A Brief History of Networking in the U.S.†

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The history of computer networking goes back 40 years. With few exceptions (*e.g.*, libraries), the U.S. Government established a creative environment or directly supported early developments. Chemical networking goes back to the year 1971, when three groups virtually simultaneously initiated access to chemical and structural databases.

This year marks the 30th anniversary of the invention of three-dimensional (3-D) color graphics (Figure 1) and the consequent development of novel molecular modeling capabilities with profound implications to chemistry and biology. The Brookhaven RAster Display (BRAD) and related color raster graphics technology[1] formed the basis for graphics workstations, desktop computers, and digital television and opened the door for novel networking. Catalytically, the BRAD display (Figure 2) system was the first system to present precise structural models in 3-D from a single image; these models are the link between human perceptions and the growing database of structural biology. Today, color graphics workstations make highly complex biological molecules comprehensible for teaching and research. Initially, the BRAD system triggered the formation of the Protein Data Bank (PDB)[2] and CRYSNET.[3−5]

While mathematicians and physicists enjoyed early access to computers, chemists tended to proceed at their own pace to make use of available computational resources. The field (i.e., hardware, software, and the user community) had to mature some before it was ready to create networks or link remote users. In 1969 an experimental four-node network was funded by the Department of Defense and later the Defense Advanced Research Projects Agency (DARPA); the ARPANET[6] was the precursor of today's Internet. Besides military networks such as SAGE (Semi-Automatic Ground Environment) developed by Lincoln Laboratories of MIT for the U.S. Air Force, the first retrieval networks were limited to serial transmission on dedicated lines until packet switching was invented in 1978 by network pioneers, Drs. Vinton Cerf and Robert Kahn. Electronic messaging and networking applications were demonstrated in October, 1972, at the International Computer Communications Conference. They coauthored the "Transport Control Protocol/Internet Protocol", better known as TCP/IP.[7,35]

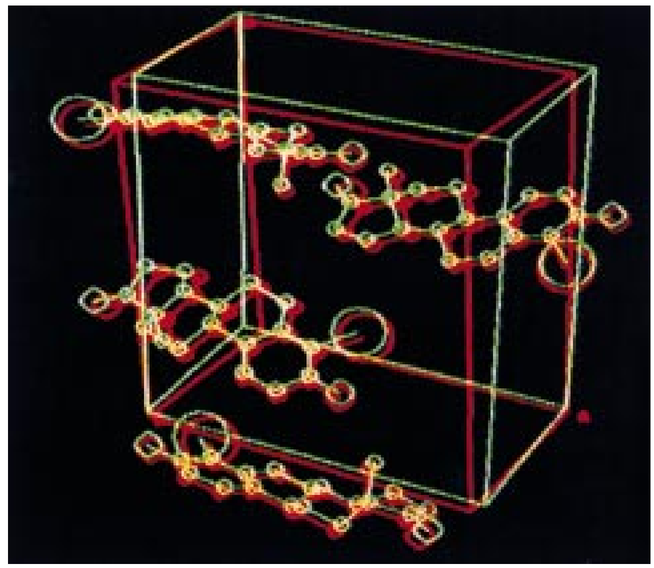

Figure 1. Depicts early (1968) 3-D color raster graphics from the BRAD[1] system using red-green stereo separation.[33]

Paul Baran, in the early 1960s a young Hughes Aircraft engineer, was another networking visionary. He worked on the design of the Minuteman missile control system and became involved with issues of vulnerability. He left Hughes and started a not-for-profit organization he called RAND (R&D). He was determined to design a communications system that would survive a nuclear attack. He conceived the idea of a parallel computer system with adaptive redundancy, which could reconfigure itself even if portions were destroyed. He also realized that the digital traffic would need to be broken up into short blocks (called packets today), which each carried its own routing information and would be able to replicate correctly if errors in transmission occurred. That design evolved into what is today called the Internet.[8,9] Project MAC at MIT was the first (1963) time-sharing computer network;[10] two linked computers supported 30 users (with teletype or Selectric typewriters) and first-of-its-kind graphics (the "KLUGE"). Just as in the early days of networking,[9] we have to differentiate between

† Presented as part of the symposium, "Networking: Yesterday, Today, and Tomorrow", held on the campus of Texas A&M University, March 2, 1998. One participant, Dr. Robert Spinrad (co-inventor of the BRAD system) played a leading role in development of both hardware and software from that cradle of creativity, Xerox PARC. The burst of human creativity generated by the ARPAnet, Internet, and now the worldwide-Web was represented by the co-founder, Dr. Robert Kahn, who spoke on current and future networking trends. The implications of these networking and computational tools for the scientific community was presented by Prof. Floyd Bloom, editor of *Science*. Current and projected developments in networking at Texas A&M and the state of Texas were presented by Dr. Richard Ewing, Dean of the College of Science and symposium sponsor.

