

Supporting Information

Substitutional Control of Non-statistical Dynamics in the Thermal Deazetization of Tetracyclic Azo compounds

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1. Table S1: Relative reaction free energies, activation free energies at 298.15 K (in kcal/mol) for (*a* –*o*) at different levels of theory.

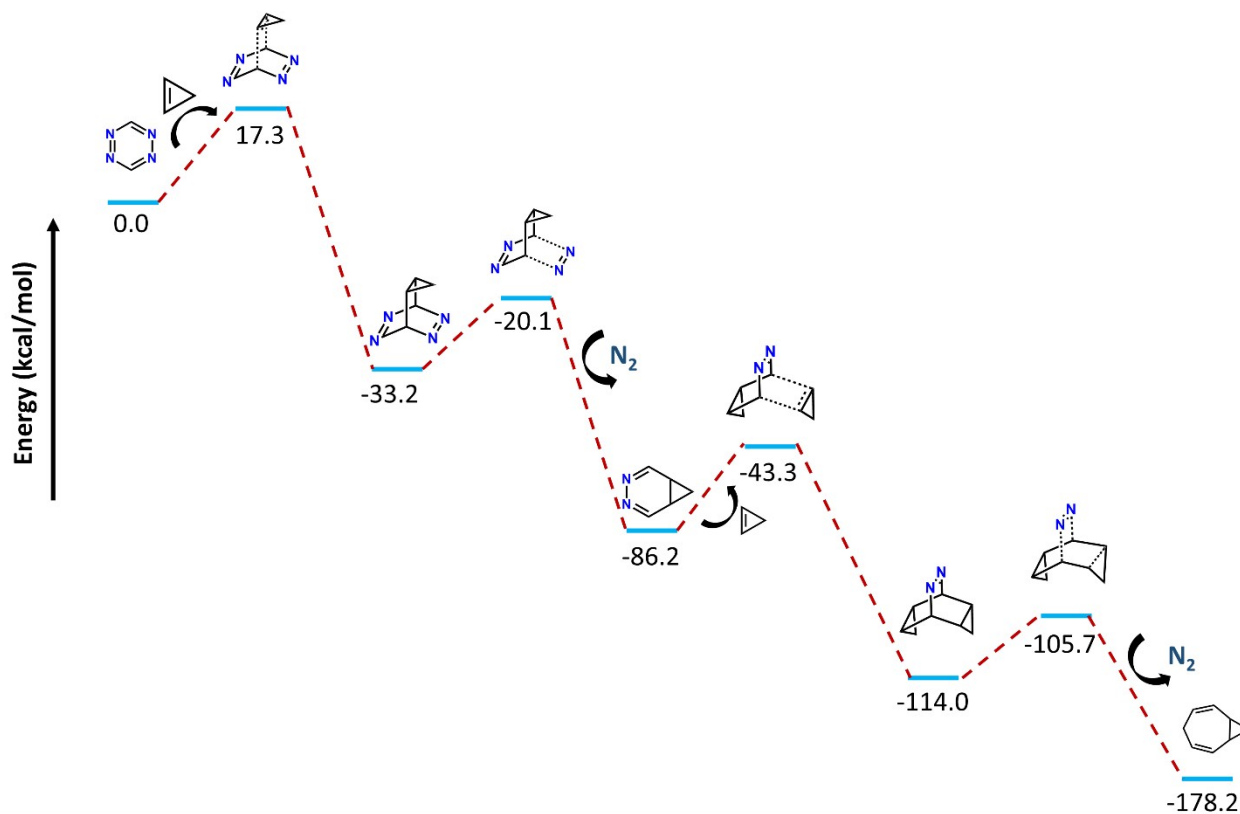
Level of Theory	Molecule	$\Delta G^\ddagger$ (kcal/mol)	ΔG_4 (kcal/mol)	ΔG_5 (kcal/mol)	$\Delta G_{4 \rightarrow 5}^\ddagger$ (kcal/mol)
B3LYP/6-31G(d) D3	a	3.4	-72.9	-72.9	22.7
B3LYP/6-31+G(d,p) D3		3.4	-76.0	-76.0	22.0
M062X/6-31G(d)		8.3	-64.2	-64.2	16.2
M062X/6-31+G(d,p)		8.2	-66.8	-66.8	16.2
DLPNO-CCSD(T)/def2-TZVP		6.5	-59.2	-59.2	15.1
B3LYP/6-31G(d) D3	b	3.1	-73.2	-71.6	21.8
B3LYP/6-31+G(d,p) D3		3.2	-76.1	-74.6	21.4
M062X/6-31G(d)		7.7	-66.4	-65.6	16.1
M062X/6-31+G(d,p)		7.7	-65.8	-64.9	15.9
DLPNO-CCSD(T)/def2-TZVP		6.0	-58.0	57.8	15.0
B3LYP/6-31G(d) D3	c	3.8	-71.2	-69.6	26.4
B3LYP/6-31+G(d,p) D3		3.9	-73.8	-72.8	25.8
M062X/6-31G(d)		8.4	-65.0	-63.5	16.2
M062X/6-31+G(d,p)		8.5	-67.0	-66.0	15.8
DLPNO-CCSD(T)/def2-TZVP		6.3	-56.5	-56.5	14.1
B3LYP/6-31G(d) D3	d	4.4	-70.5	-69.6	25.0
B3LYP/6-31+G(d,p) D3		4.4	-73.5	72.9	24.4
M062X/6-31G(d)		9.1	-64.0	-63.3	17.1
M062X/6-31+G(d,p)		9.0	-66.4	-66.0	16.8
DLPNO-CCSD(T)/def2-TZVP		7.0	-56.5	-56.8	15.2
B3LYP/6-31G(d) D3	e	3.1	-76.1	-71.4	25.0
B3LYP/6-31+G(d,p) D3		3.2	-78.6	-74.6	24.7
M062X/6-31G(d)		7.6	-68.4	-65.2	19.2
M062X/6-31+G(d,p)		7.7	-70.2	-67.7	18.4
DLPNO-CCSD(T)/def2-TZVP		6.0	-60.0	-57.9	17.9
B3LYP/6-31G(d) D3	f	2.4	-82.5	-73.8	28.4
B3LYP/6-31+G(d,p) D3		2.5	-85.0	-77.3	28.0
M062X/6-31G(d)		6.6	-77.3	-67.3	24.3
M062X/6-31+G(d,p)		6.7	-79.0	-70.1	24.0
DLPNO-CCSD(T)/def2-TZVP		5.2	-67.8	-60.5	22.7
B3LYP/6-31G(d) D3	g	3.2	-72.6	-70.4	23.3
B3LYP/6-31+G(d,p) D3		3.3	-75.0	-67.4	22.6
M062X/6-31G(d)		7.7	-66.7	-64.3	18.2
M062X/6-31+G(d,p)		7.7	-68.5	-66.7	17.7
DLPNO-CCSD(T)/def2-TZVP		5.7	-59.0	-57.3	16.6

B3LYP/6-31G(d) D3	h	3.2	-76.9	-68.4	27.1
B3LYP/6-31+G(d,p) D3		3.2	-78.9	-71.6	26.1
M062X/6-31G(d)		7.7	-70.5	-62.7	20.1
M062X/6-31+G(d,p)		7.7	-72.1	-65.3	19.3
DLPNO-CCSD(T)/def2-TZVP		5.9	-61.8	-55.3	17.5
B3LYP/6-31G(d) D3	i	3.4	-70.6	-69.4	22.9
B3LYP/6-31+G(d,p) D3		3.5	-73.3	-72.5	22.2
M062X/6-31G(d)		8.0	-64.4	-63.3	17.2
M062X/6-31+G(d,p)		8.0	-66.5	-65.7	16.8
DLPNO-CCSD(T)/def2-TZVP		6.1	-56.7	-56.4	15.7
B3LYP/6-31G(d) D3	j	3.8	-71.9	-66.6	26.5
B3LYP/6-31+G(d,p) D3		3.8	-74.4	-70.0	25.6
M062X/6-31G(d)		8.5	-65.2	-60.6	18.7
M062X/6-31+G(d,p)		8.3	-67.3	-63.4	18.2
DLPNO-CCSD(T)/def2-TZVP		6.6	-56.7	53.6	16.2
B3LYP/6-31G(d) D3	k	3.2	-74.9	-70.9	21.0
B3LYP/6-31+G(d,p) D3		3.2	-77.5	-74.0	20.5
M062X/6-31G(d)		7.8	-68.2	-65.0	16.5
M062X/6-31+G(d,p)		7.9	-70.1	-67.4	16.2
DLPNO-CCSD(T)/def2-TZVP		5.9	-57.6	-57.8	12.5
B3LYP/6-31G(d) D3	l	2.7	-81.7	-70.70	25.1
B3LYP/6-31+G(d,p) D3		2.7	-84.0	-73.7	24.7
M062X/6-31G(d)		7.5	-74.1	-64.9	18.5
M062X/6-31+G(d,p)		7.4	-75.9	-67.3	18.3
DLPNO-CCSD(T)/def2-TZVP		5.8	-64.3	-57.2	15.9
B3LYP/6-31G(d) D3	m	1.4	-83.4	-71.4	31.1
B3LYP/6-31+G(d,p) D3		2.3	-86.5	-75.0	30.5
M062X/6-31G(d)		6.6	-76.7	-65.6	21.9
M062X/6-31+G(d,p)		6.7	-78.8	-68.3	21.8
DLPNO-CCSD(T)/def2-TZVP		5.2	-65.6	-58.8	18.8
B3LYP/6-31G(d) D3	n	5.7	-72.8	-67.5	34.0
B3LYP/6-31+G(d,p) D3		3.9	-77.2	-72.9	33.1
M062X/6-31G(d)		10.6	-66.5	-62.2	15.4
M062X/6-31+G(d,p)		11.1	-67.8	-64.3	14.6
DLPNO-CCSD(T)/def2-TZVP		8.4	-56.4	-56.1	11.1
B3LYP/6-31G(d) D3	o	4.8	-75.0	-61.0	33.3
B3LYP/6-31+G(d,p) D3		4.8	-78.1	-64.2	32.9
M062X/6-31G(d)		10.0	-67.4	-54.7	16.5
M062X/6-31+G(d,p)		9.3	-70.5	-57.9	16.0
DLPNO-CCSD(T)/def2-TZVP		7.8	-58.9	-47.5	13.2

* ΔG is exactly equal to sum of the electronic energy and thermal correction to Gibbs Free energy.
Here for DLPNO- CCSD(T) calculation, the thermal correction to Gibbs Free energies are calculated

by M062X/6-31G(d) level of theory and later combined with electronic energies are calculated by DLPNO-CCSD(T) level of theory. ¹

2. Figure S1: Relative free-energy (ΔG) at 298.15 K for **1a**→**4a,5a** at M06-2X/6-31G(d) level of theory.



3. NBO Analyses:

a. Table S2: %s character of different bonds (involved in transition-state structure) for **3(a-d)** at M062X/6-31G(d) level of theory.

Molecule	%s character for C1-N6	%s character for C2-N5
3a	21.52	21.52
3b	21.35	21.17
3c	21.68	21.65
3d	21.84	21.77

b. Table S3: %s character of different bonds (in cyclopropane ring and adjacent to functional group) for **4(a-d)** and **5(a-d)** at M062X/6-31G(d) level of theory.

Molecule	%s character for C4-C9	%s character for C11-C12
4a	29.70	20.59
5a	29.70	20.59
4b	30.89	21.15
5b	29.92	21.60
4c	28.72	21.57
5c	29.70	21.83
4d	29.08	21.97
5d	29.70	22.04

c. Table S4: %s character of different bonds (ring opening bond) for **TS(a-o)** at M062X/6-31G(d) level of theory.

Molecule	%s character for C3-C4	%s character for C10-C11
TS-a	14.42	14.42
TS-b	14.51	14.47
TS-m	12.70	14.98
TS-c	14.65	14.42
TS-n	12.22	14.93
TS-d	14.89	14.47
TS-o	14.08	15.07
TS-e	15.49	14.71
TS-f	15.10	15.20
TS-g	15.41	14.69
TS-h	14.92	14.93
TS-i	14.48	14.45
TS-j	14.31	14.31
TS-k	14.41	13.29
TS-l	11.99	14.68

6. Implicit solvation study:

Absolute energies, enthalpies, free energies, entropies and lowest frequencies of relevant calculated structures.

a. Table S5: For **3a**→**4a/5a** reaction in gas phase at M062X/6-31G(d).

Structure	E _{elec} (Hartree)	E _{elec} + ZPE (Hartree)	H (Hartree)	S (cal mol ⁻¹ K ⁻¹)	G (Hartree)	Lowest Freq (cm ⁻¹)
3a	-420.0586475	-419.886205	-419.878315	81.943	-419.917249	53.67
TS-a	-420.041987	-419.873403	-419.865182	81.918	-419.904104	-528.70
4a/5a	-310.6482346	-310.488875	-310.481242	80.343	-310.519416	130.53
TS_{4a→5a}	-310.6217976	-310.463693	-310.456543	77.864	-310.493539	-409.60
N₂	-109.4874243	-109.481628	-109.478323	45.762	-109.500066	2544.22

b. Table S6: For **3a**→**4a/5a** reaction in water (PCM model) at M062X/6-31G(d).

Structure	E _{elec} (Hartree)	E _{elec} + ZPE (Hartree)	H (Hartree)	S (cal mol ⁻¹ K ⁻¹)	G (Hartree)	Lowest Freq (cm ⁻¹)
3a	-420.0661948	-419.893849	-419.885920	82.823	-419.925272	34.23
TS-a	-420.0477213	-419.879324	-419.871077	82.007	-419.910041	-524.58
4a/5a	-310.6515847	-310.492388	-310.484766	80.256	-310.522898	135.30
TS_{4a→5a}	-310.6255993	-310.467628	-310.460482	77.842	-310.497467	-408.24
N₂	-109.4878008	-109.482001	-109.478696	45.761	-109.500439	2545.82

c. Table S7: $3(a-o) \rightarrow 4(a-o)/5(a-o)$ reaction in water (SMD model) at M062X/6-31G(d).

Molecule	$\Delta G^\ddagger$ (kcal/mol)	ΔG_4 (kcal/mol)	ΔG_5 (kcal/mol)	$\Delta G_{4 \rightarrow 5}^\ddagger$ (kcal/mol)
a	11.6	-56.4	-56.4	16.0
b	11.4	-58.7	-58.6	15.3
c	11.6	-58.4	-56.0	16.1
d	11.9	-58.5	-56.9	16.9
e	11.3	-59.6	-56.7	18.6
f	9.7	-68.2	-59.3	23.0
g	11.5	-58.4	-55.8	18.1
h	11.0	-62.7	-54.7	20.0
i	11.7	-56.9	-55.4	17.0
j	11.6	-58.8	-53.7	16.5
k	11.4	-56.5	-60.0	12.4
l	10.4	-67.4	-57.0	18.5
m	10.6	-70.5	-56.4	23.6
n	11.4	-61.3	-56.2	14.7
o	12.5	-62.9	-46.7	19.7

d. Table S8: $3(a-o) \rightarrow 4(a-o)/5(a-o)$ reaction in benzene (SMD model) at M062X/6-31G(d).

Molecule	$\Delta G^\ddagger$ (kcal/mol)	ΔG_4 (kcal/mol)	ΔG_5 (kcal/mol)	$\Delta G_{4 \rightarrow 5}^\ddagger$ (kcal/mol)
a	10.9	-65.8	-65.8	16.5
b	8.8	-63.2	-61.5	16.4
c	9.2	-61.9	-59.8	16.6
d	10.0	-61.0	-59.5	17.4
e	8.5	-64.9	-61.4	19.6
f	7.3	-73.6	-63.9	24.1
g	8.7	-63.0	-60.4	18.5
h	8.4	-67.4	-59.2	20.2
i	8.9	-61.0	-59.5	17.5
j	9.3	-62.4	-57.2	19.1
k	8.7	-64.8	-61.1	16.5
l	8.1	-72.0	-61.4	18.8
m	7.5	-73.7	-61.6	22.4
n	9.4	-64.3	-56.8	16.5
o	9.0	-66.6	-52.2	16.9

e. Table S9: $3(a-o) \rightarrow 4(a-o)/5(a-o)$ reaction in chloroform (SMD model) at M062X/6-31G(d).

Molecule	$\Delta G^\ddagger$ (kcal/mol)	ΔG_4 (kcal/mol)	ΔG_5 (kcal/mol)	$\Delta G_{4 \rightarrow 5}^\ddagger$ (kcal/mol)
a	8.6	-60.0	-60.0	16.3
b	9.4	-61.8	-59.9	16.2
c	9.7	-60.9	-58.5	16.4
d	10.4	-60.2	-58.6	17.3
e	9.1	-63.1	-60.0	19.1
f	7.8	-72.0	-62.6	23.7
g	9.3	-61.6	-58.9	18.3
h	8.9	-66.0	-57.9	19.9
i	9.5	-59.8	-58.3	17.3
j	9.9	-61.3	-56.1	19.0
k	9.3	-63.5	-59.7	16.4
l	8.6	-70.9	-60.0	18.7
m	9.0	-72.6	-60.0	22.6
n	10.0	-65.1	-57.4	16.3
o	9.6	-65.6	-50.6	17.7

7. Table S10: Relative activation free energies at 298.15 K (in kcal/mol) for $3(a-d)$ and $3^\#(a-d)$ M06-2X/6-31G(d) level of theory.

Molecule	$\Delta G^\ddagger$ (kcal/mol)
3a	8.3
3[#]a	68.4
3b	7.7
3[#]b	65.5
3c	8.4
3[#]c	67.8
3d	9.1
3[#]d	64.1

8. QCT Inputs:

The reaction trajectories were simulated using ProgDyn-Gaussian16 interface from the sampled transition-states TS structures at 298.15 K. The energies and derivatives were calculated on the fly with M06-2X/6-31G(d) level.

