

# 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 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. Schafer & D. E. Lewis, *QCPE* **1977**, 11, 339) 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.* **1971**, 55, 477). The present version is dimensioned by using the external CAM\_SIZE file, which can be edited to change the number of atoms.

```
! Header file for CAMVIB, CAMISO, LIPFR and UJISO to set array
! sizes as functions of the maximum number of atoms.
!
! 31 April 1997 - AJT
! 16 October 2016 - IHW

      parameter(MAXNAT =1000)

! These should not be touched:
      parameter(MAXNC  = MAXNAT * 3)
      parameter(MAXNI  = MAXNAT * 3 + MAXNAT / 2)
      parameter(MAXNINT= MAXNC  - 6)
      parameter(MAXDIAG= MAXNC  * (MAXNC + 1) / 2)
      parameter(MAXAPO = MAXNAT + 1)

! For CAMISO:
      parameter(MAXFCMS = MAXDIAG * 3)
      parameter(MAXXYZ  = MAXNAT * 10)
```

**Figure 1.** The CAM\_SIZE file, used to dimension the arrays in CAMVIB, LIPFR, and UJISO. Parameter MAXNAT (currently set at 1000) determines the maximum number of atoms. For most purposes a much smaller number may be chosen.

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.

I PROG - 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 rotational 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, *Theochem - J. Mol. Struct.* **1983**, 11, 275-284).

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/rad<sup>2</sup> 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*, **1983**, 105, 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.* **1982**, 88, 462-466).

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 keyword DISO is specified as an option.)

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.)

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 SECDEF calculation with the CADPAC program using the PUNCH option.

GAUS - Cartesian force constants from a Gaussian job to be read from the standard input using format (3E20.10).

6E16 - Cartesian force constants to be read from the standard input using format (6E16.8). (Not normally used now.)

GRAC - Cartesian force constants from a Grace job to be read from the standard input using format (1X, 3E20.12).

GAMS - Cartesian coordinates to be read from logical unit 73 assigned to a file generated by the GAMESS program. (Not normally used now.)

BREF - minimal printout

NOPR - skips unnecessary computation and printout when valence (or internal) coordinates are not being used in a calculation.

EXPL - symmetry coordinates are to be input explicitly (see item 11).

3.

TITLE - Format (20A4)

- anything you wish, its up to you!

4. Skip to item 5 unless keyword DISO is specified as an option.

IS, IG, IFFREQ - Format (3 I 2)

where

IS is the rotational symmetry number

IG is the electronic degeneracy

IFFREQ specifies the number of pre-calculated frequencies to be read (if desired).

5. Skip to item 6 unless keyword MASS is specified as an option. (Not normally used)

IA, IFK, X, Y, Z, WT - Format (A4, A1, 4F12.6)

where

IA is any symbol you want to denote an atom whose mass is given explicitly.

IFK is a symbol that serves no purpose in CAMVIB but is significant with program CUTOFF.

X,Y,Z are Cartesian coordinates in Ångström units, or in atomic units if BOHR is specified.

WT is a mass in atomic mass units.

\*--- 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.

Skip to item 8 if keyword MASS is specified as an option.

6.

IA, IFK, X, Y, Z - Format (A4, A1, 3E20.10)

where

IA is any symbol you want to denote an atom whose mass is given explicitly.

IFK is a symbol that serves no purpose in CAMVIB but is significant with program CUTOFF.

X,Y,Z are Cartesian coordinates in Ångström units, or in atomic units if BOHR is specified.

\*--- ends this section of the data. (N.B. this is a special value for the symbol IA.)

7. (Not normally used)

If keyword AMPA (for AMPAC) is specified as an option, 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.

TIME, IPT, REFH (Unformatted) – these serve no purpose in CAMVIB

X, Y, Z are Cartesian coordinates in Ångström units, one line for each atom specified in item 6.

Skip to item 10.

8. (Not normally used)

If keyword GAMS (for GAMESS) is specified as an option, then only the isotopic symbols IA are required (one per line): the Cartesian coordinates are read from logical unit 73 and the contents of the present X, Y and Z fields are overwritten.

X, Y, Z are Cartesian coordinates in Ångström units, one line for each atom specified in item 6.

Skip to item 10.

9. (Not normally used)

If keyword CADP (for CADPAC) is 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.

CADTIT – Format(A76) – is a title

SHDG – Format(IX,A4) – is a subheading with the value 'GEOM'

X, Y, Z are Cartesian coordinates in Ångström units, one line for each atom specified in item 6.

SHDG – Format(IX,A4) – is a subheading with the value 'GRAD'

Gx, Gy, Gz – Format(IX,3E20.12) – are components of the gradient, one line for each atom specified in item 6.

SHDG – Format(IX,A4) – is a subheading with the value 'CART'

10. Skip to item 11 unless any of the keywords VALE, REDU, SYMM, ININ, or INSY is specified as an option.

Specification of valence coordinates and implicit symmetry coordinates, one lines for each coordinate.

