# APPENDICES

**Appendix 1: Input file of Tetraaza macrocyclic ligand at ground state**

```
%nprocshared=2
 Will use up to    2 processors via shared memory.
 %mem=1024MB
 %chk=C:\Users\iChemStudent\Desktop\Scratch\Ligand\ligandfull15.chk
 ---------------------------------------------------------------------
 # opt freq=raman rb3lyp/6-311++g(d,p) pop=nbo geom=connectivity polar
 ---------------------------------------------------------------------
 1/18=20,19=15,26=3,38=1,57=2/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=4,6=6,7=1111,11=2,25=1,30=1,71=1,74=-5,116=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
 6/7=2,8=2,9=2,10=2,28=1,40=1/1,7;
 7//1,2,3,16;
 1/18=20,19=15,26=3/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=4,6=6,7=1111,11=2,25=1,30=1,71=1,74=-5,116=1/1,2,3;
 4/5=5,16=3,69=1/1;
 5/5=2,38=5,98=1/2;
 7//1,2,3,16;
 1/18=20,19=15,26=3/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1,40=1/1,7;
 99/9=1/99;
 ------------------
 Title Card Required
 ------------------
 Symbolic Z-matrix:
 Charge =  2 Multiplicity = 1
 C                 -2.45086  -0.10765   0.02062
 H                 -3.51582  -0.28707   0.19916
 C                  3.6704    0.52855  -1.56712
 H                  4.7353    0.70797  -1.746
 C                 -2.35348   1.10825  -0.95707
 C                 -2.74223   0.69853  -2.39746
 H                 -2.03135  -0.01241  -2.83552
 H                 -3.73423   0.2341   -2.40314
 H                 -2.80026   1.57739  -3.05201
 N                 -0.90038   1.63503  -1.03323
 C                 -0.44034   2.71718  -0.07225
```

| | | | |
|---|---|---|---|
| C | 1.0085 | 3.10528 | -0.43636 |
| N | 1.78464 | 1.86538 | -0.76573 |
| C | 3.03522 | 1.85006 | -1.13468 |
| C | 3.90214 | 3.08065 | -1.21726 |
| H | 3.3824 | 4.01172 | -0.98585 |
| H | 4.33558 | 3.16378 | -2.22321 |
| H | -2.02395 | 0.16905 | 0.99688 |
| H | 3.24315 | 0.25173 | -2.54318 |
| C | -3.30985 | 2.21798 | -0.45446 |
| H | -4.34435 | 1.86575 | -0.52487 |
| H | -3.12753 | 2.49192 | 0.59083 |
| H | -3.2365 | 3.11979 | -1.07395 |
| H | 4.75247 | 2.9793 | -0.52808 |
| H | -1.08193 | 3.60246 | -0.1309 |
| H | -0.49593 | 2.31872 | 0.94463 |
| H | 1.01715 | 3.77557 | -1.30645 |
| H | 1.46509 | 3.64303 | 0.40242 |
| C | 3.57331 | -0.68728 | -0.58931 |
| C | 4.52964 | -1.797 | -1.09205 |
| N | 2.12015 | -1.21411 | -0.51295 |
| C | 3.96221 | -0.27767 | 0.85103 |
| H | 4.34703 | -2.07114 | -2.13724 |
| H | 5.56412 | -1.44463 | -1.02203 |
| H | 4.4566 | -2.69871 | -0.47239 |
| C | 1.66015 | -2.29648 | -1.47372 |
| H | 3.25171 | 0.43363 | 1.28909 |
| H | 4.01983 | -1.15655 | 1.50559 |
| C | 0.2112 | -2.68439 | -1.10976 |
| N | -0.56492 | -1.44445 | -0.78048 |
| H | -0.24537 | -3.22212 | -1.94856 |
| H | 0.20246 | -3.35464 | -0.23965 |
| C | -1.81554 | -1.42915 | -0.41165 |
| C | -2.6824 | -2.65979 | -0.32902 |
| H | -2.16266 | -3.59082 | -0.56058 |
| H | -3.53288 | -2.55844 | -1.01799 |
| H | -3.11558 | -2.74299 | 0.67704 |
| H | 1.99022 | -1.5448 | 0.45199 |
| H | 2.30159 | -3.18184 | -1.41458 |
| H | 1.71611 | -1.89837 | -2.49072 |
| H | -0.68527 | 1.67877 | -2.0378 |
| H | 4.95448 | 0.18618 | 0.85674 |
| H | 2.50005 | -2.01538 | -1.01698 |
| H | -1.20969 | 2.57582 | -0.78898 |