The typical input file for reaction trajectory simulations is shown below:

c. ProgDyn.conf:

```
#This is the configuration file for PROGDYN. This file is read by progdynstarterHP and
# the awk programs proggenHP, prog1stpoint, prog2ndpoint, and progdynb.
#The programs won't read anything past the first blank line,
#and this file must end with a blank line.
```

```

#The program has a number of default values but they are unlikely to be what you want.
#Do not delete lines - rather, comment out lines for unwanted options.
#The values here are read repeatedly and most can be changed in the middle of running jobs
***The keywords are case sensitive. The following keywords should always be defined:***
***method, charge, multiplicity, memory, processors, title
*** method --The following word is copied exactly to the gaussian input file.
method m062x/6-31g(d)
#To do a nonstandard route, make nonstandard 1. For normal calcs, use nonstandard 0 or else
leave it out.
#Then make a file called "nonstandard" containing the nonstandard route with no extra lines.
#nonstandard 0
# NMRoptions As is NMRtype=1 will add a section for an NMR calc at every NMRevery
intervals. If you want to combine the two use nonstandard
#NMRtype 1
#NMRmethod2 B97D/6-31G*
#NMRmethod LC-wPBE/6-31G*
#NMRmethod3 B3LYP/cc-pvtz
#NMRevery 4
#NMRrand 1
#NMRcc 1
#loadlimit 10.0
#geometry linear
#rotationmode 0
*** method2 --The options here are restricted, unrestricted, and read. restricted is the default
#If the method is U..., put unrestricted here and the .com files will have in them guess=mix.
#If you put read here, the .com files will contain guess=tcheck, which sometimes makes
things faster, sometimes not.
#The use of read requires a specifically defined checkpoint file name using the keyword
checkpoint.
method2 restricted
charge 0
multiplicity 1
#onionchargemult 1 1
processors 24
*** memory --The following "word" is copied exactly to the gaussian input file after
%mem=.
memory 8gb
*** killcheck and checkpoint -- You can use a specifically defined checkpoint file name by
putting
#the name after the keyword checkpoint. This is necessary if you use the read option with
method2.
#Defined checkpoint names are an unnecessary modest hassle and if you do not want to
bother, use killcheck 1
killcheck 1
checkpoint gl6.chk
*** diagnostics -- 0 prints out nothing extra, 1 (default) prints out extra stuff to a
#file "diagnostics", 2 adds more stuff, 3 adds velocities to a file "vellist"
#4 adds the apparent temperature to vellist, but this is meaningless with quasiclassical
calculations
diagnostics 0
*** title -- the title keyword must be followed by exactly four words

```

```

title deazitation reaction dynamics study
*** initialdis -- 0 (default) turns off displacement of the normal modes, so that all
trajectories start from the same place
# and only the energies and signs of the motion in the modes are randomized
# 1 gives a flat distribution of displacements where all of the possible values are equally
likely
# 2 (recommended) gives a QM-like gaussian distribution of displacements, so that
displacements in the middle are more likely than
# those at the end by 1/e
initialdis 2
*** timestep -- this is the time between points in the trajectory. Typical values would be
1E-15 or 0.5E-15 or 0.25E-15
timestep 1E-15
*** scaling -- this lets you scale the gaussian frequencies by a constant
scaling 1.0
temperature 298.15
*** thermostat 1 puts in a damping factor so as to bring the classical temperature toward the
desired temperature.
*** use a thermostatmult between 0.95 and 1, typically 0.995, so the damping happens
slowly - otherwise there will be
*** overadjustment in response to random variation
*** the thermostat is not exact. The second traj point ignores this, so it only applies to later
points handled by progdynb.
#thermostat 1
#thermostatmult 0.999
*** method3, method4, method5, and method6 -- These keywords let you add extra lines to
the gaussian input file.
#method3 and method4 add lines at the top of the input after the lines defining the method,
and
#this is useful to implement things like the iop for mPW1k
#method5 and method6 add lines after the geometry, after a blank line of course
#only a single term with no spaces can be added, one per method line. Here are some
examples to uncomment if needed
#method3 IOp(3/76=0572004280)
#method3 scrf=(pcm,solvent=ethanol)
#method3 scrf=(pcm,Solvent=dichloromethane)
#method3 empiricaldispersion=gd3
#add the line below with big structures to get it to put out the distance matrix and the input
orientation
#method4 iop(2/9=2000)
#method3 scf=(conver=5)
#method4 iop(3/124=3)
#method4 scrf=(pcm,solvent=dmsol,read)
#method5 radii=bondi
#method6
*** methodfile -- This keyword lets you add more complicated endings to gaussian input
files
#such as a gen basis set. Put after the keyword the number of lines in a file you create called
#methodfile that contains the test you want to add to the end of the gaussian input
methodfile 0

```

```

*** numimag --This tells the program the number of imaginary frequencies in the starting
structure.
#if 0, treats as ground state and direction of all modes is random
#if 1, motion along the reaction coordinate will start out in the direction defined by searchdir
#if 2, only lowest freq will go direction of searchdir and other imag mode will go in random
direction
numimag 1
*** searchdir -- This keyword says what direction to follow the mode associated with the
imaginary frequency.
#The choices are "negative" and "positive". Positive moves in the direction defined in the
gaussian frequency calculation
#for the imaginary frequency, while negative moves in the opposite direction. The correct
choice can be made either
#by a careful inspection of the normal modes and standard orientation geometry, or by trial
and error.
searchdir positive
*** classical -- for quassiclassical dynamics, the default, use 0. for classical dynamics, use
1
#if there are no normal modes and the velocities are to be generated from scratch, use
classical 2
classical 0
*** DRP, saddlepoint, and maxAtomMove --to run a DRP use 'DRP 1' in the line below,
otherwise leave it at 0 or comment it out
#the treatment of starting saddlepoints is not yet implemented so use saddlepoint no
#if DRP shows oscillations then decrease maxAtomMove
#DRP 1
#saddlepoint no
#maxAtomMove 0.01
*** cannonball -- The program can "fire" a trajectory from a starting position toward a
particular target, such as toward
#a ts. To use this, make a file cannontraj with numAtom lines and three numbers per line that
defines the vector
#for firing the trajectory, relative to the starting geometry's standard orientation. The number
following cannonball sets
#the extra energy being put into the structure in kcal/mol
#cannonball 10
*** keepevery --This tells the program how often to write the gaussian output file to file
dyn, after the first two points.
#Use 1 for most dynamics to start with, but use a higher number to save on disk space or
molden loading time.
keepevery 1
*** highlevel --For ONIOM jobs, the following line states the number of highlevel atoms,
#which must come before the medium level atoms. Use some high value such as 999 if not
using ONIOM
#highlevel 9999
*** fixedatom1, fixedatom2, fixedatom3, and fixedatom4 - These fix atoms in space.
#Fixing one atom serves no useful purpose and messes things up, while fixing two atoms
#fixes one distance and fixing three has the effect of fixing three distances, not just two
#in current form fixed atoms only are meant to work with no displacements, that is,
initialdis=0
#fixedatom1 16

```

```

#fixedatom2 1
#fixedatom3 4
#fixedatom4 20
#applyforce 1 lets one push atoms together or apart - a positive force pushes them together
#format is applyforce force - with the units on force the same as in the Gaussian output file
#applyforce 2 or 3 or 4 applies a polynomial force centered at dist0. 2 is just harmonic, 3 is
second order, 4 is third order
#format is applyforce 4 forcecoefficient dist0 forcecoefficient2 forcecoefficient3
#then use afatoms to choose the atoms with format afatoms firstatom secondatom [additional
atoms]
#applyforce 2 0.1 2.1
#afatoms 16 1 2 3 4 5 6
#applyforceB 2 0.01 5.2
#afatomsB 8 15
#applyforceC 2 0.01 5.2
#afatomsC 8 15
#zeroatom pushes the numbered atom toward the origin with a small harmonic potential -
good with boxon when you want to keep the reaction in the center
#zeroatom 16
*** boxon and boxsize - With boxon 1, a cubic box is set such that atoms that reach the edge
#are reflected back toward the middle. Useful for dynamics with solvent molecules. This is a
crude
#implementation that is ok for a few thousand femtoseconds but will not conserve energy
long term.
#Set the box size so as to fit the entire initial molecule but not have too much extra room.
#The dimensions of the box are two times the boxsize, e.g. boxsize 7.5 leads to a box that is
15 x 15 x 15 angstroms
#boxon 1
#boxsize 11.2
*** sphereon and spheresize and sphereforce - uses a force to push atoms within a sphere.
notice that if the atom is far outside of
#the sphere then the force is large unless sphereforce is set small
#sphereon 1
#spheresize 12.9
#sphereforce .01
#setting a value for empiricaldispersion sets its s6 value with the Grimme 2006 algorithm.
Default is 0, with no empiricaldispersion
#empiricaldispersion 0.0
*** displacements -- This keyword lets you set the initialdis of particular modes by using a
series of lines of the format
# displacements NumberOfMode InitialDisForThatMode, as in the example below. You
should be able to do as many of these as you like
# you might consider this for rotations where a straight-line displacement goes wrong at large
displacements
# The choices for InitialDisForThatMode are 0, 1, 2, and 10, where 10 does the same thing as
0 but is maintained for now because
# a previous version of the program had a bug that made 0 not work.
#displacements 2 0
#displacements 3 0
#displacements 4 0
#displacements 5 0

```

```

#displacements 6 0
#displacements 7 0
#displacements 8 0
#displacements 9 0
#displacements 10 0
*** etolerance --This sets the allowable difference between the desired energy in a trajectory
and the actual
#energy, known after point 1 from the potential energy + the kinetic energy in the initial
velocities.
#The unit is kcal/mol and 1 is a normal value for mid-sized organic systems. For very large
and floppy molecules, a larger value
#may be needed, but the value must stay way below the average thermal energy in the
molecule (not counting zpe).
#If initialdis is not 0 and few trajectories are being rejected, decrease the value.
etolerance 1
*** controlphase --It is sometimes useful to set the phase of particular modes in the
initialization of trajectories.
#The format is controlphase numberOfModeToControl positive or controlphase
numberOfModeToControl negative.
#controlphase 2 positive
*** damping -- The damping keyword lets you add or subtract energy from the system at
each point, by multiplying the velocities
#by the damping factor. A damping of 1 has no effect, and since you mostly want to change
the energy slowly, normal values range
#from 0.95 to 1.05. The use of damping lets one do simulated annealing - you add energy
until the structure is moving enough
#to sample the kinds of possibilities you are interested in, then you take away the energy
slowly.
damping 1.000
#at a damping of .9995, the energy is cut in half in 693 points
*** reversetraj --This keyword sets the trajectories so that both directions from a transition
state are explored.
reversetraj true

#updated Aug 9, 2007 to include the possibility of classical dynamics by the keyword
classical
#updated Jan 2008 to include fixed atoms, ONIOM jobs, keepevery, and box size
#update Feb 2008 to include methodfile parameter
# updated Nov 2008 to allow for start without an initial freq calc using classical = 2
# update Aug 2010 to include etolerance, damping controlphase and reversetraj

```

d. Proganal Code: (for TS-a)

```

BEGIN {
firsttitle=1
getline < "isomernumber"
isomer=$1
}
/ deazitation / {

```



```

# if ((C1C2<2.95) && (C3C4<2.01) && (C10C11<2.01) && (C1N6>2.7) &&
(C2N5>2.7)){
#   print "ts_2 formed XXXX"
#   }
  system("date '+%b:%d:%Y %T'")
  system("tail -1 Echeck | grep XXXX")
}

function Distance(Atom1,Atom2) {
  return sqrt((A[Atom1]-A[Atom2])^2 + (B[Atom1]-B[Atom2])^2 + (C[Atom1]-
C[Atom2])^2)
}

function Angle(Atom1,Atom2,Atom3) {
  value=((
Distance(Atom1,Atom3)^2+Distance(Atom1,Atom2)^2+Distance(Atom2,Atom3)^2)/(2*Dist
ance(Atom1,Atom2)*Distance(Atom2,Atom3)))
  return acos(value)
}

function asin(x) { return (180/3.141592)*atan2(x, sqrt(1-x*x)) }

function acos(x) { return (180/3.141592)*atan2(sqrt(1-x*x), x) }

function atan(x) { return (180/3.141592)*atan2(x,1) }

function Dihedral(Atom1,Atom2,Atom3,Atom4) {
  B1x=A[Atom2]-A[Atom1]
  B1y=B[Atom2]-B[Atom1]
  B1z=C[Atom2]-C[Atom1]
  B2x=A[Atom3]-A[Atom2]
  B2y=B[Atom3]-B[Atom2]
  B2z=C[Atom3]-C[Atom2]
  B3x=A[Atom4]-A[Atom3]
  B3y=B[Atom4]-B[Atom3]
  B3z=C[Atom4]-C[Atom3]
  modB2=sqrt((B2x^2)+(B2y^2)+(B2z^2))
# yAx is x-coord. etc of modulus of B2 times B1
  yAx=modB2*(B1x)
  yAy=modB2*(B1y)
  yAz=modB2*(B1z)
# CP2 is the crossproduct of B2 and B3
  CP2x=(B2y*B3z)-(B2z*B3y)
  CP2y=(B2z*B3x)-(B2x*B3z)
  CP2z=(B2x*B3y)-(B2y*B3x)
  termY=((yAx*CP2x)+(yAy*CP2y)+(yAz*CP2z))
# CP is the crossproduct of B1 and B2
  CPx=(B1y*B2z)-(B1z*B2y)
  CPy=(B1z*B2x)-(B1x*B2z)
  CPz=(B1x*B2y)-(B1y*B2x)
  termX=((CPx*CP2x)+(CPy*CP2y)+(CPz*CP2z))
}

```

```

dihed4=(180/3.141592)*atan2(termY,termX)
return dihed4
}

function killdyn(isomer) {
  system("rm -f dyn")
}

```

9. Optimized cartesian coordinates and harmonic frequencies at M062X/6-31G(d):

3a

C	0.00000000	1.24592000	0.37449800
C	0.00000000	-1.24592000	0.37449800
C	-1.31530000	-0.75553600	-0.21318300
C	-1.31530000	0.75553600	-0.21318300
N	0.00000000	-0.61462600	1.78355100
N	0.00000000	0.61462600	1.78355100
H	0.00000000	2.32373600	0.53010800
H	0.00000000	-2.32373600	0.53010800
C	-1.53159700	0.00000000	-1.49266300
C	1.31530000	-0.75553600	-0.21318300
C	1.31530000	0.75553600	-0.21318300
C	1.53159700	0.00000000	-1.49266300
H	-2.56667700	0.00000000	-1.82026900
H	-0.84248900	0.00000000	-2.31748600
H	-2.17864100	1.27278500	0.19498300
H	-2.17864100	-1.27278500	0.19498300
H	2.17864100	-1.27278500	0.19498300
H	2.17864100	1.27278500	0.19498300
H	2.56667700	0.00000000	-1.82026900
H	0.84248900	0.00000000	-2.31748600

Low frequencies (cm⁻¹): 53.67, 301.16, 360.52, 364.60, 406.66, 480.29, 585.39, 635.88, 654.72, 655.70

TS-a

C	-1.31913500	0.00000000	0.22254600
C	1.31913500	0.00000000	0.22254600
C	0.79330800	-1.28067100	-0.25271600
C	-0.79330800	-1.28067100	-0.25271600
N	0.58051700	0.00000000	1.97735100
N	-0.58051700	0.00000000	1.97735100
H	-2.34653000	0.00000000	0.56427100
H	2.34653000	0.00000000	0.56427100

C	0.00000000	-1.54506200	-1.49501300
C	0.79330800	1.28067100	-0.25271600
C	-0.79330800	1.28067100	-0.25271600
C	0.00000000	1.54506200	-1.49501300
H	0.00000000	-2.58888100	-1.78995900
H	0.00000000	-0.87491600	-2.33769200
H	-1.27015600	-2.14935400	0.19391500
H	1.27015600	-2.14935400	0.19391500
H	1.27015600	2.14935400	0.19391500
H	-1.27015600	2.14935400	0.19391500
H	0.00000000	2.58888100	-1.78995900
H	0.00000000	0.87491600	-2.33769200

Low frequencies (cm⁻¹): -528.70, 152.18, 254.72, 291.99, 350.78, 377.70, 394.48, 521.38, 555.46, 560.30

4a

C	-0.28698800	-0.38727100	1.56105300
C	-0.28698800	-0.38727100	-1.56105300
C	-0.99948000	0.70204700	-1.26357000
C	-0.99948000	0.70204700	1.26357000
H	-0.50550500	-0.88056100	2.50612400
H	-0.50550500	-0.88056100	-2.50612400
C	-0.90997500	1.53112000	0.00000000
C	0.78324000	-1.03527000	-0.76437300
C	0.78324000	-1.03527000	0.76437300
C	1.81300800	-0.25133500	0.00000000
H	-1.73588800	2.24768400	0.00000000
H	0.00000000	2.14726600	0.00000000
H	1.14752000	-1.96127200	-1.19846400
H	1.14752000	-1.96127200	1.19846400
H	2.83329600	-0.61910000	0.00000000
H	1.72232700	0.82855700	0.00000000
H	-1.74117800	1.02385100	1.99103400
H	-1.74117800	1.02385100	-1.99103400

Low frequencies (cm⁻¹): 130.53, 203.93, 291.15, 344.27, 351.58, 525.28, 580.27, 649.22, 700.24, 764.57

TS_{4a→5a}

C	-0.00082800	-1.47358100	-0.56411600
C	-0.00002900	1.47334400	-0.56443400
C	1.24906500	1.00276500	-0.17317200
H	2.11159500	1.38110900	-0.71359300
C	1.24851400	-1.00304900	-0.17355400
H	2.11064600	-1.38207500	-0.71411300

