted by author, nucleus, NMR subject or journal, from 1964 to the present ($36.00 per connect hour)*

Powder Diffraction Search-Match (PDSM)—contains over 30,000 powder diffraction patterns, provided by the Joint Committee on Powder Diffraction Standards (JCPDS), for identifying compounds based upon the characteristics of their powder diffraction pattern, as opposed to x-ray crystal identification. ($60.00 per connect hour)*

X-ray Crystallographic Search System (CRYST)—contains the bibliographic and structural files of the Crystallographic Data Centre (Cambridge, England). There are over 25,000 compounds which have space groups assigned which may be used as a search element. There are approximately 18,000 compounds which have had the atomic coordinates and cell parameters reported. ($36.00 per connect hour)†

X-ray Single Crystal Search System (XTAL)—is a search system of the **Crystal Data Determinative Tables** published by the National Bureau of Standards and the Joint Committee on Powder Diffraction Standards. The space group, density, unit cells and chemical types will be searchable. This system currently uses the Cambridge Crystallographic Data Centre file. ($36.00 per connect hour)*

EPA's Oil and Hazardous Materials-Technical Assistance Data System (OHM-TADS)—provides information pertinent to emergency spill response efforts. The OHM-TADS data base includes a wide variety of physical, chemical, biological, toxicological and commercial data on these materials, with emphasis placed on their deleterious effects on water quality. Up to 126 different fields of information are maintained for more than 1,000 materials. ($36.00 per connect hour)*

Water Drop—Distribution Registry of Organic Pollutants contains data on drinking and other types of water, date and location of water sample, compound identity, analytical method used, concentration detected, and references to published results. ($36.00 per connect hour)*

Federal Register Notices—provides a cross-reference to all of the citations of a chemical or class of chemicals cited in the Federal Registry since January 1, 1978. The title, part, subpart, and a short description of the notice of the chemical of interest is available. ($60.00 per connect hour)*

Registry of Toxic Effects of Chemical Substances (RTECS)—is provided by the National Institute of Occupational Safety and Health to the CIS. The RTECS publication, with over 40,000 toxicological measurements, is available with a set of programs to search the file on the basis of toxicological data and designators (e.g. animal type and measuring method ($36.00 per connect hour)*

Chemical Modeling Laboratory (CHEMLAB)—provides all the capabilities of the former component, CAMSEQ-II, for three-dimensional conformational analysis, molecular orbital calculations, and in addition, provides for the estimation of many properties of a chemical; such as, the partition coefficient, melting point, boiling point, solubility and others. ($60.00 per connect hour)*

Mathematical Modeling System (MLAB)—an interactive system for mathematical modeling. This component provides major capabilities in the areas of curve and distribution fitting, linear and non-linear regression, statistical analysis, differential and integral calculus, and two- and three-dimensional plotting. ($60.00 per connect hour)*

Operational soon:

Clinical Toxicology of Commercial Products (CTCP)—will be an interactive search system based upon the publication of the same name by Gleason, Hodge, Gosselin, et al. CTCP will permit searching of common commercial products by identifying the product or its constituents. The toxicity of the products in CTCP will also be available ($60.00 per connect hour)*

Partition Coefficients (LOGP)—have been provided by Pomona College (California). The data will contain partition coefficients on approximately 5,000 common chemicals. LOGP will allow searching to be done by value, solvent, and references as to the compound in question. ($36.00 per connect hour)*

*European users are given a credit of $12.00 per connect hour. The PTT will bill the communications costs directly to the user. Hourly rates include CRU's and connect minutes accumulated in a program. There is a $3.00 minimum per session.

†Non-USA users require permission from Cambridge Data System.

7/1/80

Appendix C

VIII. Computer Programs for Handling Technical Data

NBS Tech. Note 444, Reform: A General-Purpose Program for Manipulating Formatted Data Files, R. C. McClenon and J. Hilsenrath (1968).