**Appendix 2: Input file of Pd(II) tetraaza macrocyclic ligand at ground state**

```
%chk=C:\Users\iChemStudent\Desktop\Scratch\METAL\metalcomplex9.chk
 ---------------------------------------------------------------
 # opt freq=raman rb3lyp/lanl2dz pop=nbo geom=connectivity polar
 ---------------------------------------------------------------
 1/18=20,19=15,26=3,38=1,57=2/1,3;
 2/9=110,12=2,17=6,18=5,40=1/2;
 3/5=6,6=3,11=2,25=1,30=1,71=1,74=-5,116=1/1,2,3;
 4//1;
 5/5=2,38=5,98=1/2;
 6/7=2,8=2,9=2,10=2,28=1,40=1/1,7;
 7//1,2,3,16;
 1/18=20,19=15,26=3/3(2);
 2/9=110/2;
 99//99;
 2/9=110/2;
 3/5=6,6=3,11=2,25=1,30=1,71=1,74=-5,116=1/1,2,3;
 4/5=5,16=3,69=1/1;
 5/5=2,38=5,98=1/2;
 7//1,2,3,16;
 1/18=20,19=15,26=3/3(-5);
 2/9=110/2;
 6/7=2,8=2,9=2,10=2,19=2,28=1,40=1/1,7;
 99/9=1/99;
 ------------------
 Title Card Required
 ------------------
 Symbolic Z-matrix:
 Charge =  2 Multiplicity = 1
 C                 -2.51572  -0.25157   0.
 H                 -3.58068  -0.43099   0.17854
 C                  3.60554   0.38462  -1.58773
 H                  4.67044   0.56404  -1.76662
 C                 -2.41834   0.96433  -0.97769
 C                 -2.80709   0.5546   -2.41808
 H                 -2.09621  -0.15634  -2.85613
 H                 -3.79909   0.09018  -2.42376
 H                 -2.86512   1.43346  -3.07263
 N                 -0.96524   1.49111  -1.05384
 C                 -0.5052    2.57325  -0.09287
 C                  0.94364   2.96136  -0.45698
 N                  1.71978   1.72145  -0.78634
 C                  2.97036   1.70613  -1.1553
 C                  3.83728   2.93672  -1.23788
 H                  3.31754   3.86779  -1.00647
 H                  4.27072   3.01985  -2.24383
```

