CAMVIB

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CAMVIB originated in early 1980 as a program to transform cartesian force constants (generated by the HONDO ab initio quantum chemistry package) to internal force constants. It was subsequently developed over several years at the University of Cambridge as a more general program for vibrational analysis. The present version was implemented for VAX/VMS machines (e.g. UK.AC.BRISTOL.CSA) and contains calls to the VAX-specific timing routine SECNDS. The whole code is FORTRAN77 compatible and compiles successfully with the standard VAX FORTRAN compiler under VMS 4.4 and earlier versions, as well as g77. The original versions of subroutines BMAT and VIB were derived from programs RELK (L.B. Sims, 1975) and NCRDWDC (H.L. Sellers, L.B. Sims, L. Schafor & D.E. Lewis, QCPE 11, 339 (1977)) which utilise analytical s-vector expressions (E.B. Wilson, J.C. Decius & P.C. Cross, "Molecular Vibrations", McGraw-Hill, New York, 1955, pp 54-61) for B-matrix elements to solve the vibrational eigenvector/eigenvalue problem in mass-weighted cartesian coordinates (W.D. Gwinn, J.Chem.Phys. 55 (1971) 477). The present version is dimensioned by using the external CAM_SIZE file which can be edited to change the number of atoms and valence coordinates. Many of the options (specified by "keywords") have been incorporated to deal with particular problems arising in the course of the IHW's research group (into force-constant calculations, prediction of vibrational spectra and computation of isotope effects) and will not be required by the "ordinary" user who may simply want to post-process the results of a Cartesian-force-constant calculation performed using some other (probably quantum-chemical) program. What follows consists of two parts. First, a description of the data and the various options available, item by item. Second, sample data files and corresponding output files selected to demonstrate aspects of the "normal" usage of the program. These have been annotated in the hope of clarifying their meaning. (N.B. In this document the underlining symbol _ is used to denote a blank.).

Overview of CAMVIB input

1. IPROG - Format (1A4)

May have the following values:

*VIB_* to start a calculation

STOP to finish a calculation

2. OPTIONS - Format (20(A4 , 1X)

The following keywords may be specified:

BOHR - Cartesian coordinate input is in atomic units instead of Angstroms.

REDU - a redundant set of valence coordinates is to be supplied, which implies that

"symmetry" coordinates are also to be specified.

VALE - valence coordinates are to be input. (Not required if SYMM, REDU, RELX, ININ or INSY is specified.) Valence force constants are computed. If REDU or SYMM is specified, both valence and "symmetry" force constants are computed. Spurious translational and rotaitonal contributions present in the supplied Cartesian force constants to be projected out; transformed Cartesian force constants are then re-computed from the internal force constants. (cf. I.H. Williams, J.Mol.Struct. 94 (1983) 275).

SYMM - "symmetry" coordinates are to be constructed. (Not required if REDU or INSY is specified.)

IFCS - internal force constants (valence and/or symmetry) are printed out in units of: md/Å for stretching, md.Å /rad² for bending, and md/rad for stretch/bend interactions.

SCAL - valence force constants are to be scaled by a single value.

SCVD - diagonal valence force constants to be scaled individually.

SCVA - all valence force constants to be scaled by Pulay's method (see item 6; cf. P. Pulay, G. Fogarasi, G. Pongor, J.E. Boggs & A. Vargha, JACS, 105 (1983) 7037).

SCSD - diagonal symmetry force constants to be scaled individually (see item 6).

SCSA - all symmetry force constants to be scaled by Pulay's method (see item 6).

VECT - normal coordinates are to be printed out in Cartesian coordinates (both mass-weighted and unweighted). Additionally the normal coordinates are printed out in valence coordinates if VALE is specified or in "symmetry" coordinates if SYMM or REDU is specified, together with an approximate "potential energy distributions". If VECT is not specified frequencies only are computed and printed out.

RELX - compliance constants. relaxed force constants and interaction displacement

coordinates are computed. (cf. I.H. Williams, Chem. Phys. Lett. 88 (1982 462).

INCA - Cartesian force constant input : since it is the default, this option never needs to be specified explicitly.

ININ - valence force constant input.

INSY - symmetry force constant input.

OUTC - projected Cartesian force constants are written to channel 12. (Not required if DISO is specified.)

OUTI - valence force constants (unscaled) are written to channel 12.

OUTS - symmetry force constants (unscaled) are written to channel 12.

LINE - molecule is linear (with 3N-5 internal degrees of freedom for N atoms).

PRAX - geometrical coordinates are transformed to a principal-axis system with origin at the centre of mass. (Not normally required.)

DISO - data for program CAMISO is written to channel 12.

MASS - non-standard atomic masses are to be supplied. (Not required if standard isotopic masses for H, Li, Be, B, C, N, O, F, Si, P, S Br Cl are to be used.)

FULL - full printout of all matrices and eigenvectors.

