

1. HISTORICAL INTRODUCTION

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?BAWGEL
#ADATE 820705
#COMPND bis(Benzene)-chromium bromide
#FORMUL C12 H12 Cr1 1+,Br1 1-
#AUTHOR A.L.Spek,A.J.M.Duisenberg
#JRNL 189,10,1531,1981
#CREP msdb 14.74.003 nbsid 532193 batch 53 cdvol 6
#CLASS 1/74
#SYSCAT sys 0 cat 3
#CONN El= Cr 2 Br 14 V= 1 2 Ch= + 2 Ch= - 14
Res= Plot= 1 B= 5 1-3 1-4 3-6 4-7 5-8 5-9 6-10 7-10 8-11 9-12 11-13 12-13
B= 9 1 2-5
Res= Plot= 1 14
#DIAGRAM
  469 151 374 202 469 248 554 103 272 248 556 299
  640 152 186 296 272 151 640 250 101 247 185 100
  100 149 100 50 0 0 0 0 0 0 0 0
#CELL a 9.753(6) b 9.316(3) c 11.941(8) z 4 cent 1 sg Fmmm
#SYMM x,y,z
x,1/2+y,1/2+z
1/2+x,y,1/2+z
1/2+x,1/2+y,z
-x,y,z
-x,1/2+y,1/2+z
1/2-x,y,1/2+z
1/2-x,1/2+y,z
x,-y,z
x,1/2-y,1/2+z
1/2+x,-y,1/2+z
1/2+x,1/2-y,z
-x,-y,z
-x,1/2-y,1/2+z
1/2-x,-y,1/2+z
1/2-x,1/2-y,z
#DENSITY dx 1.764
#UNIS int 3 sigcc 3
#RFACT R= 0.0540.
#RADIUS C 0.68 H 0.23 Br 1.21 Cr 1.35
#TOLER 0.40
#ATOM Cr1 0.0 0.0 0.0
Br1 0.0 0.0 0.50000
C1 0.06900 0.12800 0.13400
C2 0.13900 0.0 0.13400
H1 0.09300 0.20400 0.12500
H2 0.19800 0.0 0.13000
#BOND Cr1 C1 2.100
Cr1 C2 2.090
C1 C1* 1.340
C1 C2 1.370
C1 H1 0.760
C2 H2 0.580
#MDATE 901205
#END

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Fig. 1.1.3.2. An example of a CSD BCCAB format file.

1.1.5. The impact of networking on crystallography

The growth in power of individual minicomputers inevitably helped the development of computational techniques in crystallography. Yet perhaps a more profound development was networking – the ability to exchange electronic data directly between computers. The laborious procedures for transferring information by manual keystroke or exchange of card decks and magnetic tapes were replaced by error-free programmatic procedures. Initially, data could flow easily between computers in the same laboratory; then colleagues could exchange data between scientific departments on the same campus; and before long experimental results, programs and general communications were flowing freely across national and international networks.

During the 1960s, networking was *ad hoc* and proprietary, and rarely extended effectively outside the laboratory. By the 1970s, however, a few standard networking protocols were becoming established. These included uucp, which promoted the growth of dial-up networking between university campuses, and TCP/IP, the transport protocol underlying the ARPANET, that would eventually give rise to the dominant Internet with which we are familiar today. The potential for improving the practice of crystallography through the ease of communications afforded by computer networks was very clear. However, the technology was still costly and required much effort and expertise to implement. Even towards the end of the decade, a meeting of protein crystallographers concluded (Freer & Stewart, 1979) that