H	-0.00069000	-2.15647700	-1.41008300
H	0.00056200	2.15668200	-1.41001700
C	1.54946900	-0.00040400	0.88988100
H	0.92730800	0.00007200	1.77637900
H	2.59854400	-0.00040200	1.18226400
C	-1.24909000	1.00395500	-0.17294800
C	-1.24969900	-1.00330200	-0.17294900
C	-1.54817500	0.00029400	0.89021400
H	-2.11253600	-1.38251900	-0.71224000
H	-2.59622200	0.00083900	1.18623200
H	-0.92279800	-0.00016100	1.77442500
H	-2.11176400	1.38279300	-0.71278200

Low frequencies (cm⁻¹): -409.60, 204.50, 331.95, 353.35, 362.72, 372.82, 542.81, 556.60, 708.21, 719.78

N₂

N	0.00000000	0.00000000	0.54939000
N	0.00000000	0.00000000	-0.54939000

Low frequencies (cm⁻¹): 2544.22

VRI point for 3a

C	-1.38061700	0.00000000	0.39005600
C	1.38061700	0.00000000	0.39005600
C	0.84073500	-1.26354100	0.01229600
C	-0.84073500	-1.26354100	0.01229600
N	0.55922600	0.00000000	2.41589000
N	-0.55922600	0.00000000	2.41589000
H	-2.33505900	0.00000000	0.89614600
H	2.33505900	0.00000000	0.89614600
C	0.00000000	-1.55308200	-1.18806500
C	0.84073500	1.26354100	0.01229600
C	-0.84073500	1.26354100	0.01229600
C	0.00000000	1.55308200	-1.18806500
H	0.00000000	-2.59462900	-1.48808800
H	0.00000000	-0.88185700	-2.03315200
H	-1.27566100	-2.13776400	0.49131100
H	1.27566200	-2.13776400	0.49131100
H	1.27566200	2.13776400	0.49131100
H	-1.27566100	2.13776400	0.49131100
H	0.00000000	2.59462900	-1.48808800
H	0.00000000	0.88185700	-2.03315200

Low frequencies (cm⁻¹): -269.71, -205.88, 165.88, 177.25, 206.60, 287.63, 349.06, 378.00, 435.51, 449.66

3b

C	-1.19148200	-0.08322900	1.30089100
C	-0.22531000	0.69369200	-0.87286400
C	0.67427000	-0.36771200	-0.27968600
C	0.08181600	-0.86855700	1.01738600
N	-0.25179800	1.77345400	0.23455400
N	-0.71537500	1.38645000	1.30395600
H	-1.56270000	-0.28058400	2.30478400
H	0.22029300	1.15904500	-1.74727900
C	0.40206300	-1.82659000	-0.09166200
C	-1.69820400	0.35225500	-1.06179900
C	-2.29889100	-0.06487600	0.26027000
C	-2.40889600	-0.96910800	-0.92696900
H	1.30389200	-2.39508800	0.10568800
H	-0.31287800	-2.33287500	-0.71410900
H	0.76598800	-0.91845400	1.85958500
H	-2.21549400	1.10617900	-1.64650100
H	-3.20284400	0.42739300	0.60557200
H	-3.39081400	-0.96686600	-1.38931700
H	-1.93924500	-1.93539700	-0.97330800
N	2.10706000	0.02181300	-0.24075700
O	2.43886700	1.00283300	-0.87420500
O	2.85393200	-0.66916000	0.42885500

Low frequencies (cm⁻¹): 66.55, 95.01, 174.08, 231.49, 302.23, 361.73, 388.74, 406.11, 464.92, 509.16

TS-b

C	-1.23712000	-0.14091800	1.32223600
C	-0.20631000	0.51423400	-1.03243600
C	0.64346000	-0.43255800	-0.31549900
C	0.02237000	-0.84932800	1.08952000
N	-0.16260100	1.94064800	0.20437600
N	-0.60008500	1.65848900	1.24075800
H	-1.55304500	-0.06522000	2.35439700
H	0.26582500	1.05557700	-1.83989500
C	0.37140600	-1.85659900	0.04066400
C	-1.65206900	0.29767600	-1.11390700
C	-2.27934800	-0.06506600	0.29910500
C	-2.43435000	-0.96091100	-0.88772500
H	1.27355400	-2.40623000	0.27950300
H	-0.35454000	-2.41462200	-0.52514400
H	0.73420400	-0.80864400	1.90926600
H	-2.16760000	1.06708600	-1.68029600
H	-3.15793600	0.50084200	0.59373100
H	-3.42392800	-0.92843600	-1.32989800
H	-1.99699100	-1.94446000	-0.92227800

N	2.07524800	-0.03278800	-0.25542400
O	2.41375700	0.94215300	-0.89491200
O	2.81428000	-0.69959300	0.44752300

Low frequencies (cm⁻¹): -531.05, 73.08, 118.20, 185.04, 230.19, 281.86, 316.32, 347.39, 392.36, 409.52

4b

C	-2.01090700	1.12058200	-0.69899000
C	0.04802000	-1.16613700	-0.19902200
C	0.72781900	-0.05600800	0.10325400
C	-0.92035300	1.78581200	-0.31282400
H	-2.70116400	1.63669200	-1.36221300
H	0.63642200	-2.00814200	-0.54960400
C	0.20240600	1.27641500	0.56543400
C	-1.40451900	-1.38131500	-0.10423800
C	-2.42105100	-0.25953000	-0.34149200
C	-2.23128500	-0.82990100	1.02958300
H	1.02775200	1.98637200	0.53733400
H	-0.10093800	1.22390600	1.61896700
H	-0.80048100	2.80149200	-0.68026900
H	-1.72004500	-2.35057700	-0.47426900
H	-3.31089000	-0.60032600	-0.86077600
H	-3.00809700	-1.47165800	1.42949400
H	-1.72648300	-0.21590900	1.76582400
N	2.20189100	-0.14945800	-0.04080800
O	2.68232200	-1.16721800	-0.50737500
O	2.86141700	0.80532400	0.33374200

Low frequencies (cm⁻¹): 41.68, 67.22, 160.37, 249.88, 273.58, 299.89, 363.28, 371.69, 480.24, 527.21

5b

C	-0.15517300	-1.38543700	-0.01396000
C	-1.40041500	1.39247100	-0.75040400
C	-2.47446900	0.63371000	-0.52553400
C	-1.46828000	-1.59536100	0.09352500
H	0.49170800	-2.22056800	-0.25598800
H	-1.49523600	2.20814900	-1.46273500
C	-2.55128100	-0.57668400	0.37847500
C	-0.05111600	1.26841600	-0.14716100
C	0.55595500	-0.10321700	0.18091800
C	0.21043600	0.87508100	1.26999200
H	-3.52118000	-1.05784700	0.23152200
H	-2.54033800	-0.27673600	1.43520200
H	-1.80735100	-2.61625900	-0.06187700
H	0.69200600	1.95067400	-0.54606200
H	1.04809000	1.35370800	1.76252300

H	-0.62336200	0.59337300	1.90121100
N	2.01252200	-0.15888700	-0.12721900
O	2.45916300	-1.18439600	-0.60178300
O	2.67304900	0.83905300	0.10639500
H	-3.38363200	0.88658700	-1.06526000

Low frequencies (cm⁻¹): 65.97, 125.72, 157.74, 238.76, 273.49, 309.90, 356.52, 370.66, 487.29, 516.89

TS_{4b→5b}

C	0.15477200	1.30950500	-0.00851400
C	1.41490900	-1.23050100	-0.92702600
C	0.23412300	-1.51545300	-0.24635000
C	-0.61609900	0.20659900	0.35650300
H	-0.37261200	2.07613200	-0.56431400
H	1.48390900	-1.62701600	-1.93606400
C	-0.19119400	-1.01870600	1.09012600
H	0.56466400	-0.86007100	1.84762600
H	-1.03700700	-1.56622400	1.49474300
C	2.39401000	-0.31494900	-0.56735000
C	1.52900700	1.42152000	0.08287900
C	2.49473200	0.45907800	0.70237600
H	1.97678900	2.28398200	-0.40055800
H	3.47917000	0.90236700	0.84263400
H	2.19366000	-0.03863700	1.61601000
H	3.15077500	-0.08671800	-1.31246500
N	-2.02554000	0.22243500	-0.05315700
O	-2.67309300	-0.80259300	0.10950100
O	-2.48081900	1.24845500	-0.52824400
H	-0.51482900	-2.11031400	-0.76141900

Low frequencies (cm⁻¹): -378.06, 78.97, 127.66, 229.24, 250.12, 321.22, 334.18, 366.44, 428.18, 529.73

VRI point for 3b

C	-0.79519000	0.00072900	1.37807300
C	0.27585200	0.67947500	-1.06721400
C	1.12427300	-0.18828100	-0.31489800
C	0.47159000	-0.62460500	1.15878300
N	0.33519700	2.29892800	0.30639000
N	-0.08541600	2.02581700	1.30992300
H	-1.06173400	0.21923500	2.40154700
H	0.75153600	1.33414700	-1.77986600
C	0.86004500	-1.59557200	0.09189300
C	-1.14541200	0.53453800	-1.10617400
C	-1.80323000	0.15189400	0.37619900
C	-1.95554400	-0.69569200	-0.84115700
H	1.75913300	-2.14935500	0.32857000

H	0.13312500	-2.15604400	-0.47443600
H	1.20560300	-0.55181000	1.95810800
H	-1.67598000	1.32213800	-1.63454600
H	-2.66793900	0.75349900	0.64573300
H	-2.94424700	-0.66717600	-1.28401200
H	-1.51779500	-1.68134500	-0.87632900
N	2.55270600	0.22469900	-0.22050400
O	2.89692000	1.20461000	-0.84835900
O	3.28650600	-0.43983100	0.49227800

Low frequencies (cm⁻¹): -331.80, -46.62, 75.63, 120.42, 162.80, 228.80, 245.00, 264.89, 312.00, 336.16

3c

C	-2.10318200	0.82485900	0.92023100
C	-0.90573800	-0.08931500	-1.05998300
C	-0.10640900	-0.47297600	0.18827000
C	-0.89474600	0.01620300	1.38072600
N	-0.91767800	1.45043900	-0.98721400
N	-1.49482200	1.90144800	0.00120500
H	-2.56615500	1.36151800	1.74705200
H	-0.36662800	-0.34424700	-1.97171700
C	-0.59684400	-1.45473700	1.20744400
C	-2.38853600	-0.44042500	-1.15544300
C	-3.13018600	0.17488500	0.00712200
C	-3.25665200	-1.29052100	-0.25942300
H	0.18445200	-1.80547300	1.87556700
H	-1.32407200	-2.21314600	0.98189600
H	-2.78204200	-0.27688100	-2.15434700
H	-3.99342600	0.80426200	-0.18896100
H	-4.19351500	-1.57078800	-0.73112600
H	-2.90533300	-2.03683300	0.43015200
C	1.37323500	-0.24027000	0.07329500
C	2.21130700	-1.30225400	-0.27457400
C	1.93318200	1.02161800	0.28656200
C	3.58355200	-1.11168700	-0.40617200
H	1.77716900	-2.28644600	-0.43474900
C	3.30605800	1.21410500	0.15726700
H	1.28750800	1.85461900	0.54989500
C	4.13383400	0.14940300	-0.18972000
H	4.22331500	-1.94726000	-0.67361000
H	3.72947700	2.19913500	0.32825500
H	5.20430100	0.30106600	-0.28865400
H	-0.34079600	0.50394100	2.17879200

Low frequencies (cm⁻¹): 29.98, 64.74, 90.67, 140.75, 245.42, 279.79, 283.54, 350.21, 386.99, 404.49

TS-c

C	2.16650900	-0.70157700	1.02778300
C	0.88715800	0.24372500	-1.07634200
C	0.12669800	0.52004000	0.15142500
C	0.92857900	-0.02274300	1.41313600
N	0.90117500	-1.66426900	-1.01363400
N	1.45683600	-2.07795900	-0.08179500
H	2.58288500	-1.38669500	1.75547500
H	0.32213500	0.29537700	-1.99919300
C	0.58051400	1.42791700	1.25726900
C	2.33073100	0.46973800	-1.18376200
C	3.10557800	-0.11562300	0.07038700
C	3.21887600	1.32248700	-0.32795700
H	-0.23242900	1.74126700	1.90421500
H	1.32019100	2.19554300	1.10838100
H	2.73872000	0.21042200	-2.15659800
H	3.96929500	-0.73824600	-0.14519800
H	4.16278000	1.56251000	-0.80551100
H	2.85233600	2.12310900	0.29150800
C	-1.35201700	0.26287400	0.05786300
C	-2.20214700	1.30986700	-0.30903100
C	-1.90119900	-0.99536400	0.31114700
C	-3.57341700	1.10621500	-0.42274800
H	-1.77626100	2.29213100	-0.50008900
C	-3.27483700	-1.20059200	0.20214200
H	-1.24942100	-1.81782500	0.59068500
C	-4.11328000	-0.15241800	-0.16574400
H	-4.22139200	1.92958700	-0.70771000
H	-3.68908600	-2.18360800	0.40440200
H	-5.18352700	-0.31392700	-0.25016600
H	0.33122100	-0.56131400	2.14439300

Low frequencies (cm⁻¹): -527.27, 32.52, 80.23, 90.30, 170.05, 225.74, 258.14, 281.86, 315.88, 346.87

4c

C	2.94781500	0.72950900	1.09559100
C	0.85900100	-1.11826000	-0.28481400
C	0.17184900	0.02991800	-0.17018400
C	1.88899100	1.52482900	0.92582500
H	3.59872100	0.93856100	1.94203400
H	0.27575600	-2.03706600	-0.30564500
C	0.82108200	1.40716500	-0.14117300
C	2.31924200	-1.33254700	-0.40846000
C	3.35309800	-0.43571100	0.27524900
C	3.22766400	-0.45152900	-1.22175700
H	0.04813400	2.14849000	0.07519500
H	1.21575800	1.67752900	-1.12919700
H	2.59363500	-2.38282800	-0.41433200

H	4.20863200	-0.97497100	0.66967600
H	4.01499200	-0.93554600	-1.78917100
H	2.79877000	0.41944800	-1.70155400
C	-1.31092100	-0.02149800	-0.06591900
C	-2.10833400	0.90820700	-0.74641200
C	-1.95142700	-1.00204100	0.70245100
C	-3.49633900	0.84670800	-0.67968500
H	-1.63642400	1.67549000	-1.35459900
C	-3.33909600	-1.06356900	0.77272500
H	-1.34803200	-1.70427700	1.27020600
C	-4.11855100	-0.14046500	0.08018700
H	-4.09337900	1.57098300	-1.22572300
H	-3.81288000	-1.82742800	1.38207700
H	-5.20158000	-0.18514400	0.13833700
H	1.75345800	2.33246600	1.64095900

Low frequencies (cm⁻¹): 51.27, 69.63, 116.16, 167.45, 195.02, 247.90, 272.72, 341.46, 355.85, 418.31

5c

C	-1.24242500	-0.10674700	-1.06975300
C	1.28731300	-1.78846500	-1.72714400
C	0.55223000	-1.93248300	-2.83229100
C	-1.48740500	-0.55810500	-2.30282300
H	-2.10271500	0.09663500	-0.43500000
H	1.95829500	-2.60367400	-1.46393700
C	-0.47667000	-0.95572200	-3.35697300
C	1.31205300	-0.64849600	-0.78093500
C	0.06769600	0.17677000	-0.41201600
C	1.19148400	0.79093200	-1.19938900
H	-1.01120700	-1.42556800	-4.18686400
H	0.00757200	-0.07177200	-3.79400300
H	1.96947900	-0.80427000	0.06964800
H	1.83292100	1.50410800	-0.69183000
H	1.01341900	1.00708700	-2.24587200
H	-2.53234800	-0.68113600	-2.57842500
C	-0.05662800	0.54283800	1.04137900
C	0.13569100	1.84996200	1.48810000
C	-0.41397600	-0.44026800	1.96966100
C	-0.01500200	2.16941400	2.83633600
H	0.39858700	2.62394000	0.77204100
C	-0.56669700	-0.12528600	3.31533000
H	-0.56534100	-1.45994900	1.62281800
C	-0.36494300	1.18297300	3.75296400
H	0.13855500	3.19170000	3.16881900
H	-0.83965400	-0.90052000	4.02501600
H	-0.48085600	1.43062100	4.80360700
H	0.67696300	-2.85111000	-3.40069300

Low frequencies (cm⁻¹): 26.58, 83.83, 94.28, 142.01, 196.33, 252.39, 284.21, 322.48, 350.20, 415.82

TS_{4c→5c}

C	2.16650900	-0.70157700	1.02778300
C	0.88715800	0.24372500	-1.07634200
C	0.12669800	0.52004000	0.15142500
C	0.92857900	-0.02274300	1.41313600
N	0.90117500	-1.66426900	-1.01363400
N	1.45683600	-2.07795900	-0.08179500
H	2.58288500	-1.38669500	1.75547500
H	0.32213500	0.29537700	-1.99919300
C	0.58051400	1.42791700	1.25726900
C	2.33073100	0.46973800	-1.18376200
C	3.10557800	-0.11562300	0.07038700
C	3.21887600	1.32248700	-0.32795700
H	-0.23242900	1.74126700	1.90421500
H	1.32019100	2.19554300	1.10838100
H	2.73872000	0.21042200	-2.15659800
H	3.96929500	-0.73824600	-0.14519800
H	4.16278000	1.56251000	-0.80551100
H	2.85233600	2.12310900	0.29150800
C	-1.35201700	0.26287400	0.05786300
C	-2.20214700	1.30986700	-0.30903100
C	-1.90119900	-0.99536400	0.31114700
C	-3.57341700	1.10621500	-0.42274800
H	-1.77626100	2.29213100	-0.50008900
C	-3.27483700	-1.20059200	0.20214200
H	-1.24942100	-1.81782500	0.59068500
C	-4.11328000	-0.15241800	-0.16574400
H	-4.22139200	1.92958700	-0.70771000
H	-3.68908600	-2.18360800	0.40440200
H	-5.18352700	-0.31392700	-0.25016600
H	0.33122100	-0.56131400	2.14439300

