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.*

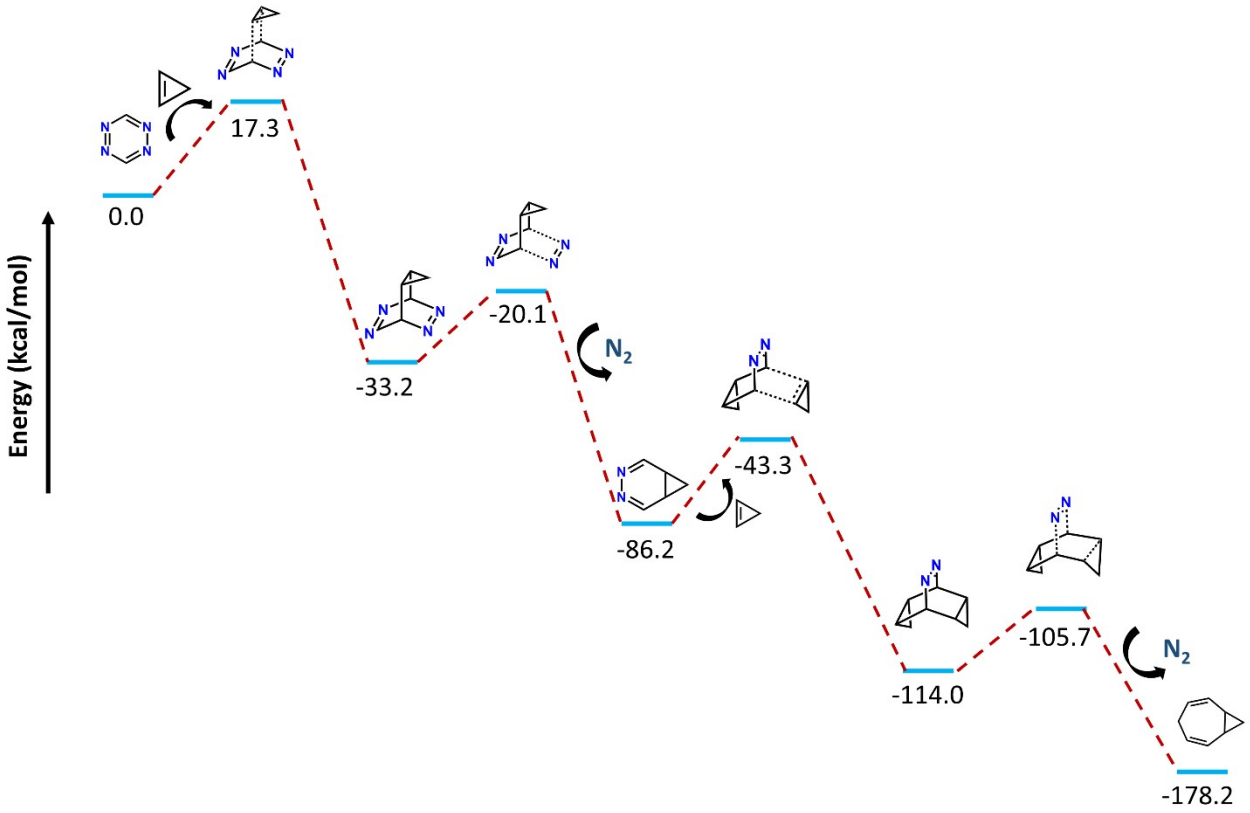
Level of Theory	Molecule	$\Delta G^{\ddagger}$ (kcal/mol)	ΔG_4 (kcal/mol)	ΔG_5 (kcal/mol)	$\Delta G^{\ddagger}_{4\rightarrow5}$ (kcal/mol)
B3LYP/6-31G(d) D3	**a**	3.4	-72.9	-72.9	22.7
B3LYP/6-31+G(d,p) D3		3.4	-76.0	-76.0	22.0
M062X/6-31G(d)		8.3	-64.2	-64.2	16.2
M062X/6-31+G(d,p)		8.2	-66.8	-66.8	16.2
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
N_2	-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
N_2	-109.4878008	-109.482001	-109.478696	45.761	-109.500439	2545.82