OBSD - calculated frequencies to be compared with supplied observed frequencies and the r.m.s. error computed.

AMPAC - geometry and force constants to be read from logical unit 9 assigned to a file (e.g. filename, RES) generated by a FORCE calculation with the AMPAC (or MOPAC) program.

CADPAC - geometry and force constants to be read from logical unit 9 assigned to a file generated by a SECDER calculation with the CADPAC program using the PUNCH option.

GBZF - Cartesian force constants to be read from logical unit 7 assigned to a file generated by a FREQ calculation with the GAUSSIAN B2 program using the PUNCH=FCS option.

BREF - minimal printout

EXPL - symmetry coordinates are to be input explicitly (see item 7).

3. TITLE - Format (20A4)

anything you wish, its up to you!

4. IA,X,Y,Z,WT - Format (A4,A1,3E20.14)

IA

specifies the required isotope: currently the following symbols are accepted:

_ _1H, _ _2H, _ _6Li, _7Li, _9BE, _10B, _11B, _12C, _13C, _14C, _14N, _15N, _16O, _17O, _18O, _19F, 28SI, _31P, _32S, _34S, 35CL, 37CL.

X,Y,Z

are Cartesian coordinates in Angstroms or atomic units if BOHR is specified.

WT

is a non-standard atomic mass. (Not required if IA is any of the above symbols). To override automatic assignment of standard isotopic masses then a symbol IA different from those listed above must be specified, e.g. DUMM or C12_ . (This facility has been used to input atoms of mass 4000 : I.H. Williams, JACS , 106 (1984) 7206).

*---

ends this section of the data. (N.B. this is a special value for the symbol IA.) If keyword AMPAC or CADPAC has been specified, then only the isotopic symbols IA are required (one per line) : the Cartesian coordinates are read from logical unit 9 and the contents of the present X,Y and Z fields are overwritten.

5. Skip to item 6 unless DISO is specified.

IS, IG - Format (2I2)

IS - rotational symmetry number

IG - electronic degeneracy

6. Skip to item 9 unless VALE, REDU, SYMM, ININ, or INSY is specified.

TYPE, (LIST(1)....LIST(4),SF,SLAB - Format (A1,4I3,F10,3,A4)

TYPE denotes the type of valence coordinate specified by the atoms in

LIST, and may be one of the following.:

S - stretching of bond LIST(1) - LIST(2) :

B - bending of angle LIST(1) - LIST(2) - LIST(3) :

W - wagging of LIST(1) out of the plane LIST(2) - LIST(4) - LIST(3). LIST(1) is bonded to the central atom LIST(4). (cf. McIntosh et al., Can.J. Chem. 56 (1978) 1289).

L - bending of collinear atoms LIST(1) - LIST(2) - LIST(3) in the plane of LIST(4); a second valence coordinate for bending of the same three collinear atoms in the plane perpendicular to this is automatically generated. If the molecule itself is linear (rather than just a subsection of atoms being collinear) then keyword LINE must be specified to ensure the correct number of internal coordinates; the molecule must also be aligned along the z-axis. For the linear bending coordinate LIST(4) is given a number of greater than NAT (the number of atoms in the molecule). e.g. LIST(4) = 4 for CO_2. The two valence coordinates generated are for bending in the xz and yz planes respectively.

T - torsion about bond LIST(1) = LIST(2). (cf. I.H. Williams, J.McKenna & L.B. Sims, J. Mol. Struct. 55 (1979) 147; I.H. Williams, J.Mol.Spec. 66 (1977) 288) N.B. all torsional coordinates must follow all stretching coordinates in the specification of the valence coordinates: this ensures the complete atomic connectivity table is available for use in generating the 8-matrix elements for torsional coordinates.

* - ends this section of the data.

SF - is a scaling factor which is ignored unless one of the keywords SCAL, SCVD, SCVA, SCSD or SCSA has been specified. If left blank or input as zero, then a value of unity is printed and assumed. If SCAL has been specified, then only the value of SF associated with the first valence coordinate is significant: this is the factor by which the entire force-constant matrix is to be multiplied. (Note that this is equivalent to multiplying all the vibrational frequencies by the square root of SF.) If SCVD or SCVA has been specified, then the value of SF input for each valence coordinate is significant. SCVD multiplies each diagonal valence force constant by its associated SF value. SCVA not only causes the diagonal valence force constants to be scaled in this manner but also scales the off-diagonal valence force constants: the force constant $F(i,j)$ coupling valence coordinates $R(i)$ and $R(j)$ is scaled by $SQRT(SF(i)*SF(j))$. This is equivalent to the scaling procedure recommended by Pulay (JACS, 105 (1983) 7037).

