```
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
C    STRFIT - GENERAL STRUCTURE FITTING PROGRAM, FITTING EFFECTIVE STRUCTURAL
C             PARAMETERS DEFINED IN THE 'CART' SCHEME TO ANY COMBINATION
C             OF ROTATIONAL CONSTANTS
C
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
C       This program was originally written in 1990 for determination of
C       effective r.0 structures of hydrogen bonded complexes, but it can also
C       be used to fit rz, rm^(1L), rm^(2L), re^(SE) and other geometries.
C
C       Citation and additional information on this program:
C             Z.Kisiel, J. Mol. Spectrosc. 218, 58-67 (2003).
C
C       This STRFIT was written independently of, but seems to embody similar
C       features to Schwendeman's STRFIT.  Once I found this out it was too late
C       to change the name.
C
C       See:  R.H.Schwendeman, "Structural parameters from rotational spectra",
C             in "Critical evaluation of chemical and physical structural
C             information", D.R.Lide and M.A.Paul, Eds., National Academy of
C             Sciences, Washingtom, D.C. (1974).
C
C       For a similar least-squares fitting approach see also:
C
C             P.Nosberger,A.Bauder, and Hs.H.Gunthard, "A versatile method
C             for molecular structure determinations from ground state
C             rotational constants",  Chem.Phys. 1,418-425(1973).
C
C       The basic least-squares engine for fitting r0 internal parameters to
C       ground state moments of inertia can be used to evaluate also:
C
C       1/ r.z, re^SE or any other geometry fitted to moments of inertia
C          modified by user supplied corrective contributions.  For example,
C          in the re^SE geometry (= semi-experimental equilibrium) the Be-B0
C          corrections from a CFOUR anharmonic force field calculation can
C          be used directly.  The much smaller rotational g-tensor contributions
C          can also be used.
C       2/ r.m(1r) and rm(1rL) geometry
C       3/ r.m(2r) and rm(2rL) geometry
C
C       For r.m(1), r.m(2) and their subvariants see:
C
C             J.K.G.Watson, A.Roytburg, W.Ulrich, J.Mol.Spectrosc.
C             196,102-119(1999)
C
C       Reviews dealing (among other topics) with re^SE evaluations:
C             J.Demaison, Molec.Phys. 105,3109-3138(2007)
C             C.Puzzarini et al., Int.Rev.Pjys.Chem. 29,273-367(2010)
C
C       Demonstration of the usefulness of rotational g-tensor corrections
C       in r_e^SE geometry evaluations:
C             A.G.Csaszar,J.Demaison,H.D.Rudolph, "Equilibrium structures of three-
C             four-, five-, six-, and seven-membered unsaturated N-containing
C             heterocycles",  J.Phys.Chem.A 119,1731-1746(2015)
C
C       Declaration scheme of internal structural coordinates
C       (colloquially called CART since it was adapted from a Wilson
C       group program of that name):
C
C             H.R.Thompson, J.Chem.Phys. 47,3407-3410(1967)
C
C
C       Main features of STRFIT:
C
```

```
C     - fit of up to MAXPAR structural parameters to up to MAXCON measured
C       rotational constants in up to MAXISO isotopic species
C
C     - each structural parameter can have up to twenty repetitions in the
C       molecule
C
C     - up to MAXCHG structural parameters can be different between the parent
C       and the substituted species
C
C     - non-linear Levenberg-Marquardt least squares fitting algorithm is used
C       (Numerical Recipes Chapt.14)
C
C     - the fit is to (equally weighted) moments of inertia or planar moments
C       and not to rotational constants, although when rotational constants
C       are to be fitted they are declared conventionally
C
C     - the spectroscopic constants that can be fitted to are A,B,C, B+C,
C       and A+B, and the three planar moments Pa,Pb,Pc (in any combination)
C
C     - the data set for STRFIT is compatible with PMIFST so the latter can
C       be used to check the 'CART' definitions
C
C     - The user only needs to specify the generic name MOLNAM on startup,
C       and the input/output files are then:
C
C         MOLNAM.STF = the input file
C
C         MOLNAM.OUT = the main output file with complete results of the fit
C         MOLNAM.PMI = the abbreviated output file containing at the top
C                      the connectivity declaration of the fitted structure
C                      for viewing with PMIFST
C         MOLNAM.XYZ = the fitted geometry in Cartesians for viewing with packages
C                      such as Chimera, JMol, MacMolPlot...