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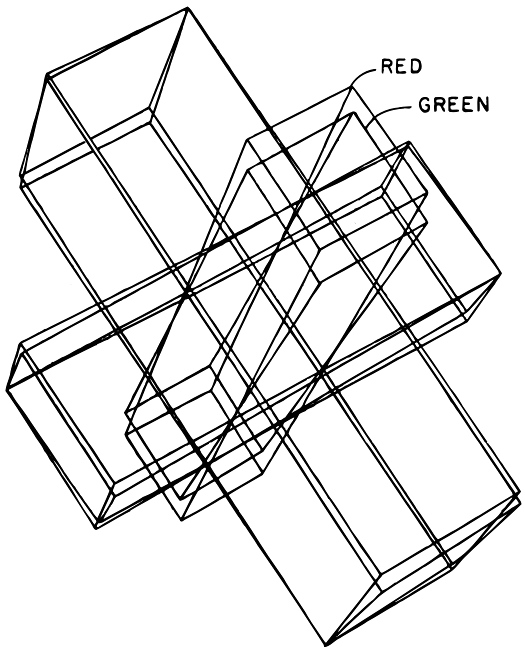

Figure 2. Presents the illustration of the BRAD[1] 3-D graphics for patent application S-36,382 by D. Ophir, B. J. Shepherd, and R. J. Spinrad. Reprinted with permission from Ophir, D.; Shepherd, B. J.; Spinrad, R. J. *Commun. A.C.M.* **1969**, *16*(6), 309−318. Copyright 1969 Association for Computing Machinery.

computer-computer and human−computer(−human) linkages.

Business and public policy decisions also helped shape the development of networking. This year also marks the 30th anniversary of the "Carter Phone" decision that broke the Bell Telephone monopoly on computer access to the telephone system in the U.S. by permitting the use of non-Bell modems. The D. C. Haynes Company was the first to develop low-cost modems which set the *de facto* standard for the communications industry. In 1971, Intel produced the first microprocessor and Ray Tomlinson of BBN invented e-mail. In 1972, the "open skies" policy permitted any entity that had the technical capability and financial resources to own and operate a satellite system. Another critical event was the suit brought against the American Telephone and Telegraph Company (AT&T) in 1974 by Microwave Communications, Inc. (MCI) and the Department of Justice, charging AT&T with monopoly. It took eight years for an agreement to be reached, but in 1982, AT&T was divested of the 22 Bell operating companies and 1984 resulted in the formation of the "Baby Bells". Specialized common carrier provisions opened competition in the telecommunications industry, permitting the sale of services by new and existing carriers. MCI was the first new entrant in this market.[11] Ultimately, these technological advances and decisions helped pave the way for the development of today's Internet. The Internet grew steadily throughout the 1970s. UNIX was developed in 1972 at Bell Laboratories and existing smaller networks such as Csnet and BitNet ("Because it's time" Net) improved connectivity. The public was drawn into the push for computer communications with the introduction of Altair 8800 computer, marketed as a hobbyist kit in 1975 by Ed Roberts and Leslie Solomon. Refined to a business by Paul Terrell in 1976, the Byte Shop opened its doors and the computer dealer was born.[12]

The 1980s brought faster progress in networking. IBM introduced the Personal Computer (PC) in 1981 and the mouse was introduced. By 1983, there were close to 1000 host computers on the Internet, and the addressing schemes were being pushed to the limit. This brought about the creation of the Domain Name System by Jonathan Postel (†1998). Original top-level domains were defined as "Commercial" −.com, "Education" −.edu, "government − US" −.gov, "Military − US" −.mil, "Major network support centers" −.net, "Organizations" −.org, "International" −.int, and "country codes" −.xx (two letter geographic abbreviation). These domain names were maintained by the Network Information Center, originally funded by DARPA.[6,9]

Computer-aided database storage and retrieval was envisioned 50+ years ago in a perceptive article, "As We May Think,"[13] published by Vannevar Bush in 1945. Peering well into the future, he envisioned a "Memex" machine which would be used by individuals to mechanize their private files and libraries. It would store records and communications and work with speed and flexibility, as a supplement to human memory.