NBS Tech. Note 446, PRECISE: A Multiple Precision Version of OMNITAB, A. E. Bean and J. Hilsenrath (1968).

NBS Tech. Note 470, Edpac: Utility Programs for Computer-Assisted Editing, Copy-Production, and Data Retrieval, C. G. Messina and J. Hilsenrath (1969).

NBS Tech. Note 500, Edit-Insertion Programs for Automatic Typesetting of Computer Printout, C. G. Messina and J. Hilsenrath (1970).

NBS Tech. Note 700, COMBO: A General-Purpose Program for Searching, Annotating, Encoding-Decoding, and Reformatting Data Files, Robert McClenon and Joseph Hilsenrath (1972).

NBS Tech. Note 738, Subroutine for the Calculation of CODEN Check Characters, D. Garvin (1972).

NBS Tech. Note 740, SETAB: An Edit/Insert Program for Automatic Typesetting of Spectroscopic and Other Computerized Tables, Robert C. Thompson and Joseph Hilsenrath (1973).

NBS Tech. Note 760, Description of the Magnetic Tape Version of the Bulletin of Thermodynamics and Thermochemistry, No. 14, R. McClenon, W. H. Evans, D. Garvin, and B. C. Duncan (1973).

NBS Tech. Note 820, Complete Clear Text Representation of Scientific Documents in Machine-Readable Form, Blanton C. Duncan and David Garvin (1974).

NBS Tech. Note 903, The NIRA Computer Program Package (Photonuclear Data Center), H. J. Vander Molen and H. M. Gerstenberg (1976).

NBS Tech. Note 928, Computer Programs for the Evaluation of Activity and Osmotic Coefficients, B. R. Staples and R. L. Nuttall (1976).

NBS Handbook 101, OMNITAB, A Computer Program for Statistical and Numerical Analysis, J. Hilsenrath, G. G. Ziegler, C. G. Messina, P. J. Walsh, and R. J. Herbold (Revised January 1968).

NBS Handbook 125, OMNIDATA, An Interactive System for Data Retrieval, Statistical and Graphical Analysis, and Data Base Management, A User's Manual, J. Hilsenrath and B. Breen (1978).

NBS Spec. Publ. 424, A Contribution to Computer Typesetting Techniques: Table of Coordinates for Hershey's Repertory of Occidental Type Fonts and Graphic Symbols, N. M. Wolcott and J. Hilsenrath (1976).

NBSIR 76-1147, A Combined Least Sum and Least Squares Approach to the Evaluation of Thermodynamic Data Networks, D. Garvin, V. B. Parker, D. D. Wagmann, and W. H. Evans (1976).

NBSIR 78-1432, Automation of the Ion Energetics Data Center, R. Thompson, W. Webb, H. M. Rosenstock (1977).

IX. NBS Magnetic Tape Series

NBS Magnetic Tape 1, OMNITAB II Magnetic Tape and Documentation Parcel, David Hogben, Sally T. Peavy, and Ruth Varner (1970).

NBS Magnetic Tape 2, Fortran Programs for Text Editing, File Manipulation and Automatic Typesetting, C. G. Messina, R. McClenon, and J. Hilsenrath (1973).

NBS Magnetic Tape 3, Bibliography and Index to the Literature in the NBS Alloy Data Center, G. C. Carter and D. J. Kahan (1973).

NBS Magnetic Tape 4, Magnetic Tape Version of the Bulletin of Thermodynamics and Thermochemistry, No. 14 (1971), Robert McClenon and Blanton Duncan (1973).

NBS Magnetic Tape 9, Crystal Data Tape, Derived from the 3rd Edition of Crystal Data Determinative Tables, H. M. Ondik and A. D. Mighell (1975).

NBS Magnetic Tape 10, Atomic Spectral-Line Intensities, W. F. Meggers, C. H. Corliss, and B. F. Scribner (1975).