| | | | |
|---|---|---|---|
| H | -2.08881 | 0.02512 | 0.97626 |
| H | 3.17829 | 0.1078 | -2.5638 |
| C | -3.37471 | 2.07405 | -0.47508 |
| H | -4.40921 | 1.72183 | -0.54549 |
| H | -3.19239 | 2.348 | 0.57022 |
| H | -3.30136 | 2.97586 | -1.09456 |
| H | 4.68761 | 2.83537 | -0.5487 |
| H | -1.14679 | 3.45853 | -0.15151 |
| H | -0.56079 | 2.17479 | 0.92401 |
| H | 0.95229 | 3.63164 | -1.32707 |
| H | 1.40023 | 3.4991 | 0.38181 |
| C | 3.50845 | -0.83121 | -0.60993 |
| C | 4.46478 | -1.94093 | -1.11266 |
| N | 2.05529 | -1.35804 | -0.53357 |
| C | 3.89735 | -0.42159 | 0.83042 |
| H | 4.28217 | -2.21507 | -2.15786 |
| H | 5.49926 | -1.58856 | -1.04265 |
| H | 4.39174 | -2.84264 | -0.493 |
| C | 1.59529 | -2.44041 | -1.49434 |
| H | 3.18685 | 0.28971 | 1.26848 |
| H | 3.95497 | -1.30048 | 1.48497 |
| C | 0.14634 | -2.82831 | -1.13038 |
| N | -0.62978 | -1.58838 | -0.8011 |
| H | -0.31023 | -3.36604 | -1.96918 |
| H | 0.1376 | -3.49857 | -0.26027 |
| C | -1.8804 | -1.57307 | -0.43227 |
| C | -2.74726 | -2.80371 | -0.34964 |
| H | -2.22752 | -3.73474 | -0.5812 |
| H | -3.59774 | -2.70237 | -1.03861 |
| H | -3.18044 | -2.88692 | 0.65642 |
| H | 1.93607 | -1.71581 | 0.42306 |
| H | 2.23673 | -3.32576 | -1.43519 |
| H | 1.65125 | -2.0423 | -2.51134 |
| H | -0.84583 | 1.84897 | -2.01042 |
| Pd | 0.54501 | 0.06651 | -0.79372 |
| H | 4.88962 | 0.04226 | 0.83612 |

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Initialization pass.

**Appendix 3: Input file of Pd(II) tetraaza macrocyclic ligand at excited state in gas**

```
%mem=3000MW

%oldchk=C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Gas\METALCOMP
LEX9 TD-UV-N
 40-GAS.chk

%chk=C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Gas\METALCOMPLE
X9 TD-UV-N40-
 NSinglet-SpinTriplet-GAS.chk
 Copying data from
"C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Gas\METALCOMPLEX9
TD-UV-N40-GAS.chk" to current chk file
"C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Gas\METALCOMPLEX9
TD-UV-N40-NSinglet-SpinTriplet-GAS.chk"
 IOpt=  2 FromEx=T IUOpen= 4 IOptOp= 5 NList=   0 IFRang= 0 IUIn= 4 IUOut= 2.
 ---------------------------------------------
 # td=(singlets,nstates=40,root=1) ub3lyp/lanl2dz
 ---------------------------------------------
 1/38=1,172=1/1;
 2/12=2,17=6,18=5,40=1/2;
 3/5=6,6=3,11=2,25=1,30=1,74=-5,116=2/1,2,3,8;
 4//1;
 5/5=2,38=5/2;
 8/6=1,10=1,107=1,108=40/1;
 9/8=1,41=40,42=1,48=1,70=2/14;
 6/7=2,8=2,9=2,10=2/1;
 99/5=1,9=1/99;
 ---------
 tdscf-DFT
 ---------
 Symbolic Z-matrix:
 Charge =  2 Multiplicity = 3
 C                  3.03101  -0.36028  -0.79409
 H                  4.08051  -0.54324  -1.0465
 C                 -3.03099   0.36027   0.79412
 H                 -4.08048   0.54323   1.04657
 C                  3.03369   0.89356   0.16512
 C                  3.48162   0.48371   1.58753
 H                  2.76544  -0.19419   2.06952
 H                  4.45212  -0.0226    1.54872
 H                  3.60864   1.36519   2.22843
 N                  1.63067   1.51246   0.32149
 C                  1.10626   2.54913  -0.64357
 C                 -0.34341   2.96803  -0.25637
```