Low frequencies (cm⁻¹): -375.04, 60.96, 75.42, 115.68, 197.50, 242.52, 290.22, 335.45, 355.35, 385.06

VRI point for 3c

C	2.18282700	-0.77145900	1.06411400
C	0.84241700	0.21583000	-1.13728200
C	0.08401600	0.39332600	0.06172600
C	0.93410800	-0.17782300	1.40254900
N	0.84625600	-1.97415700	-1.09252700
N	1.37846900	-2.37270600	-0.19284200
H	2.52936100	-1.58444300	1.68526200
H	0.28046500	0.09098400	-2.05227400

C	0.53102600	1.24877200	1.20861600
C	2.25922200	0.34676300	-1.25223300
C	3.07886500	-0.27154700	0.07390900
C	3.18211700	1.14464400	-0.38695300
H	-0.27885300	1.56775700	1.85521900
H	1.27148500	2.01935100	1.05802300
H	2.68557500	0.04261900	-2.20565100
H	3.92108700	-0.90904700	-0.18609400
H	4.12549900	1.38882300	-0.86174200
H	2.81594300	1.94740400	0.23417100
C	-1.38924400	0.09744600	-0.00330400
C	-2.24530500	1.14235200	-0.36169200
C	-1.93690400	-1.16152800	0.25749700
C	-3.61525400	0.93749900	-0.47367500
H	-1.81815400	2.12369100	-0.55288800
C	-3.31246300	-1.36801500	0.15166900
H	-1.28806000	-1.98581900	0.53832300
C	-4.15315200	-0.32205900	-0.21676200
H	-4.26298000	1.76048300	-0.75919800
H	-3.72715600	-2.35151600	0.35364600
H	-5.22336200	-0.48423000	-0.30152900
H	0.30214500	-0.73339600	2.09192000

Low frequencies (cm⁻¹): -265.26, -199.08, -26.22, 79.12, 82.02, 169.84, 182.80, 220.26, 256.87, 281.97

3d

C	-0.14315500	0.06617600	-1.01667100
C	-1.41162500	0.67454500	1.03349200
C	-0.15631900	-0.09288300	1.42954800
C	0.65039300	-0.43226800	0.20107600
N	-0.87185700	1.88277200	0.24857700
N	-0.25813200	1.58109400	-0.77465700
H	0.42616400	-0.04929400	-1.94010000
H	-1.92386600	1.08370200	1.90312100
C	0.19384300	-1.52597600	1.11743300
C	-2.38305200	0.06076300	0.03363500
C	-1.60230500	-0.34694700	-1.19313700
C	-2.41840400	-1.36126900	-0.43532900
H	1.00782100	-1.89469700	1.73304300
H	-0.51335700	-2.28629800	0.84330900
H	-3.28743600	0.64870800	-0.09333500
H	-1.99464900	-0.06532900	-2.16589600
H	-3.33912100	-1.62375600	-0.94762000
H	-2.01982800	-2.18303200	0.13137600
N	2.06938100	-0.21082300	0.21086800
C	2.48773500	1.17247600	0.05124500
H	2.27896700	1.58468200	-0.95013500
H	3.56538800	1.23291200	0.23331500

H	1.97356600	1.80026900	0.78346700
C	2.77568300	-1.10259900	-0.69208800
H	3.85123100	-1.03043400	-0.50288700
H	2.60637500	-0.87306400	-1.75907800
H	2.45902400	-2.13297800	-0.50601900
H	0.37722000	0.34520600	2.26869100

Low frequencies (cm⁻¹): 46.84, 104.48, 188.45, 207.94, 244.58, 301.70, 307.20, 316.20, 336.63, 386.62

TS-d

C	-0.10375600	-0.02746800	-1.04498400
C	-1.49663300	0.45463900	1.14326900
C	-0.21473400	-0.17672000	1.45424700
C	0.63971300	-0.46761000	0.14348300
N	-0.90280000	2.04921400	0.28955200
N	-0.30135300	1.84266800	-0.68140700
H	0.48634800	0.11703400	-1.94385100
H	-1.98504100	0.97488800	1.95757400
C	0.22024700	-1.56106500	1.07910100
C	-2.36472300	-0.03862800	0.07075100
C	-1.52512700	-0.32615100	-1.24280100
C	-2.35615600	-1.38554500	-0.58589500
H	1.05641600	-1.91105800	1.67390900
H	-0.47707100	-2.33494100	0.81003700
H	-3.27437900	0.54051600	-0.06078100
H	-1.93271600	0.08053500	-2.16411800
H	-3.27277600	-1.60115300	-1.12450800
H	-1.93401400	-2.26020900	-0.12155500
N	2.05174500	-0.19167900	0.21730700
C	2.43697100	1.19750300	0.03223100
H	2.24516700	1.58306100	-0.98316500
H	3.50870600	1.28698000	0.23583800
H	1.89655500	1.82937500	0.74077500
C	2.81778000	-1.08589200	-0.63444400
H	3.88393600	-0.97050600	-0.41545300
H	2.66964800	-0.89428800	-1.71209300
H	2.53065100	-2.12078800	-0.42681500
H	0.34393200	0.28074900	2.26629000

Low frequencies (cm⁻¹): -525.39, 83.10, 118.10, 196.95, 218.20, 248.66, 266.55, 280.60, 306.93, 328.21

4d

C	-0.00689000	1.13335200	-0.09037300
C	2.17121700	-0.97449300	-0.80906700
C	1.09727900	-1.71083700	-0.51234700
C	-0.68401300	-0.01927500	0.04896900

H	-0.56342900	2.01768500	-0.38383900
H	2.86709300	-1.38005100	-1.54072100
C	-0.03281700	-1.34291900	0.42585500
C	2.52754700	0.36142500	-0.28394200
C	1.44587800	1.38018300	0.08637900
C	2.29687100	0.75115800	1.15168500
H	-0.79271300	-2.12287400	0.34444700
H	0.29524700	-1.34505300	1.47237500
H	3.41138600	0.79458300	-0.74180100
H	1.72446700	2.40202300	-0.15328700
H	3.04756600	1.37252300	1.62811400
H	1.84396600	0.01663600	1.80615000
N	-2.06820200	-0.13198500	-0.23664300
C	-2.68540600	0.98504500	-0.91967000
H	-2.75592500	1.89219300	-0.29366700
H	-3.69971400	0.69788200	-1.21173900
H	-2.11417100	1.22553900	-1.81929100
C	-2.87800500	-0.55685400	0.89881200
H	-3.87135900	-0.85108800	0.54685000
H	-2.99467200	0.24838900	1.64358300
H	-2.42588800	-1.41626200	1.39750100
H	0.99558900	-2.66893700	-1.01597600

Low frequencies (cm⁻¹): 69.56, 98.12, 171.46, 219.72, 233.69, 263.12, 283.90, 293.68, 338.99, 363.25

5d

C	1.67306200	1.42960400	0.37127300
C	0.04344400	-1.22021300	0.29388900
C	1.30823900	-1.64807600	0.30545000
C	2.63086400	0.49959300	0.37665300
H	1.89931700	2.38050600	0.84963300
H	-0.70530200	-1.88737700	0.71995600
C	2.52917800	-0.90107200	-0.18748400
C	-0.51662200	0.05834100	-0.22807800
C	0.30959900	1.34360400	-0.20323300
C	-0.00353800	0.65498800	-1.50632700
H	3.41959100	-1.46078100	0.11127300
H	2.55925200	-0.88283800	-1.28584100
H	-0.31290700	2.21294900	-0.01496600
H	-0.74186900	1.13172200	-2.14210000
H	0.79955800	0.14280700	-2.02278800
H	1.49377700	-2.63163500	0.73171200
N	-1.92555000	0.29007100	0.00059800
C	-2.26391900	0.37463500	1.41040700
H	-3.29917500	0.71534800	1.51301500
H	-2.16906000	-0.58665500	1.94544500
H	-1.60740100	1.10201100	1.89638100
C	-2.77677600	-0.64999900	-0.70727900

H	-3.81764300	-0.31887800	-0.63405700
H	-2.49249500	-0.67211300	-1.76313000
H	-2.72241800	-1.68015000	-0.31284300
H	3.57443200	0.75616000	0.85250200

Low frequencies (cm⁻¹): 105.20, 106.27, 155.24, 199.34, 235.65, 253.18, 257.51, 296.61, 318.87, 356.37

TS_{4d→5d}

C	-0.10375600	-0.02746800	-1.04498400
C	-1.49663300	0.45463900	1.14326900
C	-0.21473400	-0.17672000	1.45424700
C	0.63971300	-0.46761000	0.14348300
N	-0.90280000	2.04921400	0.28955200
N	-0.30135300	1.84266800	-0.68140700
H	0.48634800	0.11703400	-1.94385100
H	-1.98504100	0.97488800	1.95757400
C	0.22024700	-1.56106500	1.07910100
C	-2.36472300	-0.03862800	0.07075100
C	-1.52512700	-0.32615100	-1.24280100
C	-2.35615600	-1.38554500	-0.58589500
H	1.05641600	-1.91105800	1.67390900
H	-0.47707100	-2.33494100	0.81003700
H	-3.27437900	0.54051600	-0.06078100
H	-1.93271600	0.08053500	-2.16411800
H	-3.27277600	-1.60115300	-1.12450800
H	-1.93401400	-2.26020900	-0.12155500
N	2.05174500	-0.19167900	0.21730700
C	2.43697100	1.19750300	0.03223100
H	2.24516700	1.58306100	-0.98316500
H	3.50870600	1.28698000	0.23583800
H	1.89655500	1.82937500	0.74077500
C	2.81778000	-1.08589200	-0.63444400
H	3.88393600	-0.97050600	-0.41545300
H	2.66964800	-0.89428800	-1.71209300
H	2.53065100	-2.12078800	-0.42681500
H	0.34393200	0.28074900	2.26629000

Low frequencies (cm⁻¹): -330.69, 86.39, 102.73, 193.26, 218.16, 223.71, 304.54, 309.73, 326.46, 341.26

VRI point for 3d

C	-0.25312500	0.01956500	-1.04015200
C	-1.71248600	0.52016100	1.24884100
C	-0.42784300	-0.02005700	1.52841600
C	0.48031900	-0.32511900	0.13401800
N	-1.04172200	2.36907400	0.28979600
N	-0.47065500	2.16967000	-0.65122300
H	0.32144400	0.33228700	-1.90259300

H	-2.14008800	1.19018200	1.98045900
C	0.06321800	-1.37098200	1.11873300
C	-2.54401300	0.12110300	0.15762500
C	-1.65691000	-0.17886300	-1.22672700
C	-2.52610600	-1.19296700	-0.55480600
H	0.89641200	-1.72506200	1.71373700
H	-0.63585000	-2.14675800	0.84932100
H	-3.43347400	0.72350200	-0.01289000
H	-2.08533500	0.26365200	-2.12366800
H	-3.44165900	-1.41315800	-1.09195900
H	-2.10410500	-2.07005100	-0.08940200
N	1.88145100	-0.01103800	0.24592900
C	2.26667600	1.37914300	0.06525000
H	2.07954200	1.76720300	-0.94895200
H	3.33891200	1.46711700	0.27214600
H	1.72908700	2.01048900	0.77676900
C	2.65719400	-0.90472900	-0.59767800
H	3.72176600	-0.78798100	-0.37689500
H	2.50509500	-0.71261200	-1.67446700
H	2.36658600	-1.93867600	-0.39012700
H	0.16566800	0.46490500	2.30050000

Low frequencies (cm⁻¹): -265.20, -183.86, 78.64, 123.20, 162.67, 211.85, 215.14, 248.43, 258.99, 273.03

3e

C	-0.62017400	0.35566300	1.26799500
C	0.14759000	0.37820500	-1.10659400
C	1.16614100	-0.35745600	-0.26683700
C	0.69608600	-0.40252300	1.15255800
N	0.10422900	1.77294600	-0.44393900
N	-0.26701000	1.75888100	0.72726300
H	-0.91841100	0.49888100	2.30500100
H	0.50998400	0.52572900	-2.12265600
C	1.03748700	-1.67825600	0.38988600
C	-1.30273200	-0.08195200	-1.04988300
C	-1.78635900	-0.04793600	0.38023200
C	-1.88453800	-1.31508900	-0.40951400
H	2.00260300	-2.06818000	0.69816000
H	0.34764200	-2.44594800	0.08450200
H	-1.91675000	0.38847600	-1.81123400
H	-2.70755800	0.47868400	0.61027600
H	-2.88664700	-1.54303000	-0.75853200
H	-1.32497700	-2.19788000	-0.15698400
F	2.43290000	0.07474800	-0.54429900
H	1.41647600	-0.13618800	1.91983100

Low frequencies (cm⁻¹): 88.27, 237.49, 287.35, 332.95, 387.37, 405.92, 436.80, 512.02, 573.43, 595.76

TS-e

C	-0.65696300	0.23088300	1.32759000
C	0.16391200	0.21463200	-1.18504100
C	1.12852400	-0.43135600	-0.30614000
C	0.63631300	-0.43822200	1.18693400
N	0.18921000	1.94738700	-0.41968400
N	-0.17550500	1.95697000	0.68250500
H	-0.91408000	0.57930800	2.31958600
H	0.54678800	0.50664000	-2.15494500
C	1.00306200	-1.70382300	0.44077500
C	-1.26745700	-0.07811000	-1.08204400
C	-1.76938200	-0.04857500	0.41821100
C	-1.92856600	-1.26193100	-0.44264700
H	1.96892600	-2.08460900	0.75397300
H	0.30170200	-2.47490400	0.16638000
H	-1.87557500	0.46422300	-1.79961600
H	-2.66952500	0.52597800	0.61496800
H	-2.94392700	-1.42503500	-0.78664800
H	-1.40586500	-2.17949200	-0.22989200
F	2.40557300	-0.00233200	-0.53035000
H	1.38880500	-0.12260800	1.90376600

Low frequencies (cm⁻¹): -529.76, 133.75, 217.05, 258.17, 317.63, 351.59, 380.20, 401.74, 430.21, 516.23

4e

C	1.30736600	-1.31261100	-0.48079400
C	-0.52460100	1.25750500	-0.37586700
C	-1.33208900	0.26847900	-0.01036000
C	0.12687600	-1.81063500	-0.10749500
H	2.00014300	-2.00573100	-0.95382100
H	-1.01126700	2.14881200	-0.76132000
C	-1.03133700	-1.09400500	0.54661700
C	0.95372100	1.29955600	-0.26961500
C	1.83715900	0.06371300	-0.32549400
C	1.68116900	0.83511700	0.96026400
H	-1.93847800	-1.68575900	0.39420600
H	-0.89865300	-1.03971700	1.63744000
H	1.38820000	2.16565100	-0.75854700
H	2.77967900	0.22302100	-0.83990100
H	2.52450500	1.41607100	1.31764400
H	1.08344000	0.37092700	1.73852600
F	-2.66639500	0.47037000	-0.12310200
H	-0.03960000	-2.86932100	-0.28984300

Low frequencies (cm⁻¹): 36.18, 153.17, 251.52, 319.99, 329.60, 418.22, 447.85, 506.16, 552.88, 642.61

5e

C	0.31451200	-1.41008600	-0.27759400
C	-0.80491600	1.50377800	-0.54307500
C	-1.89968400	0.78056000	-0.29566900
C	-0.99528000	-1.57618800	-0.09147500
H	0.90414600	-2.22911400	-0.68198900
H	-0.92968600	2.42356700	-1.11011000
C	-1.97107500	-0.54483800	0.43477100
C	0.59278900	1.20773900	-0.14722100
C	1.11989000	-0.20232900	0.00222100
C	0.96937600	0.65076300	1.21370500
H	-2.98335300	-0.94272100	0.32709100
H	-1.83542300	-0.40215100	1.51585600
H	1.33855800	1.87727600	-0.56414500
H	1.89009300	1.01950500	1.65161400
H	0.17589600	0.41864000	1.91425400
H	-1.41377900	-2.54501100	-0.35219100
F	2.41607400	-0.36025200	-0.42264200
H	-2.84477900	1.16589300	-0.67058100

Low frequencies (cm⁻¹): 125.74, 163.92, 269.87, 322.78, 332.70, 383.28, 412.77, 550.17, 556.14, 646.97

TS_{4e→5e}

C	0.28734400	-1.33622100	-0.35124600
C	-0.84163400	1.39251700	-0.66560200
C	0.44806000	1.44702400	-0.13876000
H	1.17898200	2.05173000	-0.66618800
C	1.18271400	-0.38220600	0.11820000
H	0.70153000	-2.01124900	-1.09410100
H	-0.99475800	1.97386900	-1.57147900
C	0.97923200	0.73414400	1.06572000
H	0.31206700	0.57194000	1.90352300
H	1.93176600	1.13400700	1.40854700
C	-1.86962800	0.52860500	-0.32612800
C	-1.08069400	-1.36059200	-0.14113500
C	-1.86452400	-0.48284000	0.77481700
H	-1.65481800	-2.07398700	-0.72380600
H	-2.85828200	-0.87781800	0.98216600
H	-1.39476300	-0.20068400	1.71080600
H	-2.74895200	0.52576800	-0.96290400
F	2.45355700	-0.48179600	-0.33352900

Low frequencies (cm⁻¹): -394.71, 157.54, 264.02, 311.19, 335.33, 347.45, 403.02, 466.61, 535.97, 557.72

