The puckering program package consists of the following programs:

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ring.f90                  ! MAIN PROGRAM
!**************************************************************************
! Puckering and planar deformations of rings
! Version January 2011
!**************************************************************************

PROGRAM ring

!     ****                                                    ****
!     ****                PROGRAM RING *2011*                 ****
!     ****                  WRITTEN BY                        ****
!     ****                 DIETER CREMER                      ****
!     ****                 DMITRY IZOTOV                      ****
!     ****                 ELFI KRAKA                         ****
!     ****                                                    ****
!     ****   *RING* CALCULATES THE MEAN PLANE (MP),           ****
!     ****   THE RING PUCKERING COORDINATES,                  ****
!     ****   THE RING DEFORMATION COORDINATES,                ****
!     ****   AND THE SUBSTITUENT POSITIONS OF A GENERAL       ****
!     ****   N-MEMBERED RING.  IN ADDITION, *RING* CALCULATES ****
!     ****   THE LEAST-SQUARES PLANE (LSP) BY AN ITERATIVE    ****
!     ****   ALGORITHM AND PROVIDES INFORMATION ABOUT THE     ****
!     ****   DEVIATION OF THE LSP FROM THE MP                 ****
!     ****                                                    ****
!     ****   REFERENCES:                                      ****
!     ****                                                    ****
!     ****   D.CREMER AND J.A.POPLE,                          ****
!     ****  "A GENERAL DEFINITION OF RING PUCKERING COORDINATES"****
!     ****   J.AMER.CHEM.SOC.,97,1358,(1975)                  ****
!     ****                                                    ****
!     ****   D.CREMER ,                                       ****
!     ****   "A GENERAL DEFINITION OF RING SUBSTITUENT POSITIONS",
!     ****   ISRAEL J.CHEM.,20,12,(1980)                      ****
!     ****                                                    ****
!     ****   H.ESSEN AND D. CREMER,                           ****
!     ****   "ON THE RELATIONSHIP BETWEEN THE MEAN PLANE AND THE****
!     ****   LEAST-SQUARES PLANE OF AN N-MEMBERED RING ",     ****
!     ****   ACTA CRYST., B40, 418, (1984)                    ****
!     ****                                                    ****
!     ****    D.CREMER,                                        ****
!     ****   "ON THE CORRECT USAGE OF THE CREMER-POPLE        ****
!     ****    PUCKERING PARAMETERS AS QUANTITATIVE DESCRIPTORS ****
!     ****    OF RING SHAPES",                                ****
!     ****   ACTA CRYST., B40, 498 , (1984)                   ****
!     ****                                                    ****
!     ****    W. ZOU, D. IZOTOV, D.CREMER,                    ****
!     ****   "DESCRIPTION OF RING DEFORMATIONS BY A NEW SET   ****
!     ****    OF COORDINATES"                                 ****
!     ****   TO BE PUBLISHED                                  ****
!     ****                                                    ****
!     ****                                                    ****
!     ****   CATCO GROUP                                      ****
!     ****   SOUTHERN METHODIST UNIVERSITY, DALLAS, TX        ****
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!     ****   http://smu.edu/catco/index.html                  ****
!     ****                                                    ****
!     ****   REVISED VERSION A, D. CREMER, DECEMBER 1974      ****
!     ****                                                    ****
!     ****   REVISED VERSION B, D. CREMER, DECEMBER 1988      ****
!     ****                                                    ****
!     ****   REVISED VERSION C, D. IZOTOV, E. KRAKA,          ****
!     ****                  AND D. CREMER, JANUARY 2011       ****
!     ****                                                    ****
!
!**********************************************************************
!
!     PROGRAM DESCIPTION
!
!     (Note that input is in free format (*)  except TITLE)
!
!     0) Print control
!        READ(IN,*) IPRINT
!
!           IPRINT = 0     short version of output
!                          (excluding B-matrix information) is written onto file output.dat
!           IPRINT = 1     long version of output with complete B-matrix information is
!                          written onto file output.dat
!           IPRINT = 2     puckering information is written onto file output.dat and B-
!                          matrix information is written
!                          onto file matrices.dat
!
!
!     1) Title:
!        READ(IN,1020) TITLE
!   1020 FORMAT(A80)
!
!     2) Control line (free format)
!        READ(IN,*) N,ICELL,ISUB,KORD,IXYZ
!
!        N           Number of ring atoms
!        ICELL = 0   Cartesin coordintes are read in
!              = 1   cell coordinates are red in
!        ISUB  = 1   in addition substituent coordinates are read in
!                    (Cartesian or cell coordinates)
!
!        KOORD = 0   Order of atoms read has to be clockwise with the ring atom with
!                    highest atomic number z being atom one.
!                    If ring atoms are equivalent the degree of substituion is desisive.
!                    If this does not lead to a good choice
!                    for ring atom 1 the puckering coordinates can be calculated and after
!                    knowing the phase angle a suitable choice can be made.
!                    Around the ring starting with the atom of Kahn-Prelog rules
!                    (non-clockwise ordering leads to wrong puckering/deformation
!                    parameters; and deviation from Kahn-Prelog causes a shift in
!                    the phase angles
!        KORD  = 1   re-ordering of ring atoms
!        IXYZ        determines the input format of the coordinates
!              = 0   just x,y,z
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```
!              = 1   Gaussian94 output, 2 integers and x,y,z
!              = 2   Gaussian98 output, 3 integers and x,y,z
!              = 3   x,y,z coordinates with numbering

