Chapter 9.2

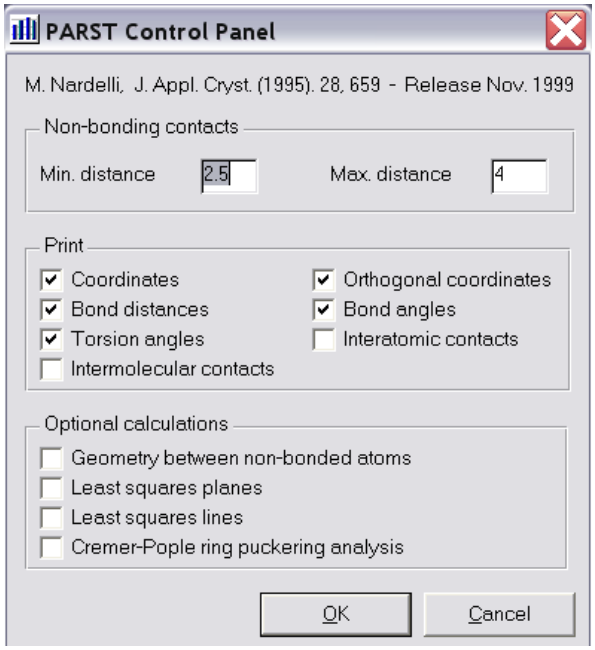
PARST

(the late) MARIO NARDELLI
DIPARTIMENTO DI CHIMICA GENERALE ED INORGANICA,
CHIMICA FISICA E CHIMICA ANALITICA
DELLA UNIVERSITA' DEGLI STUDI DI PARMA, ITALY

PARST is a system of computer routines for calculating molecular parameters from the results of crystal structure analyses. Published in: *Computer and Chemistry*, (1983), **7**, 95-98 and: *J. Appl. Cryst*. (1995). **28**, 659.

The program calculates: Niggli's reduced cell, orthogonal co-ordinates, principal axes of thermal ellipsoids, bond lengths (uncorrected and corrected for thermal motion), angles, torsions, planes, straight lines, angles formed by planes and lines, puckering and displacement asymmetry parameters of rings, spherical polar co-ordinates for stereographic projections, intramolecular and inter-molecular contacts, possible hydrogen bonds, coordinates of hydrogens in typical groups, for a given set of atoms. The s.u.'s for all these magnitudes are calculated. Comparison of the coordinates of pairs of subsets of atoms is also considered to check for lost symmetries.

The input file for PARST (*PARST.INPUT)* is created automatically by WinGX from information in the SHELXL.LST file. If this file is absent (and no file *PARST.INPUT* exists), then PARST cannot be run. The GUI shown below allows the user to customise this file, and it is also possible to run PARST from a pre-existing or edited version of *PARST.INPUT*.



9.3.1 PARST input file format

In order for users to edit the instruction file, the details of the input-file format are given below. NOTE that, in part, this file is a FORMATTED file and that the column entries may be important.

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1.Title card: TITLE (80A1)
2.Space group card: symbol of the space group (80A1)
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It is important that the character in column 1 is the symbol of the Bravais
lattice.
N.B.- Rombohedral lattices must be indicated as P when a rombohedral cell
is chosen, as R when the cell is hexagonal (obverse cell: -h+k+l = 3n )
3.Control card (free format):
N,D3,DM,NH1,NTN,LSP,LSL,NPR,NST,KL,KY,KC,KO,KB,KA,KT,KD,KE,KOR,NI
     N=Total number of atoms (max. 500)
     D3=Minimum distance for non-bonding intramol. contacts (dummy)
     DM=Maximum distance for non-bonding contacts
     NH1=Number of groups of hydrogen atoms whose coordinates must
         be calculated (max. number of H-atoms: 500-N)
     NTN=Number of torsion angles formed by non-bonded atoms
     LSP=Number of planes (max. 50)
     LSL=Number of lines (max. 50)
     NPR=Number of rings (max. 50)
     NST=Number of stereographic sets
     KL=Code for the format of the atomic parameters
     KY=0 no crystal data (cards 4 and 5 must not be given)
       =1 crystal data are printed
     KC=0 no coordinates,          =1 coordinates are printed
     KO=0 no orthog. coord.,       =1 orthog. coord. are printed
     KB=0 no bond distances,       =1 bond distances are printed
     KB=-1 only bond distances not involving hydrogens are printed
     KA=0 no angles,               =1 angles are printed
     KA=-1 only bond angles not involving hydrogens are printed
     KT=0 no torsions,             =1 torsion angles are calculated
     KT=-1 only torsion angles not involving hydrogens are printed
     KD=0 no interatomic contacts, =1 interatomic contacts are calc.
     KD=-1 only intra-contacts not involving hydrogens are printed
     KE=0 no intermolecular contacts, =1 intermolecular contacts
          less than DM and possible hydrogen bonds are calculated
     KE=-1 only inter-contacts not involving hydrogens are printed
     KOR=0  no thermal parameters in the input
     KOR=1, beta: exp[-(beta11*h**2+...+2*beta12*h*k+...)]
     KOR=2, U: exp[-2*pi**2(U11*h**2*(a*)**2+...+2*U12*h*k*
                                                (a*)*(b*)+...)]
     KOR=3, B: exp[-0.25*(B11*h**2*(a*)**2+...+2*B12*h*k*
                                                (a*)*(b*)+...)]
     KOR=4, b: exp[-(b11*h**2+...+b12*h*k+...)]
     KOR=5, U*:exp[-2*pi**2(U11*h**2*(a*)**2+...+2*U12*h*k*
                                     (a*)*(b*)*cos(gamma*)+...)]
     KOR=6, B*: exp[-0.25*(B11*h**2*(a*)**2+...+2*B12*h*k*
                                     (a*)*(b*)*cos(gamma*)+...)]
     KOR=7, anisotropic thermal parameters given in the input, but
            not processed and printed