| | | | |
|---|---|---|---|
| N | -1.1643 | 1.75887 | 0.0387 |
| C | -2.4317 | 1.70501 | 0.33542 |
| C | -3.34633 | 2.90411 | 0.35437 |
| H | -2.85396 | 3.83644 | 0.07021 |
| H | -3.77877 | 3.03076 | 1.35668 |
| H | 2.54433 | -0.08794 | -1.74444 |
| H | -2.54429 | 0.08792 | 1.74446 |
| C | 4.02064 | 1.93594 | -0.41892 |
| H | 5.04026 | 1.53632 | -0.40546 |
| H | 3.78461 | 2.20101 | -1.45638 |
| H | 4.02421 | 2.85248 | 0.18317 |
| H | -4.19473 | 2.73713 | -0.32355 |
| H | 1.73543 | 3.44679 | -0.66363 |
| H | 1.12137 | 2.1198 | -1.65441 |
| H | -0.32253 | 3.61195 | 0.63422 |
| H | -0.7683 | 3.55807 | -1.07806 |
| C | -3.0337 | -0.89356 | -0.1651 |
| C | -4.02065 | -1.93593 | 0.41896 |
| N | -1.63068 | -1.51247 | -0.32149 |
| C | -3.48165 | -0.48371 | -1.58749 |
| H | -3.78459 | -2.20102 | 1.45642 |
| H | -5.04026 | -1.5363 | 0.40554 |
| H | -4.02425 | -2.85246 | -0.18314 |
| C | -1.10626 | -2.54911 | 0.64361 |
| H | -2.76547 | 0.19419 | -2.0695 |
| H | -3.60869 | -1.36518 | -2.22839 |
| C | 0.3434 | -2.96802 | 0.25639 |
| N | 1.16431 | -1.75888 | -0.0387 |
| H | 0.7683 | -3.55805 | 1.07809 |
| H | 0.32251 | -3.61197 | -0.63419 |
| C | 2.43171 | -1.70502 | -0.33539 |
| C | 3.34635 | -2.90411 | -0.35427 |
| H | 2.85398 | -3.83644 | -0.0701 |
| H | 4.19472 | -2.7371 | 0.32369 |
| H | 3.77883 | -3.03078 | -1.35655 |
| H | -1.56625 | -1.88622 | -1.27492 |
| H | -1.73543 | -3.44677 | 0.66371 |
| H | -1.12135 | -2.11975 | 1.65443 |
| H | 1.5662 | 1.88617 | 1.27494 |
| Pd | 0. | 0. | -0.00006 |
| H | -4.45215 | 0.02262 | -1.54866 |

**Appendix 4: Input file of Pd(II) tetraaza macrocyclic ligand at excited state in solvent phase**

%oldchk=C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Methanol\METALCOMPLEX9 TD
-uv-n100-METH.chk
%mem=3000MW

%chk=C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Methanol\METALCOMPLEX9 TD-uv
-n40-METH.chk
Copying data from "C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Methanol\METALCOMPLEX9 TD-uv-n100-METH.chk" to current chk file "C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Methanol\METALCOMPLEX9 TD-uv-n40-METH.chk"
IOpt= 2 FromEx=T IUOpen= 4 IOptOp= 5 NList= 0 IFRang= 0 IUIn= 4 IUOut= 2.
---
# td=(singlets,nstates=40,root=1) ub3lyp/lanl2dz scrf=(iefpcm,solvent=methanol)
---
1/38=1,172=1/1;
2/12=2,17=6,18=5,40=1/2;
3/5=6,6=3,11=2,25=1,30=1,70=2201,72=3,74=-5,116=2/1,2,3,8;
4//1;
5/5=2,38=5,53=3/2;
8/6=1,10=1,107=1,108=40/1;
9/8=1,41=40,42=1,48=1,70=2/14;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
---
td-uv-meth
---
Symbolic Z-matrix:
Charge = 2 Multiplicity = 3

| | | | |
|---|---|---|---|
| C | 2.99862 | -0.34993 | -0.80796 |
| H | 4.04124 | -0.52536 | -1.0915 |
| C | -2.99863 | 0.34993 | 0.80794 |
| H | -4.04128 | 0.52539 | 1.09137 |
| C | 3.01021 | 0.89342 | 0.16383 |
| C | 3.45785 | 0.466 | 1.58047 |
| H | 2.73002 | -0.20747 | 2.0492 |
| H | 4.42098 | -0.05321 | 1.52936 |
| H | 3.58544 | 1.34344 | 2.22665 |
| N | 1.62326 | 1.51703 | 0.32103 |
| C | 1.10854 | 2.56135 | -0.63079 |
| C | -0.34132 | 2.97485 | -0.24394 |

