Electronic Supplementary Information

Accurate entropy calculation for large flexible hydrocarbons using multi-structural 2-dimensional torsion method

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1. The basic steps of MS-2DT calculation

Note: the users are required to install MSTor program suite before using MS-2DT method.

1. Initial conformer guess.

In MS-2DT calculation, we adopt the minimally coupled strategy, i.e. simultaneously changing every torsion pair to generate initial conformers totaling $C_n^2 \cdot 9$ or $4.5N(N-1)$. In comparison, the standard MS-T calculation generates initial conformer up to 3^N. For instance, applying MS-2DT to the molecule with 5 rotatable torsions invokes optimization for 90 initial conformers, while the

MS-T calculation invokes 243 initial conformers. Clearly, MS-2DT always produce quiet fewer conformers than MS-T calculation, especially for those molecules with many torsions.

The initial structure generation is performed using our code ***2DConfGen***. In this code, the user need to prepare two input files, one is the coordinate file (T.inp), the other is the torsion file (Tor.inp). Put the two files and this code in the same folder and then type in linux command "*bash 2DConfGen.sh*". Later on, a hint appears on the screen "*pls type the number of coupled torsions*". Once the user input the torsion number, the initial structures can be generated and stored in a new subfolder ConfGen.

2. Geometry optimization

The initial conformers are optimized in Gaussian or other programs with user-defined electronic structure method.

3. Distinguished structures sampling

From all optimized conformers, one need to sort the distinguished structures by *mvinput*.exe in MSTor suite.

4. Frequency calculation

The frequencies of all the distinguishable structures are computed with the same method as geometry optimization. One may need to abstract the coordinate of the distinguished structures. This could be done using our code ***O2F.sh.*** The user can obtain this code upon request to the corresponding author renwei@mae.cuhk.edu.hk.

5. Structural reasonableness confirmation

All the frequencies should be checked to justify the distinguishable structures. Remove the unreasonable structures and turn to step (3). If all the structures are reasonable, then proceed to the next step.

6. Entropy calculation

The hessian matrixes of the reasonable distinguishable structures are integrated with the input file for MS-T calculation generated by *msinput*.exe. Meanwhile, the periodic value M should also be computed by *mcvorm*.exe. Finally, the entropy calculation is implemented by *mstor*.exe.

2. Detailed Partition Functions

Table S1. Partition Functions of n-hexane predicted by MS-T, MS-2DT, PO, and RRHO methods

T	Partition Function			
	MS-T	MS-2DT	PO	RRHO
200	3.60295E14	3.42439E14	5.3796E15	7.65487E13
300	2.36109E16	2.23618E16	1.48166E18	3.08352E15
400	7.04101E17	6.62172E17	1.15885E20	7.57955E16
500	1.4689E19	1.3745E19	4.14857E21	1.47591E18
600	2.48851E20	2.32506E20	9.45786E22	2.50037E19
700	3.59541E21	3.37281E21	1.61822E24	3.8105E20
800	4.61452E22	4.35724E22	2.28185E25	5.29265E21
900	5.34866E23	5.0964E23	2.82085E26	6.74342E22
1000	5.65128E24	5.44196E24	3.08576E27	7.91518E23
1100	5.48704E25	5.34262E25	3.07397E28	8.5892E24
1200	4.96148E26	4.88222E26	2.82609E29	8.64527E25
1300	4.14089E27	4.11803E27	2.38134E30	8.09676E26
1400	3.24362E28	3.25506E28	1.87286E31	7.07771E27
1500	2.38102E29	2.41116E29	1.37895E32	5.79207E28
1600	1.64606E30	1.68122E30	9.53306E32	4.45055E29
1700	1.07478E31	1.1055E31	6.20574E33	3.22012E30
1800	6.64289E31	6.87415E31	3.83367E34	2.19991E31
1900	3.889E32	4.04877E32	2.23086E35	1.42285E32
2000	2.18059E33	2.28163E33	1.24458E36	8.73448E32

Table S2. Partition Functions of n-heptane predicted by MS-T, MS-2DT, PO, and RRHO methods