C
C
C       ver. 8.IV.2020                              ----- Zbigniew KISIEL -----
C                                    _____
C                                   | Institute of Physics, Polish Academy of Sciences |
C                                   | Al.Lotnikow 32/46, Warszawa, POLAND       |
C                                   |                      kisiel@ifpan.edu.pl  |
C                                   |     http://info.ifpan.edu.pl/~kisiel/prospe.htm  |
C_____/--------------------------------------------------
C
C   Modification history:
C
C       1990:  Creation
C   24.06.95:  PARAMETER dimensioning
C   10.12.99:  Fitting of B+C and A+B
C   30.08.00:  Echo of fitted structure to STRFIT.PMI
C    8.01.01:  Various incremental modifications
C    8.04.02:  Fitting also of planar moments
C   19.04.02:  Elimination of bug in writing STRFIT.PMI
C    4.06.02:  rm(1) and rm(2) model + fixed parameters + overhaul
C   29.10.02:  increase in MAXPAR and associated corrections
C   30.01.03:  fitting equal c or d constants
C    8.08.05:  correction of 'final principals' bug spotted by Stew Novick
C   14.11.08:  correction to mass used for d terms, spotted by Jean Demaison
C   25.05.09:  elimination of erroneous temporary code that crept in about 2005
C              in Laurie parameter + improvement of symmetric top performance
C   15.02.10:  allowance also for dB=B*-Bexp input and better input debugging
C   15.12.10:  optional user parameter descriptors and updated input description
C   17.02.12:  uncertainties in principal coordinates
C   12.12.12:  increased dimensioning
C    6.03.13:  allowance for exclusion from fit of some of the declared constants
C    6.05.15:  parameter repetitions with changes
c   22.05.15:  generic i/o file names and addition of .xyz output
```

```
C    8.10.16:   improved diagnostics of errors in the input data file
C   25.07.19:   electronic correction in r_e^SE evaluation + misc. updates
C    8.04.20:   some output and documentation changes
C
C++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++++
C
C    STRFIT DATA FILE STRUCTURE - specimen data file is reproduced below, with
C    lines numbered to facilitate description:
C
C        first column of the data file
C        |                             32nd column of data file (beginning of
C        |                             |      numerical input for all lines
C        |                             |      below the CART deck)
C lno.   |                             |
C  1.    buteneyne...HF, HF at the TRIPLE bond, in the bey plane
C  2.       11     0
C  3.        1  0  0  0      .000000      .000000      .000000     12.000000
C  4.        2  1  0  0     1.208600      .000000      .000000     12.000000
C  5.        3  2  1  0     1.431000   177.900000      .000000     12.000000
C  6.        4  3  2  1     1.341600   123.100000   180.000000     12.000000
C  7.        5  1  2  4     1.062000   182.300000   180.000000      1.007825
C  8.        6  4  3  2     1.087000   121.600000      .000000      1.007825
C  9.        7  4  3  2     1.087000   118.700000   180.000000      1.007825
C 10.        8  3  4  7     1.087000   121.700000     0.000000      1.007825
C 11.        9  2  3  8     0.604300   177.900000      .000000       .000001
C 12.       10  9  2  3     3.080000    90.000000   180.000000     18.998404
C 13.       11 10  9  2     0.925700   360.000000      .000000      1.007825
C 14.    TOTAL NUMBER OF PARAMETERS:     2
C 15.    atom no., parameter no.       10 1 0
C 16.    atom no., parameter no.        9 1 0
C 17.    NO OF CONSTANTS TO FIT TO:     6
C 18.    constant,species,value         1 1 5182.82917
C 19.    constant,species,value         2 1 3312.90406
C 20.    constant,species,value         3 1 2021.475817
C 21.    constant,species,value         1 2 5182.55955
C 22.    constant,species,value         2 2 3271.83826
C 23.    constant,species,value         3 2 2005.91671
C 24.    NO OF CHANGES FROM PARENT SP.:  2
C 25.    atom no.,parameter no.,value   11 4 2.0141022
C 26.    atom no.,parameter no.,value   11 1 -0.0023
C
C
C The various lines are:
C
C     line 1:  descriptive comment (truncated to 78 characters if longer)
C
C-----------------------------------------------------------------------------
C lines 2-13 - block containing the CART definition of the molecular geometry
C-----------------------------------------------------------------------------
C
C     line 2:  The number of atoms in the molecule, read in with format=(I5)
C              Optionally a second number (also in an I5 field) can be included,
C              and if equal to 1 specifies output of debugging information.