| | | | |
|---|---|---|---|
| N | -1.15336 | 1.76824 | 0.057 |
| C | -2.41791 | 1.69726 | 0.34095 |
| C | -3.35286 | 2.88367 | 0.33651 |
| H | -2.86533 | 3.81174 | 0.03079 |
| H | -3.77778 | 3.02282 | 1.33941 |
| H | 2.47066 | -0.06561 | -1.72938 |
| H | -2.47079 | 0.0656 | 1.72942 |
| C | 4.00856 | 1.93071 | -0.41116 |
| H | 5.02339 | 1.51827 | -0.39527 |
| H | 3.77021 | 2.19786 | -1.44733 |
| H | 4.00621 | 2.84472 | 0.19465 |
| H | -4.19692 | 2.68756 | -0.3375 |
| H | 1.7349 | 3.4615 | -0.6319 |
| H | 1.12328 | 2.1423 | -1.64395 |
| H | -0.31997 | 3.61655 | 0.64725 |
| H | -0.76853 | 3.56013 | -1.06731 |
| C | -3.01022 | -0.89345 | -0.1638 |
| C | -4.0086 | -1.9307 | 0.41122 |
| N | -1.62332 | -1.51714 | -0.321 |
| C | -3.45784 | -0.46605 | -1.58045 |
| H | -3.77027 | -2.19781 | 1.44741 |
| H | -5.02344 | -1.51826 | 0.3953 |
| H | -4.00625 | -2.84474 | -0.19455 |
| C | -1.10842 | -2.56112 | 0.63111 |
| H | -2.72996 | 0.20736 | -2.0492 |
| H | -3.58551 | -1.34349 | -2.2266 |
| C | 0.34133 | -2.9748 | 0.2441 |
| N | 1.15338 | -1.76827 | -0.05717 |
| H | 0.76863 | -3.55999 | 1.06749 |
| H | 0.31982 | -3.61662 | -0.647 |
| C | 2.41798 | -1.69725 | -0.34083 |
| C | 3.35303 | -2.88358 | -0.33602 |
| H | 2.86575 | -3.81145 | -0.0293 |
| H | 4.19754 | -2.6869 | 0.33725 |
| H | 3.77727 | -3.02347 | -1.33911 |
| H | -1.53191 | -1.85968 | -1.28249 |
| H | -1.73481 | -3.46125 | 0.6327 |
| H | -1.12293 | -2.14167 | 1.64412 |
| H | 1.53171 | 1.85926 | 1.28262 |
| Pd | -0.00005 | -0.00004 | -0.00021 |
| H | -4.42093 | 0.05324 | -1.52933 |

%oldchk=C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Acetonitrile\METAL COMPLEX
9 uv-ACETONITRILE.chk

%chk=C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Acetonitrile\METALC OMPLEX9 U
V-ACN-n40-triplet.chk
Copying data from "C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Acetonitrile\METALCOMPL EX9 uv-ACETONITRILE.chk" to current chk file "C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Acetonitrile\METALCOMPL EX9 UV-ACN-n40-triplet.chk"
IOpt= 2 FromEx=T IUOpen= 4 IOptOp= 5 NList= 0 IFRang= 0 IUIn= 4 IUOut= 2.
---
# td=(singlets,nstates=40,root=1) ub3lyp/lanl2dz scrf=(iefpcm,solvent= acetonitrile)
---
1/38=1,172=1/1;
2/12=2,17=6,18=5,40=1/2;
3/5=6,6=3,11=2,25=1,30=1,70=2201,72=2,74=-5,116=2/1,2,3,8;
4//1;
5/5=2,38=5,53=2/2;
8/6=1,10=1,107=1,108=40/1;
9/8=1,41=40,42=1,48=1,70=2/14;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
---
tdscf-acn
---
Symbolic Z-matrix:
Charge = 2 Multiplicity = 3