 N.B.-If there are isotropic atoms together with anisotropic ones,
     the thermal parameter for them is given as U11 (or B11, etc.)
     and zeros must be given for U22, U33, U12, U13, U23

     NI=Number of pairs of subset of atoms whose coordinates are to
     be compared.
     If NI is negative only research of missing symmetries is
     carried out.
4.Data card (free format): NNS,Z,AL
     NNS=Number of atomic species in the chemical formula
     Z  =Number of molecules in the unit cell
     AL =Wavelength (Cu or Mo K-alpha)
5.Formula card (free format): symbols of the atoms, within apices,
     followed by their numbers
6.Parameter card (free format): a,b,c,sigma(a),sigma(b),sigma(c),
     alpha,beta,gamma,sigma(alpha),sigma(beta),sigma(gamma)
7.Coordinate format card: Format of the coordinate cards (80A1);
   this card is not given if KL=4
8.Coordinate cards (thermal parameters are given only if KOR is
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   not equal to zero)
     If KL=1: ATOM(6A1),X,Y,Z,S(X),S(Y),S(Z),B11,B22,B33,B23,B13,
              B12,S(B11),S(B22),S(B33),S(B23),S(B13),S(B12)
     If KL=2: ATOM(6A1),X,Y,Z,B11,B22,B33,B23,B13,B12,S(X),S(Y),
              S(Z),S(B11),S(B22),S(B33),S(B23),S(B13),S(B12)
     If KL=3: ATOM(6A1),X,S(X),Y,S(Y),Z,S(Z),B11,S(B11),B22,S(B22),
              B33,S(B33),B23,S(B23),B13,S(B13),B12,S(B12)
     If KL=4: FORMAT UNIMOL (7X,6A1,2X,3F8.5,12X,3(5A1,3X))
              KOR must be 0
   N.B.- When KY=0, i.e. the formula card is not given, the second
         character of the atomic labels cannot be alphabetic when
         the chemical simbol requires only one character (e.g.: H,
         B, C, N, O, F, O, S,... ).
         When KY=1, i.e. the formula card is given, there is no
         restriction for the second character of the labels of these
         atoms.
9.Cards for hydrogens in calculated positions: KDG,D,SB
   (these cards mustn't be given if NH1=0)
     If KDG=1,(methyl):SB=ATOM1,ATOM2,ATOM3 (I1,1X,F6.4,3(6A1))
        ATOM1 is bonded to hydrogens and to ATOM2; ATOM2 is bonded
        to ATOM1 and to ATOM3
     If KDG=2,(methylene): as for methyl, ATOM2 and ATOM3 are bonded
        to ATOM1
     If KDG=3,(tert-C):SB=ATOM1,ATOM2,ATOM3,ATOM4 (I1,1X,F6.4,4(6A1)
        ATOM1 is bonded to hydrogen,ATOM2,ATOM3,ATOM4
     If KDG=4 (benzene): as for methylene
     If KDG=5 (alkyne): SB=ATOM1,ATOM2 (I1,1X,F6.4,2(6A1))
        ATOM1 is bonded to hydrogen and to ATOM2
     If KDG=6 (ethylenic system): as for tert-C; ATOM1 is bonded to
        two hydrogens and to ATOM2 which is planarly bonded to ATOM1
        ATOM3 and ATOM4
   N.B.- If KOR is not equal to zero, an isotropic thermal parameter
         is assigned equal to the arithmetic mean of the anisotropic
         parameters of the atom the hydrogen is attached to
     D = ATOM1-H distance (F6.4)
     SB= Labels of the non-hydrogen atoms
10.Cards for torsion angles formed by non-bonded atoms:
     ATOM1,ATOM2,ATOM3,ATOM4  (FORMAT (4(6A1))
11.Cards for LSQ-planes: NT,NFP,names of the atoms
     FORMAT (2I2,4X,12(6A1)/(12(6A1)))
     NT=Total number of atoms (max 40)
     NFP=Number of the atoms not defining the plane
12.Cards for LQ-lines: NT,NFP,names of the atoms
     FORMAT (2I2,4X,12(6A1)/(12(6A1)))
     NT=Total number of atoms (max 40)
     NFP=Number of the atoms not defining the line
