

**A computational study for the reaction mechanism of 2,2-azobis(isobutyronitrile)-initiated
oxidative cleavage of the geminal alkenes**

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1. The Optimized Geometries of The Transition States with Selected Interatomic Distances

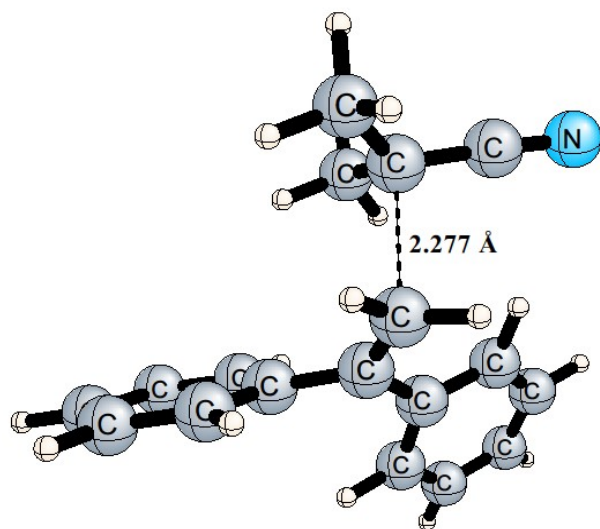


Figure S1. Computed structure of TS3a-4a at the B3LYP/6-311G(d,p) level (im. freq. = 452*i*).

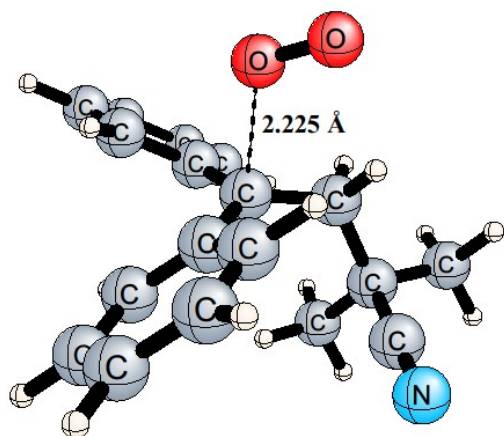


Figure S2. Computed structure of TS4a-5a at the B3LYP/6-311G(d,p) level (im. freq. = 161*i*).

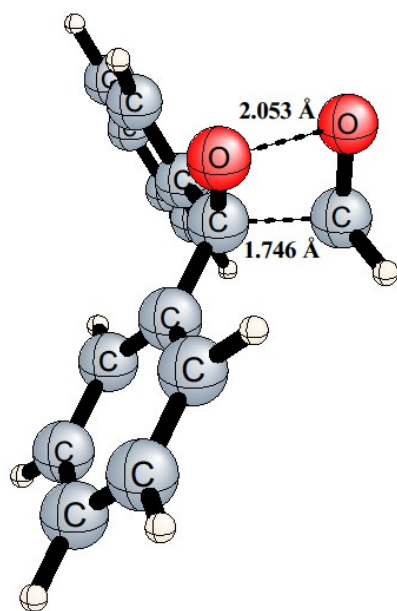


Figure S3. Computed structure of TS6a-8a at the B3LYP/6-311G(d,p) level (im. freq. = 1434*i*).

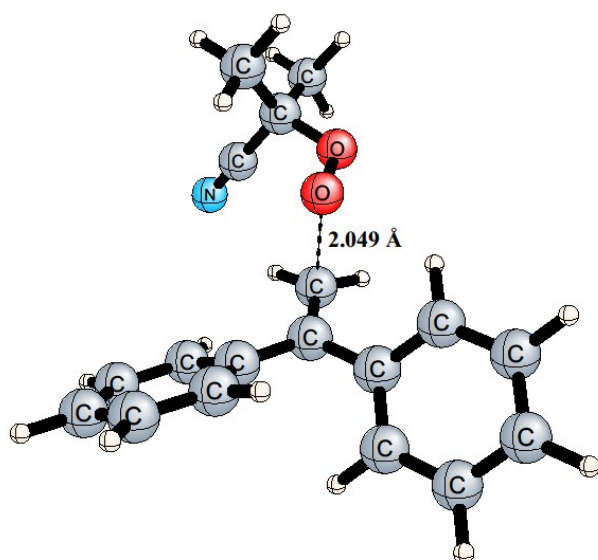


Figure S4. Computed structure of TS9-10a at the B3LYP/6-311G(d,p) level (im. freq. = 365*i*).