C
C    line 3+:  CART DEFINITION LINE:
C              N,NA,NB,NC,R,A,D,W
C
C                 this is read in free format, but N,NA,NB,NC are to be integers, and
C                 R,A,D,W are to be floating point values. There should be as many
C                 such lines as the number of atoms declared in Line 2.
C
C                 The structure of the CART line is defined in a separate set of
C                 comments further below.
C                 CART lines declare either real or dummy atoms, and the use of dummy
C                 atoms is encouraged since it may considerably simplify the declaration
C                 of the molecule. In the example above a dummy atom
```

```
C                  (carrying an infinitesimally small but non-zero mass) defines
C                  the centre of the triple bond to which the HF molecule
C                  is notionally bonded.  The program will actually use the mass in
C                  the calculation so specify as low as possible (but non-zero mass)
C                  and mass of 0.000001u is recommended.
C                  Dummy atoms should not be counted in the evaluation of the rm^2
C                  d-parameters and are identified as such if their mass is less
C                  than 0.00001u.
C
C
C-------------------------------------------------------------------------------
C lines14-16 - block defining the parameters of fit
C-------------------------------------------------------------------------------
C
C   line 14:   The total number of declared parameters.  These parameters can either
C                  be parameters of fit or are to be held fixed at declared values.
C                  The parameters can be either internal structural coordinates, or
C                  ancillary parameters such as c,d parameters of the rm(1) and
C                  rm(2) models, Laurie delta_H parameters, or empirical bond length
C                  change (mostly for use with deuteration)
C
C   Parameter of fit declaration lines 15+ can be in two different forms, 15a or 15b:
C
C
C   line 15a:   DEFINITION OF AN INTERNAL COORDINATE:
C                  N,I,J,V,AD
C
C                  this is read in with input format=(31x,3i2,f14.0,20x,A20) so that
C                  the numbers have to be EXACTLY in the columns indicated below:
C
C                          column:  32    38          51                72               91
C                                   |     |           |                 |                |
C                                   --++--+++++++++++++                  cccccccccccccccccccc
C                  Examples:
C
C  atom no., parameter no.     7 1 0                                    r(C-C)
C  atom no., parameter no.     7 2 2                                    CCH (in CH3)
C                              8 9
C  atom no., parameter no.  FIX 8 2 0    15.346                         fixed at lit.value
C
C            N - the number of atom containing the required internal coordinate in
C                its CART definition
C            I - the CART parameter for that atom corresponding to the required internal
C                (1=bond length, 2=bond angle, 3=dihedral angle)
C
C            J - the optional repeat count declaring whether this parameter
C                has any additional occurrences:
C              J = 0 means that the parameter is unique
C              J > 0 makes it possible to fit 'degenerate' parameters,
C                    occurring for more than one atom (eg. CX bond in a CX3 pyramidal
C                    segment) and the value of J defines the number
C                    of additional occurrences of the parameter (e.g. J=2 for bond
C                    lengths in a methyl group).  An additional line
C                    in format =(a31,20i2) should then be inserted immediately
C                    following the current definition line and containing
C                    the numbers of atoms also carrying this parameter.
C                    Up to twenty such additional occurrences are allowed.
C                    NOTE: symmetric +- dihedral angle values can be fitted by
C                       specifying the values which have opposite sign to that of
C                       the parent value by using a negative number for the respective
C                       atom. Regrettably, owing to current formatting restrictions,
C                       the numbers of such atoms have to be smaller
C                       than 10 (single digit)
C              J < 0 makes it possible to fit 'degenerate' parameters with changes.
C                    This feature is designed primarily for dihedral angles in
C                    order to allow implementation of local rotational symmetry based
```

```
C                        on a non-zero rotation angle for atom N.
C                        This line is to be followed by |J| lines, each containing
C                        two numbers: integer number of the atom carrying the repeated value,
C                        and the difference of this value relative to that for atom N.
C                        The entries are to start from column 32, but are free-format
C                        otherwise.  Negative atom numbers are allowed, and these will
C                        specify a reversed sign value of V (see below).  With this method
C                        there is no limitation on the atom number that is present for J>0.