13.Cards for puckered rings: NP,Names of the atoms in the right
   sequence
     FORMAT (I2,6X,12(6A1)/(12(6A1)))
     NP=Number of the atoms of the ring (max 40)
14.Cards for stereographic projections: KO,NP,NQ,names of the atoms
   in the right sequence
     FORMAT(I1,2I2,3X,12(6A1)/(12(6A1)))
     KO=1,origin at 1st atom,Z axis along ATOM1-ATOM2
     KO=2,origin at 1st atom,Z axis perpendicular to the mean plane
          through the first NQ atoms, excepting ATOM1
     KO=3,origin at the center of the first NQ atoms, Z axis perpen-
          dicular to the plane through them
     NP=Total number of atoms (max 40)
     NQ=Number of the atoms defining the projection plane inclusive
     of first atom
15.Data for intermolecular contacts (always given ): IC,NE,NT
   (Free FORMAT)
     IC=1 if the space group is acentric
       =-1 if the space group is centric
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     NE=Number of the equivalent positions (the general, X Y Z, and
        the centrosymmetric ones must be omitted)
     NT=Maximum translation required (suggested 1 when the set of
        atoms in the general position is the nearest to the origin,
        2 in the other cases)
16.Equivalent position cards: one equivalent position per card
   (38A1). Examples: 1/2-X,1/2+Y,1/2+Z
                     Y-X,-X,1/3+Z
17.Card with the total number of atoms whose coordinates are com-
   pared (free FORMAT).
18.Cards with the labels of the atoms whose coordinates are compared
   (12(6A1)). First the atoms of the first subset, then the atoms
   of the second subset exactly in the same sequence.
   Of course card 17 and cards 18 are not given if NI=0.
```

9.3.2 The output file PARST.LST

All output is directed to this file and this file is displayed after the program has run A sample output listing (edited to shorten) from a default run is shown below:

```
Ru3(CO)12   RT data collection 23/1/96   PSI-SCANS
 P

 Crystal data
 a =   8.1028(0.0006)                          alpha=  90.00(0.00)
 b =  14.8436(0.0010)                          beta = 100.65(0.00)
 c =  14.5820(0.0006)                          gamma=  90.00(0.00)
 V =   1723.64( 0.19)  cubic-Angstrom


 Niggli reduced cell:   8.103 14.582 14.844  90.00  90.00 100.65
 Niggli matrix:        65.6554    212.6347    220.3325
                        0.0000      0.0000    -21.8361
 Transformation matrix:     1.00    0.00    0.00
                            0.00    0.00    1.00
                            0.00    1.00    0.00

 Ru  3. O  12. C  12.
 M       =   639.335          (Atomic weights 1977)
 Z       =     4.00
 D(calc.)=     2.4637         Mg/m**3
 F(000)  =  1200.0
 mu      =    26.567          cm**-1 (Int.Tab. Vol.C, Table 4.2.4.2, p.193)
 Lambda  =     0.7107300      Angstrom

 Number of atoms:     27

 Atomic coordinates
 Atom              X/a                 Y/b                 Z/c
 Ru1          0.80601(    3)      0.08051(    1)      0.66201(    1)
 Ru2          1.05754(    3)     -0.02304(    1)      0.77685(    1)
 Ru3          1.05785(    3)      0.16818(    1)      0.79292(    2)
 O11          1.01745(   28)      0.10614(   17)      0.51109(   15)
.
 C33          1.25010(   40)      0.18207(   23)      0.89144(   23)
 C34          0.91222(   38)      0.16032(   20)      0.88458(   21)