Computer networking in various forms dates back some 40 years. The first on-line bibliographic search capability was demonstrated in 1960 by the Systems Development Corp. (Protosynthex) with a full text search of the Golden Book Encyclopedia.[36] In 1965 the Systems Development Corp., supported by ARPA.[37] developed the ORBIT system to provide 13 organizations with networked access to some 200 000 bibliographic records. The RECON system was developed by Lockheed Palo Alto Research Laboratory a year later to access NASA documents. Pertinent references include refs 14−21.

Thus both the branches and the roots of networking and information storage/retrieval are intimately intertwined. On the high-tech end, thanks to abundant intellectual and financial resources, ARPA led the way. On the low-tech end (teletype, telephone, ...) libraries led the way. By 1970 university libraries, the legal profession, NASA, the European Space Agency, Chemical Abstracts, the American Institute of Physics, the National Library of Medicine, DIALOG Information Services, and the Educational Resources Information Center (ERIC), among others, offered bibliographic retrieval services, some employing networks. The State University of New York (SUNY) Network went online with ERIC in October, 1968 (30 years ago!) and was subsequently described as "the first bibliographic utility accessible on-line, although terminals were dedicated to the system".[22] The OCLC (Ohio College Library Center) went on-line[23] in 1971, offering the first shared library cataloging system. The same year, MEDLINE[38] from the National Library of Medicine became available over dial-up telephone lines for textual searches (key words, authors, etc.). Commercial database companies (DIALOG, ORBIT, ABI/INFORM, LEXIS, *etc.*) quickly followed. Because of the uniform nature of bibliographic and textual databases, search techniques and algorithms (*e.g.*, inverted files) could be developed for speed and efficiency of retrieval. A review of these efforts suggests that librarians were doing more information retrieval over networks than the rest of the country combined.

The year 1971 is unique because, within weeks if not days, three numerical (nonbibliographic) databases became available on-line; all of them were chemical in nature. Two of them, the DENDRAL project[24] at Stanford University and the Chemical Information System at the NIH, accessed mass-spectral files for the identification of small-molecule compounds.[25,39] The DENDRAL project designed by Djerassi (steroids), Feigenbaum, Lederberg, *et al*., was made available to those with access to the ARPAnet for search and retrieval of mass spectral and NMR data of small molecular fragments and was subsequently accessed from as far away as Switzerland (A. Dreiding, personal communication). Concurrently, the Chemical Information System, MSSS, at the National Institutes of Health (NIH)[26] made available a similar search/retrieval system for small molecule mass-spectroscopy.[40] While neither system is operative today in its original form, the seeds were planted for more powerful systems to follow; the MSSS database has been extended by the National Institute for Standards and Technology and currently contains 130 000 spectra of 107 000 compounds.

Although some details of novel developments given here may be new, it comes as no surprise that innovative groups on the east and west coasts were using networks to establish and access scientific databases. But what about the rest of the U.S.? Who would think of similar networking events in Texas? Especially relevant to this symposium is an event that occurred in 1971 that was the first networked retrieval of structural information from a biological database (the PDB), and it occurred here at Texas A&M, using conventional hardware (ARS-33 teletype, 110 Baud modem, long distance telephone line) and novel software.

The PDB consists of spatial (atomic) coordinates and isotropic thermal (Debye–Waller or "B") factors of individual atoms of amino acids and related molecules comprising proteins (and later, nucleic acid and carbohydrate polymers).[41] A typical protein might contain 200 amino acids or 2000 non-hydrogen atoms, with an architectural complexity that far exceeds human capacity to visualize and comprehend the interactions that constitute life at the most fundamental level, atom-to-atom. Because of inherent structural complexity and the minute size of biological molecules, facile graphical inspection of macromolecular models in 3-D was and is essential; the BRAD[1] system and program DISPLAY used color raster graphics to open the door to these magnificent structures and led directly to the creation of the PDB.[42]

Program SEARCH[27] was written during the spring and summer of 1971; with it the user could call forth a specific protein crystallographic data file[43] from the PDB and extract specific nontextual (structural) information. These structure-based search procedures were necessary because of inherent hardware (32k words of memory) limitations. Likewise, program DISPLAY had a working maximum limit of 512 atoms, whereas available protein structures contain many more atoms. Simplification procedures therefore were required to accommodate computer memory limitations as well as human visualization limitation, typically in the functional range of 50–100 atom fragments. (*i.e.*, 5–10 amino acids) (Figure 3).

