ELECTRONIC SUPPLEMENTARY INFORMATION **FOR *FARADAY DISCUSSIONS***

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Multi-State Pair-Density Functional Theory

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Geometries

S1.1. LiF

Li 0.00000000 0.00000000 0.00000000
F 0.00000000 0.00000000 $z

$z = 1.00000000 + 0.20000000*t, t=0,1,2,…,35

S1.2. LiH

Li 0.00000000 0.00000000 0.00000000
H 0.00000000 0.00000000 $z

$z = 1.00000000 + 0.20000000*t, t=0,1,2,…,60

S1.3. HNCO

Geometries along the C – N dissociation of HNCO molecule with 130 deg of t(HNCO) torsion angle

```
#!/bin/bash -l
 Project=HNCO

 rOC=1.19064881 # r(CO) distance in Ang
 rHN=1.058354498 # r(HN) distance in Ang
 aNCO=100.0 # a(NCO) bond angle in deg
 aHNC=110.0 # a(HNC) bond angle in deg
 tHNCO=130.0 # t(HNCO) torsion angle in deg
 # The t(HNCO) torsion angle was varied from 130 to 180 deg
 # by 5 deg of increments
 pi=3.14159265359

 # The coordinates of O and H atoms, which do not change along the
 # separation of N and C atoms
 Oy=$(echo "scale=4;$rOC*s ($aNCO/180.0*$pi)"|bc -l)
 Oz=$(echo "scale=4;$rOC*c ($aNCO/180.0*$pi)"|bc -l)
 Hx=$(echo "scale=4;$rHN*s ($aHNC/180.0*$pi)*s ($tHNCO/180.0*$pi)"|bc -l)
 Hy=$(echo "scale=4;$rHN*s ($aHNC/180.0*$pi)*c ($tHNCO/180.0*$pi)"|bc -l)

 i=0
 while [ $i -le 35 ]
  do
   # r[$i] is the r(NC) distance at step i
   # r(NC) = [3.0 – 1.25] in Ang
   r[$i]=$(echo "scale=4;3.00-$i*0.05"|bc)
   tmp=${r[$i]}
```

```
    # Hz[$i] is the Z coordinate of atom H at step i
    Hz[$i]=$(echo "scale=4;$tmp - $rHN*c ($aHNC/180.0*$pi)"|bc -l)
    ((i=$i+1))
  done

# The $Project.xyz contains the Cartesian coordinates of HNCO for MOLCAS
# calculations
  i=0
  while [ $i -le 35 ]
   do
    echo " 4
 Angstrom
 C  0.00000  0.00000  0.00000
 O  0.00000  ${Oy} ${Oz}
 N  0.00000  0.00000  ${r[$i]}
 H  ${Hx}   ${Hy}   ${Hz[$i]}
" > $Project.xyz
  done
```

S1.4. Methylamine

(1) Eclipsed-H3 path

N	0.00204548	0.00000628	0.70120477
H	0.86019472	-0.00004443	1.22059369
H	$*x*	$*y*	$*z*
C	0.00189000	-0.00000337	-0.73696736
H	0.48596396	-0.88475017	-1.15933998
H	-1.02936906	0.00030992	-1.08536656
H	0.48647423	0.88448060	-1.15929483

$*x* = -0.68326229 - 0.08547330**t*, *t*=0,1,2,…,27
$*y* = -0.00003324 - 0.00000493**t*, *t*=0,1,2,…,27
$*z* = 1.11738313 + 0.05190680**t*, *t*=0,1,2,…,27

(2) Staggered conformation

N	-0.12310328	0.00071775	0.72548951
H	$*x*	$*y*	$*z*
H	-0.14273413	0.94922612	1.08510310
C	-0.00066683	0.00002564	-0.72911009
H	-0.50666213	0.87808667	-1.12875744
H	1.02787762	0.00059336	-1.10940810
H	-0.50604478	-0.87873942	-1.12824835

$x = -0.14067119 - 0.00215360*t, t=0,1,2,…,28
$y = -0.76201092 - 0.09350048*t, t=0,1,2,…,28
$z = 1.01424867 + 0.03539806*t, t=0,1,2,…,28

(3) 95º

N	-0.12310328	0.00071775	0.72548951
H	$x	$y	$z
H	-0.23641226	0.94561052	1.07721977
C	-0.00066683	0.00002564	-0.72911009
H	-0.50666213	0.87808667	-1.12875744
H	1.02787762	0.00059336	-1.10940810
H	-0.50604478	-0.87873942	-1.12824835

$x = -0.21301655 - 0.01102216*t, t=0,1,2,…,27
$y = -0.75919142 - 0.09315467*t, t=0,1,2,…,27
$z = 1.00815843 + 0.03465142*t, t=0,1,2,…,27

(4) 100º

N	-0.12310328	0.00071775	0.72548951
H	$x	$y	$z
H	-0.30699192	0.93665960	1.07128320
C	-0.00066683	0.00002564	-0.72911009
H	-0.50666213	0.87808667	-1.12875744
H	1.02787762	0.00059336	-1.10940810
H	-0.50604478	-0.87873942	-1.12824835

$x = -0.27277587 - 0.01834789*t, t=0,1,2,…,27
$y = -0.75158710 - 0.09222266*t, t=0,1,2,…,27
$z = 1.00312420 + 0.03403435*t, t=0,1,2,…,27

S1.5. Phenol

(1) H-O-C-C torsion angle of 1 deg

(2) H-O-C-C torsion angle of 10 deg

C	2.48389500	0.00000000	1.39346700
C	2.48082400	0.00000000	0.00170800
C	1.27241700	0.00000000	-0.70914500
C	0.04833800	0.00000000	-0.00195900
C	0.05522100	0.00000000	1.39974800
C	1.26417600	0.00000000	2.08699700
O	-1.17779400	0.00000000	-0.62950900

H 3.41532300 0.00000000 -0.54368500
H 3.41880000 0.00000000 1.93709400
H 1.25934600 0.00000000 3.16905500
H -0.88934600 0.00000000 1.92553800
H 1.27491700 0.00000000 -1.79297700
H $x $y $z

$x = -1.03911352 + 0.00693402*t, t=0,1,2,…,49
$y = -0.16442970 - 0.00822149*t, t=0,1,2,…,49
$z = -1.60610032 - 0.04882957*t, t=0,1,2,…,49

S1.6. O_2 + O collision

(1) fixed bond angle (a = 175 deg)

```
#!/bin/bash –l
  Project=O3_a175

  rO1O2=1.208 # Bond length of the O2 molecule in Ang
  a=175.0 # Bond angle of the three O atoms in deg
  pi=3.14159265359

# Coordinates which do not change along the collision
  O2y=$(echo "scale=4;$rO1O2*1.0"|bc -l)

  i=0
  while [ $i -le 15 ]
   do
   # rO1O3[$i] is the distance between one the atoms in the molecule (O1)
   # and the colliding atom (O3)
   # r(O1O3) = [2.5 – 1.0] in Ang
   rO1O3[$i]=$(echo "scale=4;2.50-$i*0.1"|bc)
   tmp=${rO1O3[$i]}
   # Coordinates of the colliding atom (O3)
   O3y[$i]=$(echo "scale=4;$tmp*s ($a/180.0*$pi)"|bc -l)
   O3z[$i]=$(echo "scale=4;$tmp*c ($a/180.0*$pi)"|bc -l)
   ((i=$i+1))
  done

# The $Project.xyz contains the Cartesian coordinates of O3 calculation for
# MOLCAS calculations
  i=0
  while [ $i -le 15 ]
   do
    echo " 3
```

```
 Angstrom
 O  0.00000  0.00000  0.00000
 O  0.00000  0.00000  ${O2y}
 O  0.00000  ${O3y[$i]} ${O3z[$i]}
" > $Project.xyz
  done
```

(2) fixed bond length (r(O1O3) = 1.4 Ang)

```
#!/bin/bash –l
  Project=O3_r14

  rO1O2=1.208 # Bond length of the O2 molecule in Ang
  a=180.0 # starting bond angle in deg
  pi=3.14159265359
  rO1O3=1.4 # The distance between one the atoms in the molecule (O1)
          # and the colliding atom (O3) in Ang

# Coordinates which do not change along the collision
  O2y=$(echo "scale=4;$rO1O2*1.0"|bc -l)

  i=0
  while [ $i -le 24 ]
   do
   # The bond angle of the three O atoms is varied from 180 to 60 deg
  # by 5 deg of decrements
   angle[$i]=$(echo "scale=4;$a-$i*5"|bc -l)
   # Coordinates of the colliding atom (O3)
   O3y[$i]=$(echo "scale=4;$rO1O3*s (($a-$i*5)/180.0*$pi)"|bc -l)
   O3z[$i]=$(echo "scale=4;$rO1O3*c (($a-$i*5)/180.0*$pi)"|bc -l)
   ((i=$i+1))
  done

# The $Project.xyz contains the Cartesian coordinates of O3 calculation for
# MOLCAS calculations
  i=0
  while [ $i -le 24 ]   #15
   do
    echo " 3
 Angstrom
 O  0.00000  0.00000  0.00000
 O  0.00000  0.00000  ${O2y}
 O  0.00000  ${O3y[$i]} ${O3z[$i]}
" > $Project.xyz
  done
```

S1.7. Spiro

This structure has the hole (the positive charge) on the left if one orients the structure so that the z-axis runs from negative at the left to positive at the right.

(1) Geometry A: $Q_\gamma^A(\xi = -0.5)$

C	0.00000000	1.26083600	-0.93407400
C	0.00000000	-0.67593100	-2.30714100
C	0.00000000	0.67593100	-2.30714100
C	0.00000000	1.10122500	-3.65628300
H	0.86839800	1.88745700	-0.77848400
H	-0.86839800	1.88745700	-0.77848400
H	0.00000000	2.08375800	-4.08145200
C	0.00000000	0.00000000	0.01551700
C	1.26695200	0.00000000	0.95314700
C	0.70302200	0.00000000	2.33794100
H	1.88873000	0.86712500	0.76467100
H	1.88873000	-0.86712500	0.76467100
C	-0.70302200	0.00000000	2.33794100
C	1.11965800	0.00000000	3.62808400
H	2.09431100	0.00000000	4.06624400
C	-1.11965800	0.00000000	3.62808400
C	0.00000000	-1.10122500	-3.65628300
C	0.00000000	-1.26083600	-0.93407400
H	0.86839800	-1.88745700	-0.77848400
H	-0.86839800	-1.88745700	-0.77848400
C	-1.26695200	0.00000000	0.95314700
H	-1.88873000	0.86712500	0.76467100
H	-1.88873000	-0.86712500	0.76467100
H	0.00000000	-2.08375800	-4.08145200
H	-2.09431100	0.00000000	4.06624400
N	0.00000000	0.00000000	4.40196100
H	0.00000000	0.00000000	5.39281700
N	0.00000000	0.00000000	-4.43484800
H	0.00000000	0.00000000	-5.43012800

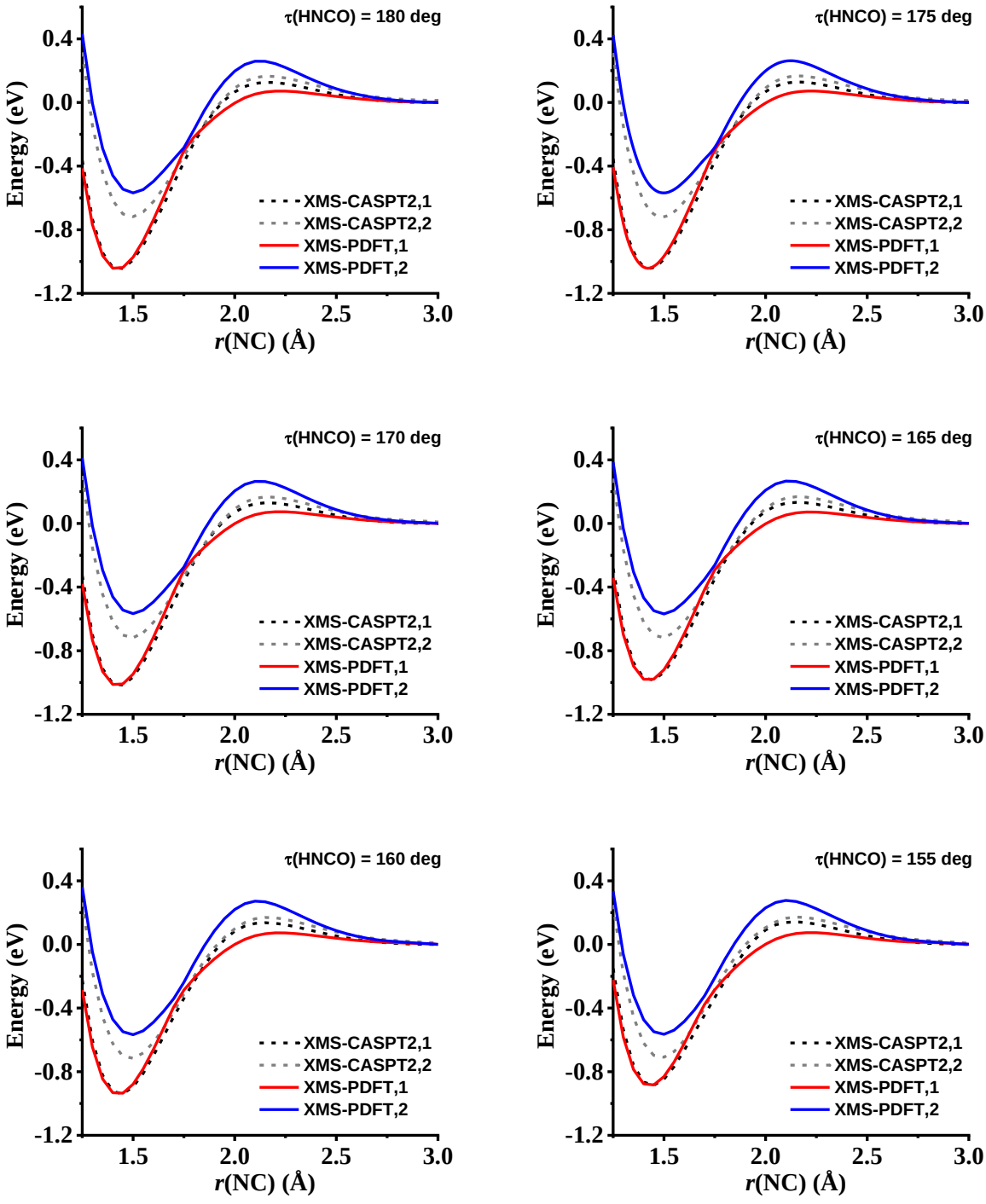
(2) Geometry B: $Q_\gamma^B(\xi = 0.5)$

C	0.00000000	1.26695200	-0.95314700
C	0.00000000	-0.70302200	-2.33794100
C	0.00000000	0.70302200	-2.33794100
C	0.00000000	1.11965800	-3.62808400
H	0.86712500	1.88873000	-0.76467100
H	-0.86712500	1.88873000	-0.76467100

H	0.00000000	2.09431100	-4.06624400
C	0.00000000	0.00000000	-0.01551700
C	1.26083600	0.00000000	0.93407400
C	0.67593100	0.00000000	2.30714100
H	1.88745700	0.86839800	0.77848400
H	1.88745700	-0.86839800	0.77848400
C	-0.67593100	0.00000000	2.30714100
C	1.10122500	0.00000000	3.65628300
H	2.08375800	0.00000000	4.08145200
C	-1.10122500	0.00000000	3.65628300
C	0.00000000	-1.11965800	-3.62808400
C	0.00000000	-1.26695200	-0.95314700
H	0.86712500	-1.88873000	-0.76467100
H	-0.86712500	-1.88873000	-0.76467100
C	-1.26083600	0.00000000	0.93407400
H	-1.88745700	0.86839800	0.77848400
H	-1.88745700	-0.86839800	0.77848400
H	0.00000000	-2.09431100	-4.06624400
H	-2.08375800	0.00000000	4.08145200
N	0.00000000	0.00000000	4.43484800
H	0.00000000	0.00000000	5.43012800
N	0.00000000	0.00000000	-4.40196100
H	0.00000000	0.00000000	-5.39281700

Other geometries are generated by using $Q_\gamma(\xi) = \left(\frac{1}{2} - \xi\right) Q_\gamma^A + \left(\frac{1}{2} + \xi\right) Q_\gamma^B$ with $\xi = -1.5 + 0.05 * t$, t=0, 1, 2,…, 60.

S2. XMS-PDFT PECs of HNCO at Other Torsion Angles



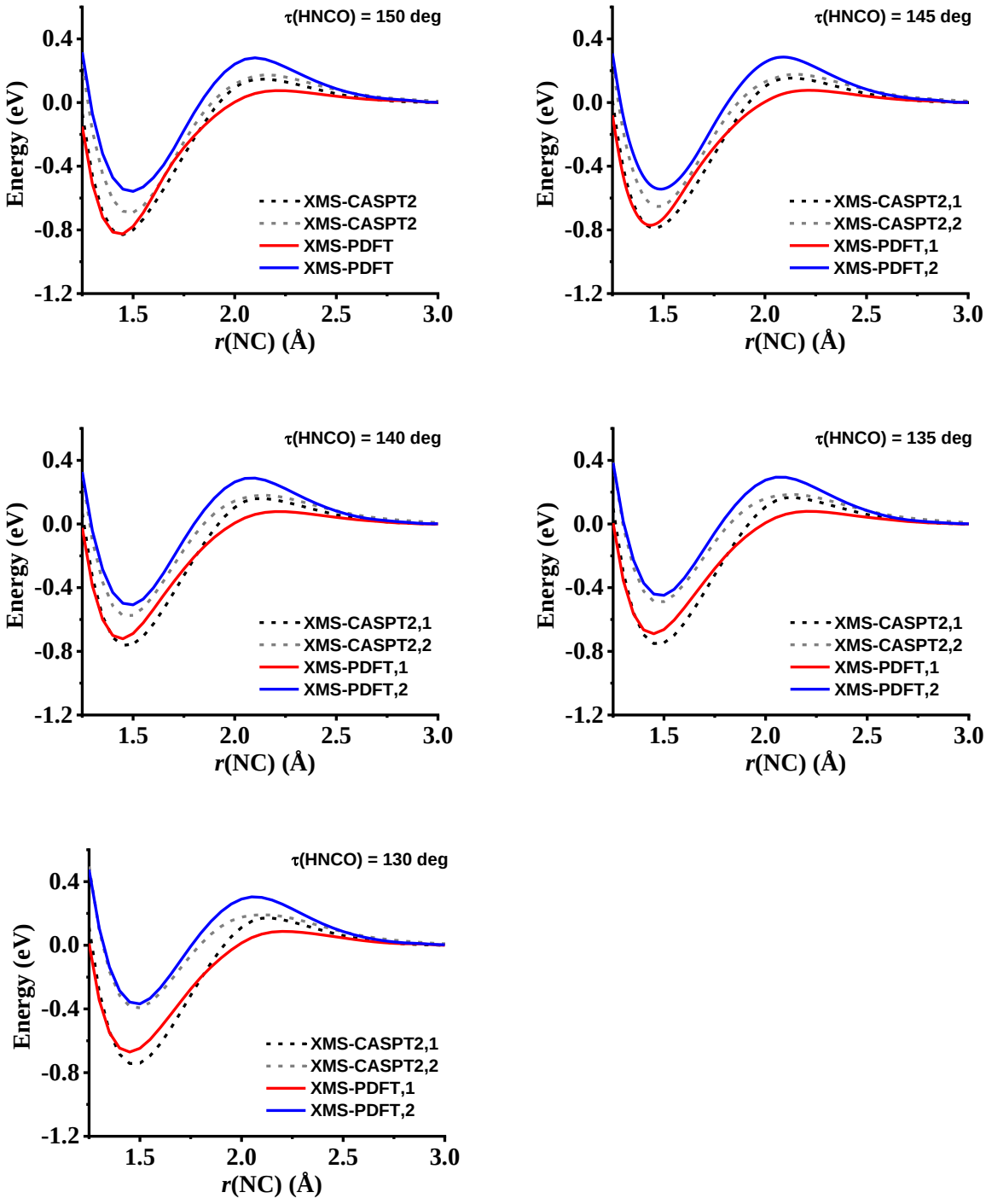


Figure S1. Comparison of XMS-PDFT with XMS-CASPT2 for the two lowest PECs along the CN bond dissociation of HNCO. The τ(HNCO), torsion angle was scanned from 180° to 130° with 5° decrements.

S3. Systems where XMS-PDFT fails

Here we provide details on systems, the $[He_2H_2]^{n+2+}$ series, $[He_2H]^{3+}$ and $[Ne_2H_2]^{5+}$, where XMS-PDFT fails. All these systems are mixed-valence systems that contain a charged noble-gas dimer plus one or two protons. We tested the tPBE functional for XMS-PDFT.

S3.1. $[He_2H_2]^{n+2+}$

The geometric diagram of this system is shown in Figure S2. The two He atoms are separated by r_1. Two protons, separated by (r_1+ 10 Å), are moving simultaneously, starting with the left proton being 1 Å away from the left He, and ending with the right proton being 1 Å away from the right He. The left-proton-He-He bond angle is varied to study if a perfect C_{2v} symmetry is the main reason why XMS-PDFT fails. For illustrative purpose, a STO-3G basis set is used, and there are only two active orbitals. We tested the case with one electron (n = 3), two electrons (n = 2) and three electrons (n = 1).