3f

C	0.36686500	0.40269500	1.25042300
C	0.36686500	0.40269500	-1.25042300
C	-0.36998400	-0.81839200	-0.74853600
C	-0.36998400	-0.81839200	0.74853600
N	1.77025200	0.24975400	-0.61386800
N	1.77025200	0.24975400	0.61386800
H	0.50596700	0.35648900	2.32916700
H	0.50596700	0.35648900	-2.32916700
C	-1.66489300	-0.93631400	0.00000000
C	-0.07956700	1.76848700	-0.75542000
C	-0.07956700	1.76848700	0.75542000
C	-1.33471300	2.09550100	0.00000000
H	-1.97981100	-1.97665700	0.00000000
H	-2.48200900	-0.23414900	0.00000000
H	0.40824000	2.58657300	-1.27551200
H	0.40824000	2.58657300	1.27551200
H	-1.57902100	3.15277100	0.00000000
H	-2.20933100	1.46992200	0.00000000
F	0.03489500	-1.94351000	-1.40079600
F	0.03489500	-1.94351000	1.40079600

Low frequencies (cm⁻¹): 77.19, 189.36, 248.40, 255.62, 316.75, 364.56, 403.52, 446.10, 490.64, 542.45

TS-f

C	0.23023800	0.41008900	1.32253600
C	0.23023800	0.41008900	-1.32253600
C	-0.43556300	-0.76787100	-0.79047600
C	-0.43556300	-0.76787100	0.79047600
N	1.94040600	0.14411200	-0.58143300
N	1.94040600	0.14411200	0.58143300
H	0.53186800	0.33833400	2.36018200
H	0.53186800	0.33833400	-2.36018200
C	-1.69548700	-0.90737200	0.00000000
C	-0.06054700	1.74447400	-0.78669200
C	-0.06054700	1.74447400	0.78669200
C	-1.26655800	2.15725000	0.00000000
H	-2.01735200	-1.94399700	0.00000000
H	-2.50101300	-0.18983700	0.00000000
H	0.49146200	2.54384900	-1.27086900
H	0.49146200	2.54384900	1.27086900
H	-1.44370100	3.22686600	0.00000000
H	-2.17710400	1.58069200	0.00000000
F	-0.00613600	-1.92195700	-1.36997800
F	-0.00613600	-1.92195700	1.36997800

Low frequencies (cm⁻¹): -540.37, 116.40, 184.52, 218.36, 243.18, 306.13, 349.38, 385.16, 391.42, 470.75

4f

C	0.09173700	0.51897100	1.61740600
C	0.09173700	0.51897100	-1.61740600
C	0.04437600	-0.76499600	-1.28967400
C	0.04437600	-0.76499600	1.28967400
H	-0.08836900	0.73823600	2.66735800
H	-0.08836900	0.73823600	-2.66735800
C	0.21273900	-1.50027200	0.00000000
C	0.38597400	1.68220400	-0.75068600
C	0.38597400	1.68220400	0.75068600
C	-0.71265500	2.39585500	0.00000000
H	1.18472700	-2.01428700	0.00000000
H	-0.53509800	-2.30236400	0.00000000
H	1.13037400	2.34527400	-1.18618100
H	1.13037400	2.34527400	1.18618100
H	-0.73087200	3.48041600	0.00000000
H	-1.68294400	1.91023300	0.00000000
F	-0.19918700	-1.65826000	-2.27823300
F	-0.19918700	-1.65826000	2.27823300

Low frequencies (cm⁻¹): 52.98, 128.07, 178.60, 310.32, 334.39, 350.60, 388.59, 433.82, 472.29, 482.78

5f

C	0.45190200	0.36518100	1.60597400
C	0.45190200	0.36518100	-1.60597400
C	0.45190200	1.65600800	-1.28301100
C	0.45190200	1.65600800	1.28301100
H	0.83429000	0.04776800	2.57405800
H	0.83429000	0.04776800	-2.57405800
C	-0.09916600	2.23833200	0.00000000
C	-0.04712300	-0.73720100	-0.74940800
C	-0.04712300	-0.73720100	0.74940800
C	0.90073000	-1.63653100	0.00000000
H	-1.18881900	2.09835400	0.00000000
H	0.06540400	3.31794000	0.00000000
H	0.63821100	-2.68971100	0.00000000
H	1.95694900	-1.39062900	0.00000000
F	-1.10785200	-1.39877800	-1.30862000
F	-1.10785200	-1.39877800	1.30862000
H	0.85572200	2.36392400	-2.00307600
H	0.85572200	2.36392400	2.00307600

Low frequencies (cm⁻¹): 67.53, 143.26, 221.47, 232.98, 259.87, 352.97, 371.69, 449.82, 494.76, 544.07

TS_{4f→5f}

C	0.43868200	1.49760600	-0.45903800
C	0.43868400	-1.49760900	-0.45903300
C	-0.70884100	-0.98131400	0.14144300
C	-0.70884100	0.98131500	0.14144500
H	0.23674300	2.20153700	-1.26113000
H	0.23674700	-2.20153900	-1.26112600
C	-0.86265400	-0.00000100	1.24222900
H	-0.12951100	-0.00000100	2.03943400
H	-1.87902500	-0.00000100	1.63154200
C	1.73409800	-1.05683700	-0.29298200
C	1.73409800	1.05683900	-0.29298400
C	2.19863400	0.00000200	0.65677500
H	2.48404800	1.46144500	-0.96493000
H	3.28194500	0.00000300	0.77343500
H	1.74756500	0.00000300	1.64503700
H	2.48405200	-1.46144900	-0.96492000
F	-1.89143000	1.44689600	-0.31691300
F	-1.89142800	-1.44689600	-0.31691700

Low frequencies (cm⁻¹): -390.67, 137.50, 164.00, 283.92, 295.52, 319.74, 357.40, 415.50, 436.33, 493.46

3g

C	-1.02086600	0.35075700	1.23970100
C	-0.01992800	0.37560800	-1.04462300
C	0.88509900	-0.43100400	-0.13162500
C	0.24083900	-0.50412500	1.22339400
N	-0.05287200	1.75675700	-0.35421800
N	-0.53081900	1.73992900	0.77688800
H	-1.39868300	0.48702300	2.25140700
H	0.42686900	0.52816800	-2.02502300
C	0.57446300	-1.76490300	0.44227100
C	-1.49499000	-0.00950200	-1.13192800
C	-2.12441600	0.05609600	0.23854300
C	-2.23626400	-1.19718500	-0.56664000
H	1.44218000	-2.27428500	0.84818400
H	-0.12876800	-2.43291700	-0.02311000
H	-1.99599600	0.49915700	-1.94962700
H	-3.01693300	0.65714800	0.38427200
H	-3.20740700	-1.34268200	-1.02901500
H	-1.78826700	-2.12206600	-0.24981000
Cl	2.59120500	0.03569200	-0.28626000
H	0.87873400	-0.33756500	2.08589400

Low frequencies (cm⁻¹): 96.27, 192.31, 242.64, 305.75, 366.88, 394.85, 411.82, 487.95, 526.97, 584.12

TS-g

C	-1.07341100	0.22827300	1.29213600
C	-0.00515100	0.21372200	-1.12631400
C	0.85077800	-0.48550400	-0.16952500
C	0.18809400	-0.51124700	1.26604600
N	0.01488300	1.93226000	-0.33149200
N	-0.44646900	1.94303700	0.73265800
H	-1.40247100	0.57603600	2.26273900
H	0.46548700	0.51194100	-2.05424300
C	0.55972600	-1.76969200	0.52073400
C	-1.45244700	-0.02039300	-1.16689400
C	-2.10471400	0.02753400	0.27467600
C	-2.24611300	-1.16678900	-0.61363000
H	1.44048700	-2.24712400	0.93466900
H	-0.15238800	-2.46792400	0.11264100
H	-1.95567000	0.55744300	-1.93650300
H	-2.98296100	0.65590900	0.38916700
H	-3.22684100	-1.26067100	-1.06679900
H	-1.81377400	-2.11854800	-0.35434900
Cl	2.55791800	-0.00938000	-0.28469700
H	0.86404400	-0.27010700	2.08098800

Low frequencies (cm⁻¹): -529.02, 116.40, 191.77, 233.68, 291.43, 321.87, 351.91, 388.91, 406.68, 478.22

4g

C	-1.75465100	1.21014900	-0.56895900
C	0.25953700	-1.17218300	-0.33485300
C	0.97575300	-0.12309800	0.06971800
C	-0.64233700	1.79957800	-0.12529500
H	-2.43348300	1.81774300	-1.16344200
H	0.79982100	-2.00677000	-0.77253700
C	0.47340800	1.16699700	0.67842700
C	-1.21055200	-1.34746100	-0.24702000
C	-2.19852900	-0.18925900	-0.36631500
C	-2.02016000	-0.91058600	0.94106300
H	1.30807900	1.86844500	0.72527600
H	0.17588400	0.99661100	1.72172600
H	-1.55228400	-2.26285500	-0.71920100
H	-3.10345600	-0.44301500	-0.90915100
H	-2.82003500	-1.56246500	1.27446400
H	-1.50528300	-0.38533900	1.73711000
Cl	2.72543400	-0.20429300	-0.10552700
H	-0.49643500	2.84580800	-0.38089200

Low frequencies (cm⁻¹): 70.07, 159.77, 252.54, 280.46, 300.99, 355.20, 405.13, 482.59, 542.50, 586.75

5g

C	-0.07792500	1.36360000	-0.18051800
C	1.22520200	-1.45010200	-0.59106500
C	2.28507000	-0.65721100	-0.42214700
C	1.22938600	1.61062900	-0.07665100
H	-0.72631400	2.16642400	-0.51900800
H	1.35696400	-2.34266700	-1.19825600
C	2.32259000	0.65013800	0.33871400
C	-0.14697400	-1.27318300	-0.05508000
C	-0.78698500	0.09442800	0.12986400
C	-0.44836600	-0.73954000	1.32481600
H	3.28735600	1.12969200	0.15500200
H	2.29556200	0.47290600	1.42269800
H	-0.85342600	-2.02251900	-0.39676900
H	-1.27190600	-1.19477700	1.86295200
H	0.37592700	-0.39994300	1.94163800
H	1.55315100	2.61551900	-0.33659200
Cl	-2.52025800	0.17310700	-0.28483800
H	3.21508600	-0.96002600	-0.89702100

Low frequencies (cm⁻¹): 117.48, 148.18, 245.31, 283.51, 309.10, 350.85, 367.13, 493.11, 539.32, 601.70

TS_{4g→5g}

C	0.06542200	-1.28360000	-0.23542600
C	-1.26332800	1.32369600	-0.73589500
C	-0.03876300	1.50902900	-0.09504500
C	0.85345200	-0.23614700	0.24417400
H	0.56093100	-1.96822500	-0.91670000
H	-1.38256800	1.86130500	-1.67301700
C	0.45152400	0.86388600	1.15939700
H	-0.27022000	0.61090100	1.92632600
H	1.30255200	1.37690100	1.60199100
C	-2.23395600	0.37655800	-0.45630900
C	-1.30644100	-1.42258700	-0.10830200
C	-2.24767100	-0.58116100	0.68939700
H	-1.76570100	-2.21632800	-0.68959000
H	-3.21734300	-1.05982200	0.81943300
H	-1.90415100	-0.21454700	1.64980100
H	-3.04134600	0.26421800	-1.17363800
Cl	2.55071800	-0.24284700	-0.22040200
H	0.67421000	2.17594800	-0.56972600

Low frequencies (cm⁻¹): -410.43, 128.73, 234.56, 264.03, 319.85, 343.60, 371.28, 413.83, 531.88, 537.64

3h

C	0.36523500	0.79200900	1.24644900
C	0.36523500	0.79200900	-1.24644900
C	-0.41614700	-0.41960700	-0.75695400
C	-0.41614700	-0.41960700	0.75695400
N	1.76129700	0.59615000	-0.61362600
N	1.76129700	0.59615000	0.61362600
H	0.50459100	0.75531200	2.32462700
H	0.50459100	0.75531200	-2.32462700
C	-1.71195700	-0.44273800	0.00000000
C	-0.03093800	2.17639100	-0.75445900
C	-0.03093800	2.17639100	0.75445900
C	-1.26530500	2.57639700	0.00000000
H	-2.16486100	-1.42912900	0.00000000
H	-2.43347600	0.35538000	0.00000000
H	0.49930100	2.96622300	-1.27752800
H	0.49930100	2.96622300	1.27752800
H	-1.43603400	3.64827800	0.00000000
H	-2.18496100	2.01943100	0.00000000
Cl	0.01174000	-1.87560600	-1.65812400
Cl	0.01174000	-1.87560600	1.65812400

Low frequencies (cm⁻¹): 45.23, 154.14, 202.52, 204.13, 297.33, 297.83, 387.31, 395.30, 440.10, 485.95

TS-h

C	0.22553800	0.80424300	1.32143900
C	0.22553800	0.80424300	-1.32143900
C	-0.46817500	-0.37381500	-0.80489500
C	-0.46817500	-0.37381500	0.80489500
N	1.94055300	0.50221900	-0.57994700
N	1.94055300	0.50221900	0.57994700
H	0.54007900	0.74150600	2.35487200
H	0.54007900	0.74150600	-2.35487200
C	-1.72758700	-0.43534500	0.00000000
C	-0.03004600	2.14544900	-0.78762300
C	-0.03004600	2.14544900	0.78762300
C	-1.21543800	2.61054200	0.00000000
H	-2.16915400	-1.42571300	0.00000000
H	-2.45693700	0.35899400	0.00000000
H	0.55275900	2.92258600	-1.27278800
H	0.55275900	2.92258600	1.27278800
H	-1.33455800	3.68829600	0.00000000
H	-2.15774400	2.08890300	0.00000000
Cl	-0.00896100	-1.85386600	-1.64870800
Cl	-0.00896100	-1.85386600	1.64870800

Low frequencies (cm⁻¹): -543.25, 89.08, 156.52, 182.24, 212.57, 290.55, 293.98, 344.51, 369.52, 427.98

4h

C	0.88804500	-0.42300200	1.56724300
C	0.88804500	-0.42300200	-1.56724300
C	-0.30782600	0.07788800	-1.25798700
C	-0.30782600	0.07788800	1.25798700
H	0.97925000	-0.94380100	2.51597600
H	0.97925000	-0.94380100	-2.51597600
C	-0.71385100	0.81335000	0.00000000
C	2.13052600	-0.35025300	-0.76287000
C	2.13052600	-0.35025300	0.76287000
C	2.54174400	0.87802200	0.00000000
H	-1.79818900	0.92399200	0.00000000
H	-0.30832300	1.83307900	0.00000000
H	2.94874400	-0.91291500	-1.20008600
H	2.94874400	-0.91291500	1.20008600
H	3.59250600	1.14544300	0.00000000
H	1.86284000	1.72286700	0.00000000
Cl	-1.60885600	-0.10928700	-2.42311600
Cl	-1.60885600	-0.10928700	2.42311600

Low frequencies (cm⁻¹): 42.30, 93.70, 209.57, 248.43, 253.19, 327.03, 348.23, 384.60, 398.41, 472.68

5h

C	-0.02077500	-0.95188900	1.54878900
C	-0.02077500	-0.95188900	-1.54878900
C	-0.63242300	-2.09928500	-1.25060500
C	-0.63242300	-2.09928500	1.25060500
H	0.54994100	-0.90121200	2.47085900
H	0.54994100	-0.90121200	-2.47085900
C	-1.41999800	-2.41862700	0.00000000
C	-0.02077500	0.31789000	-0.77000400
C	-0.02077500	0.31789000	0.77000400
C	-1.21786200	0.79477900	0.00000000
H	-1.65499600	-3.48546900	0.00000000
H	-2.39337100	-1.91174900	0.00000000
H	-1.39254300	1.86505800	0.00000000
H	-2.10864200	0.17709800	0.00000000
Cl	0.92344900	1.57412900	-1.58933300
Cl	0.92344900	1.57412900	1.58933300
H	-0.51638000	-2.91020300	1.96512700
H	-0.51638000	-2.91020300	-1.96512700

Low frequencies (cm⁻¹): 98.26, 142.12, 199.98, 240.58, 254.19, 320.44, 345.22, 370.49, 402.67, 474.04

TS_{4h→5h}

C	0.87429000	1.50191200	-0.43832100
C	0.87429800	-1.50191300	-0.43831500
C	-0.24398500	-0.99511800	0.24323200
C	-0.24399100	0.99511800	0.24323000
H	0.64930200	2.22397200	-1.21716100
H	0.64931200	-2.22397000	-1.21715800
C	-0.27009700	0.00000000	1.34975200
H	0.57318500	0.00000700	2.03038200
H	-1.20590600	-0.00000100	1.90365300
C	2.17621900	-1.06675100	-0.35577600
C	2.17621500	1.06676000	-0.35577500
C	2.72221200	0.00000500	0.53968800
H	2.87171300	1.47871800	-1.08090300
H	3.81182100	0.00000900	0.54531100
H	2.37867500	0.00000100	1.56916700
H	2.87172100	-1.47871000	-1.08089900
Cl	-1.79384200	-1.68525000	-0.18172700
Cl	-1.79385100	1.68524400	-0.18172500

Low frequencies (cm⁻¹): -399.29, 102.55, 139.41, 243.36, 255.72, 293.75, 312.64, 344.19, 381.40, 429.80

3i

C	-0.66742700	0.35425500	1.25458700
C	0.16447000	0.36481400	-1.08879200
C	1.17943100	-0.39590900	-0.24084800
C	0.61025000	-0.47137700	1.15767200
N	0.15611100	1.75468800	-0.41848500
N	-0.23989800	1.74644900	0.74545100
H	-0.97920000	0.49612600	2.28834800
H	0.52815300	0.52499300	-2.10439800
C	0.89695500	-1.73044800	0.37041200
C	-1.30722500	-0.03862000	-1.07374700
C	-1.83533300	0.02773000	0.33942600
C	-1.99057100	-1.23181000	-0.44984500
H	1.78641400	-2.24973100	0.71653500
H	0.15391600	-2.40361300	-0.01752700
H	1.29177800	-0.28202200	1.98348000
H	-1.87680500	0.45955700	-1.85265700
H	-2.72565800	0.61486500	0.54521200
H	-2.99290500	-1.38840100	-0.83651300
H	-1.51045100	-2.15128200	-0.16645500
C	2.61142200	0.03070600	-0.47574200
H	2.96394400	-0.30006300	-1.45887200
H	2.70609800	1.12032100	-0.42739700
H	3.26939600	-0.40474200	0.28274900