| | | | |
|---|---|---|---|
| C | 2.99864 | -0.34962 | -0.80778 |
| H | 4.04139 | -0.52497 | -1.09095 |
| C | -2.99861 | 0.34968 | 0.80779 |
| H | -4.04134 | 0.52505 | 1.091 |
| C | 3.00984 | 0.89371 | 0.16404 |
| C | 3.4568 | 0.46602 | 1.58081 |
| H | 2.72813 | -0.20672 | 2.04926 |
| H | 4.41947 | -0.05408 | 1.52997 |
| H | 3.58492 | 1.3434 | 2.22698 |
| N | 1.62293 | 1.51733 | 0.32085 |
| C | 1.10823 | 2.56134 | -0.63134 |
| C | -0.34173 | 2.97471 | -0.2448 |
| N | -1.15369 | 1.76813 | 0.05613 |
| C | -2.41805 | 1.69705 | 0.34073 |
| C | -3.35302 | 2.88348 | 0.33713 |
| H | -2.86595 | 3.81132 | 0.02998 |
| H | -3.77604 | 3.02323 | 1.34076 |
| H | 2.47098 | -0.06543 | -1.72943 |

| | | | |
|---|---|---|---|
| H | -2.47091 | 0.06556 | 1.72944 |
| C | 4.00856 | 1.93094 | -0.41042 |
| H | 5.02335 | 1.51837 | -0.39415 |
| H | 3.77066 | 2.19822 | -1.44667 |
| H | 4.00603 | 2.8449 | 0.19547 |
| H | -4.19831 | 2.68696 | -0.3352 |
| H | 1.73446 | 3.46157 | -0.63257 |
| H | 1.12316 | 2.14193 | -1.64436 |
| H | -0.32057 | 3.61655 | 0.64631 |
| H | -0.76884 | 3.5599 | -1.06828 |
| C | -3.00985 | -0.89371 | -0.16395 |
| C | -4.00851 | -1.93093 | 0.41062 |
| N | -1.62294 | -1.51731 | -0.32084 |
| C | -3.4569 | -0.46612 | -1.58072 |
| H | -3.77058 | -2.19809 | 1.44689 |
| H | -5.02332 | -1.51843 | 0.39431 |
| H | -4.00593 | -2.84496 | -0.19517 |
| C | -1.1082 | -2.56137 | 0.63128 |
| H | -2.72828 | 0.20663 | -2.04924 |
| H | -3.58503 | -1.34353 | -2.22683 |
| C | 0.34174 | -2.97472 | 0.24464 |
| N | 1.15369 | -1.76812 | -0.05623 |
| H | 0.76889 | -3.55997 | 1.06807 |
| H | 0.32056 | -3.6165 | -0.64651 |
| C | 2.41805 | -1.69702 | -0.34083 |
| C | 3.35302 | -2.88345 | -0.33729 |
| H | 2.86594 | -3.81131 | -0.03022 |
| H | 4.19829 | -2.68698 | 0.33507 |
| H | 3.77606 | -3.02314 | -1.34092 |
| H | -1.53116 | -1.85965 | -1.28236 |
| H | -1.73443 | -3.46161 | 0.63248 |
| H | -1.12309 | -2.14202 | 1.64432 |
| H | 1.53113 | 1.85972 | 1.28235 |
| Pd | 0. | 0. | 0.00003 |
| H | -4.41958 | 0.05397 | -1.52985 |

%oldchk=C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Water\METALCOMPLEX9 UV-wa
ter.chk