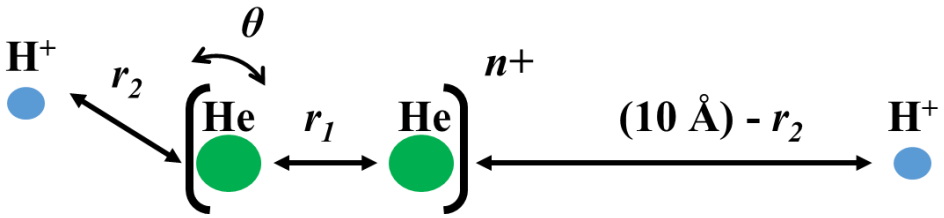


Figure S2. The geometry of $[He_2H_2]^{n+2+}$.

Figure S3 shows the potential energy curves (PECs) of the system with only one electron and the bond angle is 180 °, at four He-He distances. The XMS-PDFT curves differ from each other by showing a correct behavior of two states (r_1 = 1 Å), starting to show a "dip" (r_1 = 2 Å), show a typical "dip" (r_1 = 4 Å) and show no "dip" (r_1 = 10 Å). Nevertheless, the SA-CASSCF method gives physical PECs for all four distances.

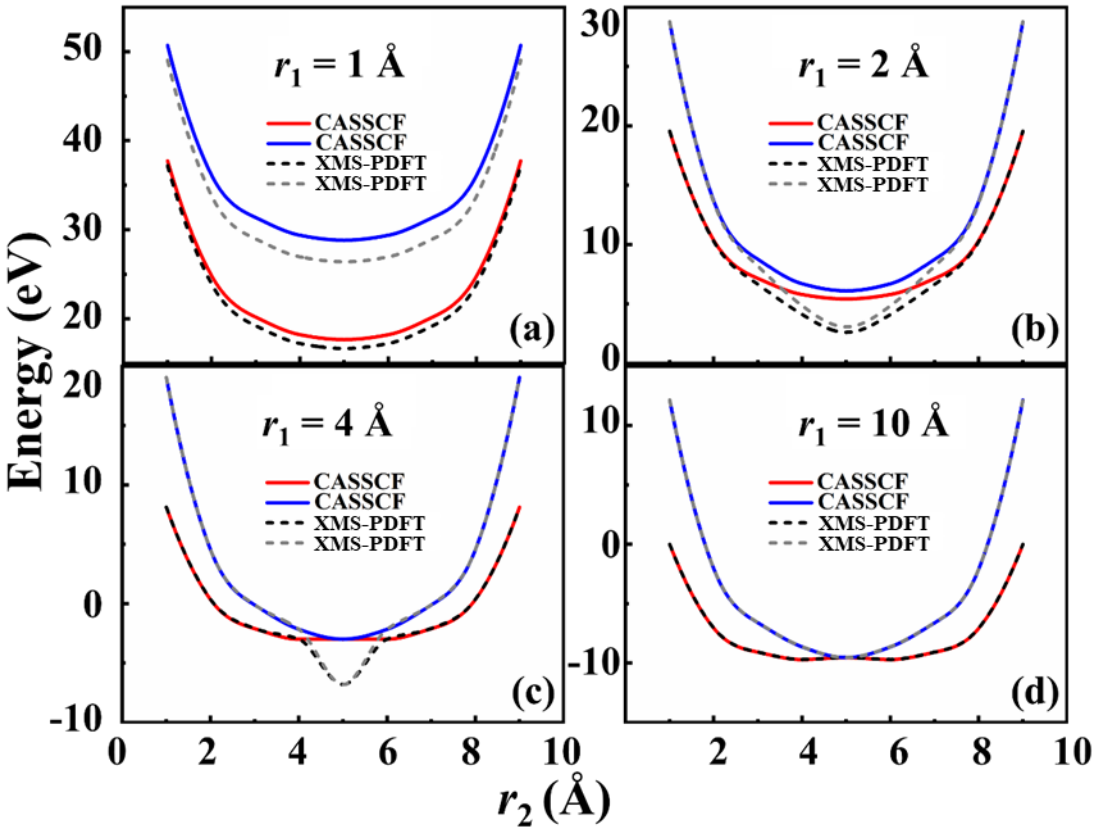


Figure S3. The potential energy curves of $[He_2H_2]^{5+}$ when the H-He-He bond angle is zero.

The active space used for this system contains only two configuration state functions (CSFs). It is then interesting two compare the rotation angle that mixes the two CSFs that form two SA-CASSCF reference states and the rotation angle that mixes the two reference states to form two intermediate states.

The reference states $|1\rangle$ and $|2\rangle$ can be written as

$$\begin{cases} |1\rangle = \cos\omega|\mathrm{CSF}_1\rangle + \sin\omega|\mathrm{CSF}_2\rangle \\ |2\rangle = -\sin\omega|\mathrm{CSF}_1\rangle + \cos\omega|\mathrm{CSF}_2\rangle \end{cases} \quad \text{(S1)}$$

and ω is the rotation angle that mixes $|\mathrm{CSF}_1\rangle$ and $|\mathrm{CSF}_2\rangle$, and can be calculated by taking the arccos function of the coefficient of the first CSF in the ground state.

The intermediate states, $|I\rangle$ and $|J\rangle$, can be written as

$$\begin{cases} |I\rangle = \cos\theta|1\rangle + \sin\theta|2\rangle \\ |J\rangle = -\sin\theta|1\rangle + \cos\theta|2\rangle \end{cases} \quad \text{(S2)}$$

Because the intermediate states are obtained by diagonalizing the Fock matrix of states defined in Eq. (10), and in the examples we are dealing with only two states, θ can be calculated as

$$\tan 2\theta = -\frac{2F_{IJ}}{F_{JJ}-F_{II}} \quad \text{(S3)}$$

or

$$\theta = \arctan\left(-\frac{2F_{IJ}}{F_{JJ}-F_{II}}\right)/2 \quad \text{(S4)}$$

We then plot ω and θ in Figure S4. We find that both angles are almost zero throughout the curve. On the contrary, θ can reach 45 ° for most of the systems studied in the paper, for example, LiF, and LiH.

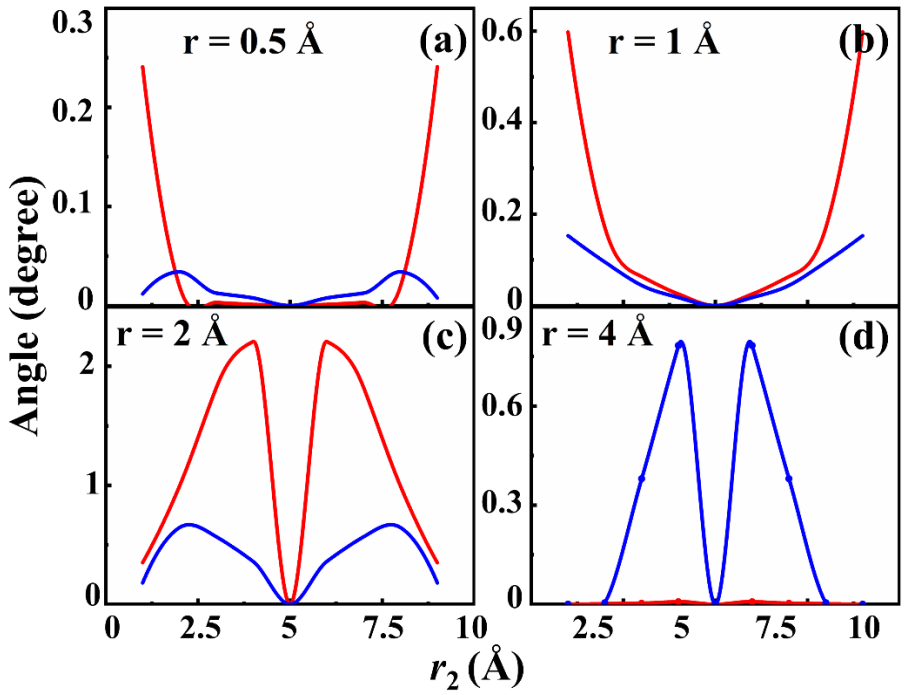


Figure S4. The rotation angle (blue) that mixes two CSFs to form SA-CASSCF adiabatic states and the rotation angle (red) that mixes the reference states to form intermediate states. Small rotation angle, θ, suggests that the off-diagonal element of the Fock matrix of states is small compared with the difference of the diagonal elements.

We also studied the PEC of $[He_2H_2]^{5+}$ when the system is not linear. We show some of the PECs for the angle being 175 ° and 90 ° in Figure S5. The XMS-PDFT curves still present unphysical "dips" of energies.

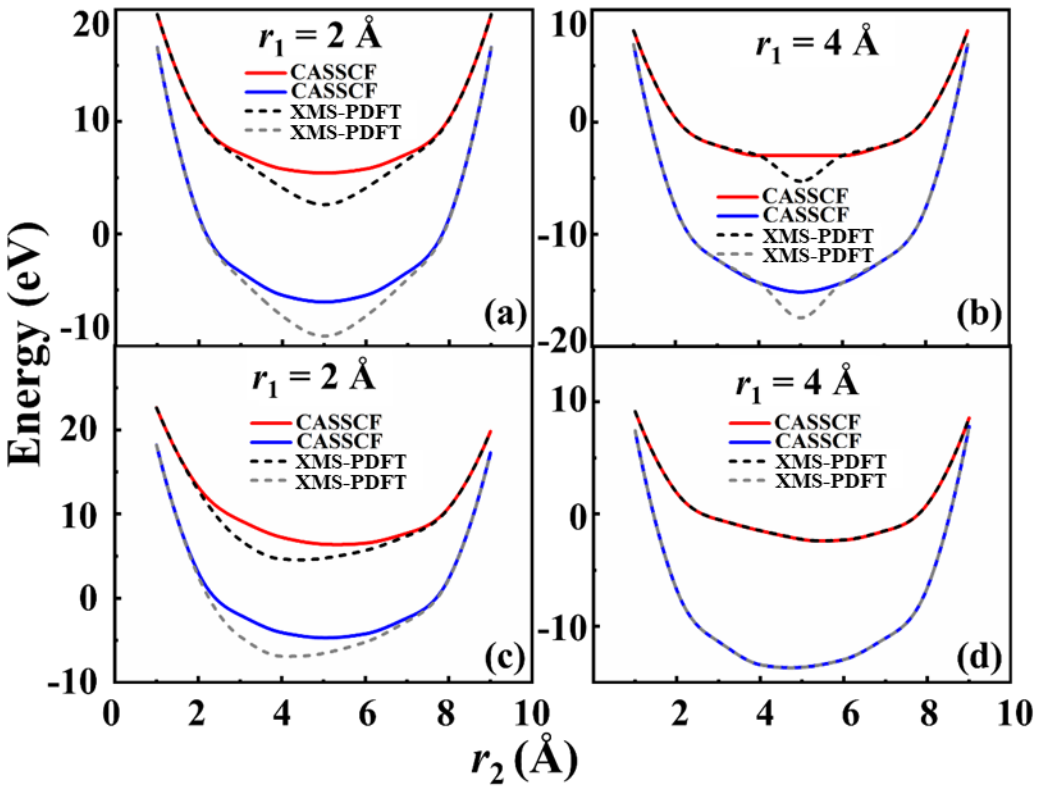


Figure S5. The potential energy curves of $[He_2H_2]^{5+}$ with the H-He-He bond angles being 175 ° in (a), (b) and 90 ° in (c), (d).

Figure S6 shows the PECs of the system with two electrons for four He-He distances. Since there are two electrons in the two orbitals, in total three states, are generated. The lowest states correspond to a He^+-He^+ pair, and the two excited states correspond to He^{2+}-He or He-He^{2+}, whoever of which has a higher energy if He^{2+} is closer to the proton. The three-state PECs also have a "dip" for weakly bonded regions (r_1 = 2 Å and 10 Å).

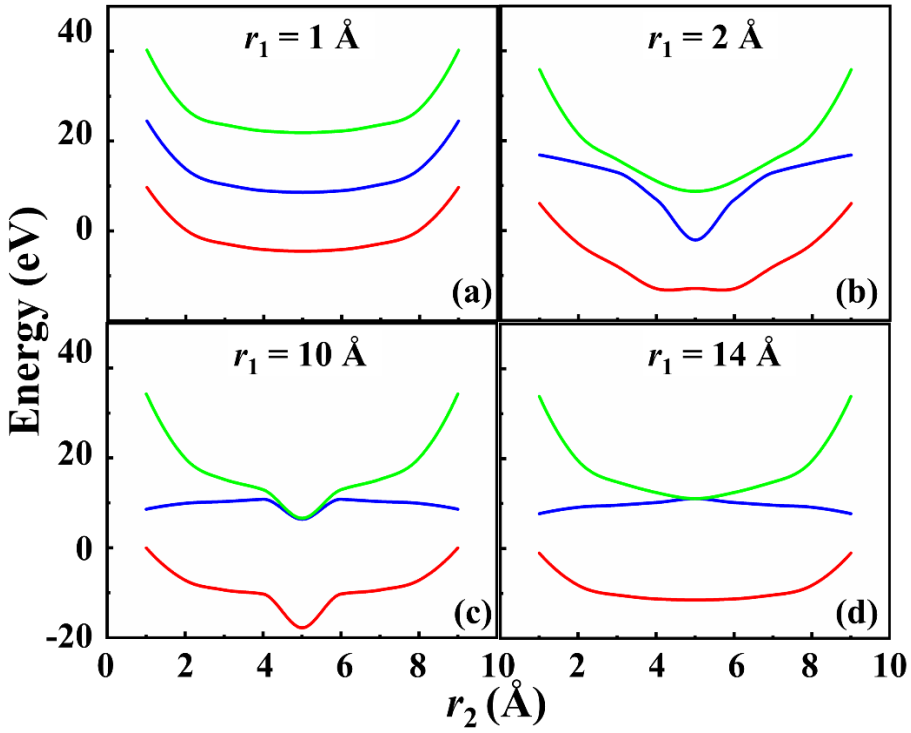


Figure S6. The potential energy curves of $[He_2H_2]^{4+}$ calculated by XMS-PDFT.

At last, we consider the three-electron case. Given three electrons in two orbitals, there are two wave functions, corresponding to He^+-He and He-He^+, respectively. A dip is also found for regions where the two He atoms are weakly bonded.

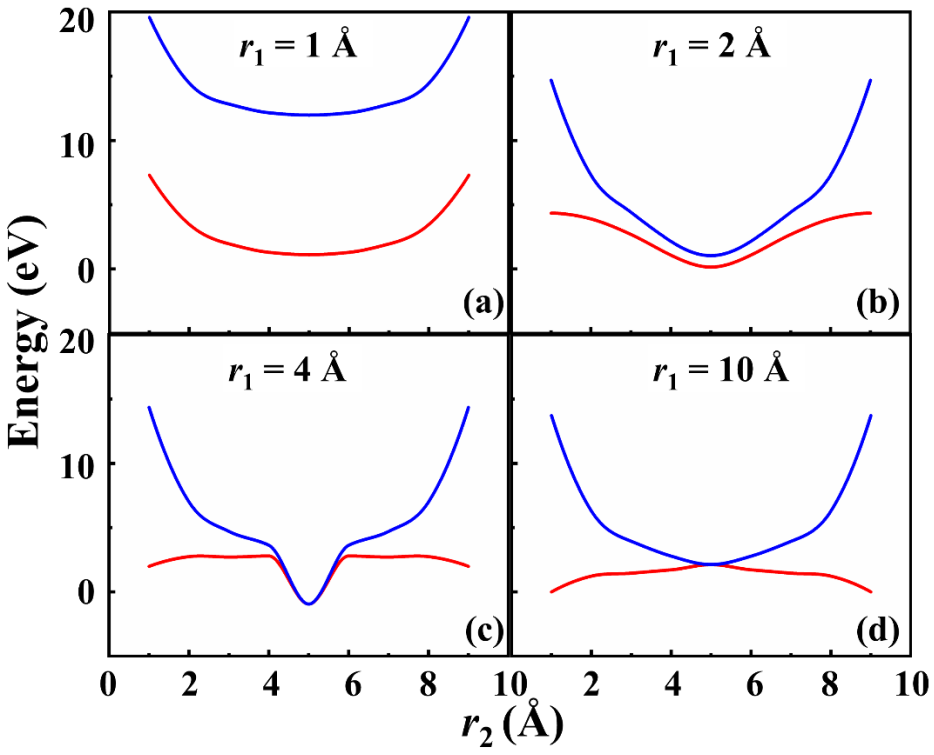


Figure S7. The XMS-PDFT potential energy curves of $[He_2H_2]^{3+}$.

The examples in this section show that the unphysical lowering of PECs does not depend on the number of electrons in a given active orbitals, nor the particular symmetry of the system.

S3.2. $[He_2H]^{4+}$

The geometric diagram of this system is shown in Figure S8. The position of the proton is quantified by its x coordinate, x_H. x_H starts at -5 Å and ends at 5 Å. x_H is 0 when the proton is equally far away from both He nuclei on its path from left to right (in other words, when the proton hits the vertical bisector of the line where the two He are in).

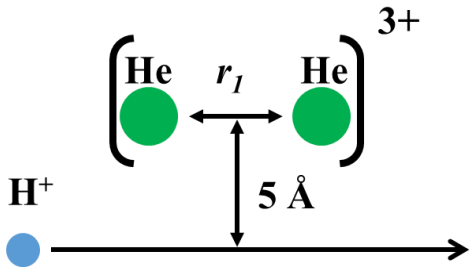


Figure S8. The geometry of $[He_2H]^{4+}$.

An active space with one electron in two orbitals is used. The basis set is STO-3G.

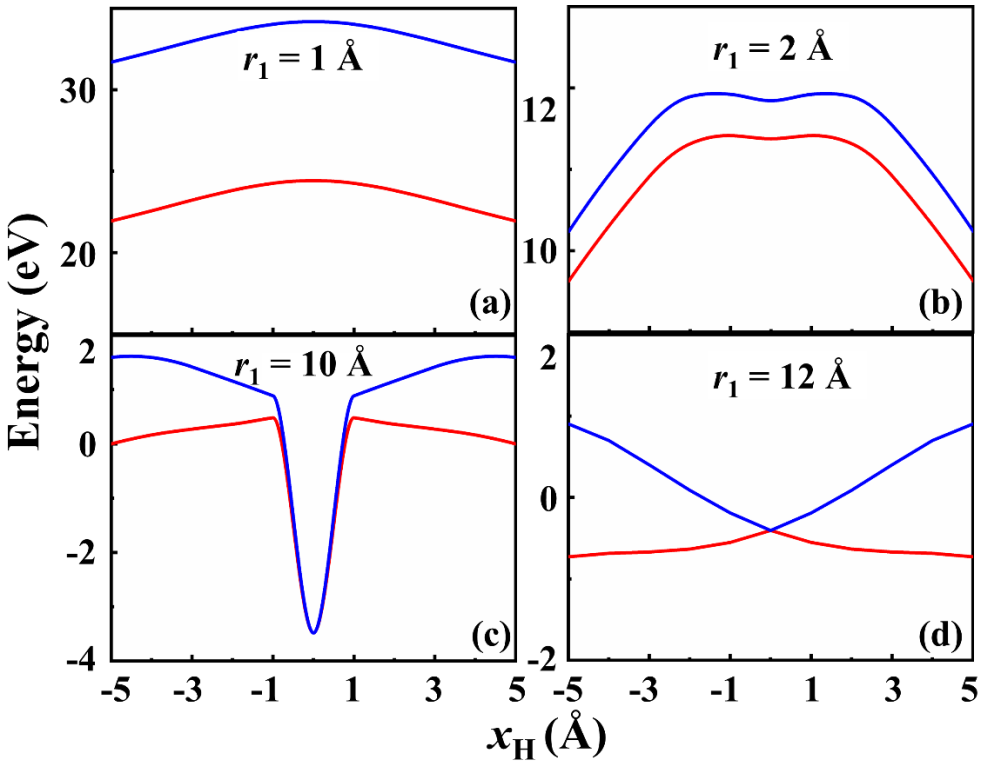


Figure S9. The XMS-PDFT potential energy curves of $[He_2H]^{4+}$.

Similar to the PECs in the previous section, this system still has unphysical lowering of energies in the PECs when the orbitals that are involved in the electron excitations are weakly bonded.

S3.3. $[Ne_2H_2]^{5+}$

The geometry of this system is the same as $He_2H_2^{5+}$, but with He replaced by Ne, as shown in Figure S10. The active space includes σ_{2s}, σ_{2s}*, σ_{2pz}, σ_{2pz}* of the Ne_2 subunit and the 1s orbitals from the two H atoms. The basis set is cc-pVTZ. The PECs are shown in Figure S11.

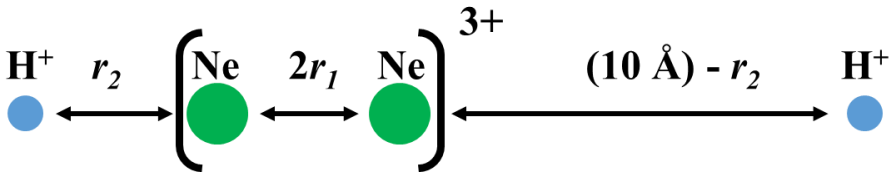


Figure S10. The geometry of $[Ne_2H_2]^{5+}$.