These procedures were well adapted to networked computing, but demonstrating program SEARCH locally at Brookhaven would have had little impact. An opportunity presented itself to use a network link over a distance (College Station, TX – Brookhaven, NY) of 3000 km on the first Monday (sixth) of September, 1971, to demonstrate[29] program SEARCH to the Brookhaven host, the late Dr. Walter Hamilton. As a direct result of this demonstration, a proposal was submitted to and funded by the U.S. National Science Foundation to create CRYSNET,[4,5] which linked the Fox Chase Cancer Institute (PA) and Texas A&M with Brookhaven in a star-type network with 3-D graphics[44] capability. By 1974 two other institutions (Johns Hopkins University, MD, and the Medical Foundation of Buffalo, NY) had joined CRYSNET, and asynchronous communication with a variety of computers (CDC 7600, IBM 360/91, DEC PDP-10) was achieved. Dr. Herbert Bernstein provided crucial technical support and his wife, Francis, helped run the PDB until very recently.

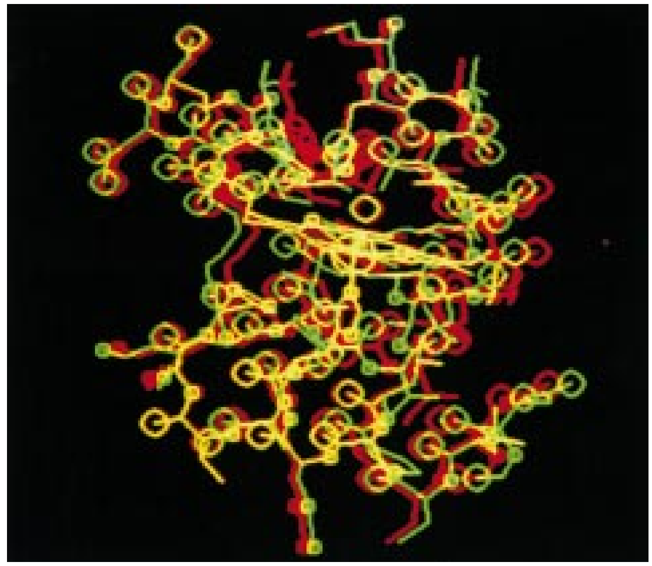

Figure 3. Illustrates the 3-D display capabilities of program DISPLAY on the BRAD system for visualization of complex molecular structures. A 15 Å scoop around the haem Fe atom in myoglobin performed by program SEARCH is shown in this photograph made in 1970.[3]

The idea of CRYSNET, to link archival data, a library of programs, and graphical modeling tools, was 25 years ahead of its time.[45] These functions are now widely and elegantly available by means of servers accessed over the worldwide-Web.[46] It arose because of need, but also because of curiosity. Of enduring value from these early efforts was the development and first use (Staph. nuclease) of 3-D graphics electron density modeling[30,31] (Figure 4); facile model building and interactive graphics tools are a crucial factor in the spectacular success of protein crystallography today. Challenged by the profound complexity of molecular structures, CRYSNET was the first to add a new dimension to networking, interactive 3-D color raster computer graphics, known today as the graphics workstation. Progress[47] in the sciences and the need for researchers to communicate rapidly continues to fuel the development of networking, now in competition with hungry commercial and ephemeral entertainment interests.

On the darker side, the opportunity for abusing the system and the mutual trust and open communication it affords has been documented.[32]

To summarize, the librarian was first, in terms of providing access to mass information and application of available