SLAB - is a symmetry-coordinate label to be supplied if implicit generation of symmetry coordinates is required, i.e. if REDU, SYMM or INSY is specified but not EXPL. It is a four character label which may be anything convenient except that certain words, viz, TRIG, TET2, TET3 and TBPH, are significant and are interpreted as described under item 7. All three valence coordinates, from which a pair of TRIG symmetry coordinates are to be constructed, should be grouped consecutively (in the order given under item 7) each with SLAB = TRIG. Similarly, all six valence coordinates, from which a set of five TET2 or TET3 symmetry coordinates are to be constructed, should also be grouped consecutively in the order given under item 7.

7. Skip to item 9 unless REDU, SYMM, or INSY is specified.

WORD, IROW(I).....IROW(NI) - Format(A4, 30I2)

Word is a label for a "symmetry" coordinates constructed as a linear combination of valence coordinates with integral coefficients IROW(1), IROW(2), etc.; e.g. SDEF_2-1-1 There are presently four built-in options allowing for implicit generation of sets of symmetry coordinates from valence coordinates specified by unit coefficients in IROW :

TRIG generates coordinates appropriate for a trigonal planar centre, e.g. X=C(Y,Z).

TET2 generates coordinates appropriate for a methylenic centre, e.g. X-CH2-Y.

TET3 generates coordinates appropriate for methyl-like centre, e.g. X-CH3 ;

TBPH generates coordinates appropriate for a trigonal bipyramidal centre having a symmetry plane containing the equatorial atoms, e.g. A - C(E1,E2,E3) -A'.

If WORD is TRIG then a set of two "symmetry" coordinates is constructed from three valence coordinates in IROW for angle bending in the plane of a trigonal atom, e.g. TRIG- - - - - - - - - - - 1_1_1. These valence coordinates should be in the order Y-C-Z, X=C-Y, X=C-Z. a "scissoring" combination and a "rocking" combination are constructed, equivalent to SCIS----------------2-1-1 ROCK--------------1-1 If WORD is TET2 or TET3 then a set of five "symmetry" coordinates is constructed for six valence coordinates in IROW for angle bending about a tetrahedral atom, e.g. TET2----------------------1-1-1-1-1-1

These valence coordinates should be in the order X-C-Y, X-C-H1, X-X-H2, Y-C-H1, Y-C-H2, H1-C-H2 for TET2 and X-C-H1, X-C-H2, X-X-H3, H1-C-H2, H1-C-H3, H2-C-H3 for TET3. The resulting "symmetry" coordinates are mutually orthogonal to the redundancy condition calculated for the actual molecular geometry. Examples of TET2 and TET3 usage are in I.H. Williams, Chem.Phys.Lett. 88 (1982) 462; D. Spangler, I.H. Williams, G.M.Maggior, J.Comput.Chem. 4 (1983) 524; J.S. Franciso & I.H. Williams, Mol. Phys., 52 (1984)743. If WORD is TBPH then a set of seven symmetry coordinates is constructed from nine valence coordinates in IROW for angle bending about a trigonal bipyramidal atom, e.g. TBPH-----------------------1-1-1-1-1-1-1-1-1.

These valence coordinates should be in the order A-C-El, A-C-E2, A-C-E3, A'-C-El, A'-C-E2, A'-C-E3, E2-C-E3, E1-C-E2, E1-C-E3.

The resulting symmetry coordinates are mutually orthogonal to the two redundancy conditions calculated for the actual molecular geometry. Examples of TBPH usage are symmetrical transition structures $H2—HC--OH2 + (I.H.Williams, Bull. Soc. Chim. Belg., 91 (1982) 356) and $HS--CH--NH3 + (I.H. Williams, JACS, 106 (1984) 7206).

XTRA - calls a user-supplied subroutine (e.g. EX03) to generate a special set of symmetry coordinates (cf. J.S. Francisco & I.H. Williams, Chem. Phys. 95 (1985) 373). Not normally used.

If the number of valence coordinates exceeds 30 then the specification of each symmetry coordinate

requires more than one line of data; second, third, fourth and fifth lines of data are read with FORMAT

30I2 to complete the array IROW if NI is. .LE. 60, .LE. 90, .LE. 120 or .LE. 140 as necessary. The total number of symmetry coordinates specified (counting TRIG as two, TET2 and TET3 as five, and TBPH as seven) must equal NINT, the number of independent internal degrees of freedom.

8. Skip to item 9 unless ININ or INSY is specified. (Not normally used.)

E(1)....E(NFI) - Format (6F12.6)

E is a linear array of dimension $(3N-6)*(3N-5)/2$ (where N is the number of atoms) into which is read the lower triangle of the matrix of valence or symmetry force constants (units of md/Å, md.Å /rad^2, etc) generated by a prior run of CAMVIB with OUTI or OUTS specified.

Now skip to item 10.

If keyword AMPA, CADP or G82F is specified, then skip to item 10.

9. E(1).....E(NFC) Format (1X, F12.8)

E is a linear array of dimensions 3N*(3N+1)/2 (where N is the number of atoms) into which is read the lower triangle of the Cartesian force constant matrix (units of hartree/bohr^2), as computed either directly (for instance by a quantum-mechanical program such as HONDO, CADPAC or GAMESS) of from a valence force field (via the program CAMVFF).