The PECs of $[Ne_2H_2]^{5+}$ have similar behaviors as those for $[He_2H_2]^{5+}$.

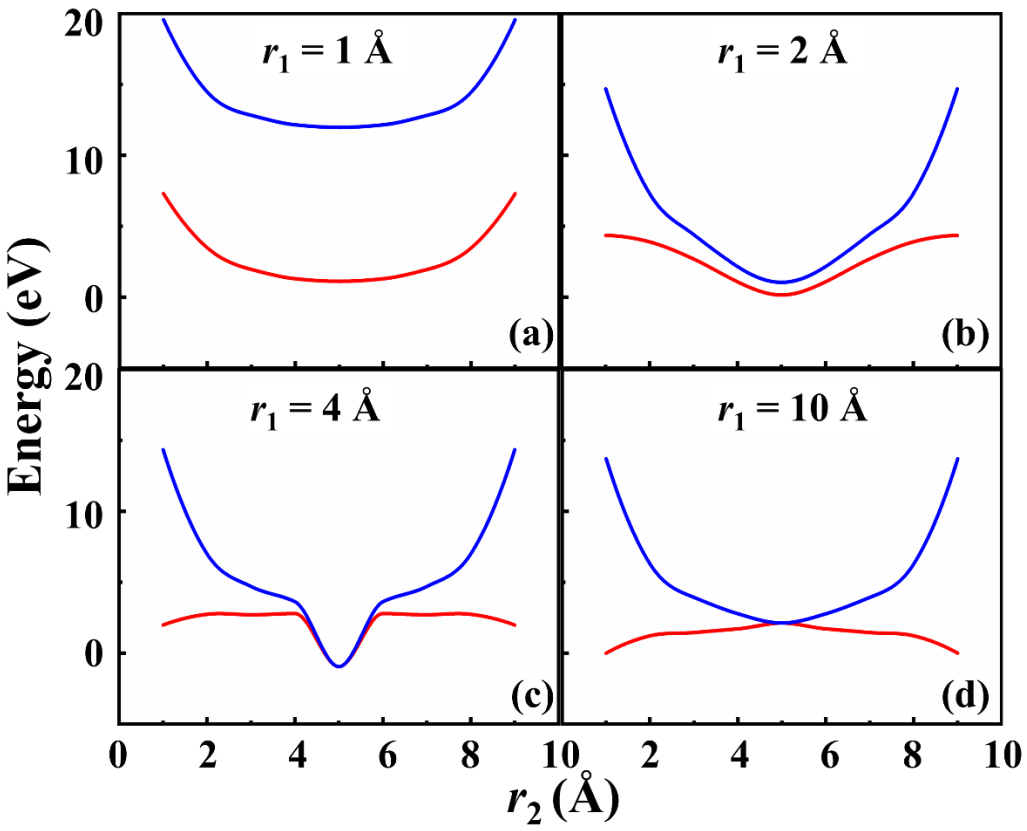


Figure S11. The XMS-PDFT potential energy curves of $[Ne_2H_2]^{5+}$.

S4. Absolute Energies

S4.1. LiF

R_{Li-F} (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (MC-PDFT)	E2 (MC-PDFT)
1.000	-106.98371802	-106.73072245	-107.00613803	-106.75666522
1.200	-107.21316271	-106.93957792	-107.21851700	-106.94802074
1.400	-107.28526235	-107.01993853	-107.28612016	-107.02450640
1.600	-107.29783084	-107.05116629	-107.29844678	-107.05642682
1.800	-107.28864864	-107.06414390	-107.29051685	-107.07172335
2.000	-107.27212201	-107.07043446	-107.27605832	-107.08134940
2.200	-107.25384641	-107.07429719	-107.26068310	-107.08967917
2.400	-107.23603143	-107.07724759	-107.24680467	-107.09851775
2.600	-107.21952868	-107.07977500	-107.23541247	-107.10850215
2.800	-107.20460777	-107.08201225	-107.22673771	-107.11967833
3.000	-107.19126713	-107.08399155	-107.22057607	-107.13183621
3.200	-107.17938454	-107.08573023	-107.21651172	-107.14480092
3.400	-107.16879549	-107.08724486	-107.21387339	-107.15830606
3.600	-107.15933521	-107.08855117	-107.21124612	-107.17136311
3.800	-107.15085481	-107.08966325	-107.20556466	-107.18109265
4.000	-107.14322615	-107.09059605	-107.19233665	-107.18234801
4.200	-107.13634105	-107.09136612	-107.17016670	-107.17199042
4.400	-107.13010731	-107.09199076	-107.14514199	-107.15446956
4.600	-107.12444738	-107.09248856	-107.12481656	-107.13734682
4.800	-107.11929435	-107.09287598	-107.11138660	-107.12406453
5.000	-107.11454723	-107.09255250	-107.10336484	-107.11443142
5.200	-107.10996936	-107.09275075	-107.09875152	-107.10732628
5.400	-107.10604616	-107.09287704	-107.09610718	-107.10181046
5.600	-107.10228531	-107.09288187	-107.09458829	-107.09729678
5.800	-107.09913322	-107.09273957	-107.09369745	-107.09344227
6.000	-107.09659486	-107.09219971	-107.09317794	-107.09003997
6.200	-107.09510996	-107.09080371	-107.09287056	-107.08697020
6.400	-107.09453854	-107.08867397	-107.09269149	-107.08415898
6.600	-107.09432411	-107.08635136	-107.09258184	-107.08155782
6.800	-107.09422959	-107.08405882	-107.09251015	-107.07913322

R_{Li-F} (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)	E1 (FMS-PDFT)	E2 (FMS-PDFT)
1.000	-107.00307934	-106.75316215	-107.00153789	-106.75255147
1.200	-107.21832561	-106.94791496	-107.21816934	-106.94796365
1.400	-107.28601692	-107.02402613	-107.28601948	-107.02384437

1.600	-107.29750119	-107.05404411	-107.29725803	-107.05331278
1.800	-107.28809545	-107.06637529	-107.28742369	-107.06503646
2.000	-107.27146968	-107.07197652	-107.27029433	-107.07009963
2.200	-107.25307190	-107.07505670	-107.25137307	-107.07278893
2.400	-107.23512844	-107.07722462	-107.23293015	-107.07474509
2.600	-107.21851758	-107.07904859	-107.21589287	-107.07654944
2.800	-107.20349826	-107.08065369	-107.20056324	-107.07832522
3.000	-107.19002442	-107.08207210	-107.18693449	-107.08007095
3.200	-107.17793886	-107.08332787	-107.17487120	-107.08172980
3.400	-107.16707002	-107.08444698	-107.16417818	-107.08325743
3.600	-107.15726825	-107.08544097	-107.15461939	-107.08465694
3.800	-107.14842090	-107.08632530	-107.14602300	-107.08591531
4.000	-107.14041998	-107.08709934	-107.13822355	-107.08706552
4.200	-107.13319079	-107.08777784	-107.13125801	-107.08797802
4.400	-107.12664755	-107.08835889	-107.12505256	-107.08863657
4.600	-107.12072835	-107.08884890	-107.11933748	-107.08924886
4.800	-107.11536954	-107.08924417	-107.11413403	-107.08974208
5.000	-107.11051881	-107.08953749	-107.10940482	-107.09011739
5.200	-107.10614489	-107.08972703	-107.10511674	-107.09036522
5.400	-107.10223567	-107.08977186	-107.10125498	-107.09047237
5.600	-107.09883407	-107.08958753	-107.09786727	-107.09036263
5.800	-107.09609622	-107.08900104	-107.09516554	-107.08979374
6.000	-107.09426130	-107.08774041	-107.09353988	-107.08836666
6.200	-107.09330784	-107.08580653	-107.09286697	-107.08617838
6.400	-107.09286186	-107.08354374	-107.09261473	-107.08375079
6.600	-107.09264605	-107.08121660	-107.09250799	-107.08133630
6.800	-107.09254031	-107.07893599	-107.09245381	-107.07900895

S4.2. LiH

$R_{\text{Li-H}}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E3 (XMS-CASPT2)	E4 (XMS-CASPT2)
1.000	-7.92561942	-7.78286211	-7.69582979	-7.68121037
1.200	-7.99036817	-7.84440506	-7.7607783	-7.74565014
1.400	-8.01639666	-7.87532284	-7.7925488	-7.7778704
1.600	-8.02282247	-7.89070354	-7.80730265	-7.79360375
1.800	-8.01946687	-7.89818961	-7.81334596	-7.80092075
2.000	-8.0114534	-7.90172052	-7.81507295	-7.80411063
2.200	-8.00149485	-7.90332313	-7.81484138	-7.80558108
2.400	-7.9910555	-7.90400624	-7.81393579	-7.80677811
2.600	-7.98090442	-7.9042265	-7.81321766	-7.80823503
2.800	-7.97150707	-7.90414228	-7.8140189	-7.80935276

3.000	-7.96307895	-7.90375456	-7.81708773	-7.80922987
3.200	-7.95577472	-7.9029782	-7.82120344	-7.80873641
3.400	-7.94967902	-7.90170851	-7.82554563	-7.80827684
3.600	-7.94481523	-7.89987051	-7.82972994	-7.80791217
3.800	-7.94111689	-7.89746635	-7.83354934	-7.80763987
4.000	-7.93842051	-7.89458459	-7.83689515	-7.80743967
4.200	-7.93655676	-7.89139727	-7.8397892	-7.80731977
4.400	-7.9352706	-7.8880518	-7.84217579	-7.80723838
4.600	-7.93440533	-7.88470656	-7.84410133	-7.80719712
4.800	-7.93382695	-7.88147668	-7.84558698	-7.8071883
5.000	-7.93344067	-7.87846031	-7.84664772	-7.80720134
5.200	-7.93318291	-7.87572062	-7.84729423	-7.80723582
5.400	-7.93301043	-7.87331438	-7.84752961	-7.80728718
5.600	-7.9328946	-7.87127883	-7.84735813	-7.80735006
5.800	-7.93281658	-7.86962549	-7.84680031	-7.80742467
6.000	-7.93276374	-7.86833807	-7.84589232	-7.80750712
6.200	-7.9327278	-7.8673726	-7.84469545	-7.80759601
6.400	-7.93270318	-7.86666979	-7.84328031	-7.80768984
6.600	-7.93268619	-7.86616843	-7.84171483	-7.80778725
6.800	-7.93267437	-7.86581487	-7.84005771	-7.80788677
7.000	-7.93266602	-7.86556708	-7.83835555	-7.80798731
7.200	-7.93266012	-7.86539356	-7.8366409	-7.80808785
7.400	-7.93265584	-7.86527192	-7.83493752	-7.80818736
7.600	-7.93265271	-7.86518643	-7.83326137	-7.80828497
7.800	-7.93265038	-7.86512613	-7.83162319	-7.80837985
8.000	-7.93264862	-7.86508342	-7.83002983	-7.80847127
8.200	-7.93264727	-7.86505304	-7.82848553	-7.80855858
8.400	-7.93264621	-7.86503132	-7.82699264	-7.80864117
8.600	-7.93264537	-7.8650157	-7.82555215	-7.80871853
8.800	-7.93264471	-7.86500442	-7.82416417	-7.80879018
9.000	-7.93264417	-7.86499622	-7.82282815	-7.80885567
9.200	-7.93264373	-7.86499022	-7.82153941	-7.80891431
9.400	-7.93264337	-7.86498583	-7.82030838	-7.80896623
9.600	-7.93264307	-7.86498256	-7.81912271	-7.80901014
9.800	-7.9326428	-7.86498013	-7.81798482	-7.80904525
10.000	-7.93264261	-7.8649783	-7.81689437	-7.80907052
10.200	-7.93264243	-7.8649769	-7.8158484	-7.80908324
10.400	-7.93264227	-7.86497584	-7.81485958	-7.80908142
10.600	-7.93264214	-7.864975	-7.81392088	-7.80905825
10.800	-7.93264203	-7.86497433	-7.8130442	-7.80900447
11.000	-7.93264193	-7.86497381	-7.81224518	-7.80890303

11.200	-7.93264185	-7.86497341	-7.81155045	-7.80872601
11.400	-7.93264178	-7.86497308	-7.81099479	-7.80843645
11.600	-7.93264173	-7.86497281	-7.8106012	-7.80801293
11.800	-7.93264167	-7.86497258	-7.81034985	-7.80747397
12.000	-7.93264164	-7.86497239	-7.81019475	-7.80685828
12.200	-7.9326416	-7.86497223	-7.81009949	-7.80621126
12.400	-7.93264158	-7.86497212	-7.81003804	-7.80554253
12.600	-7.93264156	-7.864972	-7.80999781	-7.80488515
12.800	-7.93264156	-7.86497194	-7.80997012	-7.8042154
13.000	-7.93264155	-7.86497185	-7.80995093	-7.80357841

$R_{\text{Li-H}}$ (Å)	E1 (MC-PDFT)	E2 (MC-PDFT)	E3 (MC-PDFT)	E4 (MC-PDFT)
1.000	-7.95744127	-7.81472702	-7.72552071	-7.71221549
1.200	-8.02015297	-7.87494689	-7.78917515	-7.77500893
1.400	-8.04519783	-7.90594156	-7.82066617	-7.80664637
1.600	-8.0511522	-7.92188986	-7.8354154	-7.82237424
1.800	-8.0475488	-7.93029551	-7.84145718	-7.8297202
2.000	-8.03939977	-7.93491984	-7.84311314	-7.83303015
2.200	-8.02940668	-7.93780946	-7.84258602	-7.83644143
2.400	-8.01906606	-7.94002544	-7.84150611	-7.84035495
2.600	-8.00922629	-7.94205298	-7.84078731	-7.84473026
2.800	-8.00031757	-7.9440408	-7.84483336	-7.84627814
3.000	-7.99248995	-7.9459015	-7.85606524	-7.84269743
3.200	-7.98570897	-7.94706373	-7.86461411	-7.83983791
3.400	-7.97985226	-7.94710303	-7.87131543	-7.83856494
3.600	-7.97482818	-7.94554038	-7.87698722	-7.83763291
3.800	-7.97067371	-7.94250197	-7.88184561	-7.83704661
4.000	-7.9674402	-7.93848084	-7.88599837	-7.83680923
4.200	-7.96506236	-7.93410249	-7.88946658	-7.83668577
4.400	-7.96353521	-7.92984523	-7.89229002	-7.83661726
4.600	-7.96253704	-7.9259561	-7.89445677	-7.83660962
4.800	-7.96192025	-7.92246161	-7.89585927	-7.83664995
5.000	-7.96154067	-7.9193806	-7.89638599	-7.83669873
5.200	-7.96132608	-7.9165497	-7.89583412	-7.83693432
5.400	-7.96117533	-7.91386376	-7.89406673	-7.83696195
5.600	-7.96106609	-7.91132326	-7.89126718	-7.83711638
5.800	-7.96099921	-7.90899486	-7.8876841	-7.8372744
6.000	-7.96095298	-7.90699124	-7.88375755	-7.83744793
6.200	-7.96092005	-7.90541774	-7.87987746	-7.8375875
6.400	-7.96087315	-7.90420691	-7.87623737	-7.83772822

6.600	-7.96083179	-7.90336819	-7.87294322	-7.83785308
6.800	-7.96081801	-7.90279576	-7.869988	-7.83805869
7.000	-7.96085267	-7.9024414	-7.8673396	-7.83819343
7.200	-7.96090248	-7.90227566	-7.8649564	-7.83835635
7.400	-7.96097489	-7.90225785	-7.86279941	-7.83852712
7.600	-7.96103589	-7.90233056	-7.86083067	-7.83869437
7.800	-7.96107566	-7.90242648	-7.85901995	-7.83899142
8.000	-7.9611077	-7.90254014	-7.85736552	-7.8392197
8.200	-7.96113686	-7.90261081	-7.85586521	-7.83949855
8.400	-7.96116276	-7.90270994	-7.85451066	-7.83987179
8.600	-7.96119222	-7.90284175	-7.85331174	-7.84030261
8.800	-7.9612203	-7.90297907	-7.85228921	-7.8408747
9.000	-7.96123305	-7.90306886	-7.85147642	-7.8416368
9.200	-7.96122791	-7.90312642	-7.85090468	-7.84265308
9.400	-7.96119917	-7.90315676	-7.85061239	-7.84407805
9.600	-7.96117949	-7.90315863	-7.8506543	-7.84592552
9.800	-7.96117139	-7.90314327	-7.85097585	-7.84825716
10.000	-7.96118012	-7.90314636	-7.8512086	-7.850677
10.200	-7.96116204	-7.90320926	-7.85068241	-7.85243327
10.400	-7.9611743	-7.90329038	-7.84885747	-7.85223062
10.600	-7.96117894	-7.90340105	-7.84586502	-7.84998093
10.800	-7.96109825	-7.90351427	-7.84286521	-7.84685722
11.000	-7.96104805	-7.90355821	-7.84060395	-7.84379712
11.200	-7.96083029	-7.90356368	-7.83912651	-7.8412557
11.400	-7.96072226	-7.90351662	-7.83826298	-7.83922216
11.600	-7.96054737	-7.90344623	-7.83774236	-7.83760706
11.800	-7.96022869	-7.90336055	-7.83751809	-7.83624202
12.000	-7.95995023	-7.90327442	-7.83737626	-7.83516584
12.200	-7.95964184	-7.90322782	-7.83734006	-7.83415798
12.400	-7.95907603	-7.90319569	-7.83732139	-7.83341462
12.600	-7.958772	-7.90320822	-7.83735706	-7.83261416
12.800	-7.95791224	-7.90322646	-7.83738337	-7.83216079
13.000	-7.95742197	-7.90325217	-7.83741112	-7.83150029

$R_{\text{Li-H}}$ (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)	E3 (XMS-PDFT)	E4 (XMS-PDFT)
1.000	-7.95735253	-7.81056503	-7.72541853	-7.71473334
1.200	-8.01976750	-7.87090624	-7.78904939	-7.77784636
1.400	-8.04466574	-7.90157361	-7.82056362	-7.80936508
1.600	-8.05051657	-7.91713682	-7.83557407	-7.82468966

1.800	-8.04681637	-7.92491046	-7.84219496	-7.83152006
2.000	-8.03856404	-7.92888857	-7.84474126	-7.83408878
2.200	-8.02846154	-7.93095788	-7.84538311	-7.83521133
2.400	-8.01800990	-7.93206263	-7.84518721	-7.83706329
2.600	-8.00801383	-7.93257424	-7.84465534	-7.84001972
2.800	-7.99884464	-7.93272126	-7.84713043	-7.84140731
3.000	-7.99067004	-7.93241492	-7.85203447	-7.84087495
3.200	-7.98361873	-7.93158992	-7.85691970	-7.84016350
3.400	-7.97776580	-7.93020307	-7.86112462	-7.84001098
3.600	-7.97311328	-7.92823323	-7.86469954	-7.84022478
3.800	-7.96960977	-7.92568528	-7.86747995	-7.84131315
4.000	-7.96711947	-7.92266316	-7.87000760	-7.84307465
4.200	-7.96538787	-7.91948628	-7.87257092	-7.84399797
4.400	-7.96415951	-7.91645799	-7.87479438	-7.84385394
4.600	-7.96325028	-7.91369018	-7.87627174	-7.84329522
4.800	-7.96260702	-7.91119476	-7.87700037	-7.84277812
5.000	-7.96212464	-7.90906914	-7.87720789	-7.84233084
5.200	-7.96177435	-7.90732355	-7.87693473	-7.84207701
5.400	-7.96149418	-7.90591263	-7.87620850	-7.84174873
5.600	-7.96127174	-7.90482561	-7.87513226	-7.84153173
5.800	-7.96109087	-7.90399084	-7.87377645	-7.84130768
6.000	-7.96093693	-7.90336755	-7.87223301	-7.84117906
6.200	-7.96082967	-7.90293362	-7.87058102	-7.84104218
6.400	-7.96072318	-7.90258928	-7.86883969	-7.84085601
6.600	-7.96062110	-7.90232138	-7.86706048	-7.84069982
6.800	-7.96054784	-7.90216980	-7.86528934	-7.84058437
7.000	-7.96051828	-7.90205732	-7.86353585	-7.84046851
7.200	-7.96052619	-7.90211206	-7.86182186	-7.84036566
7.400	-7.96054863	-7.90223760	-7.86015048	-7.84025715
7.600	-7.96057626	-7.90239699	-7.85851846	-7.84014514
7.800	-7.96057833	-7.90254178	-7.85693713	-7.84010160
8.000	-7.96058750	-7.90267133	-7.85540353	-7.83997374
8.200	-7.96060498	-7.90278104	-7.85392752	-7.83983530
8.400	-7.96061026	-7.90289426	-7.85250782	-7.83970760
8.600	-7.96064766	-7.90297808	-7.85114446	-7.83956035
8.800	-7.96066924	-7.90311335	-7.84984239	-7.83941907
9.000	-7.96069359	-7.90321268	-7.84860031	-7.83930891
9.200	-7.96067818	-7.90325378	-7.84741836	-7.83916079
9.400	-7.96067667	-7.90323525	-7.84629119	-7.83900342
9.600	-7.96065485	-7.90325327	-7.84522803	-7.83882567
9.800	-7.96061750	-7.90322230	-7.84424188	-7.83865231

