WEDNESDAY AFTERNOON

General

H. F. Ginsberg, Presiding

2:00 27. Chemical Carcinogenesis: A Survey of Recent Literature. O. C. Dermer, *G. Gorin*, E. M. Hodnett

2:25 28. A Workshop on the Use of Chemical Abstracts and Beilstein. *O. B. Ramsay*, B. Wallace, J. M. Doyle

2:55 29. A Dual Journal System Concept. *S. W. Terrant*, L. R. Garson

3:20 30. Computer Recognition and Segmentation of Chemically Significant Words for KWIC Indexing. D. R. Heym, *H. Siegel*, M. C. Steensland, H. V. Vo

3:40 31. Experimental Algorithmic Generation of Articulated Index Entries from Natural Language Phrases at Chemical Abstracts Service. *S. M. Cohen*, D. L. Dayton, R. Salvador

Division of Computers in Chemistry

170th National Meeting of the American Chemical Society
Chicago, Illinois, August 24–29, 1975

P. Lykos, Chairman
E. C. Olson, Vice-Chairman

MONDAY MORNING: (August 25, 1975)

Getting Started in Minicomputers—In Education

R. E. Dessy, Presiding

9:00 1. Interfacing the Student to the Computer— Why, How and How Much? G. Howard

9:30 2. Interfacing the Chemistry Department of a Liberal Arts College to a General Purpose Minicomputer for only $8K (Philosophy and Results). *J. Hix*, W. McAllister, D. Lunney, R. Morrison, C. Li

10:00 3. A Minimal Laboratory Minicomputer System for General-Purpose Use. C. Wilkins

10:30 4. A Modest Minicomputer System for Teaching Principles of Instrumentation Interfacing. J. Leone

11:00 5. A Microprocessor Based Timesharing System for Teaching Laboratories. *D. R. Deuel*, J. W. Gault

11:30 6. Problem and Concept Recognition: An Approach to Computer Aided PSI Instruction for Freshmen Chemistry. *J. C. Marshall*, A. E. Finholt, J. N. Ziemer

MONDAY AFTERNOON

Getting Started in Minicomputers—In Research

E. C. Olson, Presiding

2:00 7. Automated Analysis of Stopped-Flow Kinetics Data by Means of an Inexpensive "Off-the-Shelf" Programmable Calculator Assembly. *G. M. Harris*, S. A. Ficner

2:30 8. Building and Using a Minicomputer System. *R. E. Dessy*, S. Shaffer, P. VanVuuren, W. Nunn, M. Starling, C. Tetus

3:00 9. Hierarchical System Sharing a Mini—An Approach to Chemical Research. M. F. Burke

3:30 10. Laboratory Computerization—A Learning Process. *G. L. Kirschner*, P. W. Landis, R. A. Byers

4:00 11. Real-Time Mass Spectral Data Acquisition with a PDP-11 Computer. M. I. Levenberg

4:30 12. Trials, Tribulations, Trauma, and Triumph. J. T. Atkins

TUESDAY MORNING (August 26, 1975)

Symposium on Computer Networks and Chemistry

P. Lykos, Presiding

9:00 Introductory Remarks

9:10 13. CRYSNET: A Network for Crystallographic Computing. *T. F. Koetzle*, L. C. Andrews, F. C. Bernstein, H. J. Bernstein

9:40 14. Remote Terminal Computer Graphics. *David L. Beveridge*, Elias Guth

10:10 15. Newton. A Network of Parallel Processors. Kent R. Wilson

10:40 16. Geologic Applications of Network Conferencing: Current Experiments with the Forum System. *Jacques Vallee*, Gerald Askevold

11:10 17. A Network of Real-time Mini Computers. William J. Lennon

TUESDAY AFTERNOON

Symposium Continued

P. Lykos, Presiding

2:00 18. Laboratory Automation with Distributed Systems. Charles E. Klopfenstein

2:30 19. A Computer Utility for Interactive Instrument Control. Paul Day

3:00 20. Hierarchical Minicomputer Support as a Methodological Aid to the Laboratory Investigator. R. L. Ashenhurst

3:30 21. Computer Networking at UMR. *D. W. Beistel*, R. A. Mollenkamp

4:00 22. Computer Assembled Testing in a Large Network: The Socrates System. *William V. Willis,* Oliver Seely, Jr.