10.

Skip to item 11 unless OBSD is specified. IFR(1).....1FR(NINT) - Format (20I4)

IFR is an array containing the ordinal numbers of the calculated frequencies which are to be compared with observed frequencies. Remember that the first six calculated frequencies are the zeroes for translation and rotation, so the first genuine vibrational frequency is number seven.

OBFR(1).....OBFR(NF) - Format (8F10.4)

OBFR is an array of values of observed frequencies input in the same order as the calculated frequencies specified by IFR. The number NF is determined by the number of non-zero elements in IFR. The units are cm^{-1}.

Implementation of the script *run_camvib.sh*

In order to facilitate the use of CAMVIB, the *run_camvib.sh* script was created. It takes its input from the fort.7 file output from a calculation in Gaussian with the keywords *punch=(coord,derivatives)* specified.

run_camvib.sh requires the following files to be present, each of which will be described in turn:

> *fort.7* – the file containing the coordinates, gradient, and hessian from Gaussian.
>
> *symm_info.txt* – text file with the internal coordinates for the molecule.
>
> *vib_header.txt* – this text file contains the commands for CAMVIB and can be edited accordingly.
>
> *process_crd.awk* – AWK script which parses the *fort.7* file for coordinate data.
>
> *Process_hess.awk* – AWK script which parses the *fort.7* file for Hessian data.

The script produces the input for CAMVIB, and in the last action, runs the program. The directories used in the script itself will need to be changed in order to reflect those in the user's filesystem, however this is trivial.

Example CAMVIB input file (*.vib)

```
VIB
 REDU IFCS VECT RELX DISO FULL GAUS
  METHYL CATION
  1 1 0
  12C    -3.2073109600E-16     4.9343245540E-17    -1.7270135940E-16
   1H     8.3444103330E-16     4.9343245540E-17     2.0809731080E+00
   1H     1.8021755770E+00    -6.0205874750E-16    -1.0404865540E+00
   1H    -1.8021755770E+00     7.0074523860E-16    -1.0404865540E+00
 *
 S  1  2  0  0          C1H2
 S  1  3  0  0          C1H3
 S  1  4  0  0          C1H4
 B  2  1  3  0          TRIG
 B  2  1  4  0          TRIG
 B  3  1  4  0          TRIG
 W  2  3  4  1
 *
     0.6050901920E+00     0.4332194761E-11     0.1863129721E+00
     0.3988704486E-09    -0.4211645014E-11     0.6050794462E+00
    -0.5885475861E-01     0.1396147555E-11     0.1202783090E-09
     0.4393937524E-01    -0.1099029206E-10    -0.6210796152E-01
     0.1446574551E-11     0.9691464673E-11     0.2075177572E-01
    -0.2810385700E-09    -0.2029097949E-10    -0.3445421017E+00
    -0.1438632941E-09     0.4713621185E-11     0.3496857023E+00
    -0.2731189906E+00    -0.1411718528E-10     0.1237057117E+00
     0.7457553806E-02     0.4520217176E-11    -0.3646846014E-02
     0.2732491207E+00     0.6888282355E-11    -0.6210523332E-01
     0.1724801055E-10    -0.1967119878E-10     0.2067809284E-01
     0.2467091664E-12    -0.7637314748E-12     0.2075177572E-01
     0.1237052927E+00     0.4658526878E-11    -0.1302726323E+00
     0.2101796061E-01    -0.8454102887E-11    -0.2571663671E-02
    -0.1323920431E+00    -0.1074980990E-10     0.1203759569E+00
    -0.2731189901E+00     0.1220344137E-10    -0.1237057117E+00
     0.7457553966E-02     0.9621959021E-11     0.3646846107E-02
    -0.7586272570E-02    -0.9581580331E-11    -0.1233240341E-01
     0.2732491204E+00     0.2875157530E-12    -0.6210523332E-01
    -0.1129693408E-10     0.5061365788E-11     0.2067809284E-01
     0.8141680954E-11     0.1004924239E-10     0.2067809284E-01
     0.1691241511E-10    -0.8927842926E-11     0.2075177572E-01
    -0.1237052929E+00     0.1244636251E-10    -0.1302726325E+00
    -0.2101796052E-01    -0.1715909860E-10    -0.2571663831E-02
     0.1233240322E-01     0.3124208638E-12     0.1247216270E-01
     0.1323920433E+00     0.6036248219E-11     0.1203759571E+00
 STOP
```