10.000	-7.96056292	-7.90321061	-7.84334721	-7.83846200
10.200	-7.96063744	-7.90327670	-7.84254796	-7.83821502
10.400	-7.96061314	-7.90335725	-7.84183586	-7.83786984
10.600	-7.96073262	-7.90346997	-7.84126961	-7.83747197
10.800	-7.96075706	-7.90357926	-7.84083492	-7.83699025
11.000	-7.96077367	-7.90361883	-7.84052780	-7.83644011
11.200	-7.96077042	-7.90361200	-7.84030566	-7.83583825
11.400	-7.96075484	-7.90355506	-7.84014077	-7.83520282
11.600	-7.96072003	-7.90347492	-7.84004808	-7.83457458
11.800	-7.96070043	-7.90337859	-7.84000178	-7.83391462
12.000	-7.96069192	-7.90329666	-7.84000358	-7.83333970
12.200	-7.96068863	-7.90324485	-7.83998384	-7.83270611
12.400	-7.96068064	-7.90323166	-7.83999436	-7.83222870
12.600	-7.96069258	-7.90324992	-7.84002913	-7.83163954
12.800	-7.96070517	-7.90328172	-7.84005581	-7.83132598
13.000	-7.96071110	-7.90331350	-7.84007022	-7.83079098

$R_{\text{Li-H}}$ (Å)	E1 (FMS-PDFT)	E2 (FMS-PDFT)	E3 (FMS-PDFT)	E4 (FMS-PDFT)
1.000	-7.95805738	-7.80812846	-7.72625514	-7.70999718
1.200	-8.02032986	-7.86866962	-7.78976193	-7.77287670
1.400	-8.04511057	-7.89969415	-7.82101692	-7.80449626
1.600	-8.05085485	-7.91548933	-7.83571883	-7.81993625
1.800	-8.04707201	-7.92356231	-7.84176966	-7.82731727
2.000	-8.03875787	-7.92768424	-7.84313444	-7.83120297
2.200	-8.02857112	-7.92981226	-7.84307837	-7.83341868
2.400	-8.01800835	-7.93104435	-7.84251753	-7.83631973
2.600	-8.00792198	-7.93183514	-7.84425370	-7.83796230
2.800	-7.99891790	-7.93284743	-7.84938033	-7.83722958
3.000	-7.99141702	-7.93397767	-7.85484040	-7.83667820
3.200	-7.98336011	-7.93015621	-7.86061376	-7.84138831
3.400	-7.97846241	-7.93044037	-7.86488802	-7.84013342
3.600	-7.97346041	-7.92776063	-7.86329806	-7.83703671
3.800	-7.96997859	-7.92554940	-7.86663716	-7.83647910
4.000	-7.96740936	-7.92286984	-7.86955012	-7.83626674
4.200	-7.96564953	-7.91994263	-7.87199825	-7.83617700
4.400	-7.96455965	-7.91693382	-7.87395163	-7.83616479
4.600	-7.96390798	-7.91392559	-7.87534705	-7.83623428
4.800	-7.96357768	-7.91102772	-7.87623121	-7.83636001
5.000	-7.96358243	-7.90842616	-7.87699366	-7.83539921

5.200	-7.96371240	-7.90576976	-7.87723707	-7.83551379
5.400	-7.96375894	-7.90309801	-7.87735865	-7.83557278
5.600	-7.96339826	-7.90052385	-7.87724696	-7.83563985
5.800	-7.96265283	-7.89828807	-7.87643645	-7.83578632
6.000	-7.96186253	-7.89650818	-7.87490050	-7.83592032
6.200	-7.96115118	-7.89512123	-7.87291061	-7.83607428
6.400	-7.96060379	-7.89409313	-7.87073866	-7.83619788
6.600	-7.96019784	-7.89334510	-7.86853450	-7.83623204
6.800	-7.95992983	-7.89283596	-7.86640431	-7.83636282
7.000	-7.95978899	-7.89252662	-7.86437068	-7.83642245
7.200	-7.95974622	-7.89236504	-7.86241740	-7.83650547
7.400	-7.95977762	-7.89231180	-7.86056812	-7.83653496
7.600	-7.95983494	-7.89230697	-7.85878806	-7.83656433
7.800	-7.95988869	-7.89231487	-7.85709304	-7.83666829
8.000	-7.95971219	-7.89210802	-7.85581118	-7.83710806
8.200	-7.95978796	-7.89216011	-7.85419310	-7.83706370
8.400	-7.95986436	-7.89222006	-7.85265347	-7.83701432
8.600	-7.95993933	-7.89227852	-7.85119425	-7.83693396
8.800	-7.96003708	-7.89236780	-7.84980861	-7.83685888
9.000	-7.96010459	-7.89242870	-7.84849775	-7.83680100
9.200	-7.96011715	-7.89243324	-7.84725042	-7.83671619
9.400	-7.96012068	-7.89243810	-7.84607287	-7.83661850
9.600	-7.96005552	-7.89236695	-7.84496665	-7.83651253
9.800	-7.96013153	-7.89244785	-7.84393376	-7.83639780
10.000	-7.96016647	-7.89248117	-7.84295798	-7.83627008
10.200	-7.96024107	-7.89255419	-7.84202765	-7.83603302
10.400	-7.96039559	-7.89270743	-7.84116057	-7.83568532
10.600	-7.96054366	-7.89285835	-7.84031566	-7.83538258
10.800	-7.96067549	-7.89299154	-7.83946532	-7.83512528
11.000	-7.96075503	-7.89307244	-7.83863446	-7.83487150
11.200	-7.96077997	-7.89309974	-7.83788972	-7.83459619
11.400	-7.96074821	-7.89307174	-7.83726391	-7.83429585
11.600	-7.96069545	-7.89302213	-7.83679492	-7.83395889
11.800	-7.96064474	-7.89297411	-7.83643856	-7.83352639
12.000	-7.96061344	-7.89294413	-7.83621707	-7.83309214
12.200	-7.96058811	-7.89291911	-7.83607475	-7.83256201
12.400	-7.96059316	-7.89292450	-7.83598139	-7.83213167
12.600	-7.96061315	-7.89294445	-7.83593934	-7.83159493
12.800	-7.96063539	-7.89296657	-7.83591468	-7.83130563
13.000	-7.96065423	-7.89298561	-7.83589133	-7.83079837

S4.3. HNCO

(1) τ(HNCO) = 180 deg

R_{N-C} (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.05702148	-168.03205758	-168.27226423	-168.24122972
1.300	-168.07064062	-168.04889065	-168.28521795	-168.25719708
1.350	-168.07837138	-168.05982210	-168.29240403	-168.26763201
1.400	-168.08176005	-168.06628881	-168.29532503	-168.27389495
1.450	-168.08200251	-168.06941004	-168.29514688	-168.27705036
1.500	-168.08003120	-168.07005122	-168.29277462	-168.27791432
1.550	-168.07656917	-168.06891731	-168.28892126	-168.27714420
1.600	-168.07217626	-168.06655602	-168.28414041	-168.27528242
1.650	-168.06729988	-168.06340362	-168.27886936	-168.27282495
1.700	-168.06229314	-168.05980110	-168.27345777	-168.27012935
1.750	-168.05743729	-168.05601237	-168.26818450	-168.26748487
1.800	-168.05295429	-168.05223985	-168.26498440	-168.26329085
1.850	-168.04900984	-168.04864345	-168.26268100	-168.25893382
1.900	-168.04571411	-168.04536597	-168.26056982	-168.25520057
1.950	-168.04311948	-168.04254965	-168.25873205	-168.25213825
2.000	-168.04122017	-168.04032883	-168.25716170	-168.24979074
2.050	-168.03996147	-168.03878464	-168.25592929	-168.24824515
2.100	-168.03925209	-168.03789919	-168.25509099	-168.24750260
2.150	-168.03898242	-168.03756654	-168.25460569	-168.24751235
2.200	-168.03904163	-168.03764380	-168.25440108	-168.24806428
2.250	-168.03932906	-168.03799316	-168.25440289	-168.24895190
2.300	-168.03975901	-168.03850384	-168.25454583	-168.25001428
2.350	-168.04026392	-168.03909358	-168.25477971	-168.25110121
2.400	-168.04079294	-168.03970315	-168.25505708	-168.25213037
2.450	-168.04131128	-168.04029643	-168.25534727	-168.25305866
2.500	-168.04179030	-168.04084560	-168.25562890	-168.25386348
2.550	-168.04221908	-168.04133825	-168.25589065	-168.25454709
2.600	-168.04258775	-168.04176561	-168.25612638	-168.25512199
2.650	-168.04289476	-168.04212712	-168.25633415	-168.25560204
2.700	-168.04314126	-168.04242412	-168.25651389	-168.25599259
2.750	-168.04333061	-168.04266062	-168.25666330	-168.25630146
2.800	-168.04346966	-168.04284363	-168.25678397	-168.25653954
2.850	-168.04356475	-168.04297969	-168.25687722	-168.25671888
2.900	-168.04362285	-168.04307573	-168.25694748	-168.25685019
2.950	-168.04365038	-168.04313796	-168.25699650	-168.25694258
3.000	-168.04365132	-168.04317086	-168.25702645	-168.25700296

(2) τ(HNCO) = 175 deg

R_{N-C} (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.05669187	-168.03221804	-168.27197056	-168.24144375
1.300	-168.07033048	-168.04898438	-168.28493324	-168.25732835
1.350	-168.07808165	-168.05987519	-168.29213329	-168.26771124
1.400	-168.08149121	-168.06631683	-168.29507155	-168.27394201
1.450	-168.08175454	-168.06942241	-168.29491236	-168.27707739
1.500	-168.07980395	-168.07005369	-168.29255942	-168.27792854
1.550	-168.07636237	-168.06891329	-168.28872571	-168.27714577
1.600	-168.07198975	-168.06654754	-168.28396423	-168.27528001
1.650	-168.06713359	-168.06339189	-168.27871374	-168.27282248
1.700	-168.06214739	-168.05978655	-168.27332430	-168.27011975
1.750	-168.05731289	-168.05599458	-168.26810617	-168.26743866
1.800	-168.05285329	-168.05221683	-168.26498636	-168.26317347
1.850	-168.04893402	-168.04861297	-168.26268051	-168.25884061
1.900	-168.04565133	-168.04533919	-168.26058366	-168.25512512
1.950	-168.04306348	-168.04253130	-168.25874782	-168.25207610
2.000	-168.04117368	-168.04031455	-168.25718141	-168.24974910
2.050	-168.03992429	-168.03877255	-168.25595657	-168.24820510
2.100	-168.03922272	-168.03788832	-168.25511427	-168.24747770
2.150	-168.03895954	-168.03755732	-168.25462335	-168.24749490
2.200	-168.03902368	-168.03763564	-168.25441494	-168.24806302
2.250	-168.03931487	-168.03798587	-168.25442105	-168.24895428
2.300	-168.03974765	-168.03849728	-168.25457110	-168.25002219
2.350	-168.04025438	-168.03908779	-168.25480284	-168.25110533
2.400	-168.04078526	-168.03969771	-168.25507651	-168.25213178
2.450	-168.04130303	-168.04029008	-168.25536489	-168.25306018
2.500	-168.04178466	-168.04084096	-168.25564601	-168.25387918
2.550	-168.04221412	-168.04133390	-168.25591092	-168.25458334
2.600	-168.04258331	-168.04176154	-168.25614973	-168.25516674
2.650	-168.04289075	-168.04212327	-168.25635766	-168.25563945
2.700	-168.04313762	-168.04242047	-168.25653568	-168.25601631
2.750	-168.04332751	-168.04265737	-168.25668095	-168.25631230
2.800	-168.04346669	-168.04284056	-168.25679471	-168.25654472
2.850	-168.04356214	-168.04297753	-168.25687972	-168.25672275
2.900	-168.04362078	-168.04307634	-168.25693684	-168.25685465
2.950	-168.04364930	-168.04314594	-168.25697057	-168.25695746
3.000	-168.04365650	-168.04323374	-168.25704441	-168.25701855

(3) τ(HNCO) = 170 deg

R_{N-C} (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.05570838	-168.03266150	-168.27109728	-168.24204197
1.300	-168.06940698	-168.04924359	-168.28408742	-168.25769653
1.350	-168.07721985	-168.06002053	-168.29132993	-168.26793416
1.400	-168.08069189	-168.06639146	-168.29431865	-168.27407292
1.450	-168.08101756	-168.06945260	-168.29421431	-168.27714845
1.500	-168.07912888	-168.07005569	-168.29191813	-168.27796029
1.550	-168.07574855	-168.06889661	-168.28814201	-168.27715088
1.600	-168.07143686	-168.06651777	-168.28344017	-168.27526495
1.650	-168.06664204	-168.06335183	-168.27825208	-168.27279925
1.700	-168.06171928	-168.05973627	-168.27293496	-168.27007157
1.750	-168.05695451	-168.05592895	-168.26793715	-168.26721792
1.800	-168.05258469	-168.05211583	-168.26499018	-168.26282880
1.850	-168.04876954	-168.04846082	-168.26266508	-168.25856550
1.900	-168.04550358	-168.04522031	-168.26058745	-168.25490007
1.950	-168.04290595	-168.04246788	-168.25874627	-168.25190240
2.000	-168.04103751	-168.04026995	-168.25717323	-168.24961291
2.050	-168.03981449	-168.03873587	-168.25595408	-168.24810400
2.100	-168.03913614	-168.03785677	-168.25511008	-168.24741389
2.150	-168.03889175	-168.03752974	-168.25462187	-168.24745661
2.200	-168.03897052	-168.03761129	-168.25442685	-168.24802325
2.250	-168.03927286	-168.03796419	-168.25444018	-168.24893751
2.300	-168.03971403	-168.03847782	-168.25459228	-168.25000526
2.350	-168.04022730	-168.03907003	-168.25482674	-168.25111317
2.400	-168.04076255	-168.03968167	-168.25510249	-168.25216602
2.450	-168.04128526	-168.04027673	-168.25539192	-168.25312373
2.500	-168.04176807	-168.04082733	-168.25567496	-168.25396006
2.550	-168.04219954	-168.04132115	-168.25593718	-168.25466373
2.600	-168.04257029	-168.04174960	-168.25617007	-168.25524122
2.650	-168.04287901	-168.04211200	-168.25637295	-168.25570528
2.700	-168.04312699	-168.04240979	-168.25654602	-168.25607227
2.750	-168.04331787	-168.04264734	-168.25669595	-168.25635296
2.800	-168.04345803	-168.04283157	-168.25681395	-168.25656723
2.850	-168.04355458	-168.04297103	-168.25689998	-168.25673382
2.900	-168.04361475	-168.04307697	-168.25696770	-168.25686578
2.950	-168.04364617	-168.04316557	-168.25704689	-168.25698941
3.000	-168.04366643	-168.04332748	-168.25713030	-168.25709150

(4) τ(HNCO) = 165 deg

R_{N-C} (Å)	E1 (XMS-	E2 (XMS-	E1 (XMS-	E2 (XMS-

	CASPT2)	CASPT2)	PDFT)	PDFT)
1.250	-168.05408815	-168.03328958	-168.26966298	-168.24291292
1.300	-168.06788795	-168.04960638	-168.28269996	-168.25823446
1.350	-168.07580403	-168.06021637	-168.29001304	-168.26825620
1.400	-168.07937980	-168.06648233	-168.29308341	-168.27425650
1.450	-168.07980906	-168.06947699	-168.29306886	-168.27724160
1.500	-168.07802348	-168.07003736	-168.29086643	-168.27799487
1.550	-168.07474597	-168.06884902	-168.28718575	-168.27714975
1.600	-168.07053794	-168.06644792	-168.28258252	-168.27522893
1.650	-168.06585088	-168.06326056	-168.27750127	-168.27273273
1.700	-168.06104917	-168.05961346	-168.27232302	-168.26995974
1.750	-168.05645270	-168.05572900	-168.26780649	-168.26670907
1.800	-168.05233306	-168.05175660	-168.26500150	-168.26227501
1.850	-168.04865310	-168.04805465	-168.26265401	-168.25811513
1.900	-168.04537940	-168.04490502	-168.26056554	-168.25453350
1.950	-168.04269566	-168.04231407	-168.25870802	-168.25161021
2.000	-168.04082282	-168.04018691	-168.25716350	-168.24939266
2.050	-168.03963661	-168.03867258	-168.25597088	-168.24795273
2.100	-168.03899485	-168.03780349	-168.25513429	-168.24730013
2.150	-168.03878083	-168.03748368	-168.25465259	-168.24739187
2.200	-168.03888327	-168.03757063	-168.25445190	-168.24799451
2.250	-168.03920377	-168.03792804	-168.25446281	-168.24891211
2.300	-168.03965860	-168.03844538	-168.25461591	-168.24998390
2.350	-168.04018211	-168.03904070	-168.25485117	-168.25110085
2.400	-168.04072511	-168.03965549	-168.25512764	-168.25218109
2.450	-168.04125188	-168.04025074	-168.25541655	-168.25315437
2.500	-168.04174046	-168.04080453	-168.25569801	-168.25399251
2.550	-168.04217521	-168.04129984	-168.25596109	-168.25469534
2.600	-168.04254853	-168.04172958	-168.25619555	-168.25527034
2.650	-168.04285935	-168.04209307	-168.25639672	-168.25572954
2.700	-168.04310914	-168.04239187	-168.25656196	-168.25608714
2.750	-168.04330168	-168.04263052	-168.25669302	-168.25634937
2.800	-168.04344346	-168.04281649	-168.25680144	-168.25655046
2.850	-168.04354182	-168.04295985	-168.25689020	-168.25671437
2.900	-168.04360447	-168.04307565	-168.25696950	-168.25684208
2.950	-168.04364038	-168.04318656	-168.25705530	-168.25697808
3.000	-168.04365312	-168.04327485	-168.25708611	-168.25705631

(5) τ(HNCO) = 160 deg

$R_{N\text{-}C}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)

1.250	-168.05188621	-168.03396619	-168.26771914	-168.24390600
1.300	-168.06582609	-168.04998016	-168.28082211	-168.25884191
1.350	-168.07388444	-168.06039505	-168.28823074	-168.26860834
1.400	-168.07760403	-168.06653662	-168.29141237	-168.27444328
1.450	-168.07817762	-168.06945094	-168.29151726	-168.27732166
1.500	-168.07653757	-168.06995725	-168.28944150	-168.27800501
1.550	-168.07340904	-168.06872695	-168.28589314	-168.27711123
1.600	-168.06935918	-168.06628398	-168.28142972	-168.27514842
1.650	-168.06485833	-168.06303272	-168.27651114	-168.27259868
1.700	-168.06032840	-168.05923983	-168.27159618	-168.26967597
1.750	-168.05611182	-168.05510359	-168.26772220	-168.26590997
1.800	-168.05220071	-168.05104930	-168.26499927	-168.26153300
1.850	-168.04855862	-168.04743198	-168.26261148	-168.25750595
1.900	-168.04527902	-168.04440300	-168.26051591	-168.25403840
1.950	-168.04252409	-168.04198727	-168.25867717	-168.25120769
2.000	-168.04056158	-168.04004094	-168.25715859	-168.24909549
2.050	-168.03940118	-168.03857826	-168.25597899	-168.24773670
2.100	-168.03880478	-168.03772771	-168.25516272	-168.24715627
2.150	-168.03863068	-168.03741906	-168.25468458	-168.24731404
2.200	-168.03876496	-168.03751424	-168.25448418	-168.24797001
2.250	-168.03910994	-168.03787814	-168.25449184	-168.24891987
2.300	-168.03958326	-168.03840076	-168.25464100	-168.25000344
2.350	-168.04012064	-168.03900048	-168.25487394	-168.25111007
2.400	-168.04067380	-168.03961828	-168.25515003	-168.25217205
2.450	-168.04120911	-168.04021763	-168.25544012	-168.25313144
2.500	-168.04170293	-168.04077345	-168.25572176	-168.25396941
2.550	-168.04214217	-168.04127084	-168.25598326	-168.25467615
2.600	-168.04251899	-168.04170237	-168.25621850	-168.25525438
2.650	-168.04283269	-168.04206737	-168.25641645	-168.25572108
2.700	-168.04308498	-168.04236759	-168.25657215	-168.25608301
2.750	-168.04327977	-168.04260780	-168.25668504	-168.25634478
2.800	-168.04342379	-168.04279619	-168.25676316	-168.25652649
2.850	-168.04352460	-168.04294458	-168.25683161	-168.25669090
2.900	-168.04359052	-168.04307124	-168.25691914	-168.25685310
2.950	-168.04363185	-168.04320055	-168.25700068	-168.25697862
3.000	-168.04365272	-168.04330809	-168.25715672	-168.25713606

(6) τ(HNCO) = 155 deg

$R_{N\text{-}C}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.04919976	-168.03453023	-168.26535062	-168.24485173