C
C              V - the optional initial value for the declared parameter,
C                  which will override the value in the preceding CART deck
C             AD - the optional alphanumeric descriptor of this parameter
C                  (up to 20 characters long), which will be echoed in the output.
C                  This has to start in column 72.
C            FIX - the command to fix this parameter in the fit, details at the end
C                  of 15b below
C
C
C   line 15b:    DEFINITION OF AN ANCILLARY PARAMETER OF FIT:
C                N,M,I,V
C
C                this is read in with format=(31x,3i2,f14.0) so that the numbers have
C                to be EXACTLY in the columns indicated below:
C
C                       column:  32    38              51
C                                |     |               |
C                                --++--+++++++++++++++
C
C                Examples:
C
C    rm(1) parameter c_a.........-4 1 0    0.001
C    rm(2) parameter_d_b.........-5 2 0
C    rm(2) parameter_d_b.....FIX-5 2 0    0.001
C
C            N - the code (always negative) defining the type of the ancillary
C                parameter, and also the meaning of M,I,V
C
C               N = -4 Watson's rm(1) c parameter, in which case
C               M =  1,2,3,4,5,6 for c_a,c_b,c_c,c_ab,c_ac,c_bc
C                 =  7 for fitting of c_a = c_b
C                 =  8 for fitting of c_a = c_c
C                 =  9 for fitting of c_b = c_c
C                 = 10 for fitting c_a = c_b = c_c
C               I =  0
C               V =  optional initial value for this parameter
C
C               N = -5 Watson's rm(2) d parameter, in which case
C               M =  1,2,3 for d_a,d_b,d_c
C                 =  7 for fitting of d_a = d_b
C                 =  8 for fitting of d_a = d_c
C                 =  9 for fitting of d_b = d_c
C                 = 10 for fitting d_a = d_b = d_c
C               I =  0
C               V =  optional initial value for this parameter, which will override
C                     the value in the CART definitions
C
C               N = -6 Laurie correction term for an XH bond, in which case
C               M = the atom for which this bond is defined
C               I = the number of additional bonds subject to the same correction: if
C                    this is greater than 0 then an additional
C                    line, format=(a31,20i2) should be inserted immediately
C                    following, with numbers of atoms for which these internals
C                    are defined
C               V = optional initial value for this parameter
C
C               N = -7 experimental Laurie term defined in terms of a projection angle
```

```
C                M = the atom for which this angle is defined
C                I = the number of additional angles subject to this correction,
C                    and I>0 requires an additional line, format=(a31,20i2), specifying
C                    the numbers of atoms carrying such angles
C                V = optional initial value for this parameter
C
C                N = -8 isotopic bond length change relative to the value in
C                        the parent - this is only for use with Deuterium
C                        substitution.
C                M = the atom for which this bond is defined
C                I = the number of additional bonds subject to this correction,
C                    and I>0 requires an additional line, format=(a31,20i2), specifying
C                    the numbers of atoms carrying such bonds
C                V = optional initial value for this parameter
C
C              FIX = Any of the declared internal or ancillary parameters can be fixed
C                    instead of fitted by writing FIX in columns 29-31 of the
C                    declaration line.
C                    This is one of only two cases for which the text in
C                    in columns 1-31 is relevant (the other is XXX for an excluded
C                    spectroscopic constant).  Otherwise this field is ignored and
C                    can be used for arbitrary explanatory comments.
C
C
C-------------------------------------------------------------------------------
C lines17-23 - block defining the spectroscopic constants to be fitted to
C-------------------------------------------------------------------------------
C
C   line 17:   The total number of available spectroscopic constants.
C
C   line 18+:  DEFINITION OF THE SPECTROSCOPIC CONSTANT TO BE FITTED TO:
C              N,M,B,dI,dB
C
C              read in with format=(31x,2i2,3f14.0) so that the numbers have
C              to be EXACTLY in the columns indicated below:
C
C                       column:  32  36           50           64           78
C                                 |   |            |            |            |
C                                 ++--+++++++++++++------------+++++++++++++
C
C              Examples:
C
C Constant,species,value....... 1 1 312142.390                                   NH2CN
C Constant,species,value....... 1 1 312142.390       1.0                         NH2CN
C Constant,species,value....... 1 1 312142.390                    30000.         NH2CN
C Constant,species,value....XXX 1 1 312142.390                                   NH2CN
C Constant,species,value....... 1 1 312142.390       0.1          30000.         NH2CN
C
C          N - the code defining the type of spectroscopic constant
C              = 1,2,3 for A,B,C
C              = 4,5 for B+C and A+B
C              = 6,7,8 for P.a,P.b,P.c where P.a=(1/2)[Ib+Ic-Ia] etc.