Header section

Atom specification

Internal coordinate specification

Hessian
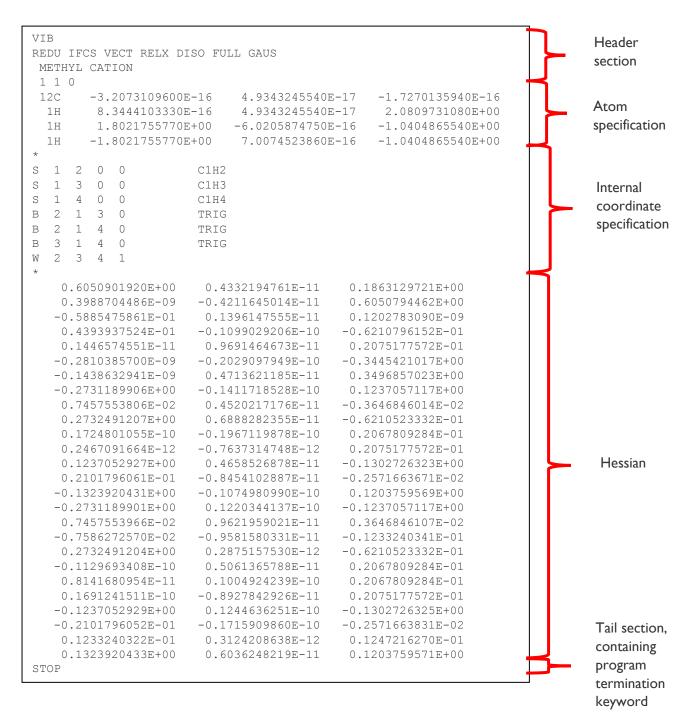
Tail section, containing program termination keyword

Figure 1. Sample input file for CAMVIB. This structure is a simple methyl cation, with four atoms. The internal coordinate input represents the individual degrees of freedom appropriate to this molecule.