c. Table S7: ***3(a-o)→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)	**$\Delta G^{\ddagger}_{4\rightarrow5}$** (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)→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)	**$\Delta G^{\ddagger}_{4\rightarrow5}$** (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)→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)	$\Delta G^{\ddagger}_{4\rightarrow5}$ (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
#oniomchargemult 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 hastle and if you do not want to bother, use killcheck 1
killcheck 1
checkpoint g16.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 that
# 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=dmso,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 appart - 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 applys a polynomical 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 (firsttitle==1) {
    printf("%s %s %s %s %s %s %s  ",$1,$2,$3,$4,$6,$7,$8)
    printf(" %s %s %s  ",$6,$7,$8) >> "fullDistList"
    runpoint=$6
    }
  firsttitle++
  }
/Standard orientation/,/Rotational constants/ {
  if (($1>.5) && ($1<99)) {
    A[$1]=$4;B[$1]=$5;C[$1]=$6
    }
  }
#/before annihilation/ {
#   printf("%s %.5f ",$1,$6)
#   }

END {
   C1C2=Distance(1,2)
   C1N6=Distance(1,6)
   C2N5=Distance(2,5)
   C3C4=Distance(3,4)
   C10C11=Distance(10,11)
  if ((C1N6<1.54) && (C2N5<1.54) && (C1C2<2.49) && (C3C4<1.51) &&
(C11C10<1.51))
    custom1="reactant"
  if ((C1C2>3.18) && (C3C4>2.56) && (C10C11<1.50)&& (C1N6>2.7) && (C2N5>2.7))
    custom1="pdt_1"
  if ((C1C2>3.18) && (C3C4<1.50) && (C10C11>2.56) && (C1N6>2.7) && (C2N5>2.7))
    custom1="pdt_2"
  if ((C1C2<2.95) && (C3C4<2.01) && (C10C11<2.01) && (C1N6>2.7) && (C2N5>2.7))
    custom1="ts_2"
printf("%s\t%.3f\t%s\t%.3f\t%s\t%.3f\t%s\t%.3f\t%s\t%.3f\t%s\t%s\n","C1C2:",C1C2,"C1N6
:",C1N6,"C2N5:",C2N5,"C3C4:",C3C4,"C10C11:",C10C11,"Reached:",custom1) >>
"fullDistList"
  if (runpoint>=2000) {
    print "Too many points.  XXXXN"
#    system("date > nogo")
    }
   if ((C1N6<1.54) && (C2N5<1.54) && (C1C2<2.49) && (C3C4<1.51) &&
(C11C10<1.51)){
    print "reactant reached XXXX"
    }
   if ((C1C2>3.18) && (C3C4>2.56) && (C10C11<1.50)&& (C1N6>2.7) &&
(C2N5>2.7)){
    print "pdt_1 formed XXXX"
    }
   if ((C1C2>3.18) && (C3C4<1.50) && (C10C11>2.56) && (C1N6>2.7) &&
(C2N5>2.7)){
    print "pdt_2 formed XXXX"
    }
```

```
#    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

$TS_{4a \rightarrow 5a}$

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

N_2

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

$TS_{4d \rightarrow 5d}$

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

$TS_{4e \rightarrow 5e}$

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

$TS_{4f \rightarrow 5f}$

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

$TS_{4g \rightarrow 5g}$

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

$TS_{4h \rightarrow 5h}$

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

$TS_{4i \rightarrow 5i}$

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

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

$TS_{4j \rightarrow 5j}$

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

$TS_{4k \rightarrow 5k}$

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

3l

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-l

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

4l

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

5l

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

$TS_{4l \rightarrow 5l}$

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

$TS_{4m \rightarrow 5m}$

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

$TS_{4n \rightarrow 5n}$

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

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

$TS_{4o \rightarrow 5o}$

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.