1.300	-168.06331436	-168.05023643	-168.27853893	-168.25938999
1.350	-168.07155271	-168.06044907	-168.28606041	-168.26889088
1.400	-168.07545738	-168.06645760	-168.28937370	-168.27455530
1.450	-168.07622183	-168.06927976	-168.28962391	-168.27732517
1.500	-168.07478325	-168.06971212	-168.28770535	-168.27793542
1.550	-168.07188016	-168.06839993	-168.28432669	-168.27698184
1.600	-168.06811199	-168.06582842	-168.28005549	-168.27496498
1.650	-168.06401145	-168.06233619	-168.27539492	-168.27229642
1.700	-168.05993583	-168.05825235	-168.27099369	-168.26900935
1.750	-168.05594834	-168.05405162	-168.26765150	-168.26487447
1.800	-168.05208719	-168.05010940	-168.26495931	-168.26061985
1.850	-168.04845286	-168.04664069	-168.26255729	-168.25675039
1.900	-168.04516984	-168.04375978	-168.26045855	-168.25342493
1.950	-168.04238909	-168.04150056	-168.25862867	-168.25071663
2.000	-168.04031749	-168.03977742	-168.25711693	-168.24871592
2.050	-168.03912660	-168.03844183	-168.25594293	-168.24746997
2.100	-168.03857380	-168.03762711	-168.25512466	-168.24700800
2.150	-168.03844606	-168.03733552	-168.25464744	-168.24724946
2.200	-168.03861863	-168.03744206	-168.25444989	-168.24795786
2.250	-168.03899337	-168.03781455	-168.25446203	-168.24892983
2.300	-168.03948928	-168.03834401	-168.25461455	-168.25001202
2.350	-168.04004372	-168.03894930	-168.25485144	-168.25112678
2.400	-168.04060963	-168.03957187	-168.25513181	-168.25219122
2.450	-168.04115479	-168.04017543	-168.25542846	-168.25314962
2.500	-168.04165538	-168.04073380	-168.25572225	-168.25397480
2.550	-168.04210016	-168.04123377	-168.25599345	-168.25467313
2.600	-168.04248133	-168.04166752	-168.25623223	-168.25525520
2.650	-168.04279858	-168.04203443	-168.25643078	-168.25572195
2.700	-168.04305399	-168.04233648	-168.25657913	-168.25608018
2.750	-168.04325161	-168.04257872	-168.25666612	-168.25634001
2.800	-168.04339843	-168.04277024	-168.25672212	-168.25652677
2.850	-168.04350230	-168.04292451	-168.25678015	-168.25668047
2.900	-168.04357221	-168.04306187	-168.25689444	-168.25683145
2.950	-168.04361917	-168.04320312	-168.25704145	-168.25702102
3.000	-168.04366399	-168.04338594	-168.25717000	-168.25710794

(7) τ(HNCO) = 150 deg

$R_{N\text{-}C}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.04619760	-168.03477560	-168.26269611	-168.24556312
1.300	-168.06052210	-168.05018153	-168.27598170	-168.25972164

1.350	-168.06898548	-168.06018865	-168.28362369	-168.26897201
1.400	-168.07313441	-168.06604630	-168.28707992	-168.27447738
1.450	-168.07417111	-168.06873580	-168.28749380	-168.27714600
1.500	-168.07305391	-168.06901442	-168.28576307	-168.27768185
1.550	-168.07055827	-168.06747773	-168.28260339	-168.27665120
1.600	-168.06728489	-168.06460360	-168.27861762	-168.27452460
1.650	-168.06361794	-168.06087578	-168.27440699	-168.27157897
1.700	-168.05974586	-168.05678997	-168.27065844	-168.26783142
1.750	-168.05581304	-168.05273642	-168.26757049	-168.26363118
1.800	-168.05196217	-168.04898174	-168.26488720	-168.25954926
1.850	-168.04832782	-168.04570100	-168.26247159	-168.25586196
1.900	-168.04504270	-168.04299607	-168.26036459	-168.25270447
1.950	-168.04225339	-168.04090121	-168.25855267	-168.25014896
2.000	-168.04012611	-168.03936968	-168.25705234	-168.24828398
2.050	-168.03884476	-168.03823826	-168.25586980	-168.24715648
2.100	-168.03831255	-168.03749682	-168.25505947	-168.24682413
2.150	-168.03823259	-168.03723224	-168.25459518	-168.24715646
2.200	-168.03844804	-168.03735441	-168.25440938	-168.24795512
2.250	-168.03885687	-168.03773801	-168.25443150	-168.24897366
2.300	-168.03937889	-168.03827604	-168.25459243	-168.25008670
2.350	-168.03995309	-168.03888824	-168.25483546	-168.25119775
2.400	-168.04053380	-168.03951639	-168.25511967	-168.25223168
2.450	-168.04108997	-168.04012436	-168.25541678	-168.25316391
2.500	-168.04159921	-168.04068673	-168.25570122	-168.25398296
2.550	-168.04205046	-168.04118990	-168.25595853	-168.25467569
2.600	-168.04243682	-168.04162625	-168.25619254	-168.25523827
2.650	-168.04275831	-168.04199545	-168.25638930	-168.25569101
2.700	-168.04301739	-168.04229976	-168.25653584	-168.25605423
2.750	-168.04321838	-168.04254456	-168.25663494	-168.25630785
2.800	-168.04336850	-168.04273989	-168.25668947	-168.25647331
2.850	-168.04347600	-168.04290068	-168.25673888	-168.25661229
2.900	-168.04355041	-168.04304784	-168.25690292	-168.25684087
2.950	-168.04360263	-168.04319477	-168.25708795	-168.25704829
3.000	-168.04363594	-168.04331539	-168.25716104	-168.25712271

$R_{N\text{-}C}$ (Å)	E1 (MC-PDFT)	E2 (MC-PDFT)	E1 (FMS-PDFT)	E2 (FMS-PDFT)
1.250	-168.26280465	-168.24562064	-168.26091730	-168.24616132
1.300	-168.27633323	-168.25999616	-168.27466340	-168.26025639
1.350	-168.28412472	-168.26947328	-168.28265075	-168.26944819
1.400	-168.28768180	-168.27520171	-168.28640233	-168.27484386

1.450	-168.28818472	-168.27806926	-168.28700955	-168.27742685
1.500	-168.28655553	-168.27874801	-168.28543064	-168.27787125
1.550	-168.28351243	-168.27776362	-168.28240024	-168.27675447
1.600	-168.27959695	-168.27556098	-168.27853123	-168.27451594
1.650	-168.27516326	-168.27259310	-168.27445657	-168.27144043
1.700	-168.27041856	-168.26936051	-168.27089242	-168.26755052
1.750	-168.26639178	-168.26551893	-168.26777196	-168.26330775
1.800	-168.26389568	-168.26081885	-168.26446595	-168.25974090
1.850	-168.26180848	-168.25665083	-168.26156002	-168.25615735
1.900	-168.25994938	-168.25323479	-168.25844165	-168.25349180
1.950	-168.25816397	-168.25053789	-168.25564122	-168.25144329
2.000	-168.25664768	-168.24859065	-168.25393787	-168.24978762
2.050	-168.25550575	-168.24739628	-168.25316859	-168.24849702
2.100	-168.25475972	-168.24696021	-168.25269684	-168.24805703
2.150	-168.25435027	-168.24722925	-168.25239936	-168.24840632
2.200	-168.25420632	-168.24797012	-168.25265460	-168.24887648
2.250	-168.25425998	-168.24896213	-168.25289590	-168.24980211
2.300	-168.25444775	-168.25006518	-168.25328081	-168.25079850
2.350	-168.25471342	-168.25117393	-168.25356625	-168.25193891
2.400	-168.25501700	-168.25222123	-168.25408476	-168.25278052
2.450	-168.25533038	-168.25315628	-168.25457662	-168.25354320
2.500	-168.25563413	-168.25396809	-168.25502430	-168.25421556
2.550	-168.25591620	-168.25465452	-168.25541842	-168.25478975
2.600	-168.25616946	-168.25522474	-168.25575742	-168.25527110
2.650	-168.25638949	-168.25569097	-168.25604338	-168.25566892
2.700	-168.25657739	-168.25606737	-168.25627990	-168.25599343
2.750	-168.25673037	-168.25636335	-168.25648965	-168.25620506
2.800	-168.25684930	-168.25659045	-168.25673800	-168.25652990
2.850	-168.25692878	-168.25675423	-168.25689670	-168.25675447
2.900	-168.25696300	-168.25685453	-168.25706695	-168.25696455
2.950	-168.25695855	-168.25688687	-168.25710908	-168.25702211

(8) τ(HNCO) = 145 deg

$R_{N\text{-}C}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.04327077	-168.03432110	-168.26004314	-168.24575980
1.300	-168.05783848	-168.04943351	-168.27341300	-168.25958280
1.350	-168.06659241	-168.05921361	-168.28115991	-168.26862384
1.400	-168.07108789	-168.06486343	-168.28475231	-168.27400299
1.450	-168.07253688	-168.06732459	-168.28534208	-168.27658714
1.500	-168.07189070	-168.06734298	-168.28383916	-168.27703788

1.550	-168.06985910	-168.06556675	-168.28098654	-168.27588189
1.600	-168.06691818	-168.06259294	-168.27743979	-168.27351897
1.650	-168.06340859	-168.05894546	-168.27380318	-168.27021174
1.700	-168.05958854	-168.05504781	-168.27048090	-168.26629015
1.750	-168.05566783	-168.05122095	-168.26749650	-168.26221489
1.800	-168.05181721	-168.04769736	-168.26477169	-168.25834087
1.850	-168.04818121	-168.04463682	-168.26234553	-168.25486441
1.900	-168.04489513	-168.04213279	-168.26021564	-168.25189799
1.950	-168.04210395	-168.04021748	-168.25842664	-168.24952856
2.000	-168.03995737	-168.03885927	-168.25694333	-168.24781323
2.050	-168.03859480	-168.03793842	-168.25576696	-168.24682987
2.100	-168.03803728	-168.03732798	-168.25494614	-168.24662502
2.150	-168.03799730	-168.03710752	-168.25447550	-168.24704521
2.200	-168.03825710	-168.03725101	-168.25428830	-168.24790755
2.250	-168.03870273	-168.03764846	-168.25431116	-168.24897972
2.300	-168.03925339	-168.03819673	-168.25447396	-168.25013636
2.350	-168.03984963	-168.03881711	-168.25472104	-168.25126732
2.400	-168.04044650	-168.03945156	-168.25501022	-168.25231374
2.450	-168.04101498	-168.04006455	-168.25531478	-168.25324232
2.500	-168.04153378	-168.04063146	-168.25561491	-168.25404019
2.550	-168.04199185	-168.04113751	-168.25589226	-168.25470551
2.600	-168.04238448	-168.04157752	-168.25613534	-168.25524537
2.650	-168.04271072	-168.04194936	-168.25633266	-168.25567888
2.700	-168.04297295	-168.04225527	-168.25650767	-168.25601111
2.750	-168.04317882	-168.04250422	-168.25663441	-168.25626721
2.800	-168.04333275	-168.04270405	-168.25672753	-168.25643234
2.850	-168.04344438	-168.04287183	-168.25679435	-168.25659891
2.900	-168.04352369	-168.04302745	-168.25693055	-168.25686050
2.950	-168.04358075	-168.04317626	-168.25706425	-168.25702908
3.000	-168.04361780	-168.04329471	-168.25710009	-168.25706897

(9) τ(HNCO) = 140 deg

$R_{N\text{-}C}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.04110023	-168.03256657	-168.25790063	-168.24500107
1.300	-168.05587683	-168.04743971	-168.27127570	-168.25859202
1.350	-168.06494030	-168.05700879	-168.27906323	-168.26750085
1.400	-168.06980997	-168.06246484	-168.28275542	-168.27281105
1.450	-168.07164704	-168.06476469	-168.28352429	-168.27533373
1.500	-168.07133282	-168.06470336	-168.28229824	-168.27568187
1.550	-168.06952363	-168.06296961	-168.27983359	-168.27435252

1.600	-168.06669705	-168.06015372	-168.27674150	-168.27176523
1.650	-168.06323287	-168.05673722	-168.27348196	-168.26834189
1.700	-168.05942550	-168.05310417	-168.27036099	-168.26451877
1.750	-168.05550504	-168.04954939	-168.26740846	-168.26066138
1.800	-168.05165181	-168.04629051	-168.26466523	-168.25703290
1.850	-168.04801373	-168.04347586	-168.26222949	-168.25378427
1.900	-168.04472787	-168.04119398	-168.26009043	-168.25103979
1.950	-168.04193828	-168.03947215	-168.25830198	-168.24886042
2.000	-168.03978832	-168.03828627	-168.25679945	-168.24732068
2.050	-168.03838479	-168.03754770	-168.25561943	-168.24650255
2.100	-168.03777061	-168.03710904	-168.25480298	-168.24642416
2.150	-168.03775061	-168.03696009	-168.25433576	-168.24691471
2.200	-168.03805224	-168.03713317	-168.25415124	-168.24780760
2.250	-168.03853572	-168.03754789	-168.25417716	-168.24888668
2.300	-168.03911619	-168.03810813	-168.25434396	-168.25005201
2.350	-168.03973604	-168.03873796	-168.25459307	-168.25119438
2.400	-168.04035063	-168.03937967	-168.25488203	-168.25225568
2.450	-168.04093255	-168.03999853	-168.25518380	-168.25320305
2.500	-168.04146165	-168.04057030	-168.25548473	-168.25402201
2.550	-168.04192768	-168.04108034	-168.25577145	-168.25471306
2.600	-168.04232665	-168.04152366	-168.25602773	-168.25527876
2.650	-168.04265815	-168.04189847	-168.25624053	-168.25572029
2.700	-168.04292496	-168.04220743	-168.25641101	-168.25603132
2.750	-168.04313509	-168.04246001	-168.25660160	-168.25625140
2.800	-168.04329322	-168.04266496	-168.25675760	-168.25647056
2.850	-168.04340936	-168.04283990	-168.25683217	-168.25663944
2.900	-168.04349376	-168.04300251	-168.25695584	-168.25683113
2.950	-168.04355521	-168.04315130	-168.25699810	-168.25695095
3.000	-168.04360364	-168.04329753	-168.25701977	-168.25696331

(10) τ(HNCO) = 135 deg

R_{N-C} (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.03995795	-168.02936021	-168.25677137	-168.24288246
1.300	-168.05479656	-168.04412482	-168.27001129	-168.25639972
1.350	-168.06404398	-168.05362399	-168.27772040	-168.26529541
1.400	-168.06913877	-168.05906682	-168.28142722	-168.27062705
1.450	-168.07117918	-168.06142802	-168.28233000	-168.27315033
1.500	-168.07101124	-168.06151231	-168.28134796	-168.27345467
1.550	-168.06928691	-168.05999760	-168.27918561	-168.27206551
1.600	-168.06650018	-168.05745232	-168.27635282	-168.26948182

1.650	-168.06304997	-168.05433556	-168.27327926	-168.26619107
1.700	-168.05924438	-168.05101259	-168.27023078	-168.26259443
1.750	-168.05532138	-168.04776391	-168.26728370	-168.25901015
1.800	-168.05146523	-168.04479609	-168.26453981	-168.25565039
1.850	-168.04782566	-168.04224889	-168.26211638	-168.25266714
1.900	-168.04454159	-168.04020351	-168.26002137	-168.25014789
1.950	-168.04175668	-168.03868610	-168.25821405	-168.24818053
2.000	-168.03961069	-168.03767515	-168.25670239	-168.24684107
2.050	-168.03819403	-168.03709977	-168.25552320	-168.24618169
2.100	-168.03752930	-168.03683318	-168.25470909	-168.24619181
2.150	-168.03750240	-168.03678720	-168.25424206	-168.24673297
2.200	-168.03783835	-168.03700113	-168.25406005	-168.24764732
2.250	-168.03835870	-168.03743697	-168.25409240	-168.24874470
2.300	-168.03896989	-168.03801114	-168.25426744	-168.24990736
2.350	-168.03961256	-168.03864964	-168.25452739	-168.25104943
2.400	-168.04024669	-168.03930086	-168.25482874	-168.25211529
2.450	-168.04084271	-168.03992603	-168.25513933	-168.25306911
2.500	-168.04138262	-168.04050301	-168.25543326	-168.25389466
2.550	-168.04185709	-168.04101731	-168.25569444	-168.25460218
2.600	-168.04226279	-168.04146419	-168.25593713	-168.25520249
2.650	-168.04259991	-168.04184223	-168.25618427	-168.25568589
2.700	-168.04287163	-168.04215458	-168.25639232	-168.25604000
2.750	-168.04308522	-168.04241041	-168.25654970	-168.25626227
2.800	-168.04324906	-168.04262192	-168.25671771	-168.25647431
2.850	-168.04337005	-168.04280407	-168.25677043	-168.25661839
2.900	-168.04345958	-168.04297236	-168.25686497	-168.25677831
2.950	-168.04352512	-168.04312032	-168.25696137	-168.25687776
3.000	-168.04357436	-168.04325750	-168.25698021	-168.25694912

(11) τ(HNCO) = 130 deg

$R_{N\text{-}C}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
1.250	-168.03937651	-168.02534017	-168.25663156	-168.23956559
1.300	-168.05417834	-168.04002114	-168.26968055	-168.25306505
1.350	-168.06349582	-168.04954573	-168.27718428	-168.26205041
1.400	-168.06870232	-168.05510398	-168.28077034	-168.26751846
1.450	-168.07084464	-168.05765681	-168.28168705	-168.27016305
1.500	-168.07074825	-168.05799582	-168.28082292	-168.27056728
1.550	-168.06906382	-168.05678207	-168.27880883	-168.26930073
1.600	-168.06629442	-168.05456666	-168.27608980	-168.26690510
1.650	-168.06284906	-168.05179405	-168.27310859	-168.26387213

1.700	-168.05904255	-168.04881578	-168.27009187	-168.26057090
1.750	-168.05511686	-168.04590051	-168.26713898	-168.25729302
1.800	-168.05125825	-168.04324411	-168.26442373	-168.25423111
1.850	-168.04761832	-168.04097928	-168.26204151	-168.25151655
1.900	-168.04433734	-168.03918170	-168.25995032	-168.24924711
1.950	-168.04155927	-168.03787550	-168.25810378	-168.24750030
2.000	-168.03942207	-168.03704191	-168.25651751	-168.24635647
2.050	-168.03800593	-168.03662039	-168.25527581	-168.24586501
2.100	-168.03731315	-168.03650815	-168.25444224	-168.24599358
2.150	-168.03726185	-168.03658641	-168.25398839	-168.24658104
2.200	-168.03762034	-168.03685561	-168.25382889	-168.24752564
2.250	-168.03817491	-168.03731732	-168.25388102	-168.24865419
2.300	-168.03881657	-168.03790735	-168.25407128	-168.24985102
2.350	-168.03948381	-168.03855761	-168.25434615	-168.25101393
2.400	-168.04013659	-168.03921711	-168.25466488	-168.25209005
2.450	-168.04074697	-168.03984921	-168.25499867	-168.25304085
2.500	-168.04129889	-168.04043140	-168.25533498	-168.25386274
2.550	-168.04178223	-168.04095102	-168.25566275	-168.25455704
2.600	-168.04219454	-168.04140081	-168.25596516	-168.25514043
2.650	-168.04253761	-168.04178238	-168.25622572	-168.25561107
2.700	-168.04281456	-168.04209846	-168.25643294	-168.25598246
2.750	-168.04303306	-168.04235914	-168.25659198	-168.25626762
2.800	-168.04320172	-168.04257656	-168.25667675	-168.25646928
2.850	-168.04332780	-168.04276583	-168.25667882	-168.25657367
2.900	-168.04342244	-168.04293871	-168.25675273	-168.25670113
2.950	-168.04349164	-168.04308494	-168.25691895	-168.25684349
3.000	-168.04354047	-168.04320863	-168.25703447	-168.25692902

S4.4. Methylamine

(1) Eclipsed-H3 path

$R_{N\text{-}H}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (MC-PDFT)	E2 (MC-PDFT)
0.602	-95.14952539	-94.95053699	-95.30222739	-95.09564919
0.702	-95.38122353	-95.18588867	-95.53265179	-95.32990009
0.802	-95.49284820	-95.30135140	-95.64405638	-95.44532499
0.902	-95.53944194	-95.35231655	-95.69116489	-95.49698250
1.002	-95.55062431	-95.36896428	-95.70330175	-95.51482019
1.102	-95.54281982	-95.36886983	-95.69881008	-95.51268238
1.202	-95.52521611	-95.36326895	-95.68401290	-95.51007383
1.302	-95.50260270	-95.35880559	-95.66481298	-95.50895192
1.402	-95.48184183	-95.35636271	-95.64333341	-95.50876417