Overview of CAMVIB output

```
SIZE PRINTOUT
 MAXAPO =      1001
 MAX ATOMS     1000
 MAX CRT-COORDS 3000
 MAX INT-COORDS 3500
 MAX DEG-FREE  2994
 MAX DIAG/MATRX 4504500
 ************************* CAMVIB : VERSION MAY 16 *************************


 OPTIONS SPECIFIED : REDU IFCS VECT RELX DISO FULL GAUS


  METHYL CATION


   ATOM     MASS          X          Y          Z     ANGSTROM


  1    C   12.000000      0.000000    0.000000    0.000000
  2    H    1.007825      0.000000    0.000000    2.080973
  3    H    1.007825      1.802176    0.000000   -1.040487
  4    H    1.007825     -1.802176    0.000000   -1.040487


 INTERNAL COORDINATES, R                               SCALING
                                                       FACTORS


   1  S 1  STRETCH   C 1 -  H 2                            1.000
   2  S 2  STRETCH   C 1 -  H 3                            1.000
   3  S 3  STRETCH   C 1 -  H 4                            1.000
   4  B 1  BEND      H 2 -  C 1 -  H 3                     1.000
   5  B 2  BEND      H 2 -  C 1 -  H 4                     1.000
   6  B 3  BEND      H 3 -  C 1 -  H 4                     1.000
   7  W 1  WAG       H 2 -  C 1  OUT OF PLANE   H 3 -  C 1 -  H 4    1.000


 B MATRIX (TRANSFORMATION FROM CARTESIANS TO INTERNALS :  R  =  B * X )


            1          2          3          4          5          6          7          8          9


    1      0.000000   0.000000  -1.000000   0.000000   0.000000   1.000000   0.000000   0.000000
 0.000000
    2     -0.866025   0.000000   0.500000   0.000000   0.000000   0.000000   0.866025   0.000000   -
 0.500000
    3      0.866025   0.000000   0.500000   0.000000   0.000000   0.000000   0.000000   0.000000
 0.000000
    4      0.720817   0.000000   0.416164  -0.480544   0.000000   0.000000  -0.240272   0.000000   -
 0.416164
    5     -0.720817   0.000000   0.416164   0.480544   0.000000   0.000000   0.000000   0.000000
 0.000000
    6      0.000000   0.000000  -0.832327   0.000000   0.000000   0.000000   0.240272   0.000000
 0.416164
    7      0.000000  -1.441633   0.000000   0.000000   0.480544   0.000000   0.000000   0.480544
 0.000000


            10         11         12
    1      0.000000   0.000000   0.000000
    2      0.000000   0.000000   0.000000
    3     -0.866025   0.000000  -0.500000
    4      0.000000   0.000000   0.000000
    5      0.240272   0.000000  -0.416164
    6     -0.240272   0.000000   0.416164
    7      0.000000   0.480544   0.000000

 REDUNDANCY CONDITION FOR COORDINATE  6 IS :

  0.00000000  0.00000000  0.00000000  1.00000000  1.00000000  1.00000000  0.00000000


 SYMMETRY COORDINATES SPECIFIED IMPLICITLY
```

```
U MATRIX (TRANSFORMATION FROM INTERNAL TO SYMMETRY COORDINATES : S = U * R )


            1        2        3        4        5        6
  R        C1H2     C1H3     C1H4     SCIS     ROCK



  S 1      1.0000   0.0000   0.0000   0.0000   0.0000   0.0000
  S 2      0.0000   1.0000   0.0000   0.0000   0.0000   0.0000
  S 3      0.0000   0.0000   1.0000   0.0000   0.0000   0.0000
  B 1      0.0000   0.0000   0.0000   0.8165   0.0000   0.0000
  B 2      0.0000   0.0000   0.0000  -0.4082   0.7071   0.0000
  B 3      0.0000   0.0000   0.0000  -0.4082  -0.7071   0.0000
  W 1      0.0000   0.0000   0.0000   0.0000   0.0000   1.0000


 UNSCALED SYMMETRY FORCE CONSTANTS (MD/A FOR STRETCHING, MD.A/RAD**2 FOR BENDING)


            1          2          3          4          5          6
   1      5.444335
   2     -0.029142   5.444314
   3     -0.029142  -0.029150   5.444314
   4      0.053587   0.053571  -0.107172   1.480353
   5      0.092815  -0.092822  -0.000017  -0.000028   1.480321
   6      0.000000   0.000000   0.000000   0.000000   0.000000   1.395748


 UNSCALED VALENCE  FORCE CONSTANTS (MD/A FOR STRETCHING, MD.A/RAD**2 FOR BENDING)


            1          2          3          4          5          6          7
   1      5.444335
   2     -0.029142   5.444314
   3     -0.029142  -0.029150   5.444314
   4      0.043753   0.043741  -0.087506   0.986902
   5      0.043753  -0.087505   0.043741  -0.493467   0.986902
   6     -0.087507   0.043765   0.043765  -0.493435  -0.493435   0.986870
   7      0.000000   0.000000   0.000000   0.000000   0.000000   0.000000   1.395748


 PROJECTED CARTESIAN FORCE CONSTANTS (HARTREE/BOHR**2)


            1          2          3          4          5          6          7          8
9


   1      0.605091
   2      0.000000   0.186316
   3      0.000000   0.000000   0.605083
   4     -0.058854   0.000000   0.000000   0.043914
   5      0.000000  -0.062105   0.000000   0.000000   0.020702
   6      0.000000   0.000000  -0.344540   0.000000   0.000000   0.349686
   7     -0.273119   0.000000   0.123706   0.007470   0.000000  -0.003647   0.273242
   8      0.000000  -0.062105   0.000000   0.000000   0.020702   0.000000   0.000000
0.020702
   9      0.123706   0.000000  -0.130272   0.021041   0.000000  -0.002573  -0.132403
0.000000   0.120355
  10     -0.273119   0.000000  -0.123706   0.007470   0.000000   0.003647  -0.007593
0.000000  -0.012344
  11      0.000000  -0.062105   0.000000   0.000000   0.020702   0.000000   0.000000
0.020702   0.000000
  12     -0.123706   0.000000  -0.130272  -0.021041   0.000000  -0.002573   0.012344
0.000000   0.012490


            10         11         12
  10      0.273242
  11      0.000000   0.020702
  12      0.132403   0.000000   0.120355