T	Partition Function			
	MS-T	MS-2DT	PO	RRHO
200	1.5176E+015	1.3029E+015	3.45875E16	1.31009E14
300	1.3659E+017	1.1434E+017	2.81692E19	7.75301E15
400	6.5984E+018	5.4281E+018	5.08989E21	2.79911E17
500	2.3347E+020	1.8964E+020	3.48059E23	8.01419E18
600	6.7893E+021	5.4689E+021	1.34313E25	1.99609E20
700	1.6972E+023	1.3609E+023	3.65163E26	4.45975E21
800	3.7232E+024	2.9814E+024	7.89694E27	9.03381E22
900	7.2548E+025	5.8162E+025	1.42806E29	1.66686E24
1000	1.2666E+027	1.0186E+027	2.25531E30	2.81044E25
1100	1.9955E+028	1.6122E+028	3.19913E31	4.34264E26
1200	2.8549E+029	2.3194E+029	4.088E32	6.16779E27
1300	3.7294E+030	3.0490E+030	4.76813E33	8.07672E28
1400	4.4713E+031	3.6801E+031	5.11798E34	9.78226E29
1500	4.9434E+032	4.0971E+032	5.09716E35	1.09932E31
1600	5.0620E+033	4.2249E+033	4.7014E36	1.1499E32
1700	4.8206E+034	4.0515E+034	4.06929E37	1.12307E33
1800	4.2855E+035	3.6267E+035	3.28211E38	1.02726E34
1900	3.5694E+036	3.0410E+036	2.51169E39	8.82594E34
2000	2.7947E+037	2.3964E+037	1.80147E40	7.14294E35

Table S3. Partition Functions of n-octane predicted by MS-T, MS-2DT, PO, and RRHO methods

T	Partition Function			
	MS-T	MS-2DT	PO	RRHO
200	7.42094E16	6.75783E16	8.01829E17	2.38022E15
300	9.81308E18	9.15931E18	2.08243E21	2.47329E17
400	6.5226E20	6.48333E20	9.09514E23	1.46501E19
500	3.00491E22	3.23238E22	1.22206E26	6.67152E20
600	1.10384E24	1.29216E24	8.22416E27	2.59416E22
700	3.44933E25	4.39401E25	3.67179E29	8.91522E23
800	9.3762E26	1.29847E27	1.23549E31	2.74001E25
900	2.25E28	3.37722E28	3.37924E32	7.57015E26
1000	4.81475E29	7.79744E29	7.88897E33	1.88677E28
1100	9.33909E30	1.62449E31	1.61731E35	4.25614E29
1200	1.64509E32	3.05964E32	2.95105E36	8.71904E30
1300	2.6343E33	5.20968E33	4.80953E37	1.62781E32
1400	3.87388E34	8.10939E34	7.16941E38	2.77969E33
1500	5.25071E35	1.15822E36	9.76163E39	4.35744E34
1600	6.58358E36	1.52258E37	1.21843E41	6.29348E35

1700	7.68295E37	1.85728E38	1.41333E42	8.40486E36
1800	8.35716E38	2.10115E39	1.52887E43	1.04152E38
1900	8.46358E39	2.20753E40	1.53206E44	1.20163E39
2000	8.05066E40	2.17074E41	1.44127E45	1.29494E40