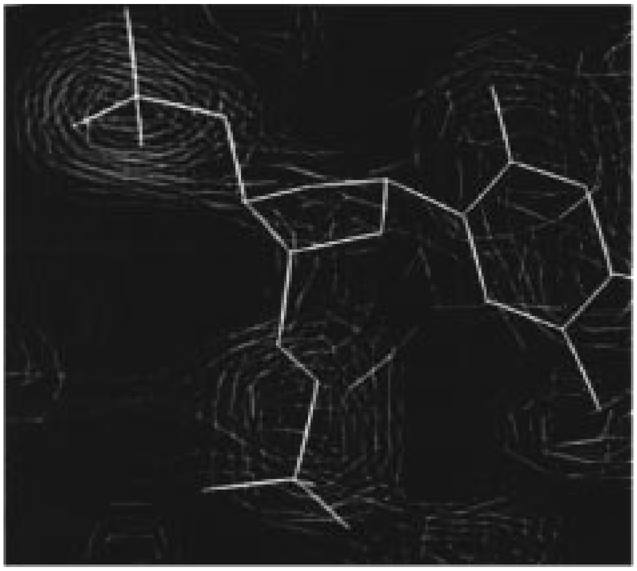

Figure 4. Depicts the first published representation of the use of computer graphics for the complete construction and publication of a macromolecular model.[30] An inhibitor was fit to density in the active site of Staph. nuclease by Dr. Marge Legg. By converting from brass models in a "Richards' Box" [34] to graphical models, this practical application of 3-D electron density modeling revolutionized protein crystallography. 3-D modeling to electron density forms the backbone of macromolecular crystallography and contributes greatly to its current success, as witnessed by the facile software that has become available since these pioneering efforts.

technology to address user needs; the U.S. Air Force created the first defense-related network, SAGE. The ARPAnet was first in terms of frontier development of hardware, software, and linkages. The National Library of Medicine was first in terms of connecting the biomedical community to the database, MEDLARS. The spectroscopic databases pressed numeric database organizations and algorithms to devise search procedures and make them available. The year 1971 marked the seminal synthesis of the database, retrieval tools, and graphics to provide the first interactive access to the Protein Data Bank, with impressive tools now available on the World Wide-Web. Each effort pressed technology to the limit, planted its seed, and opened the way for newer technologies, which repeated the patterns, each with its own life-cycle. Today, by giving sight to the investigator, structural results form the basis of new technologies (*e.g.*, structure-based drug design, mining genomic databases). Not only have the databases matured, so have powerful search engines, used by a new generation of life scientists which has never seen a teletype.

What can we conclude from this comparison? While some of the effort was directed to establishing new frontiers in human-computer (*e.g.*, Project MAC) and computer-computer interfaces (*e.g.*, ARPAnet), most of these networks were user-oriented and adapted available technology (teletype, telephone lines) to address specific topics, accepting and living within the limitations of available resources; initially, they met with modest acceptance. With the exception of ARPA projects, they also were less well funded! ARPAnet did not have to abide by the existing limits but pushed them forward with great benefit—yet it is curious that initial scientific results from the ARPA environment appear to have been minimal and of short duration.

Success has many parents but failure is an orphan. So, what factors led to the success of networking? One can point to impressive enhancements in hardware (graphics workstations)[48] and novel applications of information theory (*e.g.*, packet switching, data compression, error correction). In the academic environment, one can identify two essential ingredients: bright minds and facile, low-cost access to resources. The latter is contrary to free-market pricing of resources according to demand, conflicting with the increasing commercialization of science, and therefore suggests that the value of frontier exploration must not be judged by the bottom line.

Contrary to charging for computing at Texas A&M, Brookhaven provided free access to state-of-the-art computational and graphics resources. And, thanks to the beaches and Long Island summers that pleased wives, children, and ur-wizards (who stayed up all night, every night), visits to Brookhaven were a great stimulus and opened up new research opportunities. From this came the convergence, in 1971 here at Texas A&M, of the three crucial components of structural biology: data, graphics, and the network to link them. So a recipe for success can be distilled: Challenge minds, give them free access to resources, but do keep an eye on them. These results were possible also because of the freedom Texas A&M provided to pursue structural studies (even though it took a decade or more for the efforts to mature) and 30+ years of support by the Robert A. Welch Foundation.

Today, the world has an impressive resource at its fingertips, so long as the information is textual (i.e., alphanumeric) or two-dimensional. Facile, 3-D modeling is still beyond the reach[49] of most chemists and biochemists; workable solutions are available but their use is rather the exception. The future promises breakthroughs of information processing comparable to the impact the fast Fourier transform algorithm had on signal processing (especially for X-ray crystallography), to process the abundance of information now available digitally—and then calculate the inverse transform to help identify glaring gaps in the information database for future research. Considering the phenomenal growth of networking and its effect on our creative lives, what will the next 40 years bring?