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```
FREQUENCIES (CM-1) AND CARTESIAN COORDINATES OF NORMAL MODES

 FREQUENCY              MASS-WEIGHTED CARTESIANS              UNWEIGHTED CARTESIANS

            ATOM     X          Y          Z            X          Y          Z



    0.0000
             1    -0.036861  -0.195280   0.795578     -0.017238  -0.091322   0.372047
             2    -0.182715   0.079721   0.230560     -0.294841   0.128644   0.372047
             3     0.075334   0.019264   0.379545      0.121564   0.031086   0.612458
             4     0.075334  -0.268763   0.081576      0.121564  -0.433694   0.131636


                                       LINEAR COMPONENTS   -0.159863  -0.846911   3.450345
                                       ANGULAR COMPONENTS  -0.427160  -1.078179   0.521103



    0.0000
             1     0.666003  -0.074116  -0.208211      0.260502  -0.028990  -0.081440
             2     0.059780   0.289406  -0.060340      0.080685   0.390608  -0.081440
             3     0.259623   0.127470   0.055039      0.350411   0.172044   0.074286
             4     0.259623  -0.481312  -0.175719      0.350411  -0.649621  -0.237166


                                       LINEAR COMPONENTS    2.888389  -0.321433  -0.902990
                                       ANGULAR COMPONENTS  -0.974204  -0.834984   1.101416



    0.0000
             1    -0.333223   0.014625  -0.109597     -0.102530   0.004500  -0.033722
             2    -0.021511  -0.201515  -0.031762     -0.022839  -0.213956  -0.033722
             3    -0.134097   0.725693  -0.096763     -0.142376   0.770494  -0.102737
             4    -0.134097  -0.511463   0.033240     -0.142376  -0.543038   0.035292


                                       LINEAR COMPONENTS   -1.445155   0.063427  -0.475313
                                       ANGULAR COMPONENTS   0.644759   0.470406   2.238279



    0.0000
             1    -0.403511  -0.197144  -0.318114     -0.137569  -0.067213  -0.108455
             2    -0.550519   0.131211  -0.092190     -0.647645   0.154359  -0.108455
             3     0.099852  -0.193835   0.283302      0.117468  -0.228033   0.333283
             4     0.099852  -0.108774  -0.467682      0.117468  -0.127964  -0.550193


                                       LINEAR COMPONENTS   -1.749987  -0.854995  -1.379628
                                       ANGULAR COMPONENTS  -0.590202  -2.717378  -0.153894



    0.0000
             1    -0.184633  -0.559950  -0.079541     -0.065090  -0.197402  -0.028041
             2     0.244765   0.277308  -0.023051      0.297749   0.337336  -0.028041
             3    -0.202643  -0.389487  -0.281362     -0.246509  -0.473799  -0.342269
             4    -0.202643  -0.374645   0.235260     -0.246509  -0.455745   0.286187


                                       LINEAR COMPONENTS   -0.800735  -2.428447  -0.344962
                                       ANGULAR COMPONENTS  -1.377497   1.869360  -0.026851



    0.0000
             1    -0.214206   0.634428   0.054031     -0.081052   0.240057   0.020444
             2    -0.003800   0.713382   0.015658     -0.004961   0.931433   0.020444
             3    -0.091216  -0.035040  -0.034812     -0.119097  -0.045751  -0.045452
             4    -0.091216  -0.126766   0.066128     -0.119097  -0.165512   0.086341


                                       LINEAR COMPONENTS   -0.928992   2.751455   0.234326
                                       ANGULAR COMPONENTS  -1.659341   0.365243   0.165951
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 1386.0316
          1    -0.000006   0.000000    0.298533    -0.000002   0.000000    0.090279
          2     0.000014   0.000000    0.087577     0.000015   0.000000    0.091387
          3    -0.373211   0.000000   -0.558845    -0.389446   0.000000   -0.583156
          4     0.373215   0.000000   -0.558859     0.389451   0.000000   -0.583170


                              LINEAR COMPONENTS    0.000000   0.000000    0.000000
                              ANGULAR COMPONENTS   0.000000   0.000000    0.000000



 1386.0614
          1     0.298531   0.000000    0.000006     0.090279   0.000000    0.000002
          2    -0.774327   0.000000    0.000002    -0.808011   0.000000    0.000002
          3    -0.127904   0.000000   -0.373227    -0.133468   0.000000   -0.389463
          4    -0.127890   0.000000    0.373206    -0.133453   0.000000    0.389441


                              LINEAR COMPONENTS    0.000000   0.000000    0.000000
                              ANGULAR COMPONENTS   0.000000   0.000000    0.000000



 1428.1288
          1     0.000000  -0.448609    0.000000     0.000000  -0.143952    0.000000
          2     0.000000   0.515994    0.000000     0.000000   0.571337    0.000000
          3     0.000000   0.515994    0.000000     0.000000   0.571337    0.000000
          4     0.000000   0.515994    0.000000     0.000000   0.571337    0.000000


                              LINEAR COMPONENTS    0.000000   0.000000    0.000000
                              ANGULAR COMPONENTS   0.000000   0.000000    0.000000



 3012.3790
          1     0.000000   0.000000   -0.000006     0.000000   0.000000   -0.000002
          2     0.000000   0.000000   -0.577334     0.000000   0.000000   -0.577334
          3    -0.500008   0.000000    0.288677    -0.500008   0.000000    0.288677
          4     0.500008   0.000000    0.288677     0.500008   0.000000    0.288677