3. Details of the *2DconfGen* Code

```
#!bin/bash
read -p "pls type the number of coupled torsions: " N
declare -i N
K=1
for n in $( seq 1 $(($N-1)))
 do
 Ln1=$((6*$n)) #! Line 1
 Tor1="$(head -n $Ln1 Tors.inp | tail -n 5)"
 m=$(($n+1))
 if [ "$m" -le "$N" ];then
 for m in $( seq $m $N )
  do
   cp T.inp $K.inp #! Generate input
   echo "" >> $K.inp
   echo "#torsion 1 definition" >> $K.inp
   echo "$Tor1" >> Tor1.txt
   echo "$Tor1" >> $K.inp    #!export Tor1 to inp.
   Ln2=$((6*$m))
   Tor2="$(head -n $Ln2 Tors.inp | tail -n 5)"
   echo "$Tor2" >> Tor2.txt
   echo "#torsion 2 definition" >> $K.inp
   echo "$Tor2" >> $K.inp
   echo "%nproc=12" >> $K.inp
```

```
    echo "%mem=2000mb" >> $K.inp
    echo "# opt=(vtight,maxcyc=200) scf=maxcyc=500 AM1" >> $K.inp
    echo "0 1" >> $K.inp
    echo "" >> $K.inp
    K=$((K+1))
   done
  fi
done
#############  mkdir for $K.inp    ###############
mkdir Raw
mkdir ConfGen
mv T.inp Raw
mv Tors.inp Raw
for inp in *.inp
  do
   A="$(cut -d'.' -f1 <<<"$inp")"
   mkdir $A
   cp $A.inp $A
   cd $A
   export PATH="~/mstor_2017/exe:$PATH"
      ConfGen.exe <$A.inp
      for com in *.com
       do
        NM=$((A*9))
        echo "$NM" >> NM.txt
        B0="$(cut -d'.' -f1 <<<"$com")"
        B="$(cut -d'.' -f1 <<<"$com" | cut -c 7-)"
        echo "$B" >> B.txt
        Name=$((NM+$B))
        echo "$Name" >> Name.txt
```

```
        if [ "$Name" -lt "10" ];then
            C="s00000${Name}"
            echo "$C" >> C.txt
            cp $B0.com  $C.com
          elif [ "$Name" -ge "10" ] && [ "$Name" -lt "100" ];then
            C="s0000${Name}"
            echo "$C" >> C.txt
            cp $B0.com  $C.com
          else
            C="s000${Name}"
            echo "$C" >> C.txt
            cp $B0.com  $C.com
        fi
        mv $C.com ../ConfGen
    done
 cd ..
done
 cd 1
 mv s*.com ../ConfGen
 cd ..
 cd ConfGen
  for com in *.com
  do
   CFN="$(cut -d'.' -f1 <<<"$com")"  #! ConFormer Name
   sed -i -e '3c %chk='$CFN'.chk' $CFN.com
   sed -i -e '6c '$CFN" $CFN.com
   #chk="$(head -n 3 $CFN.com | tail -n 1)"
   #echo "$chk" >>chk.txt
   #crd="$(head -n 6 $CFN.com | tail -n 1)"
   #echo "$crd" >>crd.txt
```

```
#sed -i -e 's/%chk='$CFN'.chk/'$chk'/g' $CFN.com
#sed -i -e 's/'$CFN'/'$crd'/g' $CFN.com
done
```

4. Sample Inputs (n-hexane)

4A. MS-2DT (T and Tor files)

T.inp

```
20 2
C      -2.86421400    1.44361000    0.00039600
C      -1.33790200    1.42972900    0.00085800
H      -3.25778800    2.46199300    0.00126100
H      -3.25730500    0.93282600   -0.88260200
H      -3.25785200    0.93111900    0.88216300
C      -0.76298200    0.01490800   -0.00021300
H      -0.96340200    1.97025300   -0.87537900
H      -0.96394400    1.96869600    0.87828200
C       0.76298200   -0.01490800    0.00021300
H      -1.13668700   -0.52807800    0.87678900
H      -1.13616900   -0.52654900   -0.87837600
H       1.13668700    0.52807800   -0.87678900
H       1.13616900    0.52654900    0.87837600
C       1.33790200   -1.42972900   -0.00085800
H       0.96394400   -1.96869600   -0.87828200
H       0.96340200   -1.97025300    0.87537900
C       2.86421400   -1.44361000   -0.00039600
H       3.25778800   -2.46199300   -0.00126100
H       3.25785200   -0.93111900   -0.88216300
H       3.25730500   -0.93282600    0.88260200
```

Tor.inp

```
#torsion 1 definition
 2 6
 7
 1 3 4 5 2 7 8
 3
 0. 120. -120.
#torsion 2 definition
 6 9
 10
 1 3 4 5 2 7 8 6 10 11
 3
 0. 120. -120.
#torsion 3 definition
 9 14
 13
 1 3 4 5 2 7 8 6 10 11 9 12 13
 3
 0. 120. -120.
```