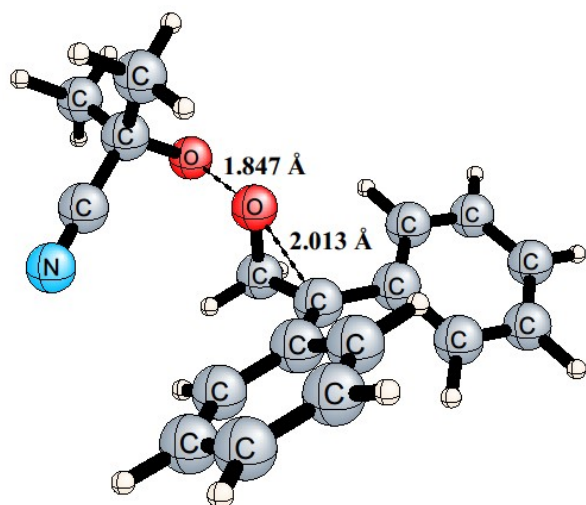


Figure S5. Computed structure of TS10a/11a at the B3LYP/6-311G(d,p) level (im. freq. = 469*i*).

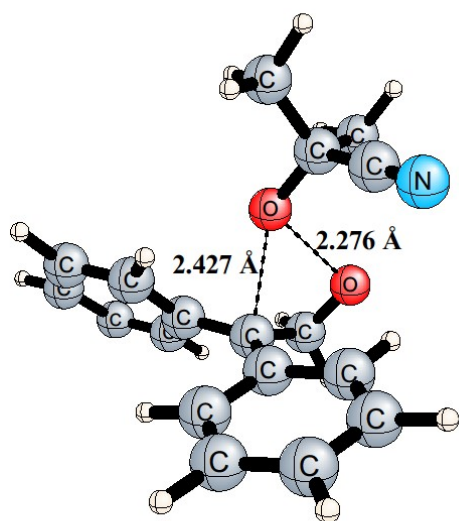


Figure S6. Computed structure of TS10a-15a at the B3LYP/6-311G(d,p) level (im. freq. = 117*i*).

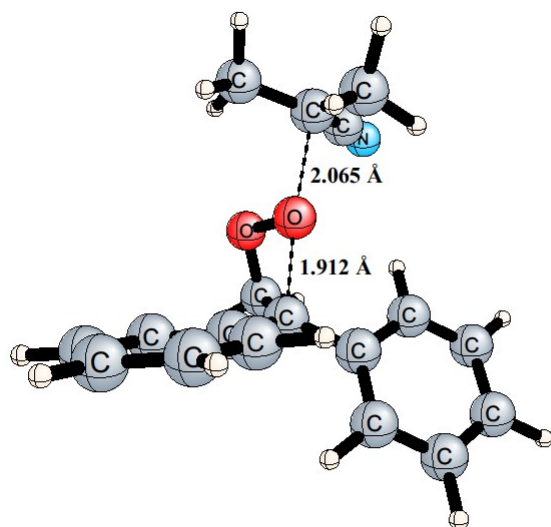


Figure S7. Computed structure of TS10a-6a at the B3LYP/6-311G(d,p) level (im. freq. = 727*i*).

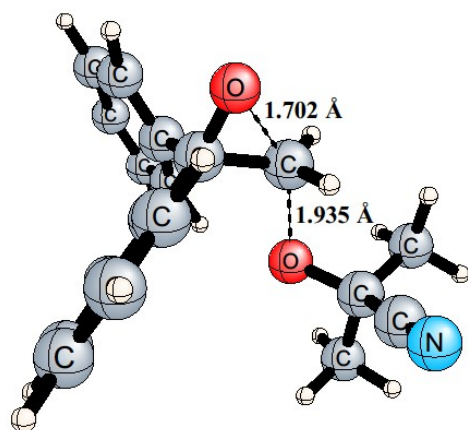


Figure S8. Computed structure of TS11a-13a at the B3LYP/6-311G(d,p) level (im. freq. = 835*i*).