NBS Magnetic Tape 12, Tables of Coordinates for Hershey's Repertory of Type Fonts and Graphic Symbols, Norman M. Wolcott and Joseph Hilsenrath (1977).

EPA/NIH Mass Spectral Data Base, S. R. Heller and G. W. A. Milne (1977). One year lease fee from $500. Write for further information to:

Office of Standard Reference Data
National Bureau of Standards
Building 221 - Room A323
Washington, D. C. 20234
Telephone: (301) 921-3442

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7. AUTHOR(S)

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13. Type of Report & Period Covered

Final

14. Sponsoring Agency Code

15. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

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.)*

A brief description is given of 51 interactive physico-chemical numerical data systems, most of which are on-line on international computer networks. The systems are listed under five headings: those useful for identification of substances from spectroscopic data; those providing thermodynamic and transport properties of pure components and mixtures; those which perform metallurgical calculations and draw phase diagrams; systems producing complete tables of thermodynamic properties of individual substances; and those for chemical process simulation, optimization, and design. References to published descriptions of the systems, where they exist, are also given.

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)*

Chemical data; data banks; data bases; data networks; interactive systems; numerical data bases; on-line data; physical data; spectroscopic data systems

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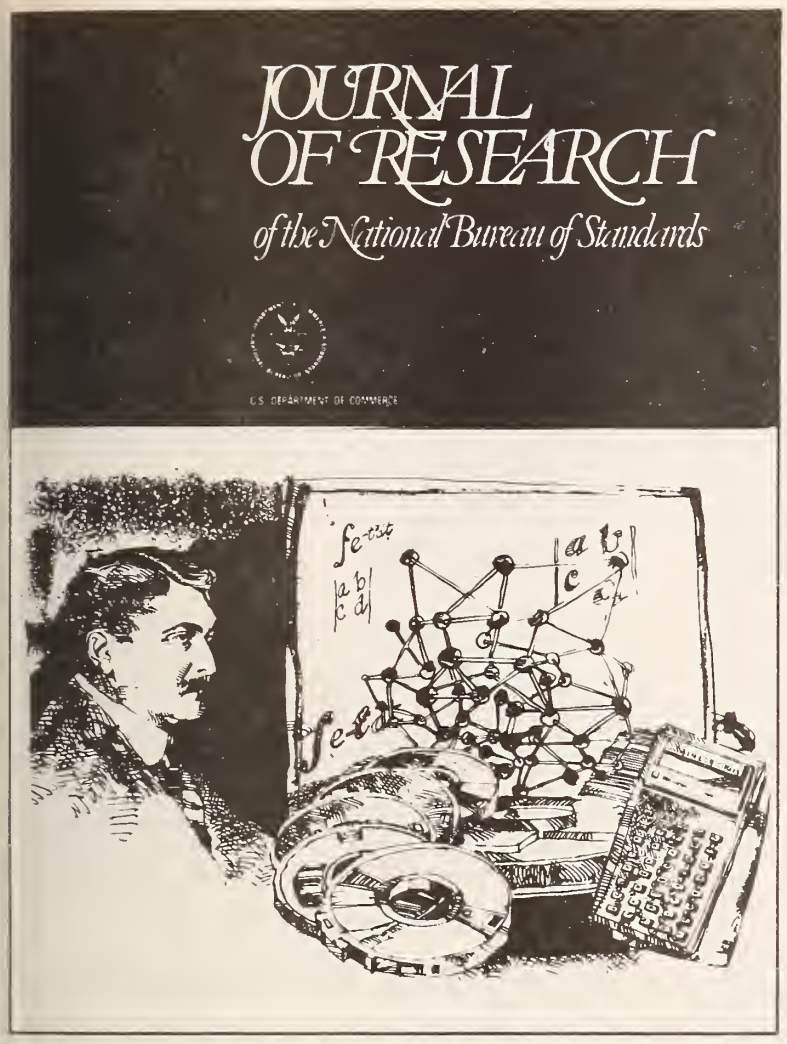

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