4:30 23. The Impact of a Computer Network on College Chemistry Departments—The Iowa Regional Network. Warren T. Zemke

WEDNESDAY MORNING (August 27, 1975)

Symposium Continued

P. Lykos, Presiding

9:00   Introductory Remarks

9:10 24. Providing the Computing Needs of Chemists via a Network—A Hierarchy of Hardware, Software, and Support Functions. J. R. Denk

9:40 25. *Ab Initio* Calculations Via a Remote Terminal and a Case History in Computer Resource Sharing. *D. G. Hopper,* P. J. Fortune, A. C. Wahl, T. O. Tiernan

10:10 26. Computer Identification and Interpretation of Unknown Mass Spectra. *R. Venkataraghavan,* Gail M. Pesyna, F. W. McLafferty

10:40 27. Networking and a Collaborative Research

Community: A Case Study Using the Dendral Programs. *Raymond E. Carhart,* Suzanne M. Johnson, Dennis H. Smith, Bruce G. Buchanan, Geoffrey Dromey, Joshua Lederberg

11:10 28. Computing in a Network Environment. James C. Emery

WEDNESDAY AFTERNOON

Planning the National Resource for Computational Chemistry (NRCC): A User-Oriented Facility (Cosponsored by NAS/NRC Planning Committee for NRCC)

J. Bigeleisen, Presiding

2:00   Introductory Remarks

2:10 29. The Atlas Computer Laboratory: A British National Computing Resource. J. Howlett

2:40 30. The Unique Role of NRCC in Chemistry. L. C. Snyder

3:00 31. Phase I: Personnel Funding, Computing, and Site Requirements. W. T. Wipke

3:20 32. Organization and Administrative Structure to Serve the User Community. J. Bigeleisen

4:00   Informal Panel Discussion

———NEWS AND NOTES———

CAS FORUM

Chemical Abstracts Service will hold the 22nd in its series of open forums Tuesday, August 26, at 8 P.M., in the Grand Ballroom of the Palmer House during the American Chemical Society's fall meeting in Chicago. Topic of discussion will be the American Chemical Society Composition System.

SYMPOSIUM ON MANAGEMENT OF DATA ELEMENTS

The Second National Symposium on the Management of Data Elements in Information Processing will be held at the National Bureau of Standards (NBS) in Gaithersburg, Maryland, October 23-24, 1975. The symposium is sponsored by the NBS Institute for Computer Sciences and Technology (ICST) and the American National Standards Institute (ANSI) Committee X3L8.

The symposium will include presentations on timely data management and data standardization topics such as: the role of the data manager, communications needs for data standards, data element directories, standard codes for character and control, use of check characters, data elements in bibliographic data bases, product coding, and coding for clinical medicine.

The registration fee for the symposium is $50, received in advance, which includes a copy of the proceedings mailed after the symposium. Papers presented at the meeting and discussions will be available on cassette tapes after the meeting.

For additional registration information, contact: Mrs. Hazel McEwen, Institute for Computer Sciences and Technology, NBS, Washington, D.C. 20234; phone (301) 921-3157.

COOPERATIVE PROGRAM IN COMPUTER PERIPHERALS

Dr. Ruth M. Davis, Director of the Institute for Computer Sciences and Technology of the National Bureau of Standards, and Mr. T. D. Puckorious, Commissioner of the Automated Data and Telecommunication Service of the General Services Administration, have announced joint approval of a cooperative program of work in computer interface standards.

Both NBS and GSA share a strong concern that Federal agencies be able to successfully procure and use the least expensive ADP equipment and services that satisfy their requirements. The development and use of computer interface standards which facilitate the competitive procurement of computer peripheral equipment has long been actively supported by both agencies and is an important part of the newly approved cooperative program.

This new cooperative program includes four tasks. First, the collective Federal Government experience with multivendor computer systems will be assimilated and made available to Federal agencies. Second, technical guidelines will be prepared to assist Federal agencies to successfully plan, select, and operate multi-vendor configurations. A government-wide interagency task group is being formed to address these two tasks.

The third task, already underway, is the identification of existing similarities and differences in the device level interface employed with high-density disk drives. Expected follow-on efforts that are part of this task will focus on other commonly used peripheral devices, such as magnetic tape, memory, printers, card readers, punches, and display devices. It is anticipated that the results of these efforts will serve to further Federal and national standards activities in the interface area.