C
C              When B+C and A+B are declared, the fit is actually to
C              4*505379.01/(B+C) = 4*I.bI.c/(I.b+I.c) =ca. I.b+I.c or to
C              4*505379.01/(A+B) = 4*I.aI.b/(I.a+I.b) =ca. I.a+I.b
C
C          M = the number of the isotopic species
C          B = the value Bobs of the experimentally determined constant, in MHz for
C              rotational constants and uA**2 for planar moments.
C              The constants should be declared in increasing order of
C              isotopic species number, although all constants for
C              a given species are not required.
C
C              It is optionally possible to specify EITHER fourth OR fifth numbers,
C              dI or dB (usually only one allowed), such that:
```

```
C
C          dI - vibration-rotation correction dI=Icorr-Iobs (in uA**2)
C               to the experimental moment of inertia defined by N and B (even if
C               experimental rotational constants are specified). In this case
C               the dB field should be left blank.
C
C          dB - vibration-rotation correction dB=Bcorr-Bobs (in MHz)
C               to the experimental rotational constant defined by N and M.
C
C               --> this is most often (Be-B0) from anharmonic force field calculations
C                   and used for r_e^SE structure evaluation
C
C               In this case the space corresponding to dI is normally to be left blank.
C               BUT if a value is placed in this position then it is assumed to be
C               the (dimensionless) rotational g-factor, g_bb, for rotational constant B.
C               STRFIT will then subtract from the pertinent rotational constant
C               an electronic correction dB_el (in MHz) = 0.000544617 * g_bb * B,
C               where B is taken to be B+dB.
C
C               The structure will then be fitted to corrected quantities
C                 Icorr=Iobs+dI, Iobs=conv/Bobs or to
C                 Icorr=conv/(Bobs+dB)            or to
C                 Icorr=conv/(Bobs+dB-dB_el)
C               where Iobs is the moment of inertia derived from the preceding
C               rotational constant, or to P=Pobs+dI if planar moment has been
C               specified
C
C               The main purpose of the dI option is evaluation of r* (r_z)
C               structures by using dI's from a harmonic force field
C
C               The main purpose of the dB option is evaluation of
C               semi-experimental equilibrium (r_e^SE) structures to either
C               the specified B = B0_exp + (Be-B0)_calc
C               or to          B = B0_exp + (Be-B0)_calc - dB_el
C
C       XXX = Any of the input rotational constants can be excluded from the fit
C             by writing XXX in columns 29-31 of the declaration line.
C             This is one of two only two cases for which the text in
C             in columns 1-31 is relevant.  Otherwise this field is ignored and
C             can be used for arbitrary explanatory comments.
C
C
C-------------------------------------------------------------------------------
C lines24-26 - Block defining the isotopic changes
C-------------------------------------------------------------------------------
C
C               There is to be one such block for each substituted isotopic species
C               represented in the spectroscopic constants.  Species 1 is taken to
C               be the parent species, the first isotopic block is to be for
C               species number 2, and successive such blocks are to be for
C               successively numbered species.
C               Each block begins with a repeat count line (line 24), which is
C               followed by the declaring lines.
C
C   line 24:    The number of changes relative to the parent for a given
C               isotopic species
C
C   line 25+ - DEFINITION OF ISOTOPIC CHANGE:
C               N,M,V
C
C               read in with format=(31x,2i2,3f14.0) so that the numbers have
C               to be EXACTLY in the columns indicated below:
C
C                   column:  32  36             49
C                            |   |              |
C                            ++--+++++++++++++++
```

```
C
C             N = the number of the isotopic atom
C             M = the number of the changed parameter (1,2,3,4 for
C                 bond length, bond angle, dihedral angle and atomic mass resp.),
C             V = the value of this parameter in the substituted species.