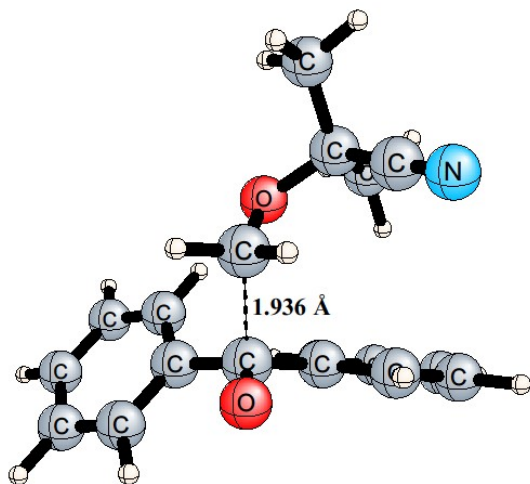


Figure S9. Computed structure of TS13a-14 at the B3LYP/6-311G(d,p) level (im. freq. = 290*i*).

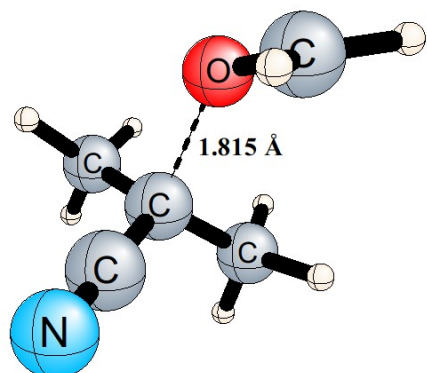


Figure S10. Computed structure of TS14-7 at the B3LYP/6-311G(d,p) level (im. freq. = 609*i*).

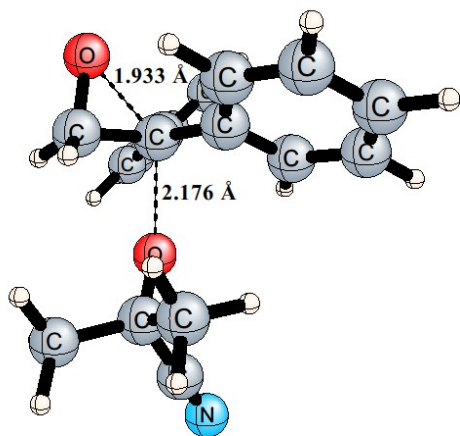


Figure S11. Computed structure of TS11a-15a at the B3LYP/6-311G(d,p) level (im. freq. = 552*i*).

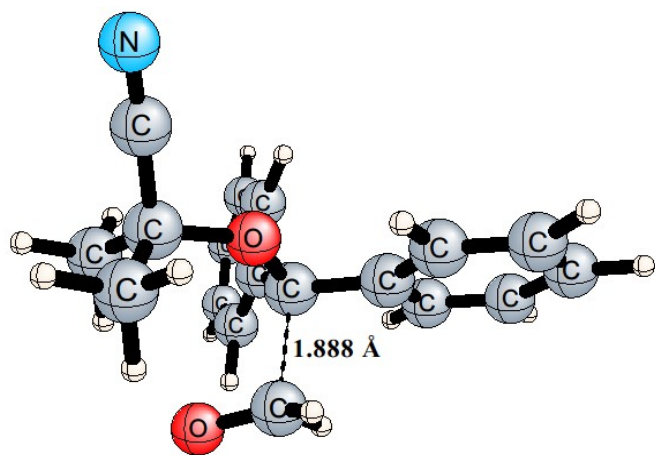


Figure S12. Computed structure of TS15a-16a at the B3LYP/6-311G(d,p) level (im. freq. = 305*i*).