Low frequencies (cm⁻¹): 96.86, 212.89, 238.84, 275.76, 328.45, 378.17, 402.42, 426.11, 486.95, 579.01

TS-i

C	-0.70850300	0.23234200	1.31379200
C	0.17269000	0.19697800	-1.16925500
C	1.13496700	-0.46652600	-0.28188500
C	0.56375900	-0.48132800	1.20323100
N	0.22176000	1.93716600	-0.39423500
N	-0.16476300	1.95234000	0.70059200
H	-0.97971200	0.57837100	2.30328500
H	0.56115600	0.52097900	-2.12835100
C	0.87185900	-1.74417400	0.45109400
C	-1.27041400	-0.04764300	-1.11233100
C	-1.80944700	0.00244100	0.37815400
C	-2.01151000	-1.19597900	-0.49406100
H	1.77525800	-2.23671300	0.79709100
H	0.11397500	-2.44185200	0.13816300
H	1.28482900	-0.21935300	1.97380500
H	-1.83789400	0.52512600	-1.84027100
H	-2.68544300	0.62000500	0.55508300
H	-3.02597400	-1.29443200	-0.86520200
H	-1.55511500	-2.14610300	-0.27421900
C	2.57545400	-0.04766300	-0.48643300
H	2.96987600	-0.45233400	-1.42476200
H	2.66025400	1.04332500	-0.52167500
H	3.20667600	-0.41425400	0.32871700

Low frequencies (cm⁻¹): -526.62, 127.49, 199.50, 228.30, 254.83, 314.53, 331.30, 374.64, 394.64, 416.09

4i

C	-1.32608500	1.28286600	-0.56020700
C	0.50915400	-1.23157100	-0.35650300
C	1.33810200	-0.25567100	0.03116800
C	-0.16739600	1.77958000	-0.11997400
H	-1.95875800	1.94236800	-1.15092200
H	0.96218300	-2.10240600	-0.82854900
C	0.89062200	1.04673300	0.67592700
C	-0.96874500	-1.30608900	-0.24452800
C	-1.87359000	-0.07912300	-0.35631900
C	-1.73956500	-0.81571900	0.94849900
H	1.76426600	1.70021500	0.76671700
H	0.55994500	0.87275800	1.70870100
H	0.05972400	2.81227500	-0.37414900
H	-1.38587000	-2.19182500	-0.71389700
H	-2.79987700	-0.26276100	-0.89182000
H	-2.58421600	-1.40829800	1.28284800
H	-1.18855100	-0.32960200	1.74452600
C	2.82450700	-0.38769800	-0.16790900

H	3.35504100	-0.30407900	0.78910800
H	3.09005400	-1.34525200	-0.62344200
H	3.20403600	0.41676100	-0.81004900

Low frequencies (cm⁻¹): 90.44, 167.79, 229.40, 267.05, 309.04, 328.96, 377.27, 403.96, 518.62, 581.52

5i

C	0.31348500	-1.38694100	-0.25464900
C	-0.86458900	1.47753200	-0.55675200
C	-1.95540400	0.73971400	-0.33839300
C	-0.99656100	-1.58255400	-0.08689400
H	0.88930900	-2.22500400	-0.64713400
H	-0.98953000	2.38894100	-1.13818700
C	-2.02034700	-0.57959600	0.39940100
C	0.52603800	1.22331700	-0.10972000
C	1.13290900	-0.17464500	0.02308500
C	0.86190200	0.65675600	1.24560400
H	-3.01589000	-1.00790100	0.25416600
H	-1.93303500	-0.42583000	1.48412800
H	-1.38413600	-2.56504900	-0.34697700
H	1.23631100	1.95930700	-0.47707100
H	1.71751700	1.07464900	1.76756400
H	0.03882800	0.36696900	1.88826000
C	2.58116100	-0.31120100	-0.40450900
H	3.06139600	-1.14638100	0.11764200
H	2.65628900	-0.49521900	-1.48155400
H	3.14588400	0.59749300	-0.17527300
H	-2.89451300	1.10373200	-0.74859600

Low frequencies (cm⁻¹): 127.94, 157.16, 230.14, 265.55, 314.20, 331.81, 365.76, 379.78, 535.24, 560.35

TS_{4i→5i}

C	0.28273300	-1.31424500	-0.31404900
C	-0.88880900	1.36705800	-0.69121900
C	0.37054500	1.45712200	-0.10578700
C	1.19238600	-0.35349600	0.13300300
H	0.67346400	-2.01064400	-1.05350000
H	-1.02047300	1.93666000	-1.60796500
C	0.86975700	0.73598800	1.10284000
H	0.16160300	0.52002500	1.89274700
H	1.76202000	1.19453800	1.53038100
C	-1.90421200	0.46980500	-0.38966200
C	-1.09191200	-1.36811900	-0.12313100
C	-1.93940700	-0.49935500	0.74556700
H	-1.63442000	-2.10757200	-0.70501200
H	-2.93258500	-0.91664300	0.90704400

H	-1.53085800	-0.17478500	1.69507900
H	-2.74912100	0.42713700	-1.07042800
C	2.63218900	-0.43257200	-0.31415300
H	3.24968000	-0.89462100	0.46706400
H	2.74172200	-1.02269400	-1.22774200
H	3.04783900	0.56236100	-0.50318100
H	1.09150900	2.11313100	-0.58493000

Low frequencies (cm⁻¹): -397.19, 145.42, 170.78, 268.75, 299.41, 337.84, 357.65, 379.49, 428.60, 543.13

3j

C	-0.35672800	0.43462700	-1.23929300
C	-0.35672800	0.43462700	1.23929300
C	0.39281900	-0.80869200	0.75944800
C	0.39281900	-0.80869200	-0.75944800
N	-1.75552000	0.25179800	0.61494100
N	-1.75552000	0.25179800	-0.61494100
H	-0.50694200	0.41109100	-2.31931800
H	-0.50694200	0.41109100	2.31931800
C	1.69168700	-0.80321700	0.00000000
C	0.04350400	1.82023100	0.75481800
C	0.04350400	1.82023100	-0.75481800
C	1.27779500	2.22190800	0.00000000
H	2.18722300	-1.77135600	0.00000000
H	2.39543500	0.00891500	0.00000000
H	-0.48457900	2.61456000	1.27436300
H	-0.48457900	2.61456000	-1.27436300
H	1.44512700	3.29474000	0.00000000
H	2.19792800	1.66626900	0.00000000
C	0.00861200	-2.04180600	1.55112800
H	0.35865400	-1.95635200	2.58561300
H	-1.07966100	-2.16677500	1.57115200
H	0.45062400	-2.94663600	1.12635100
C	0.00861200	-2.04180600	-1.55112800
H	-1.07966100	-2.16677500	-1.57115200
H	0.35865400	-1.95635200	-2.58561300
H	0.45062400	-2.94663600	-1.12635100

Low frequencies (cm⁻¹): 46.44, 179.03, 198.67, 244.38, 246.99, 285.13, 328.68, 329.98, 401.64, 433.41

TS-j

C	0.20958700	0.44668600	1.31319100
C	0.20958700	0.44668600	-1.31319100
C	-0.45444300	-0.75833300	-0.80368100
C	-0.45444300	-0.75833300	0.80368100
N	1.94863900	0.16263500	-0.58051200

N	1.94863900	0.16263500	0.58051200
H	0.54394500	0.39413700	2.34345500
H	0.54394500	0.39413700	-2.34345500
C	-1.72106500	-0.77707200	0.00000000
C	-0.04236900	1.78990200	-0.79159600
C	-0.04236900	1.78990200	0.79159600
C	-1.22120900	2.26648700	0.00000000
H	-2.21125700	-1.74669300	0.00000000
H	-2.42566400	0.03730700	0.00000000
H	0.54430600	2.56727300	-1.27289600
H	0.54430600	2.56727300	1.27289600
H	-1.32673800	3.34605400	0.00000000
H	-2.16941900	1.75633100	0.00000000
C	-0.04750200	-2.01917900	-1.54085900
H	-0.38390400	-1.97268800	-2.58206100
H	1.04237500	-2.13180600	-1.54239400
H	-0.48547200	-2.91456100	-1.09448400
C	-0.04750200	-2.01917900	1.54085900
H	1.04237500	-2.13180600	1.54239400
H	-0.38390400	-1.97268800	2.58206100
H	-0.48547200	-2.91456100	1.09448400

Low frequencies (cm⁻¹): -526.49, 105.44, 152.56, 155.56, 217.40, 239.77, 287.49, 324.33, 326.03, 367.88

4j

C	0.68443300	0.01848200	1.55627500
C	0.68443300	0.01848200	-1.55627500
C	-0.54704300	-0.41503800	-1.26830000
C	-0.54704300	-0.41503800	1.26830000
H	1.12888500	-0.33794400	2.48456000
H	1.12888500	-0.33794400	-2.48456000
C	-1.30386800	-0.05545700	0.00000000
C	1.56293200	0.91482000	-0.76437300
C	1.56293200	0.91482000	0.76437300
C	1.06408100	2.10944200	0.00000000
H	-2.25291100	-0.60369900	0.00000000
H	-1.58990700	1.00349100	0.00000000
H	2.54977600	1.03961800	-1.19948500
H	2.54977600	1.03961800	1.19948500
H	1.68481900	2.99895300	0.00000000
H	0.00000000	2.30920900	0.00000000
C	-1.27479900	-1.34308900	-2.20380500
H	-2.22916100	-0.90672400	-2.52464900
H	-0.68354900	-1.56690100	-3.09562100
H	-1.51408900	-2.28977400	-1.70290000
C	-1.27479900	-1.34308900	2.20380500
H	-0.68354900	-1.56690100	3.09562100
H	-2.22916100	-0.90672400	2.52464900

H	-1.51408900	-2.28977400	1.70290000
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Low frequencies (cm⁻¹): 72.44, 107.98, 210.65, 226.58, 253.03, 273.16, 306.00, 371.59, 379.22, 389.12

5j

C	-0.24956200	-0.55974300	1.53222000
C	-0.24956200	-0.55974300	-1.53222000
C	-1.46821100	-1.02735800	-1.25064000
C	-1.46821100	-1.02735800	1.25064000
H	0.19871800	-0.90259700	2.46464300
H	0.19871800	-0.90259700	-2.46464300
C	-2.27429400	-0.76076100	0.00000000
C	0.61598900	0.38696700	-0.77133600
C	0.61598900	0.38696700	0.77133600
C	0.00000000	1.52449700	0.00000000
H	-3.14693300	-1.41941600	0.00000000
H	-2.68445200	0.25797300	0.00000000
H	0.54096900	2.46744300	0.00000000
H	-1.07847500	1.62813700	0.00000000
C	1.92645800	0.65049000	1.49525200
H	1.72109100	0.94215000	2.53093500
H	2.55243300	-0.24854700	1.51786000
H	2.50417400	1.45623200	1.03985200
C	1.92645800	0.65049000	-1.49525200
H	2.55243300	-0.24854700	-1.51786000
H	1.72109100	0.94215000	-2.53093500
H	2.50417400	1.45623200	-1.03985200
H	-1.91585900	-1.70543100	1.97366300
H	-1.91585900	-1.70543100	-1.97366300

Low frequencies (cm⁻¹): 120.14, 147.63, 165.83, 170.05, 253.18, 301.57, 342.60, 344.07, 374.08, 381.82

TS_{4j→5j}

C	-0.49480500	-1.48026000	-0.46614700
C	-0.49481000	1.48025700	-0.46613800
C	0.68798200	1.00214200	0.12267000
C	0.68798900	-1.00214700	0.12266300
H	-0.34483400	-2.19781100	-1.27074300
H	-0.34483600	2.19781700	-1.27072700
C	0.74687200	-0.00000700	1.23071300
H	-0.04760800	-0.00001400	1.96722200
H	1.71308200	-0.00000500	1.73985200
C	-1.79373400	1.04680200	-0.30070700
C	-1.79373100	-1.04680800	-0.30071000
C	-2.28695200	-0.00000500	0.64515600
H	-2.53597700	-1.44807000	-0.98513000

H	-3.37416200	-0.00000600	0.72226000
H	-1.86926100	-0.00000500	1.64602200
H	-2.53598100	1.44806500	-0.98512600
C	1.98459300	-1.67436400	-0.25343400
H	2.27913500	-2.38666300	0.52835400
H	1.89336700	-2.22240700	-1.19489400
H	2.81340300	-0.96804200	-0.35716000
C	1.98457000	1.67438300	-0.25343400
H	2.81335000	0.96805500	-0.35735400
H	1.89326900	2.22257100	-1.19480400
H	2.27920600	2.38655700	0.52843200

Low frequencies (cm⁻¹): -382.63, 81.46, 123.43, 124.83, 250.13, 288.14, 295.90, 330.75, 350.13, 370.35

3k

C	0.03807000	0.40252600	-1.05416900
C	-0.92408200	0.32657900	1.24665000
C	-2.03559700	0.04132300	0.24960500
C	-1.43900400	0.04180900	-1.13881400
N	-0.43609400	1.72441800	0.81009800
N	0.02852600	1.76437900	-0.32590800
H	0.47745200	0.58405400	-2.03310900
H	-1.29777300	0.44323800	2.26234400
C	-2.16800900	-1.16972000	-0.62092400
C	0.34336800	-0.51688400	1.21945400
C	0.95954200	-0.43869800	-0.17245100
C	0.63044700	-1.77119600	0.45266900
H	-3.15492400	-1.28237700	-1.05855200
H	-1.71617300	-2.11792400	-0.39135600
H	-1.94868000	0.60019100	-1.91791400
H	-2.93289200	0.62392500	0.43529700
H	1.50523400	-2.30423000	0.81038200
H	-0.11119700	-2.41837100	0.02267900
C	2.36290600	-0.10924000	-0.30395600
N	3.48924800	0.13337100	-0.40691900
H	1.00134400	-0.32268000	2.06094800

Low frequencies (cm⁻¹): 59.30, 138.96, 160.60, 296.67, 354.27, 361.73, 400.99, 434.68, 538.54, 555.44

TS-k

C	0.05056500	0.23425600	-1.14389600
C	-0.96962800	0.22267900	1.29456500
C	-2.01659500	0.03786100	0.28805300
C	-1.39816900	0.02448000	-1.17276300
N	-0.32709600	1.92807600	0.75891700
N	0.11224400	1.93164800	-0.31506900

H	0.51501700	0.55759800	-2.06668700
H	-1.28912700	0.55877200	2.27254200
C	-2.19384000	-1.12597400	-0.63531600
C	0.28273500	-0.53320000	1.26050400
C	0.91965500	-0.50777300	-0.21779800
C	0.59510200	-1.78559400	0.51054100
H	-3.18856800	-1.18796500	-1.06279300
H	-1.76999200	-2.09495300	-0.43368000
H	-1.90650200	0.63673800	-1.91150200
H	-2.88902600	0.66800100	0.43320900
H	1.47579500	-2.30041900	0.87812700
H	-0.15892400	-2.45297900	0.13105400
C	2.32531500	-0.17552500	-0.31329200
N	3.45255100	0.07712000	-0.37579900
H	0.97658800	-0.28995000	2.05981200

Low frequencies (cm⁻¹): -540.42, 91.93, 139.51, 185.49, 263.14, 297.89, 345.89, 375.82, 384.98, 454.62

4k

C	0.34262600	-1.18805100	-0.31507200
C	-1.61996800	1.21240500	-0.60305500
C	-2.09081300	-0.17693500	-0.38486000
C	-1.12013700	-1.35666800	-0.24641100
H	0.87996300	-2.01750400	-0.76848800
H	-2.26969500	1.81407100	-1.23449000
C	-1.94507900	-0.89040500	0.92457700
C	-0.51357900	1.79390300	-0.13402500
C	1.07944900	-0.14269800	0.10034900
C	0.55704000	1.14663400	0.71622200
H	-2.75545800	-1.53619700	1.24341700
H	-1.43592600	-0.37591400	1.73016000
H	-1.46888100	-2.26980600	-0.71657700
H	-2.98581200	-0.42759100	-0.94509000
H	1.39515600	1.83967900	0.81576500
H	0.20707300	0.96448300	1.73953000
C	2.50566700	-0.22583400	-0.07301700
N	3.65716800	-0.26516200	-0.19500600
H	-0.33782300	2.83081100	-0.40743000

Low frequencies (cm⁻¹): 73.47, 147.95, 182.44, 240.13, 285.24, 327.35, 348.56, 500.09, 530.90, 579.63

5k

C	1.10337200	-1.44814500	-0.61198200
C	-0.14065400	1.38569600	-0.19240900
C	-0.88531700	0.13401600	0.12644100
C	-0.25514300	-1.26771500	-0.04468800

H	1.20984100	-2.32915000	-1.24007100
H	-0.76910700	2.19815400	-0.54725700
C	-0.52624000	-0.72659400	1.32108500
C	1.17069700	1.60766500	-0.08799300
C	2.17604400	-0.67146600	-0.44788000
C	2.24315600	0.62468800	0.32944400
H	-1.34817200	-1.15588700	1.88243200
H	0.30953100	-0.38216100	1.91736400
H	-0.97420200	-2.00639500	-0.38380100
H	3.21806400	1.08520100	0.15206300
H	2.20956800	0.43806000	1.41118500
H	1.51652100	2.60127000	-0.36130200
H	3.09146300	-0.97707300	-0.94841200
C	-2.29810500	0.18893500	-0.19103900
N	-3.42719400	0.22364400	-0.44115400