 Orthogonal coordinates (Angstrom)
 Orthogonalization matrix:
 a  b cosgamma        c cosbeta         8.10280   0.00000  -2.69489
 0  b singamma  -c sinbeta cosalpha*    0.00000  14.84360   0.00000
 0       0       c sinbeta sinalpha*   0.00000   0.00000  14.33082

 Atom              X                   Y                   Z
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 Ru1          4.7469(0.0002)      1.1951(0.0002)      9.4871(0.0001)
 Ru2          6.4755(0.0002)     -0.3420(0.0002)     11.1329(0.0001)
 Ru3          6.4347(0.0003)      2.4964(0.0002)     11.3632(0.0003)
 O11          6.8669(0.0023)      1.5755(0.0025)      7.3243(0.0021)
.
 C33          7.7270(0.0033)      2.7026(0.0034)     12.7751(0.0033)
 C34          5.0077(0.0031)      2.3797(0.0030)     12.6768(0.0030)

 Displacement parameters, U(I,J)x10**4
 exp(-2*pi**2(U11*h**2*(a*)**2+...+2*U12*h*k*(a*)*(b*)+...)
 Atom    U11        U22        U33        U23        U13        U12
 Ru1     259(   1)  325(   1)  283(   1)    1(   1)   17(   1)   13(   1)
 Ru2     305(   1)  312(   1)  307(   1)   22(   1)   34(   1)   38(   1)
 Ru3     308(   1)  314(   1)  354(   1)  -46(   1)   43(   1)  -43(   1)
 O11     500(  13)  659(  15)  423(  12)    4(  11)  188(  11)   -5(  12)
.
 C33     414(  17)  520(  19)  474(  18)  -88(  15)   76(  15)  -75(  14)
 C34     402(  16)  397(  16)  396(  16)  -73(  12)   31(  13) -105(  12)

 Principal axes of the thermal ellipsoids, Uequiv. (x10**4 A**2) and
 Bequiv.(A**2)
 Atom      R1         R2         R3        Uequiv.     Bequiv.  Rmax/Rmin
 Ru1     330(   2)  310(   2)  239(   1)  293(   1)  2.31(0.01)   1.38
 Ru2     348(   3)  328(   3)  258(   1)  311(   1)  2.46(0.01)   1.35
.
 C33     598(  20)  451(  23)  361(  18)  470(  11)  3.71(0.09)   1.65
 C34     506(  16)  444(  21)  262(  16)  404(  10)  3.19(0.08)   1.93

 Bond distances (Angstrom)
 (Corrections following Busing & Levy, Acta Cryst.(1964).17,142)
                 uncorrected    lower    upper    riding  non-correlated
                  distance      bound    bound    motion     motion
 Ru1    - Ru2    2.8389(   3)   2.8389   2.8846   2.8398     2.8617
 Ru1    - Ru3    2.8393(   3)   2.8394   2.8860   2.8412     2.8627
.
 O33    - C33    1.1208(  38)   1.1275   1.3750   1.1620     1.2512
 O34    - C34    1.1254(  43)   1.1290   1.3086   1.1512     1.2188
 Number of bond distances:     27


 Bond angles (deg)
 (s.u. following Cruickshank, Internat. Tables, II, 1959, p.331)
                                  Angle      s.u.
 Ru2   - Ru1   - Ru3              60.21      0.01
 Ru2   - Ru1   - C11              90.61      0.09
 Ru2   - Ru1   - C12             160.34      0.09
.
 Ru3   - C32   - O32             178.96      0.29
 Ru3   - C33   - O33             179.04      0.30
 Ru3   - C34   - O34             173.26      0.28
 Number of angles:     57

 Torsion angles (deg)
 (right-hand rule, Klyne & Prelog.(1960). Experientia,16,521)
 (s.u. following Stanford & Waser, Acta Cryst.(1972).A28,213)
                                    Angle      s.u.
 Ru3   -Ru1   -Ru2   -C21           -89.97     0.09
 Ru3   -Ru1   -Ru2   -C22            -0.86     0.28
C11   -Ru1   -Ru2   -Ru3            87.12     0.09
.
 C31   -Ru3   -C34   -O34           178.07    16.27
 C32   -Ru3   -C34   -O34           -49.03     2.36
 C33   -Ru3   -C34   -O34            55.92     2.36
 Number of torsion angles:    132
```