4B. MS-T (C6.inp)

```
20 3
C       -2.86421400    1.44361000    0.00039600
C       -1.33790200    1.42972900    0.00085800
H       -3.25778800    2.46199300    0.00126100
H       -3.25730500    0.93282600   -0.88260200
H       -3.25785200    0.93111900    0.88216300
C       -0.76298200    0.01490800   -0.00021300
H       -0.96340200    1.97025300   -0.87537900
H       -0.96394400    1.96869600    0.87828200
C        0.76298200   -0.01490800    0.00021300
H       -1.13668700   -0.52807800    0.87678900
H       -1.13616900   -0.52654900   -0.87837600
H        1.13668700    0.52807800   -0.87678900
H        1.13616900    0.52654900    0.87837600
C        1.33790200   -1.42972900   -0.00085800
H        0.96394400   -1.96869600   -0.87828200
H        0.96340200   -1.97025300    0.87537900
C        2.86421400   -1.44361000   -0.00039600
H        3.25778800   -2.46199300   -0.00126100
H        3.25785200   -0.93111900   -0.88216300
H        3.25730500   -0.93282600    0.88260200
#torsion 1 definition
 2 6
 7
 1 2 3 4 5 7 8
 3
 0. 120. -120.
#torsion 2 definition
 6 9
 10
 1 2 3 4 5 7 8 6 10 11
 3
 0. 120. -120.
#torsion 3 definition
 9 14
```

```
 13
 1 2 3 4 5 7 8 6 10 11 9 12 13
 3
 0. 120. -120.
%nproc=24
%mem=2000mb
# opt=tight Int=(Grid=99974) M062x/6-311+G(2df,2p)
0  1
```

4C. Hessian Projection Out (Mesmer input, C6.xml)

```
<?xml version="1.0" encoding="utf-8" ?>
<?xml-stylesheet type='text/xsl' href='../../mesmer2.xsl' media='other'?>
<?xml-stylesheet type='text/xsl' href='../../mesmer1.xsl' media='screen'?>
<me:mesmer xmlns="http://www.xml-cml.org/schema" xmlns:me="http://www.chem.leeds.ac.uk/mesmer"
xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance">
  <moleculeList>
 <molecule id="C6" xmlns="http://www.xml-cml.org/schema">
 <atomArray>
  <atom id="a1" elementType="C" x3="-2.860074" y3="1.441741" z3="0.000401"/>
  <atom id="a2" elementType="C" x3="-1.336020" y3="1.427878" z3="0.000867"/>
  <atom id="a3" elementType="H" x3="-3.253923" y3="2.457509" z3="0.001204"/>
  <atom id="a4" elementType="H" x3="-3.251993" y3="0.931200" z3="-0.880426"/>
  <atom id="a5" elementType="H" x3="-3.252546" y3="0.929594" z3="0.880049"/>
  <atom id="a6" elementType="C" x3="-0.761721" y3="0.015703" z3="-0.000219"/>
  <atom id="a7" elementType="H" x3="-0.961800" y3="1.967484" z3="-0.873061"/>
  <atom id="a8" elementType="H" x3="-0.962347" y3="1.965917" z3="0.875996"/>
  <atom id="a9" elementType="C" x3="0.761721" y3="-0.015703" z3="0.000219"/>
  <atom id="a10" elementType="H" x3="-1.135669" y3="-0.526281" z3="0.874338"/>
  <atom id="a11" elementType="H" x3="-1.135136" y3="-0.524719" z3="-0.875969"/>
  <atom id="a12" elementType="H" x3="1.135669" y3="0.526281" z3="-0.874338"/>
  <atom id="a13" elementType="H" x3="1.135136" y3="0.524719" z3="0.875969"/>
  <atom id="a14" elementType="C" x3="1.336020" y3="-1.427878" z3="-0.000867"/>
  <atom id="a15" elementType="H" x3="0.962347" y3="-1.965917" z3="-0.875996"/>
  <atom id="a16" elementType="H" x3="0.961800" y3="-1.967484" z3="0.873061"/>
```

```
 <atom id="a17" elementType="C" x3="2.860074" y3="-1.441741" z3="-0.000401"/>
 <atom id="a18" elementType="H" x3="3.253923" y3="-2.457509" z3="-0.001204"/>
 <atom id="a19" elementType="H" x3="3.252546" y3="-0.929594" z3="-0.880049"/>
 <atom id="a20" elementType="H" x3="3.251993" y3="-0.931200" z3="0.880426"/>
</atomArray>
<bondArray>
 <bond atomRefs2="a4 a1" order="1"/>
 <bond atomRefs2="a19 a17" order="1"/>
 <bond atomRefs2="a15 a14" order="1"/>
 <bond atomRefs2="a11 a6" order="1"/>
 <bond atomRefs2="a12 a9" order="1"/>
 <bond atomRefs2="a7 a2" order="1"/>
 <bond atomRefs2="a18 a17" order="1"/>
 <bond id="b5" atomRefs2="a14 a17" order="1"/>
 <bond id="b4" atomRefs2="a14 a9" order="1"/>
 <bond atomRefs2="a14 a16" order="1"/>
 <bond atomRefs2="a17 a20" order="1"/>
 <bond id="b3" atomRefs2="a6 a9" order="1"/>
 <bond id="b2" atomRefs2="a6 a2" order="1"/>
 <bond atomRefs2="a6 a10" order="1"/>
 <bond atomRefs2="a9 a13" order="1"/>
 <bond id="b1" atomRefs2="a1 a2" order="1"/>
 <bond atomRefs2="a1 a3" order="1"/>
 <bond atomRefs2="a1 a5" order="1"/>
 <bond atomRefs2="a2 a8" order="1"/>
</bondArray>
<propertyList>
 <property title="program">
  <scalar>Gaussian 09, Revision D.01</scalar>
 </property>
 <property title="basis">
  <scalar>6-311+G(2df,2p) (5D, 7F)</scalar>
 </property>
 <property title="method">
  <scalar>M062x</scalar>
```