C                 When the parameter is not a mass (N not equal to 4) then V declares
C                 the change relative to the value in the parent species
C
C-------------------------------------------------------------------------------
C
C       GENERAL NOTES:
C
C               - As noted in several places above the input is in the
C                 old-fashioned fixed format, so it is necessary to keep input
C                 numbers within the specified columns.
C
C               - Columns 1-31 can be used for any clarifying comments, which are
C                 up to the user and are not echoed to the output
C
C               - Columns to the right of the input fields can be also be used for
C                 comments, which are not echoed to the output.
C                 Usually columns 78 and higher are safe for this purpose except in
C                 the definitions of parameters of fit where the descriptive
C                 alphanumeric parameter extends up to and inclusive of column 91
C
C               - The input file is not read past the last set of isotopic changes,
C                 so the rest of the file can be used for any purpose - usually
C                 storage of alternative data and of results.
C
C               - STRFIT does not write to the input file so it will not corrupt it
C
C               - Additional blocks of comments are allowed before all lines
C                 with a repeat count: i.e. those that specify:
C                     the number of atoms,
C                     the number of parameters,
C                     the number of spectroscopic constants
C                     the number of isotopic changes.
C                 These comment lines have to have a '!' character in the first
C                 column, and there is no limit on their number. Such lines are
C                 echoed at the top of the output file.
C
C       WARNING: There is a known problem with symmetric top molecules
C                which break symmetry on isotopic substitution.  This is
C                associated with the way the program implements parallel axes for
C                the rm(1r) scheme and the resulting possibility of perpendicular
C                axis switching.  Steps have been taken to stabilise such behaviour,
C                and those are marked by the string May2009 in the code
C
C
C-------------------------------------------------------------------------------
C     CART = Thompson J.Chem.Phys. 47,3407(1967) definitions:
C-------------------------------------------------------------------------------
C
c  1.  Atom N in the molecule is defined in terms of three other neighbouring
C        atoms: NA, NB, and NC, and a bond length R(N-NA), a bond angle
C        A(N-NA-NB) and a dihedral angle D(N-NA-NB-NC)
C
C  1a. Atoms are declared in the sequence of increasing N (starting from N=1)
C        and the numbers of the defining atoms NA, NB, NC all have to be smaller
C        than N (and all different)
C
C  1b. For N=1 set NA,NB,NC, R,A,D to zero
C        For N=2 set    NB,NC,   A,D to zero
C        For N=3 set        NC,     D to zero
C
C  2.  For a right handed coordinate system dihedral angles are defined
```

```
C        by viewing the configuration
C            i/ from the NC direction along the NB-NA axis if NC is bonded to NB
C           ii/ from the NC direction along the NA-NB axis if NC is bonded to NA
C        The angle is defined positive for a clockwise rotation
C        of atom NC into the plane N-NA-NB.
C
C   3.  In the calculation of initial Cartesian coordinates the atom N=1
C        defines the origin, the line N=1 to N=2 defines the X axis and
C        atoms N=1, N=2, N=3 define the XY plane.
C
C
C-------------------------------------------------------------------------------
C    C O M P I L A T I O N:
C-------------------------------------------------------------------------------
C
C     If you want to compile this program then please note that it is crucially
C     dependent on the use of 'static memory allocation'.  Please read the following
C     notes copied from the PROSPE webpage (and also use the data files from
C     the webpage for testing):
C
C     Most contemporary compilers no longer use default static memory allocation
C     that preserves values of variables previously set in some subroutine. Many
C     programs assume this to be the case so that you need to use an appropriate
C     keyword to enforce static allocation. For example on the f77 compiler on
C     SGI machines this is the -static option, whereas with Intel Visual Fortran
C     you have to use option -Qsave. Note that with some compilers optimization
C     options used not to be safe. With good compilers this is no longer the
C     case, but if problems crop up it is still good to check by disabling
C     optimization.
C
C     Command line example for gfortran:
C     gfortran -fno-automatic strfit.for -o strfit
C
C     Command line example for Intel Visual Fortran 9:
C     ifort -nopdbfile -nodebug -traceback -arch=pn1 -tune=pn1 -O2 -Qsave
C                     -ccdefault:fortran -fpscomp:filesfromcmd strfit.for
C
C     Command line example for Intel Visual Fortran 11:
C     ifort -nopdbfile -nodebug -traceback -O3 -Qsave -ccdefault:fortran
C                                       -fpscomp:filesfromcmd strfit.for
C
C_____
```