1.502	-95.45946915	-95.35880512	-95.62100990	-95.50744611
1.602	-95.43888968	-95.36344836	-95.59587821	-95.50898501
1.702	-95.42040405	-95.36825284	-95.57715911	-95.51325047
1.802	-95.40416305	-95.37256521	-95.56029301	-95.51715858
1.902	-95.39019932	-95.37624482	-95.54541484	-95.52057018
2.002	-95.37813808	-95.37810167	-95.53255079	-95.52345341
2.102	-95.38068719	-95.36852444	-95.52582977	-95.52167061
2.202	-95.38272056	-95.36078640	-95.52775001	-95.51267713
2.302	-95.38432248	-95.35464790	-95.52927465	-95.50540196
2.402	-95.38557136	-95.34985845	-95.53047424	-95.49964552
2.502	-95.38653613	-95.34617558	-95.53140914	-95.49519643
2.602	-95.38727590	-95.34337833	-95.53213235	-95.49180714
2.702	-95.38784024	-95.34127528	-95.53269797	-95.48927699
2.802	-95.38826965	-95.33970710	-95.53313887	-95.48741864
2.902	-95.38859622	-95.33854530	-95.53348650	-95.48607354
3.002	-95.38884458	-95.33768863	-95.53376420	-95.48511120
3.102	-95.38903331	-95.33705887	-95.53398531	-95.48443557
3.202	-95.38917626	-95.33659647	-95.53416234	-95.48396609
3.302	-95.38928386	-95.33625674	-95.53430487	-95.48364371
3.402	-95.38936411	-95.33600664	-95.53441926	-95.48342567
3.502	-95.38942328	-95.33582192	-95.53451025	-95.48328286
3.602	-95.38946633	-95.33568497	-95.53458293	-95.48318933
4.602	-95.38956080	-95.33529921	-95.53476491	-95.48303817
5.602	-95.38954952	-95.33526716	-95.53476399	-95.48305288
7.602	-95.38953741	-95.33525593	-95.53476067	-95.48305559

$R_{N\text{-}H}$ (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
0.602	-95.30222741	-95.09564912
0.702	-95.53265180	-95.32990009
0.802	-95.64405638	-95.44532499
0.902	-95.69116489	-95.49698250
1.002	-95.70330175	-95.51482019
1.102	-95.69881011	-95.51268254
1.202	-95.68401290	-95.51007383
1.302	-95.66481298	-95.50895192
1.402	-95.64333341	-95.50876417
1.502	-95.62100992	-95.50744608
1.602	-95.59587821	-95.50898501
1.702	-95.57715911	-95.51325047

1.802	-95.56029301	-95.51715858
1.902	-95.54541484	-95.52057018
2.002	-95.53255079	-95.52345341
2.102	-95.52583150	-95.52167051
2.202	-95.52775001	-95.51267713
2.302	-95.52927464	-95.50540197
2.402	-95.53047423	-95.49964552
2.502	-95.53140913	-95.49519643
2.602	-95.53213235	-95.49180714
2.702	-95.53269797	-95.48927699
2.802	-95.53313887	-95.48741864
2.902	-95.53348650	-95.48607354
3.002	-95.53376420	-95.48511119
3.102	-95.53398531	-95.48443557
3.202	-95.53416234	-95.48396609
3.302	-95.53430487	-95.48364371
3.402	-95.53441926	-95.48342567
3.502	-95.53451025	-95.48328286
3.602	-95.53458293	-95.48318933
4.602	-95.53476491	-95.48303817
5.602	-95.53476399	-95.48305288
7.602	-95.53476067	-95.48305559

(2) Staggered conformation

$R_{N\text{-}H}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (MC-PDFT)	E2 (MC-PDFT)
0.616	-95.18280783	-94.98380007	-95.33867873	-95.13391203
0.716	-95.39262409	-95.19761416	-95.54743304	-95.34697320
0.816	-95.49227946	-95.30162737	-95.64697924	-95.45126622
0.916	-95.53213950	-95.34662454	-95.68699633	-95.49648934
1.016	-95.53947447	-95.36064847	-95.69661707	-95.50932228
1.116	-95.52945970	-95.36045045	-95.68882379	-95.51159411
1.216	-95.51055551	-95.35672757	-95.67287464	-95.50997731
1.316	-95.48949636	-95.35297185	-95.64787676	-95.50356065
1.416	-95.46646566	-95.35482799	-95.62596102	-95.50414174
1.516	-95.44421049	-95.35944299	-95.60459156	-95.50820997
1.616	-95.42385965	-95.36497728	-95.58439402	-95.51294953
1.716	-95.40578189	-95.37006872	-95.56587347	-95.51747058
1.816	-95.38979014	-95.37268916	-95.54930250	-95.52134436
1.916	-95.38045033	-95.37255550	-95.53496005	-95.52371633
2.016	-95.38160273	-95.36344830	-95.52926222	-95.51994338

2.116	-95.38385862	-95.35466396	-95.53140354	-95.51087702
2.216	-95.38578484	-95.34749995	-95.53325838	-95.50250238
2.316	-95.38732778	-95.34184384	-95.53475332	-95.49568718
2.416	-95.38853596	-95.33746689	-95.53593655	-95.49032452
2.516	-95.38946900	-95.33413187	-95.53686060	-95.48621320
2.616	-95.39018229	-95.33162176	-95.53757949	-95.48311583
2.716	-95.39072354	-95.32975061	-95.53814053	-95.48083297
2.816	-95.39113212	-95.32836600	-95.53858124	-95.47917503
2.916	-95.39143943	-95.32734697	-95.53892883	-95.47798304
3.016	-95.39166983	-95.32659966	-95.53920494	-95.47714485
3.116	-95.39184184	-95.32605265	-95.53942322	-95.47655992
3.216	-95.39196944	-95.32565228	-95.53959431	-95.47615895
3.316	-95.39206327	-95.32535879	-95.53972943	-95.47588340
3.416	-95.39213145	-95.32514301	-95.53983565	-95.47569875
3.516	-95.39218033	-95.32498375	-95.53992017	-95.47557796
3.616	-95.39221482	-95.32486571	-95.53998723	-95.47549971
4.116	-95.39227753	-95.32459828	-95.54013840	-95.47538612
5.116	-95.39227413	-95.32451097	-95.54015439	-95.47537920
7.116	-95.39225728	-95.32449164	-95.54016355	-95.47540053

$R_{\text{N-H}}$ (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)	E1 (FMS-PDFT)	E2 (FMS-PDFT)
0.616	-95.33867858	-95.13390943	-95.33867918	-95.13390286
0.716	-95.54743379	-95.34696913	-95.54743307	-95.34696691
0.816	-95.64697983	-95.45126220	-95.64697794	-95.45125978
0.916	-95.68699680	-95.49648863	-95.68699398	-95.49643108
1.016	-95.69661854	-95.50930975	-95.69661916	-95.50930784
1.116	-95.68882555	-95.51158282	-95.68882777	-95.51157749
1.216	-95.67288158	-95.50995954	-95.67288461	-95.50995529
1.316	-95.64818428	-95.50317723	-95.64858981	-95.50273263
1.416	-95.62602300	-95.50409709	-95.62587605	-95.50421735
1.516	-95.60466260	-95.50817382	-95.60442677	-95.50825854
1.616	-95.58450038	-95.51291171	-95.58409473	-95.51282758
1.716	-95.56605876	-95.51742757	-95.56525371	-95.51720723
1.816	-95.54969320	-95.52130224	-95.54855648	-95.52086386
1.916	-95.53613663	-95.52380639	-95.53469865	-95.52324921
2.016	-95.53057683	-95.51976121	-95.52834073	-95.51973832
2.116	-95.53172927	-95.51036728	-95.52912908	-95.51067244
2.216	-95.53248222	-95.50198770	-95.53025279	-95.50280296
2.316	-95.53400215	-95.49612777	-95.53118461	-95.49651746

2.416	-95.53593118	-95.49033304	-95.53192988	-95.49163151
2.516	-95.53693728	-95.48613102	-95.53252637	-95.48790659
2.616	-95.53767768	-95.48299700	-95.53301724	-95.48511222
2.716	-95.53824847	-95.48069259	-95.53342793	-95.48304629
2.816	-95.53869360	-95.47902272	-95.53376329	-95.48154987
2.916	-95.53904364	-95.47782351	-95.53404803	-95.48047074
3.016	-95.53932145	-95.47698032	-95.53428850	-95.47970165
3.116	-95.53954092	-95.47639113	-95.53449125	-95.47915914
3.216	-95.53971331	-95.47598691	-95.53466124	-95.47877896
3.316	-95.53984933	-95.47570892	-95.53479936	-95.47851375
3.416	-95.53995622	-95.47552332	-95.53490921	-95.47833249
3.516	-95.54004116	-95.47540117	-95.53499972	-95.47820983
3.616	-95.54010852	-95.47532160	-95.53507325	-95.47812838
4.116	-95.54025984	-95.47520623	-95.53525569	-95.47798322
5.116	-95.54027611	-95.47519899	-95.53529622	-95.47794477
7.116	-95.54028533	-95.47521997	-95.53531241	-95.47795777

(3) 95º

$R_{N\text{-}H}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (MC-PDFT)	E2 (MC-PDFT)
0.616	-95.18312897	-94.98369492	-95.33761039	-95.12504382
0.716	-95.39294446	-95.19750643	-95.54639691	-95.33819063
0.816	-95.49259731	-95.30150964	-95.64597841	-95.44258500
0.916	-95.53246135	-95.34649319	-95.68642291	-95.48882478
1.016	-95.53980943	-95.36049659	-95.69469620	-95.50484851
1.116	-95.52981716	-95.36026608	-95.68560710	-95.50711952
1.216	-95.51094127	-95.35649116	-95.66742427	-95.50550099
1.316	-95.48966786	-95.35235253	-95.65064444	-95.50574377
1.416	-95.46529190	-95.35074266	-95.62349969	-95.50024849
1.516	-95.44365257	-95.35638860	-95.60209383	-95.50432364
1.616	-95.42364902	-95.36219517	-95.58195344	-95.50909975
1.716	-95.40591858	-95.36728976	-95.56357616	-95.51357813
1.816	-95.39115196	-95.37098607	-95.54732334	-95.51726582
1.916	-95.38228388	-95.37035591	-95.53382775	-95.51906217
2.016	-95.38206489	-95.36260541	-95.52753004	-95.51499811
2.116	-95.38385560	-95.35427857	-95.52875867	-95.50691101
2.216	-95.38559105	-95.34730219	-95.53037997	-95.49899468
2.316	-95.38703466	-95.34174496	-95.53176638	-95.49238878
2.416	-95.38818434	-95.33742726	-95.53288709	-95.48714623
2.516	-95.38908067	-95.33413027	-95.53377017	-95.48310616
2.616	-95.38977013	-95.33164538	-95.53446136	-95.48005978

2.716	-95.39029557	-95.32979126	-95.53500149	-95.47780684
2.816	-95.39069356	-95.32841827	-95.53542718	-95.47617396
2.916	-95.39099374	-95.32740722	-95.53576330	-95.47499940
3.016	-95.39121923	-95.32666549	-95.53603021	-95.47417582
3.116	-95.39138853	-95.32612189	-95.53624194	-95.47360141
3.216	-95.39151482	-95.32572347	-95.53640938	-95.47320767
3.316	-95.39160707	-95.32543194	-95.53654153	-95.47293928
3.416	-95.39167438	-95.32521738	-95.53664613	-95.47275903
3.516	-95.39172285	-95.32505882	-95.53672721	-95.47264517
3.616	-95.39175715	-95.32494121	-95.53679374	-95.47257119
4.116	-95.39181982	-95.32467450	-95.53693846	-95.47246606
5.116	-95.39181668	-95.32458725	-95.53695581	-95.47246354
7.116	-95.39179996	-95.32456772	-95.53696725	-95.47248589

R_{N-H} (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
0.616	-95.33761147	-95.12501644
0.716	-95.54639767	-95.33816447
0.816	-95.64597849	-95.44256052
0.916	-95.68642185	-95.48880373
1.016	-95.69469378	-95.50483446
1.116	-95.68560519	-95.50711723
1.216	-95.66743037	-95.50548888
1.316	-95.65068698	-95.50564121
1.416	-95.62351073	-95.50023816
1.516	-95.60207477	-95.50433985
1.616	-95.58193248	-95.50912539
1.716	-95.56356436	-95.51362370
1.816	-95.54735432	-95.51739588
1.916	-95.53409069	-95.51965099
2.016	-95.52784647	-95.51628776
2.116	-95.52798349	-95.50779530
2.216	-95.52758746	-95.50031934
2.316	-95.52970276	-95.49299044
2.416	-95.53240475	-95.48721343
2.516	-95.53360731	-95.48310695
2.616	-95.53439477	-95.48003920
2.716	-95.53496983	-95.47778367
2.816	-95.53541293	-95.47614773
2.916	-95.53575730	-95.47497409

3.016	-95.53603411	-95.47414135
3.116	-95.53624843	-95.47356841
3.216	-95.53641836	-95.47317399
3.316	-95.53655305	-95.47290371
3.416	-95.53665888	-95.47272277
3.516	-95.53674286	-95.47260527
3.616	-95.53681041	-95.47253060
4.116	-95.53695759	-95.47242248
5.116	-95.53697789	-95.47241556
7.116	-95.53699082	-95.47243585

(3) 100º

$R_{N\text{-}H}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (MC-PDFT)	E2 (MC-PDFT)
0.616	-95.18293654	-94.98084683	-95.33687912	-95.12805416
0.716	-95.39278233	-95.19467154	-95.54576621	-95.34137450
0.816	-95.49249808	-95.29860173	-95.64549036	-95.44580229
0.916	-95.53246400	-95.34341940	-95.68612683	-95.49199483
1.016	-95.53994083	-95.35711920	-95.69463106	-95.50788465
1.116	-95.53012217	-95.35622075	-95.68591364	-95.50925465
1.216	-95.51411960	-95.35398630	-95.67281779	-95.50497529
1.316	-95.49217163	-95.35096639	-95.65248295	-95.50430943
1.416	-95.46822008	-95.34869630	-95.62600837	-95.49850944
1.516	-95.44702889	-95.35353445	-95.60482377	-95.50181958
1.616	-95.42767999	-95.35849694	-95.58506920	-95.50588401
1.716	-95.41098541	-95.36242605	-95.56728208	-95.50947761
1.816	-95.39788481	-95.36436012	-95.55202654	-95.51182686
1.916	-95.38974244	-95.36293017	-95.54026634	-95.51190971
2.016	-95.38672322	-95.35792104	-95.53365092	-95.50870599
2.116	-95.38647979	-95.35158004	-95.53184314	-95.50297326
2.216	-95.38712598	-95.34565206	-95.53203526	-95.49665492
2.316	-95.38794478	-95.34068430	-95.53270108	-95.49093300
2.416	-95.38870739	-95.33672323	-95.53340507	-95.48620315
2.516	-95.38935071	-95.33365310	-95.53402908	-95.48247559
2.616	-95.38986869	-95.33131777	-95.53454968	-95.47962721
2.716	-95.39027506	-95.32956484	-95.53497254	-95.47750270
2.816	-95.39058930	-95.32826152	-95.53531779	-95.47595457
2.916	-95.39082998	-95.32729923	-95.53559666	-95.47483983
3.016	-95.39101328	-95.32659183	-95.53582155	-95.47405684
3.116	-95.39115150	-95.32607369	-95.53600518	-95.47351158
3.216	-95.39125504	-95.32569413	-95.53615221	-95.47313873

3.316	-95.39133177	-95.32541570	-95.53627009	-95.47288565
3.416	-95.39138793	-95.32521075	-95.53636372	-95.47271701
3.516	-95.39142789	-95.32505980	-95.53643844	-95.47260767
3.616	-95.39145659	-95.32494731	-95.53649808	-95.47254264
4.116	-95.39150620	-95.32469353	-95.53663343	-95.47245007
5.116	-95.39149977	-95.32460981	-95.53665026	-95.47244539
7.116	-95.39148291	-95.32459032	-95.53666712	-95.47247022

R_{N-H} (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)
0.616	-95.33999431	-95.13330542
0.716	-95.54876193	-95.34618576
0.816	-95.64832984	-95.45023508
0.916	-95.68873880	-95.49606687
1.016	-95.69686204	-95.51153680
1.116	-95.69046080	-95.51110838
1.216	-95.67455574	-95.50922170
1.316	-95.65352507	-95.50699228
1.416	-95.62880722	-95.50200589
1.516	-95.60769179	-95.50510511
1.616	-95.58799918	-95.50898678
1.716	-95.57028271	-95.51250085
1.816	-95.55511567	-95.51494901
1.916	-95.54337608	-95.51539793
2.016	-95.53625063	-95.51259464
2.116	-95.53318618	-95.50697726
2.216	-95.53208775	-95.50068619
2.316	-95.53310900	-95.49454841
2.416	-95.53504840	-95.48934448
2.516	-95.53631723	-95.48542084
2.616	-95.53709968	-95.48250739
2.716	-95.53763693	-95.48035993
2.816	-95.53803623	-95.47880209
2.916	-95.53834503	-95.47768323
3.016	-95.53858760	-95.47689830
3.116	-95.53877869	-95.47635633
3.216	-95.53894083	-95.47597334
3.316	-95.53906305	-95.47572131
3.416	-95.53916199	-95.47555042
3.516	-95.53924249	-95.47544016

3.616	-95.53930589	-95.47537275
4.116	-95.53946162	-95.47526297
5.116	-95.53948102	-95.47525434
7.116	-95.53950066	-95.47528083

S4.5. Phenol

(1) τ(HOCC) = 1 deg, 2 states

$R_{O\text{-}H}$ (Å)	E1 (MC-PDFT)	E2 (MC-PDFT)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)
0.459	-305.94535127	-305.75846343	-305.94535572	-305.75846011
0.508	-306.30453402	-306.11793793	-306.30453859	-306.11793434
0.558	-306.55388742	-306.36758856	-306.55389187	-306.36758512
0.608	-306.72649878	-306.54048316	-306.72650305	-306.54047985
0.658	-306.84541539	-306.65967623	-306.84541954	-306.65967314
0.708	-306.92645789	-306.74099094	-306.92646182	-306.74098790
0.757	-306.98059396	-306.79539590	-306.98059778	-306.79539301
0.807	-307.01551214	-306.83058000	-307.01551585	-306.83057727
0.857	-307.03887634	-306.85462294	-307.03888333	-306.85461773
0.907	-307.05014156	-306.86620719	-307.05014875	-306.86620177
0.957	-307.05432716	-306.87070739	-307.05433465	-306.87070185
1.007	-307.05349298	-306.87017847	-307.05350064	-306.87017279
1.057	-307.04914743	-306.86612709	-307.04915525	-306.86612133
1.106	-307.04239311	-306.85965048	-307.04240096	-306.85964469
1.156	-307.03404005	-306.85155684	-307.03404780	-306.85155113
1.206	-307.02467811	-306.84242995	-307.02468553	-306.84242440
1.256	-307.01474396	-306.83270149	-307.01475096	-306.83269638
1.306	-307.00455028	-306.82268370	-307.00455661	-306.82267910
1.356	-306.99112663	-306.84613668	-306.99112675	-306.84613538
1.406	-306.98118879	-306.84967194	-306.98118899	-306.84967057
1.456	-306.97149400	-306.85317766	-306.97149422	-306.85317620
1.506	-306.96170877	-306.85545983	-306.96170913	-306.85545889
1.555	-306.95315806	-306.85966229	-306.95315833	-306.85966056
1.605	-306.94463486	-306.86255291	-306.94463523	-306.86255091
1.655	-306.93659241	-306.86519300	-306.93659286	-306.86519052
1.705	-306.92905893	-306.86758784	-306.92905950	-306.86758458
1.755	-306.92005380	-306.86783917	-306.92005409	-306.86783818
1.805	-306.91558688	-306.87170804	-306.91558803	-306.87170169
1.855	-306.90966285	-306.87346860	-306.90966473	-306.87345842
1.905	-306.90427986	-306.87505186	-306.90428315	-306.87503373
1.955	-306.89942491	-306.87648760	-306.89943298	-306.87644516
2.004	-306.89504656	-306.87790805	-306.89509237	-306.87770925

2.054	-306.88166449	-306.89010135	-306.89124485	-306.87883882
2.104	-306.87997311	-306.88778412	-306.88786354	-306.87984083
2.154	-306.88079969	-306.88484846	-306.88493251	-306.88071158
2.204	-306.88158910	-306.88227438	-306.88264543	-306.88123188
2.254	-306.88230265	-306.88004671	-306.88263530	-306.87975997
2.304	-306.88294114	-306.87813118	-306.88412287	-306.87732144
2.354	-306.88351075	-306.87649392	-306.88415491	-306.87610323
2.404	-306.88401864	-306.87509990	-306.88408089	-306.87506546
2.454	-306.88447215	-306.87391577	-306.88448917	-306.87390727
2.503	-306.88487599	-306.87291565	-306.88488263	-306.87291256
2.553	-306.88523404	-306.87207479	-306.88523719	-306.87207347
2.603	-306.88555655	-306.87136814	-306.88555818	-306.87136750
2.653	-306.88584106	-306.87077949	-306.88584194	-306.87077912
2.703	-306.88609857	-306.87028865	-306.88609907	-306.87028842
2.753	-306.88632688	-306.86988214	-306.88632719	-306.86988201
2.803	-306.88653366	-306.86954603	-306.88653390	-306.86954599
2.853	-306.88671930	-306.86926938	-306.88671946	-306.86926938
2.903	-306.88688562	-306.86904187	-306.88688573	-306.86904188
2.952	-306.88703371	-306.86885789	-306.88703375	-306.86885786