</property>
<property title="File Format">
<scalar>g03</scalar>
</property>
<property title="Energy" dictRef="me:ZPE">
<scalar units="kJ/mol" convention="computational" zeroPointVibEnergyAdded="false"> 0 </scalar>
</property>
<property title="Hessian" dictRef="me:hessian">
<matrix rows="60" matrixType="squareSymmetricLT"units="Hartree/Bohr2">
4.77968762E-01 -4.65629449E-03 5.76087539E-01 -2.39340566E-05 2.06944389E-05
5.67179436E-01 -2.02573081E-01 -3.83629833E-03 -4.21322453E-05 4.95051648E-01
-8.55949306E-04 -8.01333081E-02 -1.10945337E-06 3.68732471E-02 5.10842420E-01
-3.95298226E-05 -1.16760428E-06 -8.01302480E-02 7.03193251E-06 -7.00870252E-05
5.94092836E-01 -7.87956040E-02 8.61506611E-02 6.03318884E-05 -1.03907198E-02
3.30061477E-02 2.70428868E-05 8.68797487E-02 8.71373116E-02 -2.82141378E-01
-1.84326348E-04 -1.72045626E-03 2.56224068E-03 3.36856877E-06 -9.56745595E-02
3.04458382E-01 6.16261480E-05 -1.84189636E-04 -4.72554093E-02 -3.64308723E-06
1.32843660E-05 -1.50645476E-03 -6.60852919E-05 2.02628012E-04 4.61541248E-02
-7.69780225E-02 -4.22063476E-02 -7.34718707E-02 -1.35499121E-02 -1.61260159E-02
-2.90922151E-02 3.60003720E-03 4.61850985E-03 1.03097222E-02 8.67802579E-02
-4.25395213E-02 -1.05001351E-01 -9.94857794E-02 -2.18092362E-04 -7.95694988E-04
3.89880662E-04 -1.10967662E-02 -1.34742120E-02 -2.53844442E-02 4.72391176E-02
1.09743535E-01 -7.39322968E-02 -9.93252796E-02 -2.21727572E-01 1.81142614E-04
6.22712966E-04 1.07141489E-03 1.08794184E-03 7.97352873E-04 6.51075000E-04
8.17898508E-02 1.10006288E-01 2.37931280E-01 -7.70549948E-02 -4.23907518E-02
7.34855455E-02 -1.35721087E-02 -1.61769215E-02 2.90549640E-02 3.60719361E-03
4.63934138E-03 -1.02999288E-02 3.49202799E-03 6.47989179E-03 -9.11305309E-03
8.68704604E-02 -4.27239243E-02 -1.05356815E-01 9.96545350E-02 -2.17650988E-04
-7.94271259E-04 -3.93064556E-04 -1.11106946E-02 -1.35203076E-02 2.53520707E-02
6.47124640E-03 7.76255301E-03 -1.31564137E-02 4.74438669E-02 1.10140127E-01
7.39454680E-02 9.94934927E-02 -2.21265111E-01 -1.89818109E-04 -6.35495811E-04
1.08716678E-03 -1.10610794E-03 -8.19991353E-04 6.87979750E-04 9.14012952E-03
1.32123233E-02 -2.05972280E-02 -8.17999148E-02 -1.10194143E-01 2.37422143E-01
-1.75702167E-02 3.60137929E-02 2.52746382E-05 -9.19592871E-02 3.55153582E-02
2.57245931E-05 -6.99886726E-03 4.29949069E-04 -1.94981647E-06 1.79099554E-03