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(36) A network is implied but cannot be verified on the basis of available information.
(37) The Advanced Research Projects Administration needed a robust communication network; the result, ARPAnet, has been compellingly described (cf. ref 9).
(38) Development and progress with networks linking libraries is documented in numerous proceedings and annual reviews of the American Society for Information Science.
(39) In the 1970s, mass spectroscopy was limited to the analysis of fragmentation patterns (mass, intensity) of volatile small molecules bombarded by a beam of electrons in a vacuum. In 1976 here at Texas A&M, Ronald MacFarlane (ref 25) described for the first time in a paper in *Science* a method to create a molecular ion for the mass analysis of biological macromolecules—now a powerful and common method in the arsenal of the biochemist.
(40) "An interactive conversational mass spectral retrieval system, available over ordinary telephone lines using a teletype-writer terminal from a central computer in the Division of Computer Research and Technology at the National Institutes of Health (NIH) has been used extensively by many researchers since September, 1971". Cf. Heller, S. R.; Fales, H. M.; Milne, G. W. A. An Interactive Mass Spectral Search System. *Anal. Chem.* **1972**, *44*, 4, 725.
(41) At this writing, the PDB (http://www.pdb.bnl.gov/) contains 8295 coordinate entries: 93% (7682) proteins, 7% (601) nucleic acids, and <1% (12) carbohydrates.
(42) Contrary to other databases, for the first years, the PDB had no budget, no committee. Its relationship to the crystallographic community was discussed at a meeting of the American Crystallographic Association in 1971. Fortunately, a decision was implicitly made and kept that access would remain free (excepting cost of distribution media). Free access to information is a crucial aspect of education and academic research. The implications of the failure of some industrial laboratories to publish atomic coordinates deserves serious discussion in another forum.
(43) In 1970 the structures of only eight proteins were available in the PDB. The proceedings of the Cold Spring Harbor Symposium (ref 28) in 1971 provides an historical record of what had been done and what was yet to come in protein crystallography. Notable in the proceedings of this symposium was the contribution of Prof. Tony North and his group at the University of Leeds. Though one of the pioneers in creating molecular graphics hardware and software, especially the two-color 3-D illustrations in the proceedings, Prof. North subsequently was denied proper recognition for his pioneering accomplishments in computer graphics. A reviewer of one of numerous unfunded research proposals over the last 20 years remarked how a pioneer on the frontier had to be more concerned about "arrows in the back".
(44) Myopic advice initially caused a switch to monochromatic CRT displays for the CRYSNET system but color raster graphics ultimately prevailed: lower cost, greater availability, and the anti-aliasing algorithm were contributing factors to its superiority. Initial computer memory limitations permitted use of only two of the three primary color output of television technology. Likewise, the size of the displayed model was limited—but the technology introduced by the BRAD system ultimately proved superior to then-prevalent monochromatic displays and set the standard now fully developed in the graphics workstation and lap top computers.
(45) Why, then, did CRYSNET not survive? The simple answer is lack of sustaining funding. Ironically, the same year that CRYSNET expired because it was judged "pedestrian" by a review panel of "experts", the first paper was published describing software (program FIT[4,31]) for modeling structure into electron density in the protein (S. nuclease) here at Texas A&M. The following year, Jim Hogle accomplished the Herculean task of using program FIT to model two molecules into the asymmetric unit of monoclinic lysozyme, in a month's time, working all night, every night, on a single-user PDP-11 system with monochromatic graphics. This break-through for protein crystallography was just the opposite of "pedestrian". Also, the untimely death of Dr. Walter Hamilton in 1972 at age 41 surely deprived this novel effort of his leadership. More complex was the lack of enthusiasm within the crystallographic community. Successful crystallographers in the 1970s had made workable arrangements with their institutional computing centers and had little incentive to change.
(46) Cf. http://www.pdb.bnl.gov/pdb-bin/pdbmain, http://expasy.hcuge.ch/sprot/sprot-top.html, and http://biology.ncsa.uiuc.edu/.
(47) Productive academic and research scientists in the 1970s and 1980s generally resisted networking; they tended to look on computers as a necessary tool and were generally reluctant to make the transition from a batch processing central computer to the laboratory minicomputer (*e.g.*, VAX) and saw little need to network. Without sustaining funding, networks could not survive. ARPAnet is the significant exception, as one traces its trajectory to Internet, the worldwide-Web, JAVA, and future supersystems.
(48) Molecular graphics was and is a small component of the workstation market. We should not forget the sustaining interest of Dr. David Evans (†1998) and the technically superior graphics hardware of Evans & Sutherland. Likewise, the introduction of low-end graphics workstations within the budget of a larger number of investigators helped expand the technology to the user community. Currently, the emergence of facile graphics capabilities of MacIntosh and PC platforms makes quality graphics more affordable to those fated to live on monthly incomes. What impact will the advent of digital television have? Do we march in front of the elephant or behind?
(49) This has both figurative and literal significance. While visual input is essential, our spatial perceptions are sometimes better served by manipulating hand-held molecular models.

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