(2) τ(HOCC) = 10 deg, 2 states

$R_{O\text{-}H}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (MC-PDFT)	E2 (MC-PDFT)
0.800	-306.56153635	-306.37609952	-307.01167202	-306.82646973
0.850	-306.58431773	-306.39918061	-307.03450013	-306.84956334
0.900	-306.59658408	-306.41174736	-307.04691014	-306.86223413
0.950	-306.60133532	-306.41679013	-307.05186859	-306.86744560
1.000	-306.60076360	-306.41649608	-307.05153416	-306.86735452
1.050	-306.59648525	-306.41249672	-307.04747274	-306.86352513
1.100	-306.58965441	-306.40592198	-307.04083711	-306.85710912
1.150	-306.58113762	-306.39764899	-307.03247079	-306.84894799
1.200	-306.57160209	-306.38848101	-307.02298929	-306.83965028
1.250	-306.56143946	-306.37849698	-307.01285395	-306.82965012
1.300	-306.55105199	-306.36836972	-307.00546981	-306.82376657
1.350	-306.54073968	-306.35905214	-306.99524283	-306.81453932
1.400	-306.52895914	-306.40297974	-306.98203113	-306.84957646
1.450	-306.51929006	-306.40702652	-306.97227044	-306.85302472
1.500	-306.51005835	-306.41085375	-306.96283870	-306.85635821
1.550	-306.50131409	-306.41440270	-306.95380948	-306.85949684
1.600	-306.49311363	-306.41763736	-306.94522842	-306.86241128
1.650	-306.48548928	-306.42055246	-306.93714255	-306.86509365

1.700	-306.47845539	-306.42315724	-306.92956984	-306.86754597
1.750	-306.47201349	-306.42547451	-306.92253496	-306.86979330
1.800	-306.46607535	-306.42753886	-306.91605097	-306.87187027
1.850	-306.46082779	-306.42936828	-306.91010727	-306.87383392
1.900	-306.45623265	-306.43091719	-306.90467933	-306.87580896
1.950	-306.45209085	-306.43226720	-306.89965920	-306.87808950
2.000	-306.44846730	-306.43341263	-306.89460499	-306.88127206
2.050	-306.44538235	-306.43431898	-306.88879339	-306.88469466
2.100	-306.44291375	-306.43487767	-306.88447736	-306.88512064
2.150	-306.44127101	-306.43482126	-306.88302425	-306.88349059
2.200	-306.44064908	-306.43384790	-306.88285796	-306.88144964
2.250	-306.44076022	-306.43203891	-306.88311884	-306.87949004
2.300	-306.44103498	-306.42995779	-306.88351282	-306.87773301
2.350	-306.44105102	-306.42934513	-306.88393737	-306.87619902
2.400	-306.44097303	-306.42960212	-306.88435242	-306.87487891
2.450	-306.44100259	-306.42933567	-306.88474180	-306.87374869
2.500	-306.44110492	-306.42879260	-306.88509978	-306.87278996
2.550	-306.44123985	-306.42821048	-306.88542636	-306.87198202
2.600	-306.44138719	-306.42766974	-306.88572183	-306.87130379
2.650	-306.44153503	-306.42719094	-306.88598782	-306.87073534
2.700	-306.44167871	-306.42677575	-306.88622909	-306.87026139
2.750	-306.44181010	-306.42641733	-306.88644421	-306.86986791
2.800	-306.44193086	-306.42611096	-306.88663880	-306.86954208
2.850	-306.44203893	-306.42584882	-306.88681331	-306.86927245
2.900	-306.44213537	-306.42562494	-306.88696940	-306.86905061
2.950	-306.44221711	-306.42543264	-306.88710335	-306.86886635
3.000	-306.44229252	-306.42526942	-306.88722680	-306.86871903
3.050	-306.44235861	-306.42512995	-306.88733705	-306.86860013
3.100	-306.44241620	-306.42501063	-306.88743610	-306.86850385
3.150	-306.44246609	-306.42490840	-306.88752494	-306.86842522
3.200	-306.44250902	-306.42482063	-306.88760387	-306.86836094
3.250	-306.44254563	-306.42474512	-306.88767313	-306.86831013

$R_{O\text{-}H}$ (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)	E1 (FMS-PDFT)	E2 (FMS-PDFT)
0.800	-307.0138919	-306.8290119	-307.00890344	-306.83057214
0.850	-307.0367721	-306.8522147	-307.03186947	-306.85358959
0.900	-307.049196	-306.8649627	-307.04438485	-306.86614990
0.950	-307.0541577	-306.8702469	-307.04943958	-306.87124529
1.000	-307.0538329	-306.8702404	-307.04920619	-306.87105227

1.050	-307.049804	-306.8665232	-307.04526778	-306.86715830
1.100	-307.0432336	-306.8602557	-307.03878264	-306.86072647
1.150	-307.0349738	-306.852291	-307.03060341	-306.85261367
1.200	-307.0256433	-306.843252	-307.02134918	-306.84344535
1.250	-307.0123912	-306.8408751	-307.01147907	-306.83369078
1.300	-307.0022054	-306.8430154	-307.00134762	-306.82373305
1.350	-306.9920548	-306.8460762	-306.99139083	-306.81421188
1.400	-306.9820424	-306.8494733	-306.98201132	-306.84942107
1.450	-306.9722819	-306.8529132	-306.97224054	-306.85286464
1.500	-306.9628531	-306.8562348	-306.96279842	-306.85619154
1.550	-306.9538281	-306.8593568	-306.95375735	-306.85932204
1.600	-306.9452539	-306.8622468	-306.94516423	-306.86222169
1.650	-306.9371745	-306.8648922	-306.93706053	-306.86487799
1.700	-306.9296127	-306.867292	-306.92946980	-306.86729078
1.750	-306.9225951	-306.8694562	-306.92241749	-306.86947241
1.800	-306.9161398	-306.8714014	-306.91591588	-306.87144019
1.850	-306.9102481	-306.8731354	-306.90996627	-306.87320487
1.900	-306.9049289	-306.8746677	-306.90457202	-306.87477812
1.950	-306.9001918	-306.8760032	-306.89972832	-306.87617487
2.000	-306.8960449	-306.8771314	-306.89541461	-306.87740781
2.050	-306.8925324	-306.8780109	-306.89163103	-306.87846846
2.100	-306.88977	-306.8785321	-306.88837276	-306.87934869
2.150	-306.8879929	-306.8784745	-306.88571302	-306.87994983
2.200	-306.887472	-306.8776335	-306.88392503	-306.87996914
2.250	-306.888222	-306.8761485	-306.88337520	-306.87901254

(2) τ(HOCC) = 10 deg, 3 states

$R_{O\text{-}H}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E3 (XMS-CASPT2)
0.800	-306.56357008	-306.37866225	-306.32617027
0.850	-306.58637421	-306.40183971	-306.34959990
0.900	-306.59866388	-306.41450546	-306.36249658
0.950	-306.60344358	-306.41965990	-306.36787147
1.000	-306.60289233	-306.41945976	-306.36787191
1.050	-306.59863637	-306.41556199	-306.36416920
1.100	-306.59182209	-306.40908700	-306.35794513
1.150	-306.58331900	-306.40095933	-306.35036772
1.200	-306.57186931	-306.38659392	-306.38147366
1.250	-306.56170898	-306.38759605	-306.37610388
1.300	-306.55133639	-306.39252126	-306.36662759
1.350	-306.54104399	-306.39765070	-306.35666355

1.400	-306.53097930	-306.40282413	-306.34668224
1.450	-306.52249108	-306.41031895	-306.33972470
1.500	-306.51340723	-306.41386488	-306.34127251
1.550	-306.50478086	-306.41716768	-306.34285131
1.600	-306.49667981	-306.42021069	-306.34432128
1.650	-306.48913673	-306.42298671	-306.34564154
1.700	-306.48216543	-306.42550363	-306.34680172
1.750	-306.47576145	-306.42777981	-306.34781501
1.800	-306.46989920	-306.42984141	-306.34871076
1.850	-306.46445330	-306.43169209	-306.34954375
1.900	-306.45934735	-306.43336746	-306.35014424
1.950	-306.45434641	-306.43515531	-306.35058001
2.000	-306.44956976	-306.43704078	-306.35100046
2.050	-306.44710910	-306.43802085	-306.35137835
2.100	-306.44530960	-306.43844447	-306.35171216
2.150	-306.44352472	-306.43876625	-306.35200312
2.200	-306.44213962	-306.43881254	-306.35225470
2.250	-306.44155662	-306.43824091	-306.35247244
2.300	-306.44161474	-306.43720691	-306.35266000
2.350	-306.44189288	-306.43611055	-306.35281747
2.400	-306.44221951	-306.43510057	-306.35295675
2.450	-306.44254020	-306.43421076	-306.35307285
2.500	-306.44283778	-306.43343960	-306.35316927
2.550	-306.44310640	-306.43277698	-306.35324698
2.600	-306.44334676	-306.43220969	-306.35331357
2.650	-306.44355976	-306.43172551	-306.35336849
2.700	-306.44374760	-306.43131298	-306.35341353
2.750	-306.44391249	-306.43096167	-306.35344989
2.800	-306.44405709	-306.43066259	-306.35347927
2.850	-306.44418342	-306.43040812	-306.35350286
2.900	-306.44429351	-306.43019154	-306.35352134
2.950	-306.44438953	-306.43000705	-306.35353619
3.000	-306.44447271	-306.42984980	-306.35354718
3.050	-306.44454701	-306.42971653	-306.35356180
3.100	-306.44460920	-306.42960183	-306.35357105
3.150	-306.44466225	-306.42950352	-306.35357047
3.200	-306.44470768	-306.42941901	-306.35357557
3.250	-306.44474528	-306.42934538	-306.35357260

$R_{O\text{-}H}$ (Å)	E1 (MC-PDFT)	E2 (MC-PDFT)	E3 (MC-PDFT)

0.800	-307.01652808	-306.83077070	-306.78575646
0.850	-307.03922832	-306.85378781	-306.81083866
0.900	-307.05142958	-306.86631012	-306.82615785
0.950	-307.05532818	-306.87046383	-306.83371851
1.000	-307.05432869	-306.86978264	-306.83593511
1.050	-307.04954212	-306.86511672	-306.83199866
1.100	-307.04241935	-306.85811056	-306.82670171
1.150	-307.03384197	-306.85031181	-306.82562973
1.200	-307.02433388	-306.84337091	-306.83562013
1.250	-307.01427892	-306.83037921	-306.82883934
1.300	-307.00396319	-306.83263860	-306.81874955
1.350	-306.99359921	-306.83698947	-306.80883737
1.400	-306.98330304	-306.84235347	-306.79965892
1.450	-306.96850509	-306.86003294	-306.78731453
1.500	-306.95913986	-306.86306329	-306.78722549
1.550	-306.95032243	-306.86582158	-306.78782532
1.600	-306.94198387	-306.86838821	-306.78858273
1.650	-306.93412898	-306.87078056	-306.78933775
1.700	-306.92676651	-306.87302816	-306.79003756
1.750	-306.91990394	-306.87519824	-306.79066628
1.800	-306.91352070	-306.87743977	-306.79122412
1.850	-306.90748509	-306.88011899	-306.79171521
1.900	-306.90125691	-306.88401166	-306.79214302
1.950	-306.89383511	-306.88849346	-306.79252192
2.000	-306.88929131	-306.88800767	-306.79285878
2.050	-306.88727512	-306.88589959	-306.79316057
2.100	-306.88553961	-306.88463062	-306.79343267
2.150	-306.88577374	-306.88204177	-306.79367779
2.200	-306.88620615	-306.87968302	-306.79390158
2.250	-306.88669364	-306.87759496	-306.79410528
2.300	-306.88718085	-306.87577666	-306.79429389
2.350	-306.88764504	-306.87421217	-306.79446591
2.400	-306.88807750	-306.87287305	-306.79462803
2.450	-306.88847324	-306.87173184	-306.79477471
2.500	-306.88883388	-306.87076372	-306.79491310
2.550	-306.88915982	-306.86995061	-306.79503720
2.600	-306.88945486	-306.86926706	-306.79515458
2.650	-306.88972046	-306.86869559	-306.79526337
2.700	-306.88995959	-306.86821855	-306.79536446
2.750	-306.89017472	-306.86782235	-306.79545851
2.800	-306.89036879	-306.86749380	-306.79554640

2.850	-306.89054357	-306.86722291	-306.79562837
2.900	-306.89070013	-306.86700004	-306.79570368
2.950	-306.89083958	-306.86681681	-306.79577253
3.000	-306.89096364	-306.86666886	-306.79583492
3.050	-306.89107636	-306.86654822	-306.79589568
3.100	-306.89117629	-306.86645200	-306.79594919
3.150	-306.89126587	-306.86637430	-306.79599796
3.200	-306.89134608	-306.86631147	-306.79604303
3.250	-306.89141609	-306.86626227	-306.79608091

$R_{O\text{-}H}$ (Å)	E1 (FMS-PDFT)	E2 (FMS-PDFT)	E3 (FMS-PDFT)
0.800	-307.01142088	-306.83176939	-306.78575388
0.850	-307.03419959	-306.85458974	-306.81082311
0.900	-307.04650037	-306.86688578	-306.82610535
0.950	-307.05073175	-306.87058291	-306.83354638
1.000	-307.04995630	-306.86954866	-306.83551557
1.050	-307.04538909	-306.86469022	-306.83126722
1.100	-307.03840015	-306.85764236	-306.82563421
1.150	-307.02992440	-306.84952546	-306.82367493
1.200	-307.02319491	-306.84046953	-306.82514455
1.250	-307.01437161	-306.83143379	-306.82520084
1.300	-307.00406434	-306.83223713	-306.81838081
1.350	-306.99370890	-306.83660183	-306.80874946
1.400	-306.98344530	-306.84193130	-306.79963098
1.450	-306.96853881	-306.85996672	-306.78691887
1.500	-306.95913023	-306.86293643	-306.78693927
1.550	-306.95028481	-306.86567255	-306.78755767
1.600	-306.94192344	-306.86820384	-306.78831260
1.650	-306.93404883	-306.87052906	-306.78905704
1.700	-306.92667185	-306.87265227	-306.78974218
1.750	-306.91981111	-306.87458185	-306.79035362
1.800	-306.91348034	-306.87632985	-306.79089267
1.850	-306.90768448	-306.87790112	-306.79136438
1.900	-306.90243075	-306.87929800	-306.79177254
1.950	-306.89769826	-306.88018590	-306.79252921
2.000	-306.89355876	-306.88120515	-306.79286556
2.050	-306.89005933	-306.88194354	-306.79316667
2.100	-306.88747523	-306.88211454	-306.79343803
2.150	-306.88633469	-306.88116594	-306.79368239

2.200	-306.88633603	-306.87936908	-306.79390546
2.250	-306.88671320	-306.87746136	-306.79410848
2.300	-306.88717256	-306.87571278	-306.79429467
2.350	-306.88763184	-306.87417741	-306.79446786
2.400	-306.88806509	-306.87285271	-306.79462968
2.450	-306.88846312	-306.87171938	-306.79477601
2.500	-306.88882641	-306.87075555	-306.79491410
2.550	-306.88915440	-306.86994489	-306.79503796
2.600	-306.88945111	-306.86926299	-306.79515516
2.650	-306.88971784	-306.86869252	-306.79526381
2.700	-306.88995772	-306.86821621	-306.79536480
2.750	-306.89017349	-306.86782055	-306.79545875
2.800	-306.89036796	-306.86749237	-306.79554658
2.850	-306.89054305	-306.86722179	-306.79562851
2.900	-306.89069980	-306.86699918	-306.79570378
2.950	-306.89083937	-306.86681612	-306.79577260
3.000	-306.89096353	-306.86666831	-306.79583498
3.050	-306.89107630	-306.86654779	-306.79589571
3.100	-306.89117628	-306.86645165	-306.79594921
3.150	-306.89126588	-306.86637401	-306.79599798
3.200	-306.89134612	-306.86631123	-306.79604304
3.250	-306.89141614	-306.86626208	-306.79608092

S4.6. O_2 + O collision

(1) α(O2O1O3) = 175°, $^3A'$

$R_{O1\text{-}O3}$ (Å)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E3 (XMS-CASPT2)
1.000	-224.70852007	-224.62631333	-224.62381963
1.100	-224.81808622	-224.76823482	-224.76541124
1.200	-224.88468211	-224.83822449	-224.83579673
1.300	-224.93208133	-224.86798987	-224.86693474
1.400	-224.96571783	-224.88595354	-224.86699034
1.500	-224.98939863	-224.92903329	-224.90999136
1.600	-225.00747525	-224.96379456	-224.94703013
1.700	-225.02178752	-224.98534568	-224.97389522
1.800	-225.03465552	-225.00187481	-224.99610110
1.900	-225.04545556	-225.02058207	-225.00872526
2.000	-225.05383638	-225.03568403	-225.01602195
2.100	-225.05974998	-225.04820721	-225.02203319
2.200	-225.06411573	-225.05633922	-225.02591179
2.300	-225.06715310	-225.06175269	-225.02852138

2.400	-225.06918031	-225.06540788	-225.03048302
2.500	-225.07049229	-225.06785724	-225.03214052

R_{O1-O3} (Å)	E4 (XMS-CASPT2)	E5 (XMS-CASPT2)	E6 (XMS-CASPT2)
1.000	-224.53039558	-224.50339197	-224.48183239
1.100	-224.66083056	-224.63008376	-224.60973368
1.200	-224.74832878	-224.71673654	-224.69779796
1.300	-224.81710127	-224.79015032	-224.77147020
1.400	-224.85892253	-224.84557412	-224.82967976
1.500	-224.88948265	-224.88345210	-224.87623001
1.600	-224.93347279	-224.92389648	-224.91523859
1.700	-224.97171969	-224.95070375	-224.93306156
1.800	-224.99055416	-224.96900619	-224.96185811
1.900	-225.00437845	-224.98250658	-224.98002950
2.000	-225.01395227	-224.99997795	-224.99122046
2.100	-225.02044356	-225.01162290	-224.99784846
2.200	-225.02478416	-225.01940988	-225.00207748
2.300	-225.02767496	-225.02465446	-225.00486403
2.400	-225.02955086	-225.02804602	-225.00669260
2.500	-225.03075974	-225.03003958	-225.00787927

R_{O1-O3} (Å)	E1 (MC-PDFT)	E2 (MC-PDFT)	E3 (MC-PDFT)
1.000	-224.83221808	-224.75717963	-224.75619494
1.100	-224.93997876	-224.89969141	-224.89929604
1.200	-225.00477613	-224.96865191	-224.96904289
1.300	-225.05008094	-224.99109618	-224.99384563
1.400	-225.08128309	-225.00165407	-224.98507231
1.500	-225.10014102	-225.03904658	-225.02171968
1.600	-225.11518376	-225.07155320	-225.05602942
1.700	-225.12841092	-225.09427578	-225.08153336
1.800	-225.13992833	-225.10872837	-225.10345171
1.900	-225.14993173	-225.12793234	-225.11850422
2.000	-225.15757332	-225.14230796	-225.12603988
2.100	-225.16314617	-225.15255151	-225.13117399
2.200	-225.16710135	-225.15977586	-225.13478187
2.300	-225.16987178	-225.16483133	-225.13739189
2.400	-225.17178100	-225.16833401	-225.13948726

2.500	-225.17307030	-225.17074185	-225.14152375

R_{O1-O3} (Å)	E4 (MC-PDFT)	E5 (MC-PDFT)	E6 (MC-PDFT)
1.000	-224.65825741	-224.63794917	-224.63016700
1.100	-224.78677541	-224.76496325	-224.75749149
1.200	-224.87380383	-224.85159321	-224.84341020
1.300	-224.94393707	-224.92189567	-224.91205593
1.400	-224.97927436	-224.98248067	-224.95830721
1.500	-225.00310930	-225.00206648	-224.99639713
1.600	-225.04044796	-225.03539676	-225.04848521
1.700	-225.07778394	-225.06388517	-225.05828032
1.800	-225.09971699	-225.08162360	-225.07409702
1.900	-225.11295821	-225.09615104	-225.09509491
2.000	-225.12224461	-225.11159326	-225.10457033
2.100	-225.12870089	-225.12247992	-225.11074698
2.200	-225.13318405	-225.13011232	-225.11490902
2.300	-225.13635722	-225.13542450	-225.11772699
2.400	-225.13881467	-225.13908648	-225.11962274
2.500	-225.14108819	-225.14159306	-225.12087828

R_{O1-O3} (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)	E3 (XMS-PDFT)
1.000	-224.83250743	-224.75934136	-224.75502522
1.100	-224.94016629	-224.89958376	-224.89663297
1.200	-225.00477849	-224.96964743	-224.96701900
1.300	-225.05022430	-224.99414802	-224.99229720
1.400	-225.08192476	-225.01362530	-224.98678361
1.500	-225.09956796	-225.03939116	-225.02463676
1.600	-225.11679038	-225.07589138	-225.06016776
1.700	-225.12694312	-225.09733367	-225.08685247
1.800	-225.13895337	-225.11038609	-225.10516892
1.900	-225.14974799	-225.12621896	-225.11666465
2.000	-225.15669258	-225.14124963	-225.12457317
2.100	-225.16313838	-225.15221948	-225.13065623
2.200	-225.16704109	-225.15970734	-225.13494303
2.300	-225.16986940	-225.16480883	-225.13707463
2.400	-225.17178731	-225.16832584	-225.14148380
2.500	-225.17305860	-225.17074047	-225.14151522