Low frequencies (cm⁻¹): 110.70, 142.14, 160.43, 230.35, 304.62, 314.29, 350.56, 488.98, 532.56, 571.73

TS_{4k→5k}

C	0.11961800	-1.32075600	-0.21165400
C	-1.10211600	1.33203700	-0.76419500
C	0.09580800	1.50218500	-0.07023300
C	0.93964700	-0.29037000	0.27876000
H	0.60878300	-2.02242900	-0.88110100
H	-1.17683800	1.86724800	-1.70673700
C	0.52580600	0.83171000	1.18666000
H	-0.22331900	0.59302700	1.93005800
H	1.37653000	1.31868800	1.65926200
C	-2.10094900	0.40669200	-0.51167400
C	-1.25252400	-1.42962800	-0.10860500
C	-2.19091500	-0.53624600	0.64104700
H	-1.72240500	-2.21556000	-0.69180500
H	-3.18198000	-0.97683900	0.73878400
H	-1.86939400	-0.17046500	1.60881200
H	-2.87893700	0.30294700	-1.26258300
C	2.32180000	-0.29969400	-0.11137100
N	3.44240500	-0.29117200	-0.40800000
H	0.83367700	2.16600900	-0.51109700

Low frequencies (cm⁻¹): -375.79, 107.92, 154.66, 220.02, 311.20, 333.47, 351.51, 370.60, 504.06, 545.27

3I

C	-0.37142100	0.70762100	1.24834300
C	-0.37142100	0.70762100	-1.24834300
C	-0.00920700	2.09959400	-0.75559400
C	-0.00920700	2.09959400	0.75559400

N	-1.75880500	0.46554200	-0.61337500
N	-1.75880500	0.46554200	0.61337500
H	-0.51879000	0.66862000	2.32561400
H	-0.51879000	0.66862000	-2.32561400
C	1.21130000	2.53866800	0.00000000
C	0.44481900	-0.49476200	-0.76961200
C	0.44481900	-0.49476200	0.76961200
C	1.73784000	-0.47711000	0.00000000
H	1.34215300	3.61607800	0.00000000
H	2.15387000	2.02136200	0.00000000
H	-0.56256000	2.87419600	1.27730700
H	-0.56256000	2.87419600	-1.27730700
H	2.24912100	-1.43419500	0.00000000
H	2.40213700	0.36602500	0.00000000
C	0.13290500	-1.71929600	1.47771800
N	-0.10152100	-2.68998000	2.05983300
C	0.13290500	-1.71929600	-1.47771800
N	-0.10152100	-2.68998000	-2.05983300

Low frequencies (cm⁻¹): 31.19, 99.30, 137.50, 141.89, 191.35, 293.12, 349.58, 358.94, 394.82, 397.96

TS-I

C	0.24092500	0.72260800	1.32156200
C	0.24092500	0.72260800	-1.32156200
C	-0.50496600	-0.44105600	-0.82193500
C	-0.50496600	-0.44105600	0.82193500
N	1.92932100	0.36016400	-0.58034600
N	1.92932100	0.36016400	0.58034600
H	0.56549800	0.64979600	2.35166700
H	0.56549800	0.64979600	-2.35166700
C	-1.76037300	-0.44532900	0.00000000
C	0.01837300	2.07082600	-0.78985400
C	0.01837300	2.07082600	0.78985400
C	-1.14833800	2.57717400	0.00000000
H	-2.26509200	-1.40538100	0.00000000
H	-2.43508900	0.39259600	0.00000000
H	0.62888300	2.82924200	-1.27010600
H	0.62888300	2.82924200	1.27010600
H	-1.22343300	3.65888800	0.00000000
H	-2.11284900	2.09882500	0.00000000
C	-0.17473900	-1.68683900	-1.48090700
N	0.08102500	-2.68020300	-2.01436400
C	-0.17473900	-1.68683900	1.48090700
N	0.08102500	-2.68020300	2.01436400

Low frequencies (cm⁻¹): -558.19, 74.74, 99.96, 130.05, 152.43, 203.20, 269.07, 299.58, 341.88, 368.30

4I

C	-0.79816600	-0.42990300	1.55785000
C	-0.79816600	-0.42990300	-1.55785000
C	-2.04249400	-0.37369500	-0.76782600
C	-2.04249400	-0.37369500	0.76782600
H	-0.87198600	-0.98040100	2.49220900
H	-0.87198600	-0.98040100	-2.49220900
C	-2.47048000	0.84419500	0.00000000
C	0.39873900	0.10398800	-1.26030200
C	0.39873900	0.10398800	1.26030200
C	0.75824500	0.87352400	0.00000000
H	-3.52742200	1.08445800	0.00000000
H	-1.81334000	1.70470000	0.00000000
H	-2.85141700	-0.95430100	1.19746800
H	-2.85141700	-0.95430100	-1.19746800
H	1.83453600	1.05545800	0.00000000
H	0.29034000	1.86401000	0.00000000
C	1.46362200	-0.07706700	2.21119400
N	2.33397700	-0.20181600	2.96492200
C	1.46362200	-0.07706700	-2.21119400
N	2.33397700	-0.20181600	-2.96492200

Low frequencies (cm⁻¹): 55.32, 85.74, 143.51, 175.96, 223.42, 234.11, 301.17, 311.47, 344.71, 474.17

5I

C	0.38572400	0.78550600	1.55674200
C	0.38572400	0.78550600	-1.55674200
C	-0.16485000	-0.36604300	-0.78302100
C	-0.16485000	-0.36604300	0.78302100
H	0.88381700	0.49556900	2.47727400
H	0.88381700	0.49556900	-2.47727400
C	-1.44841000	-0.28043000	0.00000000
C	0.32860000	2.08235500	-1.25139300
C	0.32860000	2.08235500	1.25139300
C	-0.24665100	2.70669300	0.00000000
H	-2.08429600	-1.15821900	0.00000000
H	-1.96333800	0.67136600	0.00000000
H	-0.00123000	3.77088800	0.00000000
H	-1.34345600	2.66761000	0.00000000
C	0.10274200	-1.65023300	-1.40268000
N	0.31406100	-2.66092100	-1.92225900
C	0.10274200	-1.65023300	1.40268000
N	0.31406100	-2.66092100	1.92225900
H	0.78580300	2.76674800	-1.96108200
H	0.78580300	2.76674800	1.96108200

Low frequencies (cm⁻¹): 88.97, 114.47, 138.45, 164.31, 181.06, 253.29, 289.66, 318.24, 340.16, 470.03

TS_{41→51}

C	-0.78329100	-1.50308900	-0.45121400
C	-0.78329100	1.50308900	-0.45121400
C	0.32563300	1.00249000	0.26785300
C	0.32563300	-1.00249000	0.26785300
H	-0.53884000	-2.21695400	-1.23208000
H	-0.53884000	2.21695400	-1.23208000
C	0.30222600	0.00000000	1.37842600
H	-0.56455700	0.00000000	2.02472000
H	1.21689700	0.00000000	1.96735200
C	-2.08489200	1.07212800	-0.39506900
C	-2.08489200	-1.07212800	-0.39506900
C	-2.65400600	0.00000000	0.48277700
H	-2.76236300	-1.47794800	-1.14068100
H	-3.74296500	0.00000000	0.45636100
H	-2.33855600	0.00000000	1.52032200
H	-2.76236300	1.47794800	-1.14068100
C	1.61691000	-1.53161600	-0.07169200
N	2.66071100	-1.96370300	-0.32778500
C	1.61691000	1.53161600	-0.07169200
N	2.66071100	1.96370300	-0.32778500

Low frequencies (cm⁻¹): -342.38, 88.72, 95.40, 163.33, 164.40, 227.12, 291.74, 303.65, 334.47, 371.70

3m

C	0.96839800	1.16394400	0.60465800
C	1.10438900	-1.27036800	0.03819700
C	-0.16209700	-0.70528800	-0.56225800
C	-0.19803400	0.79192300	-0.30417900
N	0.94627000	-0.97678600	1.54720300
N	0.86707500	0.21454500	1.82249700
H	0.84981300	2.17282100	0.99417300
H	1.14093600	-2.35107600	-0.06487900
C	-0.27367200	0.25986800	-1.69532000
C	2.42269400	-0.58608400	-0.31078500
C	2.36809200	0.86871000	0.09389300
C	2.72818600	0.50262200	-1.30948000
H	-1.28844200	0.34220800	-2.07385000
H	0.49567200	0.33882100	-2.44183000
H	3.27519800	-1.17527900	0.01081800
H	3.14459200	1.27168900	0.73624300
H	3.78843100	0.58495900	-1.52534400
H	2.11951400	0.77081500	-2.15492900
N	-1.37924600	-1.50684100	-0.24465200

O	-1.20689100	-2.57252700	0.30563100
O	-2.45088500	-1.02938200	-0.56076000
N	-1.47227000	1.42107800	0.18596200
O	-1.62738100	1.41794800	1.38960700
O	-2.21562300	1.91259800	-0.63270600

Low frequencies (cm⁻¹): 55.39, 61.25, 84.38, 148.22, 181.20, 207.67, 267.68, 300.96, 356.87, 372.22

TS-m

C	0.95496400	1.30678900	0.40842300
C	1.12661800	-1.29620100	-0.04747500
C	-0.11325700	-0.76320600	-0.59576600
C	-0.19773000	0.84907700	-0.36318300
N	0.89426600	-0.87919800	1.75665400
N	0.82009500	0.25980200	1.96107700
H	0.82469600	2.25690500	0.90949100
H	1.14556600	-2.36817100	0.08972100
C	-0.30117600	0.21736300	-1.70106300
C	2.40635600	-0.61653600	-0.29573900
C	2.31411200	0.92720700	0.00103900
C	2.74495400	0.41123900	-1.33403400
H	-1.32620000	0.24125900	-2.05672400
H	0.44280900	0.33479400	-2.47057400
H	3.25405900	-1.13742700	0.13784500
H	3.09024400	1.34693000	0.63319900
H	3.81139200	0.50033700	-1.50804100
H	2.16621500	0.56861700	-2.22847300
N	-1.32139300	-1.55566300	-0.21252300
O	-1.14324900	-2.51314400	0.51122300
O	-2.39582800	-1.17702500	-0.63522400
N	-1.48229300	1.43849200	0.14678900
O	-1.54060100	1.62965600	1.34542800
O	-2.34439100	1.71030500	-0.65938200

Low frequencies (cm⁻¹): -556.72, 43.96, 76.13, 104.45, 150.02, 190.56, 206.37, 272.82, 288.75, 312.82

4m

C	0.66039000	0.96798600	-1.56236200
C	0.66039000	0.96798600	1.56236200
C	-0.03315800	-0.12776600	1.24807800
C	-0.03315800	-0.12776600	-1.24807800
H	0.43758600	1.41558800	-2.52575700
H	0.43758600	1.41558800	2.52575700
C	0.00000000	-0.96485200	0.00000000
C	1.70866000	1.62768200	0.76501700
C	1.70866000	1.62768200	-0.76501700

C	2.73785600	0.84407200	0.00000000
H	-0.87479300	-1.61313500	0.00000000
H	0.86194800	-1.64392800	0.00000000
H	2.05982900	2.55798600	1.19711800
H	2.05982900	2.55798600	-1.19711800
H	3.75557000	1.21656100	0.00000000
H	2.64553100	-0.23610300	0.00000000
N	-0.96969800	-0.61449400	2.29587700
O	-1.13956200	0.06979800	3.28787500
O	-1.50218300	-1.69234800	2.10360500
N	-0.96969800	-0.61449400	-2.29587700
O	-1.13956200	0.06979800	-3.28787500
O	-1.50218300	-1.69234800	-2.10360500

Low frequencies (cm⁻¹): 39.16, 43.97, 50.25, 98.02, 191.91, 237.99, 257.61, 318.14, 323.42, 353.33

5m

C	-1.22353300	-1.53929900	-0.18463600
C	-1.03417800	1.54139900	-0.49622200
C	-2.34690600	1.32706600	-0.41264700
C	-2.49721400	-1.14598600	-0.12748300
H	-0.99055800	-2.51538400	-0.59318900
H	-0.66771200	2.34687700	-1.12535200
C	-3.02574400	0.19775000	0.32814100
C	0.03408900	0.75819000	0.17435700
C	-0.03804400	-0.77814600	0.27127100
C	-0.02952300	0.09606900	1.49643100
H	-4.09778200	0.23854100	0.12575000
H	-2.93266400	0.32057300	1.41403200
H	0.90135200	0.11030100	2.05338600
H	-0.94273900	0.14930900	2.07467500
N	1.37597900	1.33027500	-0.18666000
O	1.67444900	1.25858000	-1.36159500
O	2.01773400	1.86195300	0.68998700
N	1.26037900	-1.46970600	-0.01417500
O	1.24193200	-2.38422600	-0.80939700
O	2.24954100	-1.05640400	0.55978500
H	-3.23764700	-1.85268600	-0.49199900

Low frequencies (cm⁻¹): 59.47, 73.77, 95.77, 143.05, 179.92, 211.70, 239.38, 283.88, 300.75, 337.19

TS_{4m→5m}

C	1.24083400	1.46860000	-0.29256800
C	1.02319100	-1.51195500	-0.49089600
C	-0.04330200	-0.96686800	0.24436500
C	0.08188900	0.98235300	0.33555800

H	1.07002900	2.24848400	-1.02484600
H	0.72919000	-2.14627900	-1.31939800
C	-0.04107100	-0.04728100	1.40285700
H	0.77252100	-0.11548700	2.11260000
H	-1.00751500	-0.02095800	1.89848200
C	2.34869800	-1.18224600	-0.36955700
C	2.50344500	0.94048600	-0.20323500
C	2.95044900	-0.23087900	0.61659100
H	3.24635600	1.34887300	-0.88205800
H	4.03610700	-0.31028500	0.64427900
H	2.57305500	-0.28994700	1.63151300
H	3.02278700	-1.58014900	-1.12221700
N	-1.18699900	1.63571900	-0.06314100
O	-2.20398600	1.27205100	0.50005200
O	-1.13857200	2.49660300	-0.92170100
N	-1.38430800	-1.48171700	-0.14431100
O	-2.21920500	-1.56956600	0.73285500
O	-1.54175800	-1.81477900	-1.30431500

Low frequencies (cm⁻¹): -387.53, 39.25, 71.71, 98.03, 147.25, 232.17, 233.87, 277.60, 307.57, 332.02

3n

C	0.37998100	1.90969200	1.24176200
C	0.37998100	1.90969200	-1.24176200
C	-0.45639500	0.71238200	-0.76761000
C	-0.45639500	0.71238200	0.76761000
N	1.76531300	1.68116300	-0.61512600
N	1.76531300	1.68116300	0.61512600
H	0.52722500	1.87360300	2.32046400
H	0.52722500	1.87360300	-2.32046400
C	-1.74109600	0.83417300	0.00000000
C	0.05296700	3.31852200	-0.75483300
C	0.05296700	3.31852200	0.75483300
C	-1.14928100	3.80921700	0.00000000
H	-2.31629200	-0.08637300	0.00000000
H	-2.36654200	1.70599100	0.00000000
H	0.63401600	4.07526100	-1.27412600
H	0.63401600	4.07526100	1.27412600
H	-1.22829700	4.89237100	0.00000000
H	-2.11455700	3.33675600	0.00000000
C	-0.23157600	-0.54498600	-1.56303100
C	-1.30256400	-1.19428100	-2.18083000
C	1.05431400	-1.07425200	-1.72989000
C	-1.10450900	-2.35048400	-2.93145100
H	-2.30344900	-0.78345400	-2.08385200
C	1.25353000	-2.23008300	-2.47736500
H	1.90609000	-0.57360600	-1.27906900
C	0.17506200	-2.87515600	-3.07840100

H	-1.95223400	-2.83685600	-3.40453100
H	2.25731400	-2.62836000	-2.58961000
H	0.33297300	-3.77739900	-3.66114500
C	-0.23157600	-0.54498600	1.56303100
C	-1.30256400	-1.19428100	2.18083000
C	1.05431400	-1.07425200	1.72989000
C	-1.10450900	-2.35048400	2.93145100
H	-2.30344900	-0.78345400	2.08385200
C	1.25353000	-2.23008300	2.47736500
H	1.90609000	-0.57360600	1.27906900
C	0.17506200	-2.87515600	3.07840100
H	-1.95223400	-2.83685600	3.40453100
H	2.25731400	-2.62836000	2.58961000
H	0.33297300	-3.77739900	3.66114500

Low frequencies (cm⁻¹): 16.51, 24.07, 38.34, 70.29, 106.06, 141.59, 150.22, 238.27, 259.34, 264.75

TS-n

C	0.21909200	1.93508200	1.31529200
C	0.21909200	1.93508200	-1.31529200
C	-0.50894700	0.75884000	-0.82590600
C	-0.50894700	0.75884000	0.82590600
N	1.94850400	1.70162100	-0.58125600
N	1.94850400	1.70162100	0.58125600
H	0.54655300	1.87368500	2.34650600
H	0.54655300	1.87368500	-2.34650600
C	-1.75462600	0.83047500	0.00000000
C	-0.00634600	3.29014200	-0.78697100
C	-0.00634600	3.29014200	0.78697100
C	-1.16680400	3.82046500	0.00000000
H	-2.30645700	-0.10237700	0.00000000
H	-2.40358100	1.68772400	0.00000000
H	0.61235600	4.04375400	-1.26632200
H	0.61235600	4.04375400	1.26632200
H	-1.21175300	4.90449500	0.00000000
H	-2.14471100	3.37120600	0.00000000
C	-0.25040400	-0.52561800	-1.56287000
C	-1.31060000	-1.26292300	-2.09804300
C	1.05262500	-0.99852700	-1.76048200
C	-1.08284900	-2.44265500	-2.80059100
H	-2.32786800	-0.90093800	-1.98094300
C	1.28147000	-2.18048000	-2.45785100
H	1.89593700	-0.44062500	-1.36743500
C	0.21562500	-2.90918200	-2.97885900
H	-1.92274500	-2.99421800	-3.21207900
H	2.29945400	-2.53334000	-2.59232300
H	0.39633300	-3.83107600	-3.52290200
C	-0.25040400	-0.52561800	1.56287000