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

where

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.* **1978**, 56, 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<sub>2</sub>. 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.* **1979**, 55, 147-150; I. H. Williams, *J. Mol. Spectrosc.* **1977**, 66, 288-301) 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.

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  $\text{SQRT}(\text{SF}(i)*\text{SF}(j))$ . This is equivalent to the scaling procedure recommended by Pulay (JACS **1983**, *105*, 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 6. 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 10) 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 10.

\* - ends this section of the data.

11. Skip to item 12 unless any of the keywords REDU, SYMM, or INSY are specified as options.

WORD, IROW(1).....IROW(NI) - Format(A4, 30I2)

*[If necessary, up to four more continuation lines may be supplied:*

*IROW(1).....IROW(NI) - Format(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.  $X-CH_2-Y$ .

TET3 generates coordinates appropriate for methyl-like centre, e.g.  $X-CH_3$  ;

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- - - - - I \_ I \_ I.

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

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.* **1982**, 88, 462-466; D. Spangler, I. H. Williams, G. M. Maggiora, *J. Comput. Chem.* **1983**, 4, 524-541; J. S. Francisco & I. H. Williams, *Mol. Phys.* **1984**, 52, 743-748.

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.

These valence coordinates should be in the order A-C-E1, A-C-E2, A-C-E3, A'-C-E1, 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  $[\text{H}_2\text{O}-\text{CH}_3-\text{OH}_2]^+$  (I. H. Williams, *Bull. Soc. Chim. Belg.* **1982**, 91, 356) and  $[\text{H}_3\text{N}-\text{CH}_3-\text{NH}_3]^+$  (I. H. Williams, *JACS* **1984**, 106, 7206-7212).

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.* **1985**, 95, 373). *Not available in this version of CAMVIB.*

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 3012 to complete the array IROW if NI is  $\leq 60$ ,  $\leq 90$ ,  $\leq 120$  or  $\leq 140$  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.

I2. Skip to item I3 unless ININ or INSY is specified.

(Not normally used.)

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

where

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  $\text{md}/\text{\AA}$ ,  $\text{md}\cdot\text{\AA}/\text{rad}^2$ , etc.) generated by a prior run of CAMVIB with OUTI or OUTS specified.

Skip to item I4.



13.

E(1).....E(NFC) - Format (6E12.8) – unless an alternative format is specified, as below.

where

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<sup>2</sup>), as computed by an electronic structure code such as GAUSSIAN, CADPAC or GAMESS.

If keyword GAUS (for GAUSSIAN) is specified as an option, then the format is (3E20.10).

If keyword GRAC (for GRACE) is specified as an option, then the format is (1X, 3E20.12).

If keyword 6E16 is specified as an option, then the format is (6E16.8).

14.

Skip to item 16 unless keyword OBSD is specified as an option.

IFR(1).....IFR(NINT) - Format (20I4)

where

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.

15.

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

where

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<sup>-1</sup>.

16. Go to item 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 a file containing coordinate and Hessian information, for example, the *fort.7* file output from a calculation in Gaussian with the keywords *punch=(coord,derivatives)* specified. Due to the nature of the script, it can be used with output from numerous electronic structure codes, only requiring minor editing in some circumstances.

*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)

[illegible]

**Figure 2.** Sample input file for CAMVIB. This structure is a simple methyl cation, with four atoms. The labels after each of the bond-stretching valence coordinates serve only to clarify the output (FULL) of force constants (IFCS) and normal modes (VECT) in the valence-coordinate representation. The Cartesian coordinates and Hessian were obtained from a Gaussian calculation (GAUS) and output from this calculation will be used by UJISO or LIPFR (DISO). Owing to the trigonal planar geometry of this system, the three in-plane H-C-H angles are not independent. There is a local redundancy, which is eliminated by the use of symmetry combinations (rocking and scissoring) generated implicitly in consequence of the keyword REDU and the significant label TRIG after each of these valence coordinates. The sixth independent internal coordinate is the out-of-plane wagging coordinate. Relaxed force constants (and compliance constants) are calculated (RELX).

## 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
no scaling factors specified, so default = 1.0

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 :

0.000000000  0.000000000  0.000000000  1.000000000  1.000000000  1.000000000  0.000000000

elimination of local redundancy: all 3 HCH angles cannot increase together

SYMMETRY COORDINATES SPECIFIED IMPLICITLY

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

      R      1      2      3      4      5      6
      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	0.020702	0.000000	0.000000
12	-0.123706	0.000000	-0.130272	-0.021041	0.000000	-0.002573	0.012344	0.000000	0.012490
10	0.273242								
11	0.000000	0.020702							
12	0.132403	0.000000	0.120355						

## 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	
non-zero values indicate a combination of translational and rotational motion								
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	

continued...

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
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
<b>zero values indicate pure vibrational motion</b>							
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

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	ClH2	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	ClH3	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	ClH4	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	ClH2	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	ClH3	-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	ClH4	-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							
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 *****													

**Figure 3.** Annotated sample output file for CAMVIB calculation on methyl cation corresponding to the input file shown in Figure 2.