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TITLE 00001
*p6122 CIFIO 05-Mar87 p6122 00002
00003
SG NAME 00004
LATT NP 00005
SYST HEXAGONAL 00006
BRAV HEXAGONAL 00007
HALL p_61_2_(0_0_-1) 00008
HERM p_61_2_2 00009
*EOS 00010
00011
SYMMETRY R11 2 3 T1 R21 2 3 T2 R31 2 3 T3 00012
SYOP 1 0 0 .0000000 0 1 0 .0000000 0 0 1 .0000000 1 00013
SYOP -1 0 0 .0000000 0 -1 0 .0000000 0 0 1 .5000000 2 00014
SYOP 0 -1 0 .0000000 -1 0 0 .0000000 0 0 -1 .8333330 3 00015
SYOP 0 1 0 .0000000 1 0 0 .0000000 0 0 -1 .3333330 4 00016
SYOP -1 -1 0 .0000000 0 -1 0 .0000000 0 0 -1 .0000000 5 00017
SYOP -1 1 0 .0000000 0 1 0 .0000000 0 0 -1 .5000000 6 00018
SYOP 1 0 0 .0000000 -1 1 0 .0000000 0 0 -1 .1666670 7 00019
SYOP -1 0 0 .0000000 -1 1 0 .0000000 0 0 -1 .6666670 8 00020
SYOP 0 -1 0 .0000000 1 -1 0 .0000000 0 0 1 .3333330 9 00021
SYOP 0 1 0 .0000000 -1 1 0 .0000000 0 0 1 .8333330 10 00022
SYOP -1 -1 0 .0000000 1 0 0 .0000000 0 0 1 .1666670 11 00023
SYOP -1 1 0 .0000000 -1 0 0 .0000000 0 0 1 .6666670 12 00024
*EOS 00025
00026
FORMULA EL NUM 00036
FORL s .50000o .50000c 1.0000 00037
*EOS 00038
00039
CONDITIONS 00040
CELLPAREX .7107 566.00 00041
INT PAREX .7107 566.00 .147 .681 92 00042
HKL PARE 0 2 0 4 0 12 00043
EQUIV PARE 92 525 00044
*EOS 00045
00046
ATOMS NAME X U11 Y U22 Z U33 U U12 P U13 U23 MUL AT DT 00052
UALL .03500 00053
ATCO s .20140 .79860 .91667 1.00000 6 s 200054
ATCE s .00040 .00040 .00000 .00000 00055
UIJ s .04100 .04100 .01000 .02500 -.00400 -.00400 00056
UIJE s .00800 .00800 .00700 .00700 .00500 .00500 00057
ATCO o .50100 .50100 .66667 1.00000 6 o 200058
ATCE o .00300 .00300 .00000 .00000 00059
UIJ o .08900 .08900 .09000 .06300 .00900 -.00900 00060
UIJE o .01800 .01800 .02000 .01900 .00800 .00800 00061
ATCO c 1 .49200 .09700 .03780 1.00000 12 c 200062
ATCE c 1 .00300 .00300 .00110 .00000 00063
UIJ c 1 .03170 .03170 .03170 .01585 .00000 .00000 00064
UIJE c 1 .00000 .00000 .00000 .00000 .00000 .00000 00065
*EOS 00066
00067
CELL DIMENSIONS A B C ALPHA BETA GAMMA Z 00068
CELLPARE 8.5300 8.5300 20.3700 90.0000 90.0000 120.0000 12.000069
ERRSPARE .0100 .0100 .0100 .0100 .0100 .0100 00070
VOL PARE 1283.571 3.0775 .5595 00071
PHYS PARE 566.0000 00072
*EOS 00073
00074
END 00081

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Fig. 1.1.4.1. An abbreviated example of a Standard Crystallographic File Structure (SCFS) format file.

The possibility and usefulness of establishing a computer network for communication among crystallographic laboratories was discussed. The implications for rapid updating and the ease with which programs and data could be transferred among the groups was clearly recognized by all present; however, immediate implementation of a network was not deemed practical by a majority of the participants.

By the mid-1980s, the establishment of a global computer network was well under way. There was still some diversity of transmission protocols on an international scale: uucp, BITNET and X.25 Coloured Book protocols were still competing with TCP/IP, so that communication between different networks had to be managed through gateways. Nevertheless, there was sufficient standardization that it was feasible to communicate with colleagues world-wide by e-mail, to transfer files by ftp and to log in to remote computers by telnet. E-mail, in particular, allowed for the rapid transmission of ASCII text in an arbitrary format. In many respects, this established a goal for other exchange formats to achieve. The establishment of anonymous ftp sites permitted the free exchange of software and data to any user; no special privileges on the host computer were needed. Such availability of electronic information fitted particularly well with the scientific ethic of open exchange of information.