C	-1.31060000	-1.26292300	2.09804300
C	1.05262500	-0.99852700	1.76048200
C	-1.08284900	-2.44265500	2.80059100
H	-2.32786800	-0.90093800	1.98094300
C	1.28147000	-2.18048000	2.45785100
H	1.89593700	-0.44062500	1.36743500
C	0.21562500	-2.90918200	2.97885900
H	-1.92274500	-2.99421800	3.21207900
H	2.29945400	-2.53334000	2.59232300
H	0.39633300	-3.83107600	3.52290200

Low frequencies (cm⁻¹): -547.08, 37.05, 41.12, 46.94, 86.57, 107.90, 154.47, 168.53, 223.24, 244.81

4n

C	1.97919000	-0.33244000	1.55288900
C	1.97919000	-0.33244000	-1.55288900
C	0.78875000	0.21733000	-1.26430200
C	0.78875000	0.21733000	1.26430200
H	2.05583600	-0.87213000	2.49487300
H	2.05583600	-0.87213000	-2.49487300
C	0.50526700	1.01762900	0.00000000
C	3.23149800	-0.30826700	-0.76522100
C	3.23149800	-0.30826700	0.76522100
C	3.71015400	0.89420000	0.00000000
H	-0.55378900	1.28284000	0.00000000
H	1.05121700	1.96851900	0.00000000
H	4.02349000	-0.90872900	-1.20166100
H	4.02349000	-0.90872900	1.20166100
H	4.77628400	1.09254200	0.00000000
H	3.09045200	1.78153800	0.00000000
C	-0.33683200	0.04714500	-2.22231400
C	-1.19635900	1.11405700	-2.51530700
C	-0.55927000	-1.17572100	-2.86768600
C	-2.22848300	0.97030500	-3.43640000
H	-1.04115400	2.07574400	-2.03327000
C	-1.59261100	-1.32247600	-3.78703600
H	0.07209900	-2.02429800	-2.62104300
C	-2.43109900	-0.24929200	-4.07721200
H	-2.87480400	1.81481800	-3.65590200
H	-1.75169300	-2.28299900	-4.26794800
H	-3.24082300	-0.36445300	-4.79095200
C	-0.33683200	0.04714500	2.22231400
C	-1.19635900	1.11405700	2.51530700
C	-0.55927000	-1.17572100	2.86768600
C	-2.22848300	0.97030500	3.43640000
H	-1.04115400	2.07574400	2.03327000
C	-1.59261100	-1.32247600	3.78703600
H	0.07209900	-2.02429800	2.62104300

C	-2.43109900	-0.24929200	4.07721200
H	-2.87480400	1.81481800	3.65590200
H	-1.75169300	-2.28299900	4.26794800
H	-3.24082300	-0.36445300	4.79095200

Low frequencies (cm⁻¹): 23.84, 45.95, 59.60, 75.33, 115.01, 125.90, 169.56, 185.81, 227.76, 250.92

5n

C	-0.21727700	2.12144500	1.53939700
C	-0.21727700	2.12144500	-1.53939700
C	-0.22694100	3.42507200	-1.24815100
C	-0.22694100	3.42507200	1.24815100
H	-0.69455900	1.82233600	2.47025800
H	-0.69455900	1.82233600	-2.47025800
C	0.31037300	4.08643100	0.00000000
C	0.37982900	0.98005800	-0.78582900
C	0.37982900	0.98005800	0.78582900
C	1.64481000	1.16467300	0.00000000
H	0.00000000	5.13460200	0.00000000
H	1.40811000	4.11368600	0.00000000
H	2.35623400	0.34637900	0.00000000
H	2.10239500	2.14601200	0.00000000
H	-0.71086000	4.08251100	-1.96673900
H	-0.71086000	4.08251100	1.96673900
C	0.12782000	-0.34772900	1.44716500
C	1.15726400	-1.19275600	1.85894300
C	-1.19407600	-0.74412000	1.68076800
C	0.87615800	-2.40851500	2.47992600
H	2.19121000	-0.89602300	1.71022700
C	-1.47914300	-1.95543500	2.29865000
H	-2.00357300	-0.09009900	1.36386600
C	-0.44132100	-2.79523800	2.69934600
H	1.69219500	-3.05087600	2.79702400
H	-2.51169600	-2.24762200	2.46451100
H	-0.66015000	-3.74321600	3.18095300
C	0.12782000	-0.34772900	-1.44716500
C	1.15726400	-1.19275600	-1.85894300
C	-1.19407600	-0.74412000	-1.68076800
C	0.87615800	-2.40851500	-2.47992600
H	2.19121000	-0.89602300	-1.71022700
C	-1.47914300	-1.95543500	-2.29865000
H	-2.00357300	-0.09009900	-1.36386600
C	-0.44132100	-2.79523800	-2.69934600
H	1.69219500	-3.05087600	-2.79702400
H	-2.51169600	-2.24762200	-2.46451100
H	-0.66015000	-3.74321600	-3.18095300

Low frequencies (cm⁻¹): 6.80, 40.36, 68.52, 92.91, 106.77, 116.54, 176.31, 188.13, 233.79, 246.88

TS_{4n→5n}

C	2.12078300	1.48809200	-0.40561000
C	2.12081700	-1.48796900	-0.40568300
C	1.07383100	-1.01951600	0.40371400
C	1.07376800	1.01958000	0.40371300
H	1.83059700	2.21963700	-1.15588100
H	1.83059600	-2.21948600	-1.15597200
C	1.24006000	0.00004000	1.48916900
H	2.17609300	0.00009100	2.03127200
H	0.41522700	-0.00002300	2.19822800
C	3.42731100	-1.04375300	-0.48758100
C	3.42728400	1.04388300	-0.48749300
C	4.09759200	0.00003600	0.34552900
H	4.02908500	1.45143800	-1.29480000
H	5.17739200	0.00006400	0.19904500
H	3.89400000	-0.00003600	1.41052100
H	4.02910800	-1.45125600	-1.29491600
C	-0.29287400	1.55415700	0.16862800
C	-1.13884300	1.88254600	1.23459900
C	-0.77288700	1.73784100	-1.13540100
C	-2.41188800	2.39514500	1.00689900
H	-0.78906700	1.76029500	2.25585800
C	-2.04506600	2.24800900	-1.36573200
H	-0.14445000	1.44888100	-1.97345100
C	-2.87069700	2.58022900	-0.29424800
H	-3.04601300	2.65319100	1.84971100
H	-2.39866000	2.37318600	-2.38475600
H	-3.86665200	2.97375500	-0.47216200
C	-0.29276300	-1.55416900	0.16865500
C	-1.13871600	-1.88259000	1.23461700
C	-0.77275200	-1.73786800	-1.13538000
C	-2.41173800	-2.39524200	1.00691100
H	-0.78889200	-1.76037000	2.25585800
C	-2.04490500	-2.24809500	-1.36572300
H	-0.14431500	-1.44885200	-1.97341200
C	-2.87052700	-2.58035000	-0.29424100
H	-3.04584900	-2.65333900	1.84971800
H	-2.39848400	-2.37329600	-2.38474800
H	-3.86646000	-2.97392900	-0.47216000

Low frequencies (cm⁻¹): -325.60, 31.35, 36.16, 70.00, 87.58, 108.69, 137.79, 184.02, 223.99, 236.48

3o

C	-0.40873600	0.98354400	1.23690700
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C	-0.40873600	0.98354400	-1.23690700
C	0.40613300	-0.23451100	-0.76447700
C	0.40613300	-0.23451100	0.76447700
N	-1.79485500	0.76759100	-0.61604600
N	-1.79485500	0.76759100	0.61604600
H	-0.54993600	0.95314800	2.31855000
H	-0.54993600	0.95314800	-2.31855000
C	1.69440800	-0.14391400	0.00000000
C	-0.05942300	2.38719800	-0.75427700
C	-0.05942300	2.38719800	0.75427700
C	1.15564600	2.84565900	0.00000000
H	2.19740700	-1.10711300	0.00000000
H	2.36254400	0.69686000	0.00000000
H	-0.62272700	3.15730800	-1.27332900
H	-0.62272700	3.15730800	1.27332900
H	1.26915900	3.92561400	0.00000000
H	2.10324900	2.33860600	0.00000000
N	0.27090400	-1.43414300	1.54225100
N	0.27090400	-1.43414300	-1.54225100
C	-1.09177800	-1.81524300	-1.87654900
H	-1.07285500	-2.80802500	-2.33636100
H	-1.58293300	-1.12023800	-2.57985500
H	-1.70503400	-1.86307300	-0.97716800
C	1.10328100	-1.40023100	-2.73413800
H	0.76715700	-0.65718800	-3.48028000
H	1.08560600	-2.38458300	-3.21200800
H	2.13517400	-1.16824200	-2.45820000
C	-1.09177800	-1.81524300	1.87654900
H	-1.58293300	-1.12023800	2.57985500
H	-1.07285500	-2.80802500	2.33636100
H	-1.70503400	-1.86307300	0.97716800
C	1.10328100	-1.40023100	2.73413800
H	1.08560600	-2.38458300	3.21200800
H	0.76715700	-0.65718800	3.48028000
H	2.13517400	-1.16824200	2.45820000

Low frequencies (cm⁻¹): 12.56, 75.42, 113.91, 157.47, 191.34, 204.09, 208.92, 223.63, 243.94, 258.37

TS-o

C	-0.23486500	1.01239700	1.31382600
C	-0.23486500	1.01239700	-1.31382600
C	0.44355200	-0.19025600	-0.82030600
C	0.44355200	-0.19025600	0.82030600
N	-1.97420800	0.81256700	-0.58147600
N	-1.97420800	0.81256700	0.58147600
H	-0.55394800	0.96686500	2.35000100
H	-0.55394800	0.96686500	-2.35000100
C	1.69487600	-0.19178900	0.00000000

C	0.02664200	2.35819900	-0.78528200
C	0.02664200	2.35819900	0.78528200
C	1.21148200	2.83382600	0.00000000
H	2.14070600	-1.18175100	0.00000000
H	2.41023900	0.61286500	0.00000000
H	-0.56069300	3.13635900	-1.26478700
H	-0.56069300	3.13635900	1.26478700
H	1.31565500	3.91360300	0.00000000
H	2.16036800	2.32535700	0.00000000
N	0.22866200	-1.42169100	1.52854200
N	0.22866200	-1.42169100	-1.52854200
C	-1.14716100	-1.72381200	-1.88409500
H	-1.18155800	-2.73638800	-2.29769200
H	-1.57589900	-1.03522700	-2.63308800
H	-1.78344400	-1.69361600	-0.99988900
C	1.10065500	-1.52867500	-2.68766000
H	0.84338200	-0.81167500	-3.48845200
H	1.02812600	-2.53911100	-3.10208000
H	2.13736000	-1.35161400	-2.38943200
C	-1.14716100	-1.72381200	1.88409500
H	-1.57589900	-1.03522700	2.63308800
H	-1.18155800	-2.73638800	2.29769200
H	-1.78344400	-1.69361600	0.99988900
C	1.10065500	-1.52867500	2.68766000
H	1.02812600	-2.53911100	3.10208000
H	0.84338200	-0.81167500	3.48845200
H	2.13736000	-1.35161400	2.38943200

Low frequencies (cm⁻¹): -544.32, 55.28, 90.40, 108.35, 156.26, 195.43, 203.07, 224.47, 242.32, 244.06

4o

C	1.17072100	0.34390200	1.55980200
C	1.17072100	0.34390200	-1.55980200
C	-0.06874600	-0.07989900	-1.26081200
C	-0.06874600	-0.07989900	1.26081200
H	1.30887800	0.90774400	2.47685000
H	1.30887800	0.90774400	-2.47685000
C	-0.42696600	-0.85398200	0.00000000
C	2.40901300	0.17730100	-0.76527900
C	2.40901300	0.17730100	0.76527900
C	2.76270400	-1.06852500	0.00000000
H	-1.51146400	-0.96951800	0.00000000
H	0.00664600	-1.85950500	0.00000000
H	3.26127300	0.68879100	-1.20253500
H	3.26127300	0.68879100	1.20253500
H	3.80307200	-1.37616200	0.00000000
H	2.05704900	-1.88977300	0.00000000
N	-1.19713700	0.23616400	2.06108600

N	-1.19713700	0.23616400	-2.06108600
C	-1.01442500	1.26023100	-3.06743100
H	-1.99195800	1.51419800	-3.48780900
H	-0.35992200	0.94241700	-3.89852900
H	-0.58526700	2.15320000	-2.60722000
C	-1.87333200	-0.92630500	-2.62298700
H	-1.29120700	-1.38440200	-3.44052300
H	-2.84843300	-0.62439600	-3.01708700
H	-2.03765400	-1.68708600	-1.85728000
C	-1.01442500	1.26023100	3.06743100
H	-0.35992200	0.94241700	3.89852900
H	-1.99195800	1.51419800	3.48780900
H	-0.58526700	2.15320000	2.60722000
C	-1.87333200	-0.92630500	2.62298700
H	-2.84843300	-0.62439600	3.01708700
H	-1.29120700	-1.38440200	3.44052300
H	-2.03765400	-1.68708600	1.85728000

Low frequencies (cm⁻¹): 45.16, 68.81, 94.30, 103.88, 181.53, 209.11, 227.46, 237.33, 258.67, 266.97

5o

C	1.05714000	-1.61348300	-0.19230900
C	1.29710800	1.35738800	-0.66711000
C	2.57186500	0.99270100	-0.52137400
C	2.37672100	-1.43691900	-0.09061100
H	0.72819700	-2.58696700	-0.55269900
H	1.07651200	2.15078500	-1.37792800
C	3.08389000	-0.16123100	0.30908900
C	0.05337900	0.83060600	-0.02495200
C	-0.07985100	-0.70610000	0.16358700
C	0.07574400	0.20447200	1.34986900
H	4.15608200	-0.27993900	0.13343900
H	2.98550400	0.03578800	1.38353200
H	-0.83280400	0.36077300	1.92687100
H	0.98652000	0.15979300	1.93377500
N	-1.04154800	1.74580200	-0.34958600
N	-1.38047700	-1.30825400	0.00889300
C	-0.88394100	2.94937700	0.46023400
H	0.14147300	3.32152600	0.38969400
H	-1.55934100	3.72574200	0.08899000
H	-1.10836700	2.77308100	1.52772100
C	-2.42739800	1.30945700	-0.28504100
H	-2.63784800	0.54068200	-1.02471700
H	-2.73673400	0.93139700	0.70293900
H	-3.04278700	2.18402500	-0.52078600
C	-1.64160900	-2.36339300	0.97072300
H	-2.69162400	-2.66455200	0.89538200
H	-1.01886000	-3.26248900	0.81633100

H	-1.45925100	-1.99067700	1.98226900
C	-1.66564000	-1.73073200	-1.35089600
H	-1.37343800	-0.93864900	-2.04638900
H	-1.14257800	-2.65638100	-1.64629200
H	-2.74189400	-1.90982300	-1.45562200
H	3.30898400	1.52210000	-1.12040900
H	3.01198500	-2.27191500	-0.37850000

Low frequencies (cm⁻¹): 62.15, 99.93, 141.39, 148.23, 185.34, 207.42, 221.63, 247.54, 258.39, 267.78

TS_{40→50}

C	1.19403900	-1.51315200	0.37347700
C	1.19333000	1.51377800	0.37359400
C	0.04831700	1.00875100	-0.29141700
C	0.04880300	-1.00850400	-0.29141600
H	0.98245200	-2.26767800	1.12762100
H	0.98140600	2.26813800	1.12780800
C	0.07376400	0.00011500	-1.39369400
H	0.93503300	0.00031800	-2.04859800
H	-0.84773800	-0.00013200	-1.97372200
C	2.49931300	1.10477500	0.30526000
C	2.49984700	-1.10359500	0.30513900
C	3.05322200	0.00077100	-0.54285900
H	3.19052000	-1.54858900	1.01655600
H	4.14422800	0.00103300	-0.52103900
H	2.74879800	0.00076200	-1.58768200
H	3.18976300	1.54998000	1.01676300
N	-1.23871800	1.47942200	0.03081300
N	-1.23804100	-1.47980500	0.03082700
C	-1.86248100	2.34511800	-0.95404200
H	-1.71021400	1.94720000	-1.95988900
H	-2.94023400	2.39765800	-0.76624600
H	-1.45559200	3.37036900	-0.92742600
C	-1.48109400	1.92046500	1.38630900
H	-1.09601900	2.93358900	1.59737300
H	-2.56113700	1.93230800	1.56897900
H	-1.01454800	1.22106300	2.08440000
C	-1.47984700	-1.92127500	1.38630600
H	-2.55983400	-1.93375600	1.56925000
H	-1.09414700	-2.93422900	1.59705100
H	-1.01349600	-1.22177600	2.08443000
C	-1.86081300	-2.34628700	-0.95397000
H	-1.45251000	-3.37098700	-0.92752200
H	-2.93844000	-2.40029800	-0.76589100
H	-1.70937600	-1.94804800	-1.95981800

Low frequencies (cm⁻¹): -243.11, 50.98, 64.22, 91.81, 106.86, 161.30, 197.56, 221.00, 232.39, 238.48

10. REFERENCES

1. Neese, F. Software Update: The ORCA Program System—Version 5.0. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2022**, *12* (5). <https://doi.org/10.1002/wcms.1606>.