!     2a)   For ICELL=1, input of unit cell parameters a, b, c, alpha, beta, yamma
!           READ(IN,*) (CELL(I),I=1,6)

!     2b)  For NSUB = 1, number of substituents located at each
!                        ring atom is read in
!           READ(IN,*) (NSUB(I),I=1,N)

!     2c)   For KOORD = 1,  new numbering of the ring atoms clockwise around the ring is
!           given
!           READ(IN,*) (IORD(I),I=1,N)

!     3)    Input of ring (and substituent) coordinates
!           in a format determined by IXYZ (see above)
!           if (ixyz.eq.0) read(IN,*) (X(I,J),J=1,3)
!           if (ixyz.eq.1) read(IN,*) IDD1,IDD2, (X(I,J),J=1,3)
!           if (ixyz.eq.2) read(IN,*) IDD1,IDD2,IDD3, (X(I,J),J=1,3)
!           if (ixyz.eq.3) read(IN,*) IDD1, (X(I,J),J=1,3)
!
!      If there is another molecule to be analysed, go back to 1) otherwise end the job
!       with a line
!
!      4)   READ(IN,1020) TITLE
!           with TITLE equals EOF
!
!
!*************************************************************************
!
!    COMPILATION
!    For the compilation of the program use the makefile enclosed and the following
!    two commands
!
!   csh
!   make ring
!
!   (If new subroutines are added the makefile has to be changed accordingly)
!
! ************************************************************************
!
!   EXECUTION OF PROGRAM
!   To run the program, prepare an input file called input.dat according to
!   the description given above and use the command
!
!   ./ring
!
!   A set of input examples covering the various program options can be found on in the
file
!   input_examples.dat. The corresponding output files are contained in
!   output_examples.dat and matrices_examples.dat.
!
! ************************************************************************
!
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```
!   INPUT EXAMPLE
!
!     0
!     Pyranoid ring of sucrose, neutron diffraction data + substituents
!     6  1  2  1  0
!   10.8633  8.7050  7.7585  90.  102.945  90.
!     1  1  2  0  2  0
!     4  5  6  1  2  3
!     0.2854   0.6367   0.5645
!     0.3740   0.6709   0.4420
!     0.3592   0.5511   0.2953
!     0.3772   0.3988   0.3686
!     0.2996   0.3579   0.4849
!     0.3125   0.4747   0.6360
!     0.1714   0.3463   0.39165
!     0.3347   0.2451   0.5388
!     0.3080   0.7477   0.7028
!     0.3488   0.8141   0.3563
!     0.4575   0.5708   0.1855
!     0.2638   0.5613   0.2093
!
! ***************************************************************************
!
!       DEFINING THE NUMBERING OF RING ATOMS
!
!       The pseudorotation phase angles of the puckering and / or the deformation
!
!       coordinates depend on the numbering of the ring atoms. Accordingly, it is
!       desirable to apply a set of rules that make it possible to obtain
!       comparable phase angles.
!
!       1) Ring atoms can be ordered according to their atomic numbers, their
!       degree of substitution, their position on a symmetry element (rotational
!       axis or mirror plane), and their out-of-plane deviation:
!
!       a) If their ring atoms with different atomic numbers that with the highest
!       atomic number should be atom #1.
!
!       b) If, after applying rule a) there is a still a choice between different
!       ring atoms that ring atom should be #1, which has the largest number of
!       substituent bonds or the highest substituents.
!
!       c) In cases of symmetry, it is sometimes more attractive to take atom #1 as
!       the atom located on a symmetry element. Example 1,3-dioxilane: Two O atoms
!       are located in the ring that could be taken as atom #1. In the envelope or
!       twist forms of the ring, the C atom between the O atoms can be located in a
!       mirror plane or on a C_2 axis.
!
!       2) Atom 1 must be positioned in the 9-o'clock location of a coordinate
!       system, i.e. on the -x axis.
!
!       3) Puckered rings have two faces, a top and a bottom face. Apart from
!       defining atom #1, one has to define the top face of the ring. This is the
!       one with the higher ranking substituents.
!
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!       4) The ring atoms are numbered by looking from the top onto the ring and
!       numbering the atoms in sequence clockwise around the ring starting with
!       atom #1.
!
!       5) Any deviation from rules 1), 2), 3) leads to a change in the phase
!       angles, which are shifted by a given value that can be directly calculated
!       from  N, the size of the ring, and the number of places atom 1 is shifted
!       clockwise around the ring.
!
!
!       Examples:
!
!       a) Cyclopentane, envelope form: The atom at the apex of the ring has to be
!       #1 and must stand up. Its positive out-of-plane deviation determines the
!       top-face of the ring.
!
!
!       Note: If the Cartesian coordinates of the ring atoms are not ordered
!       according to the above rules, they can be reordered utilizing the reorder-
!       command.
!