2.97397913E-04 3.88122225E-04 1.79073619E-03 2.98440230E-04 -3.85670425E-04
4.94486939E-01 4.55133353E-03 -3.92100269E-04 2.21928151E-06 3.67809651E-02
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        <me:PotentialPoint angle= "  0" potential= "0  " />
        <me:PotentialPoint angle= " 30" potential= "0.4" />
        <me:PotentialPoint angle= " 60" potential= "1.1" />
        <me:PotentialPoint angle= " 90" potential= "0.9" />
        <me:PotentialPoint angle= "120" potential= "0.4" />
        <me:PotentialPoint angle= "150" potential= "0.3" />
        <me:PotentialPoint angle= "180" potential= "0.4" />
        <me:PotentialPoint angle= "210" potential= "0.6" />
        <me:PotentialPoint angle= "240" potential= "0.8" />
        <me:PotentialPoint angle= "270" potential= "0.8" />
        <me:PotentialPoint angle= "300" potential= "0.5" />
        <me:PotentialPoint angle= "330" potential= "0.1" />
        <me:PotentialPoint angle= "360" potential= "0  " />
      </me:HinderedRotorPotential>
      <me:periodicity>1</me:periodicity>
      <me:PlotStates/>
  </me:ExtraDOSCMethod>
  <me:ExtraDOSCMethod name="HinderedRotorQM1D">
  <me:bondRef>b2</me:bondRef>
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UseSineTerms="yes">
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        <me:PotentialPoint angle= " 60" potential= "2.6" />
        <me:PotentialPoint angle= " 90" potential= "1.3" />
        <me:PotentialPoint angle= "120" potential= "0.9" />
        <me:PotentialPoint angle= "150" potential= "2.7" />
```

```
        <me:PotentialPoint angle= "180" potential= "4.9" />
        <me:PotentialPoint angle= "210" potential= "2.3" />
        <me:PotentialPoint angle= "240" potential= "0.6" />
        <me:PotentialPoint angle= "270" potential= "1.6" />
        <me:PotentialPoint angle= "300" potential= "3.5" />
        <me:PotentialPoint angle= "330" potential= "1.7" />
        <me:PotentialPoint angle= "360" potential= "0  " />
      </me:HinderedRotorPotential>
      <me:periodicity>1</me:periodicity>
      <me:PlotStates/>
     </me:ExtraDOSCMethod>
 <me:ExtraDOSCMethod name="HinderedRotorQM1D">
  <me:bondRef>b3</me:bondRef>
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UseSineTerms="yes">
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        <me:PotentialPoint angle= " 60" potential= "2.6" />
        <me:PotentialPoint angle= " 90" potential= "1.3" />
        <me:PotentialPoint angle= "120" potential= "0.9" />
        <me:PotentialPoint angle= "150" potential= "2.7" />
        <me:PotentialPoint angle= "180" potential= "4.9" />
        <me:PotentialPoint angle= "210" potential= "2.3" />
        <me:PotentialPoint angle= "240" potential= "0.6" />
        <me:PotentialPoint angle= "270" potential= "1.6" />
        <me:PotentialPoint angle= "300" potential= "3.5" />
        <me:PotentialPoint angle= "330" potential= "1.7" />
        <me:PotentialPoint angle= "360" potential= "0  " />
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      <me:periodicity>1</me:periodicity>
      <me:PlotStates/>
     </me:ExtraDOSCMethod>
  <me:ExtraDOSCMethod name="HinderedRotorQM1D">
  <me:bondRef>b4</me:bondRef>
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UseSineTerms="yes">
```