R_{O1-O3} (Å)	E4 (XMS-PDFT)	E5 (XMS-PDFT)	E6 (XMS-PDFT)
1.000	-224.66873302	-224.64447683	-224.61436505
1.100	-224.79907849	-224.77128207	-224.74331048
1.200	-224.87958754	-224.86002339	-224.83175438
1.300	-224.94801579	-224.92727467	-224.90374449
1.400	-224.97698891	-224.96924738	-224.95437001
1.500	-225.01579472	-225.00160808	-224.98800758
1.600	-225.04154578	-225.03478393	-225.02895431
1.700	-225.07832390	-225.05966140	-225.04599943
1.800	-225.10070928	-225.07951506	-225.07379045
1.900	-225.11295777	-225.09582722	-225.09030745
2.000	-225.12222402	-225.11148691	-225.10271958
2.100	-225.12868983	-225.12234301	-225.11078947
2.200	-225.13343832	-225.13010367	-225.11481698
2.300	-225.13615554	-225.13525074	-225.11775492
2.400	-225.14092184	-225.13907834	-225.11959847
2.500	-225.13999079	-225.13946857	-225.12085320

(2) α(O2O1O3) = 175°, $^3A''$

R_{O1-O3} (Å)	E1 (MC-PDFT)	E2 (MC-PDFT)	E3 (MC-PDFT)
1.000	-224.98450204	-224.83014041	-224.75613707
1.100	-225.08506315	-224.93837332	-224.89850066
1.200	-225.12380135	-225.00374966	-224.96753229
1.300	-225.12914178	-225.04973145	-224.98789950
1.400	-225.11474546	-225.08073435	-224.99374713
1.500	-225.10756765	-225.09708462	-225.03638521
1.600	-225.11742601	-225.08774474	-225.07859041
1.700	-225.12971797	-225.09394483	-225.08217906
1.800	-225.14105162	-225.10921484	-225.10057472
1.900	-225.15079190	-225.11959230	-225.11370346
2.000	-225.15829860	-225.12677598	-225.12291112
2.100	-225.16326251	-225.13142517	-225.12891140
2.200	-225.16711699	-225.13493696	-225.13331517
2.300	-225.16988539	-225.13753728	-225.13648483
2.400	-225.17179690	-225.13961217	-225.13891859
2.500	-225.17308852	-225.14162731	-225.14114818

R_{O1-O3} (Å)	E4 (MC-PDFT)	E5 (MC-PDFT)	E6 (MC-PDFT)
1.000	-224.66570848	-224.63714945	-224.68985818
1.100	-224.79277197	-224.76395321	-224.81787465
1.200	-224.87553564	-224.85102810	-224.87315510
1.300	-224.94257632	-224.92201805	-224.90983027
1.400	-224.98155560	-224.96887745	-224.96505682
1.500	-225.02214305	-225.00440704	-225.01525466
1.600	-225.05649290	-225.03916503	-225.04898068
1.700	-225.10062309	-225.06503276	-225.07018955
1.800	-225.10460393	-225.08302694	-225.07267292
1.900	-225.09429002	-225.09487989	-225.11019673
2.000	-225.11000295	-225.10521002	-225.11494646
2.100	-225.12242653	-225.11099608	-225.09911930
2.200	-225.13016777	-225.11507549	-225.10703213
2.300	-225.13548066	-225.11789005	-225.11232176
2.400	-225.13914149	-225.11978487	-225.11594582
2.500	-225.14164639	-225.12103971	-225.11842266

R_{O1-O3} (Å)	E1 (XMS-PDFT)	E2 (XMS-PDFT)	E3 (XMS-PDFT)
1.000	-224.98178569	-224.83403196	-224.75568257
1.100	-225.08693060	-224.93741799	-224.89694206
1.200	-225.12699060	-225.00220947	-224.96933162
1.300	-225.13497479	-225.04653523	-224.98535330
1.400	-225.12375320	-225.07406809	-224.99777584
1.500	-225.11450620	-225.09166219	-225.03835395
1.600	-225.12093029	-225.09397128	-225.07260303
1.700	-225.13257330	-225.10148516	-225.09368721
1.800	-225.14188272	-225.10873692	-225.10263902
1.900	-225.15123670	-225.11894181	-225.11377004
2.000	-225.15762128	-225.12766099	-225.12290635
2.100	-225.16328057	-225.13112243	-225.12911200
2.200	-225.16705451	-225.13502108	-225.13373930
2.300	-225.16979331	-225.13857804	-225.13757790
2.400	-225.17176316	-225.14170344	-225.14115048
2.500	-225.17309285	-225.14157306	-225.14010018

R_{O1-O3} (Å)	E4 (XMS-PDFT)	E5 (XMS-PDFT)	E6 (XMS-PDFT)

1.000	-224.70123804	-224.65185072	-224.63954466
1.100	-224.82968229	-224.78014991	-224.76588634
1.200	-224.89311765	-224.85475469	-224.85171347
1.300	-224.95314122	-224.92209915	-224.90443343
1.400	-224.98679026	-224.96877727	-224.95614019
1.500	-225.02768707	-225.00925060	-224.99926703
1.600	-225.06143786	-225.04352214	-225.03443083
1.700	-225.08855542	-225.06406440	-225.05183932
1.800	-225.10079599	-225.08461864	-225.07286365
1.900	-225.10909759	-225.09716623	-225.09421439
2.000	-225.11439884	-225.11006065	-225.10375541
2.100	-225.12229709	-225.10866549	-225.09904482
2.200	-225.13009450	-225.11510779	-225.10703018
2.300	-225.13539406	-225.11774883	-225.11231262
2.400	-225.13905516	-225.11972887	-225.11594156
2.500	-225.13958793	-225.12101116	-225.11841815

R_{O1-O3} (Å)	E4 (XMS-PDFT)	E5 (XMS-PDFT)	E6 (XMS-PDFT)
1.000	-224.70123804	-224.65185072	-224.63954466
1.100	-224.82968229	-224.78014991	-224.76588634
1.200	-224.89311765	-224.85475469	-224.85171347
1.300	-224.95314122	-224.92209915	-224.90443343
1.400	-224.98679026	-224.96877727	-224.95614019
1.500	-225.02768707	-225.00925060	-224.99926703
1.600	-225.06143786	-225.04352214	-225.03443083
1.700	-225.08855542	-225.06406440	-225.05183932
1.800	-225.10079599	-225.08461864	-225.07286365
1.900	-225.10909759	-225.09716623	-225.09421439
2.000	-225.11439884	-225.11006065	-225.10375541
2.100	-225.12229709	-225.10866549	-225.09904482
2.200	-225.13009450	-225.11510779	-225.10703018
2.300	-225.13539406	-225.11774883	-225.11231262
2.400	-225.13905516	-225.11972887	-225.11594156
2.500	-225.13958793	-225.12101116	-225.11841815

(3) R_{O1-O3} = 1.4 Å

Angle (deg)	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E3 (XMS-CASPT2)
60.0	-224.73104883	-224.70452115	-224.66496573
65.0	-224.75042002	-224.73622372	-224.72930925

70.0	-224.81919925	-224.80913266	-224.78758086
75.0	-224.88945600	-224.87138783	-224.82839448
80.0	-224.94771332	-224.90826748	-224.85582041
85.0	-224.98895294	-224.93369328	-224.87267047
90.0	-225.01762602	-224.95093519	-224.88199112
95.0	-225.03662722	-224.96214885	-224.88669900
100.0	-225.04856591	-224.96904107	-224.88856320
105.0	-225.05513048	-224.97270677	-224.88927264
110.0	-225.05730602	-224.97377904	-224.89060714
115.0	-225.05587184	-224.97286672	-224.89501967
120.0	-225.05150827	-224.96992970	-224.89673971
125.0	-225.04442949	-224.96546672	-224.90486660
130.0	-225.03502110	-224.95976098	-224.91298977
135.0	-225.02355963	-224.95300750	-224.92088311
140.0	-225.01052295	-224.94538528	-224.92884361
145.0	-224.99614148	-224.93767130	-224.93522700
150.0	-224.98023953	-224.94331753	-224.92764517
155.0	-224.96431793	-224.94783234	-224.91777052
160.0	-224.95872660	-224.93991088	-224.90710746
165.0	-224.96127535	-224.92173616	-224.89547317
170.0	-224.96208716	-224.90120248	-224.88198737
175.0	-224.96571745	-224.88595528	-224.86698863
180.0	-224.96618911	-224.87586174	-224.85825793

Angle (deg)	E4 (XMS-CASPT2)	E5 (XMS-CASPT2)	E6 (XMS-CASPT2)
60.0	-224.64018547	-224.63059029	-224.62798376
65.0	-224.71755765	-224.70802301	-224.68664763
70.0	-224.76274903	-224.75212380	-224.73603913
75.0	-224.78873569	-224.78169504	-224.75956500
80.0	-224.80055775	-224.79484351	-224.77437558
85.0	-224.80395446	-224.79840210	-224.78702631
90.0	-224.80498890	-224.79917334	-224.79576819
95.0	-224.81993962	-224.79943089	-224.78906668
100.0	-224.83370565	-224.80300589	-224.78412002
105.0	-224.84810665	-224.81616429	-224.77921405
110.0	-224.85660779	-224.82394099	-224.77396766
115.0	-224.86433454	-224.82709542	-224.77735096
120.0	-224.86861220	-224.82367195	-224.78497504
125.0	-224.87254221	-224.82556170	-224.79233490

130.0	-224.87486123	-224.82274286	-224.79929342
135.0	-224.87625967	-224.81940557	-224.80485174
140.0	-224.87719556	-224.82078192	-224.80577360
145.0	-224.87741838	-224.82529599	-224.80811396
150.0	-224.87656037	-224.83173197	-224.81368539
155.0	-224.87465761	-224.83705334	-224.81934214
160.0	-224.87181599	-224.84056596	-224.82418088
165.0	-224.86862711	-224.84325850	-224.82785368
170.0	-224.86508757	-224.84679489	-224.82979935
175.0	-224.85891753	-224.84557203	-224.82967088
180.0	-224.84028909	-224.83872561	-224.83354000

Angle (deg)	E1 (MC-PDFT)	E2 (MC-PDFT)	E3 (MC-PDFT)
60.0	-224.84523870	-224.82403730	-224.79077993
65.0	-224.86296468	-224.85975931	-224.85553660
70.0	-224.92645946	-224.92717669	-224.91035324
75.0	-225.00411420	-224.97953833	-224.94921887
80.0	-225.06267868	-225.01714251	-224.97539828
85.0	-225.10424723	-225.04345534	-224.99182501
90.0	-225.13333290	-225.06158952	-225.00130487
95.0	-225.15301131	-225.07353303	-225.00631250
100.0	-225.16571901	-225.08065661	-225.00855659
105.0	-225.17269079	-225.08399684	-225.00960085
110.0	-225.17505310	-225.08496483	-225.01081002
115.0	-225.17395504	-225.08500162	-225.01363748
120.0	-225.16971874	-225.08265509	-225.01795638
125.0	-225.16270704	-225.07863360	-225.02346928
130.0	-225.15330146	-225.07334480	-225.03003891
135.0	-225.14178163	-225.06706097	-225.03740029
140.0	-225.12839406	-225.06031459	-225.04525491
145.0	-225.11334815	-225.05389503	-225.05290316
150.0	-225.09701849	-225.05964246	-225.04403925
155.0	-225.08090428	-225.06557020	-225.03452029
160.0	-225.07467448	-225.06047227	-225.02406084
165.0	-225.07656162	-225.03863025	-225.01210182
170.0	-225.07935851	-225.01855630	-224.99773483
175.0	-225.08128257	-225.00165491	-224.98507285
180.0	-225.08172101	-224.99361625	-224.97640589

Angle (deg)	E4 (MC-PDFT)	E5 (MC-PDFT)	E6 (MC-PDFT)
60.0	-224.77033478	-224.76519045	-224.74866227
65.0	-224.83212752	-224.83385989	-224.82158561
70.0	-224.88780318	-224.88604435	-224.85058145
75.0	-224.91236596	-224.91188534	-224.87510313
80.0	-224.92393783	-224.92311513	-224.89039263
85.0	-224.92722417	-224.90406830	-224.92305889
90.0	-224.91805859	-224.92549322	-224.92202590
95.0	-224.93482197	-224.92316571	-224.91711220
100.0	-224.95032655	-224.92452476	-224.91268424
105.0	-224.96278826	-224.93077383	-224.90787332
110.0	-224.97323195	-224.93746438	-224.89922305
115.0	-224.98078048	-224.94065814	-224.89914169
120.0	-224.98555074	-224.94098935	-224.90756375
125.0	-224.98916441	-224.93937759	-224.91634058
130.0	-224.99186746	-224.93685633	-224.92546883
135.0	-224.99386726	-224.93590017	-224.93132246
140.0	-224.99510777	-224.93913159	-224.93084544
145.0	-224.99560485	-224.94616879	-224.93668017
150.0	-224.99510954	-224.95340200	-224.94120316
155.0	-224.99396062	-224.96003437	-224.94604933
160.0	-224.99264239	-224.96586899	-224.95062542
165.0	-224.99250223	-224.97103242	-224.95443143
170.0	-224.99073540	-224.97614917	-224.95717168
175.0	-224.97927455	-224.98247687	-224.95830129
180.0	-224.95520217	-224.96985677	-224.96159936

Angle (deg)	E1 (XMS-PDFT)	E2 (XMS-PDFT)	E3 (XMS-PDFT)
60.0	-224.84472589	-224.82534840	-224.79554861
65.0	-224.86607874	-224.86253894	-224.85452360
70.0	-224.92876979	-224.92503497	-224.91359042
75.0	-225.00466484	-224.98003004	-224.95107172
80.0	-225.06270243	-225.01727949	-224.97541980
85.0	-225.10472196	-225.04360024	-224.99262670
90.0	-225.13327616	-225.06157114	-225.00067275
95.0	-225.15341321	-225.07365221	-225.00578893
100.0	-225.16621897	-225.08071363	-225.00938135

105.0	-225.17306104	-225.08396862	-225.01001015
110.0	-225.17520356	-225.08498691	-225.00977795
115.0	-225.17479300	-225.08505128	-225.01314189
120.0	-225.16995561	-225.08272430	-225.02074940
125.0	-225.16302106	-225.07860034	-225.02414422
130.0	-225.15274063	-225.07341924	-225.03093194
135.0	-225.14116988	-225.06698805	-225.03711230
140.0	-225.13064235	-225.06104514	-225.04563893
145.0	-225.11699800	-225.05731010	-225.05373021
150.0	-225.09934584	-225.06021436	-225.04410269
155.0	-225.08253992	-225.06543343	-225.03464654
160.0	-225.07189851	-225.05841746	-225.02451203
165.0	-225.07625936	-225.04409867	-225.01352831
170.0	-225.08073188	-225.03065929	-225.00496961
175.0	-225.08363771	-225.00890382	-224.98987014
180.0	-225.08263982	-225.00085474	-224.97893677

Angle (deg)	E4 (XMS-PDFT)	E5 (XMS-PDFT)	E6 (XMS-PDFT)
60.0	-224.76877500	-224.75431329	-224.75020514
65.0	-224.83618380	-224.83278982	-224.80645069
70.0	-224.89181142	-224.87719533	-224.85193532
75.0	-224.91206810	-224.90329014	-224.87799802
80.0	-224.92535410	-224.91696975	-224.89555074
85.0	-224.92935136	-224.91966347	-224.90468917
90.0	-224.92930569	-224.92324982	-224.91536956
95.0	-224.93640425	-224.92673372	-224.91365469
100.0	-224.95037148	-224.92818965	-224.91029835
105.0	-224.96411244	-224.93473717	-224.89782503
110.0	-224.97372834	-224.94215052	-224.89027352
115.0	-224.98079146	-224.94469662	-224.89056510
120.0	-224.98829849	-224.94474862	-224.90036812
125.0	-224.99073869	-224.94342551	-224.90812384
130.0	-224.99349160	-224.93958754	-224.91531503
135.0	-224.99481374	-224.94021589	-224.92193698
140.0	-224.99579159	-224.94441621	-224.92533902
145.0	-224.99544097	-224.94444009	-224.93492585
150.0	-224.99433907	-224.95539428	-224.93933709
155.0	-224.99547871	-224.95981228	-224.94652770
160.0	-224.99856505	-224.96370734	-224.94969985

165.0	-224.99478037	-224.96709902	-224.94988160
170.0	-224.98165364	-224.96972597	-224.95249047
175.0	-224.97458116	-224.96598784	-224.95968061
180.0	-224.96158811	-224.96052297	-224.95318809

S4.7. Spiro

ξ	E1 (XMS-CASPT2)	E2 (XMS-CASPT2)	E1 (MC-PDFT)	E2 (MC-PDFT)
0.00	-611.02464104	-611.02126657	-612.13250625	-612.12958252
0.05	-611.02494038	-611.02130382	-612.11813840	-612.11500060
0.10	-611.02554251	-611.02121544	-612.09980815	-612.09606229
0.15	-611.02611114	-611.02083132	-612.08975017	-612.08513577
0.20	-611.02655535	-611.02017553	-612.08465732	-612.07903959
0.25	-611.02686587	-611.01930811	-612.08186906	-612.07518890
0.30	-611.02706606	-611.01827902	-612.08019961	-612.07240523
0.35	-611.02715992	-611.01711243	-612.07908441	-612.07014984
0.40	-611.02715271	-611.01582388	-612.07825043	-612.06815842
0.45	-611.02704749	-611.01442323	-612.07755393	-612.06629297
0.50	-611.02684596	-611.01291565	-612.07691341	-612.06447487
0.55	-611.02654911	-611.01130514	-612.07628073	-612.06265838
0.60	-611.02615785	-611.00959470	-612.07562616	-612.06081534
0.65	-611.02567156	-611.00778470	-612.07492938	-612.05892682
0.70	-611.02509089	-611.00587659	-612.07417788	-612.05697964
0.75	-611.02441567	-611.00387137	-612.07336202	-612.05496603
0.80	-611.02364561	-611.00176938	-612.07247515	-612.05288018
0.85	-611.02278061	-610.99957031	-612.07151280	-612.05071637
0.90	-611.02182031	-610.99727421	-612.07047106	-612.04847094
0.95	-611.02076431	-610.99488149	-612.06934687	-612.04614246
1.00	-611.01961247	-610.99239213	-612.06813819	-612.04372855
1.05	-611.01836434	-610.98980578	-612.06684315	-612.04122733
1.10	-611.01702255	-610.98712055	-612.06546805	-612.03863256
1.15	-611.01558059	-610.98433943	-612.06399562	-612.03595245
1.20	-611.01404057	-610.98145950	-612.06243239	-612.03318002
1.25	-611.01240247	-610.97848130	-612.06077731	-612.03031601
1.30	-611.01066600	-610.97540453	-612.05903032	-612.02735787
1.35	-611.00883039	-610.97222891	-612.05718954	-612.02430671
1.40	-611.00689449	-610.96895257	-612.05525378	-612.02115998
1.45	-611.00485899	-610.96557705	-612.05322361	-612.01791778
1.50	-611.00272203	-610.96209991	-612.05109683	-612.01457839

ξ	E1 (XMS-PDFT)	E2 (XMS-PDFT)	E1 (FMS-PDFT)	E2 (FMS-PDFT)
0.00	-612.13250704	-612.12958326	-612.07505433	-612.07194597
0.05	-612.12387706	-612.12071048	-612.07512304	-612.07178735
0.10	-612.10890888	-612.10510676	-612.07529129	-612.07135120
0.15	-612.09764558	-612.09297493	-612.07549184	-612.07070473
0.20	-612.09065397	-612.08498779	-612.07566682	-612.06990450
0.25	-612.08641285	-612.07968824	-612.07578648	-612.06898031
0.30	-612.08365665	-612.07582283	-612.07584364	-612.06793988
0.35	-612.08177425	-612.07280480	-612.07582591	-612.06679533
0.40	-612.08038966	-612.07026656	-612.07572830	-612.06555098
0.45	-612.07928950	-612.06800063	-612.07554757	-612.06421013
0.50	-612.07834624	-612.06588242	-612.07528173	-612.06277401
0.55	-612.07748170	-612.06383617	-612.07492932	-612.06124376
0.60	-612.07664597	-612.06181395	-612.07448937	-612.05962061
0.65	-612.07580527	-612.05978291	-612.07396053	-612.05790423
0.70	-612.07493781	-612.05772175	-612.07334280	-612.05609524
0.75	-612.07402723	-612.05561472	-612.07263678	-612.05419436
0.80	-612.07306210	-612.05345108	-612.07183746	-612.05219906
0.85	-612.07203421	-612.05122274	-612.07095029	-612.05011264
0.90	-612.07093701	-612.04892347	-612.06996900	-612.04793120
0.95	-612.06976567	-612.04654855	-612.06889715	-612.04565722
1.00	-612.06851659	-612.04409505	-612.06773335	-612.04329022
1.05	-612.06718657	-612.04155926	-612.06647804	-612.04083001
1.10	-612.06577751	-612.03893386	-612.06513235	-612.03826924
1.15	-612.06427846	-612.03622792	-612.06368900	-612.03561996
1.20	-612.06269152	-612.03343286	-612.06215099	-612.03287470
1.25	-612.06101619	-612.03054830	-612.06051892	-612.03003422
1.30	-612.05925031	-612.02757255	-612.05879141	-612.02709759
1.35	-612.05739315	-612.02450508	-612.05696843	-612.02406502
1.40	-612.05544306	-612.02134360	-612.05504902	-612.02093484
1.45	-612.05339962	-612.01808859	-612.05303311	-612.01770801
1.50	-612.05126094	-612.01473746	-612.05091927	-612.01438230