*************************************************************************
 adds.f90             contains a set of service subroutines from the original
                      f77 version

!Deck TRANSF
      SUBROUTINE TRANSF
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
!      ****   SUBROUTINE *TRANSF* TRANSFORMS CELL COORDINATES    ****
!      ****   TO CARTESIAN COORDINATES USING THE CELL DATA A, B, ****
!      ****   C, ALPHA, BETA, GAMMA STORED IN VECTOR CELL OF     ****
!      ****   COMMON/XRAY/                                       ****
!      ****   REFERENCE:                                         ****
!      ****   J.S.ROLLETT, COMPUTING METHODS IN CRISTALLOGRAPHY, ****
!      ****   PERGAMON PRESS, OXFORD (1965)                      ****

!Deck LSPIT
      SUBROUTINE LSPIT
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
!
!      ****  *LSPIT* calculates least-squares plane(LSP) by an   **
!      ****          iterative algorithm described by            ****
!      ****          Esser and Cremer.                           ****

!DECK EULER
      SUBROUTINE EULER(AL,BE,GE,TOLD)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
!
!     Calculate Euler angles alpha, beta, gamma between old and new plane:
!
!     Coordinate system of old plane defined by UM, UN, UL
!     Coordinate system of NEW plane defined by UX, UY, UZ
!     In both cases the geometrical center of the ring is the origin
!
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```
!     alpha: angle between UN and UZ ( 0.LE.AL.LE.Pi)
!     beta : angle in UL,UM-plane from UL to the projection of UZ on the
!            UL,UM-plane ( 0.LE.BE.LE.TWO*Pi)
!     gamma: angle in UX,UY-plane from the positive direction of line of
!            nodes (intersection of UL,UM- and UX,UY-plane) and UY
!            ( 0.LE.GA.LE.TWO*Pi )

!Deck SUBSTI
      SUBROUTINE SUBSTI
      Implicit double precision (a-h,o-z)
!      ****   SUBROUTINE *SUBSTI* CALCULATES THE RELATIVE DIREC- ****
!      ****   TIONS OF SUBSTITUENT AND/OR RING BONDS IN TERMS OF ****
!      ****   POLAR AngleS ALPHA AND BETA                        ****

      END
!Deck OUTPUT
           SUBROUTINE OUTPUT
       IMPLICIT DOUBLE PRECISION (A-H,O-Z)
!      ****   SUBROUTINE *OUTPUT* WRITES THE CALCULATED CARTE-   ****
!      ****   SIAN AND PUCKERING COORDINATES AS WELL AS THE PO-  ****
!      ****   LAR AngleS OF SUBSTITUENT AND RING BONDS           ****

!Deck DISTAN
      SUBROUTINE DISTAN(C,N,NN)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
!      ****   SUBROUTINE *DISTAN* EVALUATES THE DISTANCE MATRIX  ****

      END
!Deck Angle
      SUBROUTINE Angle(R,N)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
!      ****   SUBROUTINE *Angle* CALCULATES AND WRITES THE INTER-****
!      ****   NAL RING AngleS                                    ****

!Deck DIHEDL
      SUBROUTINE DIHEDL(C,N)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
!      ****   SUBROUTINE *DIHEDL* CALCULATES AND WRITES THE DIHE-****
!      ****   DRAL AngleS OF THE RING                            ****

!Deck OUTMATD
      SUBROUTINE OUTMATD(R,N)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
!      ****   SUBROUTINE *OUTMAT* PRINTS THE LOWER TRIAngle OF   ****
!      ****   MATRIX R

!Deck OutMat
      Subroutine OutMat(X,M,N,MM,NN)
      Implicit Real*8(A-H,O-Z)
      COMMON/IO/ IN,IOUT, IOUT1
!
!     Print matrix X.
!

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 checkbmatrpla.f90

! calculates planar deformation B-matrix numerically via finite differences
! the derivatives of Q can be calculated only by right differences,
!   because Q >= 0 !!!

*************************************************************************
 checkbmatrpuck.f90      ! calculates B-matrix numerically
 checkde.f90             ! calculates de, d2e matrices numerically
 checkdr.f90             ! calculates DR-matrix numerically

*************************************************************************
 interfaces.f90          ! defines fortran 90 modeules

*************************************************************************
 planardef.f90

! computes 2d deformational coordinates of a n-member planar ring
! rings are assumed to be numbered clock-wise,  1st atom placed at 9 o'clock
! Please note that the first  t(n),tau(n),omega(n) values to be used are  n=2,
! however, vectors start with n=1
!

*************************************************************************
 puckdef.f90              ! calculates puckering coordinates

*************************************************************************
 readdata.f90             ! reads input data and controls output

*************************************************************************

*************************************************************************
 standorient.f90           ! brings the molecule to the standard orientation

*************************************************************************
 types.f90                 ! defined types

*************************************************************************
 utils.f90                 ! utillities

*************************************************************************
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