%chk=C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Water\METALCOMPLEX9 UV-water
-n40-triplet.chk
Copying data from "C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Water\METALCOMPLEX9 UV-water.chk" to current chk file "C:\Users\iChemStudent\Desktop\Scratch\METAL\UV\Water\METALCOMPLEX9 UV-water-n40-triplet.chk"
IOpt= 2 FromEx=T IUOpen= 4 IOptOp= 5 NList= 0 IFRang= 0 IUIn= 4 IUOut= 2.
---
# td=(singlets,nstates=40,root=1) ub3lyp/lanl2dz scrf=(iefpcm,solvent=
water)
---
1/38=1,172=1/1;
2/12=2,17=6,18=5,40=1/2;
3/5=6,6=3,11=2,25=1,30=1,70=2201,72=1,74=-5,116=2/1,2,3,8;
4//1;
5/5=2,38=5,53=1/2;
8/6=1,10=1,107=1,108=40/1;
9/8=1,41=40,42=1,48=1,70=2/14;
6/7=2,8=2,9=2,10=2/1;
99/5=1,9=1/99;
---
tdscf-water
---
Symbolic Z-matrix:
Charge = 2 Multiplicity = 3

| | | | |
|---|---|---|---|
| C | 2.99864 | -0.34962 | -0.80778 |
| H | 4.04139 | -0.52497 | -1.09095 |
| C | -2.99861 | 0.34968 | 0.80779 |
| H | -4.04134 | 0.52505 | 1.091 |
| C | 3.00984 | 0.89371 | 0.16404 |
| C | 3.4568 | 0.46602 | 1.58081 |
| H | 2.72813 | -0.20672 | 2.04926 |
| H | 4.41947 | -0.05408 | 1.52997 |
| H | 3.58492 | 1.3434 | 2.22698 |
| N | 1.62293 | 1.51733 | 0.32085 |
| C | 1.10823 | 2.56134 | -0.63134 |
| C | -0.34173 | 2.97471 | -0.2448 |
| N | -1.15369 | 1.76813 | 0.05613 |
| C | -2.41805 | 1.69705 | 0.34073 |
| C | -3.35302 | 2.88348 | 0.33713 |
| H | -2.86595 | 3.81132 | 0.02998 |
| H | -3.77604 | 3.02323 | 1.34076 |
| H | 2.47098 | -0.06543 | -1.72943 |

| | | | |
|---|---|---|---|
| H | -2.47091 | 0.06556 | 1.72944 |
| C | 4.00856 | 1.93094 | -0.41042 |
| H | 5.02335 | 1.51837 | -0.39415 |
| H | 3.77066 | 2.19822 | -1.44667 |
| H | 4.00603 | 2.8449 | 0.19547 |
| H | -4.19831 | 2.68696 | -0.3352 |
| H | 1.73446 | 3.46157 | -0.63257 |
| H | 1.12316 | 2.14193 | -1.64436 |
| H | -0.32057 | 3.61655 | 0.64631 |
| H | -0.76884 | 3.5599 | -1.06828 |
| C | -3.00985 | -0.89371 | -0.16395 |
| C | -4.00851 | -1.93093 | 0.41062 |
| N | -1.62294 | -1.51731 | -0.32084 |
| C | -3.4569 | -0.46612 | -1.58072 |
| H | -3.77058 | -2.19809 | 1.44689 |
| H | -5.02332 | -1.51843 | 0.39431 |
| H | -4.00593 | -2.84496 | -0.19517 |
| C | -1.1082 | -2.56137 | 0.63128 |
| H | -2.72828 | 0.20663 | -2.04924 |
| H | -3.58503 | -1.34353 | -2.22683 |
| C | 0.34174 | -2.97472 | 0.24464 |
| N | 1.15369 | -1.76812 | -0.05623 |
| H | 0.76889 | -3.55997 | 1.06807 |
| H | 0.32056 | -3.6165 | -0.64651 |
| C | 2.41805 | -1.69702 | -0.34083 |
| C | 3.35302 | -2.88345 | -0.33729 |
| H | 2.86594 | -3.81131 | -0.03022 |
| H | 4.19829 | -2.68698 | 0.33507 |
| H | 3.77606 | -3.02314 | -1.34092 |
| H | -1.53116 | -1.85965 | -1.28236 |
| H | -1.73443 | -3.46161 | 0.63248 |
| H | -1.12309 | -2.14202 | 1.64432 |
| H | 1.53113 | 1.85972 | 1.28235 |
| Pd | 0. | 0. | 0.00003 |
| H | -4.41958 | 0.05397 | -1.52985 |