```
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        <me:PotentialPoint angle= " 30" potential= "1.4" />
        <me:PotentialPoint angle= " 60" potential= "2.6" />
        <me:PotentialPoint angle= " 90" potential= "1.3" />
        <me:PotentialPoint angle= "120" potential= "0.9" />
        <me:PotentialPoint angle= "150" potential= "2.7" />
        <me:PotentialPoint angle= "180" potential= "4.9" />
        <me:PotentialPoint angle= "210" potential= "2.3" />
        <me:PotentialPoint angle= "240" potential= "0.6" />
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        <me:PotentialPoint angle= "300" potential= "3.5" />
        <me:PotentialPoint angle= "330" potential= "1.7" />
        <me:PotentialPoint angle= "360" potential= "0  " />
      </me:HinderedRotorPotential>
      <me:periodicity>1</me:periodicity>
      <me:PlotStates/>
     </me:ExtraDOSCMethod>
  <me:ExtraDOSCMethod name="HinderedRotorQM1D">
  <me:bondRef>b5</me:bondRef>
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UseSineTerms="yes">
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        <me:PotentialPoint angle= " 30" potential= "0.4" />
        <me:PotentialPoint angle= " 60" potential= "1.1" />
        <me:PotentialPoint angle= " 90" potential= "0.9" />
        <me:PotentialPoint angle= "120" potential= "0.4" />
        <me:PotentialPoint angle= "150" potential= "0.3" />
        <me:PotentialPoint angle= "180" potential= "0.4" />
        <me:PotentialPoint angle= "210" potential= "0.6" />
        <me:PotentialPoint angle= "240" potential= "0.8" />
        <me:PotentialPoint angle= "270" potential= "0.8" />
        <me:PotentialPoint angle= "300" potential= "0.5" />
        <me:PotentialPoint angle= "330" potential= "0.1" />
        <me:PotentialPoint angle= "360" potential= "0  " />
      </me:HinderedRotorPotential>
      <me:periodicity>1</me:periodicity>
```

```
        <me:PlotStates/>
       </me:ExtraDOSCMethod>
</molecule>
  </moleculeList>
  <me:modelParameters>
    <me:grainSize units="cm-1">50</me:grainSize>
    <me:energyAboveTheTopHill>200.0</me:energyAboveTheTopHill>
  </me:modelParameters>
  <me:control>
    <me:calcMethod units="kJ/mol" xsi:type="me:thermodynamicTable">
      <me:Tmin>200</me:Tmin>
      <me:Tmid>1000</me:Tmid>
      <me:Tmax>2000</me:Tmax>
      <me:Tstep>100</me:Tstep>
      <!--Note that the unit must be 'kJ/mol' because of the limitation of code for NASA format fitting-->
    </me:calcMethod>
  </me:control>
</me:mesmer>
```

4D. RRHO input (KistheIp: C6.kinp)

```
*MASS (in amu)
86.10955
*END
*NUMBER OF SYMMETRY
1
*END
*FREQUENCIES (in cm-1)
64.6010
91.5785
132.6101
144.2429
228.7660
242.4985
296.9076
```

371.2710

466.8539

728.1623

741.8102

799.3167

902.6702

903.5398

910.7327

1008.3927

1037.4848

1067.6185

1090.0252

1095.2703

1169.5526

1207.4040

1251.9286

1267.0203

1306.1615

1327.4335

1332.7362

1335.9889

1387.8091

1405.2416

1412.3337

1414.4100

1488.2362

1489.2609

1496.3891

1502.8694

1503.1004

1503.5825

1512.3169

1517.4574

3016.1411

3021.8183

3033.7917

3036.5379

3041.1314

3041.5755

3044.0015

3055.9592

3071.7629

3081.9869

3109.3021

3109.8417

3117.6485

3117.6768

*END

*ELECTRONIC DEGENERACY

1

*END

*MOMENT OF INERTIA (in Amu.bohr**2)

123.1258133263348

1575.9041869992557

1632.6442080254546

*END

*LINEAR

not linear

*END

*POTENTIAL ENERGY (in hartree)

-237.0250298

*END