                              LINEAR COMPONENTS    0.000000   0.000000    0.000000
                              ANGULAR COMPONENTS   0.000000   0.000000    0.000000



 3218.9221
          1    -0.000116   0.000000    0.334855    -0.000036   0.000000    0.102445
          2     0.000000   0.000000   -0.769371     0.000000   0.000000   -0.812213
          3     0.332922   0.000000   -0.193160     0.351461   0.000000   -0.203916
          4    -0.332521   0.000000   -0.192929    -0.351037   0.000000   -0.203672


                              LINEAR COMPONENTS    0.000000   0.000000    0.000000
                              ANGULAR COMPONENTS   0.000000   0.000000    0.000000



 3218.9230
          1    -0.334857   0.000000   -0.000116    -0.102446   0.000000   -0.000036
          2     0.000952   0.000000    0.000267     0.001005   0.000000    0.000282
          3     0.577142   0.000000   -0.332663     0.609279   0.000000   -0.351187
          4     0.577373   0.000000    0.332797     0.609523   0.000000    0.351329


                              LINEAR COMPONENTS    0.000000   0.000000    0.000000
                              ANGULAR COMPONENTS   0.000000   0.000000    0.000000
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EIGENVECTORS IN INTERNAL COORDINATES AND POTENTIAL ENERGY DISTRIBUTION


      FREQUENCY (CM-1) :     0.00          0.00          0.00          0.00
0.00          0.00


                    VECTOR  P.E.D.  VECTOR  P.E.D.  VECTOR  P.E.D.  VECTOR  P.E.D.  VECTOR
P.E.D.   VECTOR  P.E.D.


   1    C1H2           0.000   0.00   0.000   0.00   0.000   0.00   0.000   0.00
0.000   0.00   0.000   0.00
   2    C1H3           0.000   0.00   0.000   0.00   0.000   0.00   0.000   0.00
0.000   0.00   0.000   0.00
   3    C1H4           0.000   0.00   0.000   0.00   0.000   0.00   0.000   0.00
0.000   0.00   0.000   0.00
   4    SCIS           0.000   0.00   0.000   0.00   0.000   0.00   0.000   0.00
0.000   0.00   0.000   0.00
   5    ROCK           0.000   0.00   0.000   0.00   0.000   0.00   0.000   0.00
0.000   0.00   0.000   0.00
   6                   0.000   0.00   0.000   0.00   0.000   0.00   0.000   0.00
0.000   0.00   0.000   0.00


      FREQUENCY (CM-1) :  1386.03       1386.06       1428.13       3012.38
3218.92       3218.92


                    VECTOR  P.E.D.  VECTOR  P.E.D.  VECTOR  P.E.D.  VECTOR  P.E.D.  VECTOR
P.E.D.   VECTOR  P.E.D.


   1    C1H2           0.001   0.00   0.000   0.00   0.000   0.00  -0.575   0.34    -
0.863   0.66   0.000   0.00
   2    C1H3          -0.001   0.00   0.001   0.00   0.000   0.00  -0.575   0.34
0.432   0.17   0.747   0.50
   3    C1H4          -0.001   0.00  -0.001   0.00   0.000   0.00  -0.575   0.34
0.431   0.17  -0.748   0.50
   4    SCIS           0.437   0.25   0.757   0.75   0.000   0.00   0.000   0.00
0.050   0.00  -0.086   0.00
   5    ROCK           0.757   0.75  -0.437   0.25   0.000   0.00   0.000   0.00
0.086   0.00   0.050   0.00
   6                   0.000   0.00   0.000   0.00   0.928   1.00   0.000   0.00
0.000   0.00   0.000   0.00


 SYMMETRY COMPLIANCE CONSTANTS (A/MD FOR STRETCHING, RAD**2/MD.A FOR BENDING)


            1          2          3          4          5          6
   1     0.183947
   2     0.000859   0.183948
   3     0.000859   0.000859   0.183948
   4    -0.006628  -0.006625   0.013255   0.676954
   5    -0.011480   0.011480   0.000002   0.000013   0.676969
   6     0.000000   0.000000   0.000000   0.000000   0.000000   0.716462


 RELAXED PRIMARY SYMMETRY FORCE CONSTANTS (DIAGONAL ELEMENTS) AND
 INTERACTION DISPLACEMENT COORDINATES (OFF-DIAGONAL ELEMENTS)


            1          2          3          4          5          6
   1     5.436340
   2     0.004668   5.436320
   3     0.004668   0.004670   5.436320
   4    -0.009791  -0.009787   0.019580   1.477206
   5    -0.016957   0.016958   0.000004   0.000019   1.477173
   6     0.000000   0.000000   0.000000   0.000000   0.000000   1.395748
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VALENCE  COMPLIANCE CONSTANTS (A/MD FOR STRETCHING, RAD**2/MD.A FOR BENDING)


            1          2          3          4          5          6          7
  1      0.183947
  2      0.000859   0.183948
  3      0.000859   0.000859   0.183948
  4     -0.005412  -0.005410   0.010823   0.451302
  5     -0.005412   0.010823  -0.005410  -0.225644   0.451302
  6      0.010823  -0.005413  -0.005413  -0.225659  -0.225659   0.451317
  7      0.000000   0.000000   0.000000   0.000000   0.000000   0.000000   0.716462


RELAXED PRIMARY VALENCE  FORCE CONSTANTS (DIAGONAL ELEMENTS) AND
INTERACTION DISPLACEMENT COORDINATES (OFF-DIAGONAL ELEMENTS)


            1          2          3          4          5          6          7
  1      5.436340
  2      0.004668   5.436320
  3      0.004668   0.004670   5.436320
  4     -0.011991  -0.011987   0.023981   2.215809
  5     -0.011991   0.023981  -0.011987  -0.499984   2.215809
  6      0.023981  -0.011994  -0.011994  -0.500000  -0.500000   2.215736
  7      0.000000   0.000000   0.000000   0.000000   0.000000   0.000000   1.395748


***************************** THE END *****************************
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Figure 2. Sample output for the <.vib> file included in Fig. 1. Each of the related vibrational parameters is considered individually and are printed out to provide the user with significant information on the system.