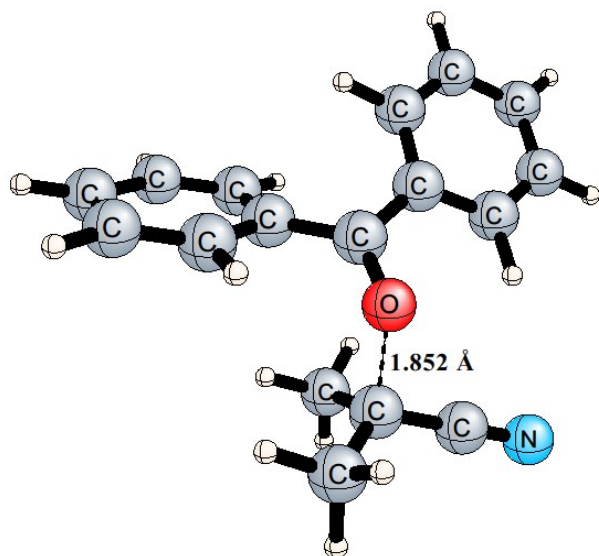


Figure S13. Computed structure of TS16a-8a at the B3LYP/6-311G(d,p) level (im. freq. = 573*i*).

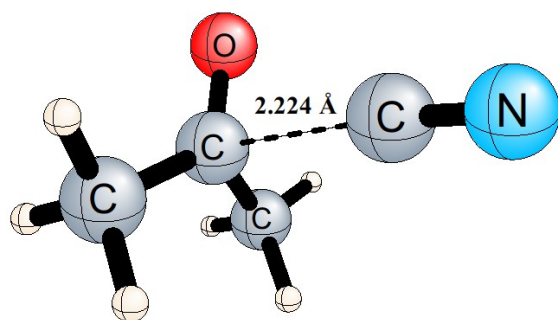


Figure S14. Computed structure of TS12-17 at the B3LYP/6-311G(d,p) level (im. freq. = 300*i*).

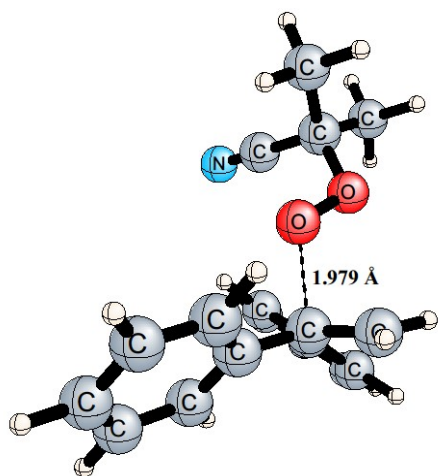


Figure S15. Computed structure of TS18a-3a at the B3LYP/6-311G(d,p) level (im. freq. = 304*i*).

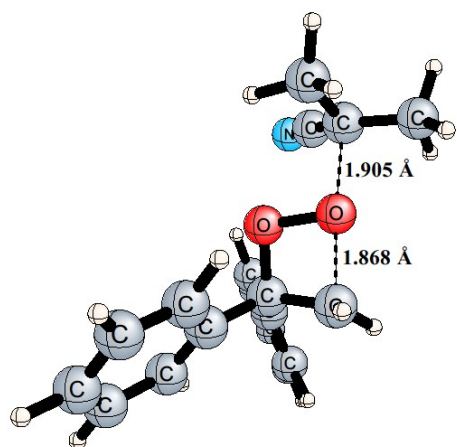


Figure S16. Computed structure of TS18a-6a at the B3LYP/6-311G(d,p) level (im. freq. = 888*i*).

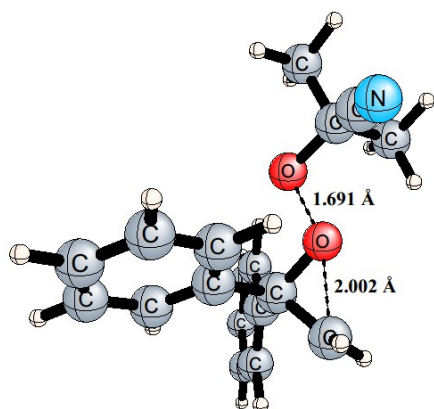


Figure S17. Computed structure of TS18a-11a at the B3LYP/6-311G(d,p) level (im. freq. = 597*i*).

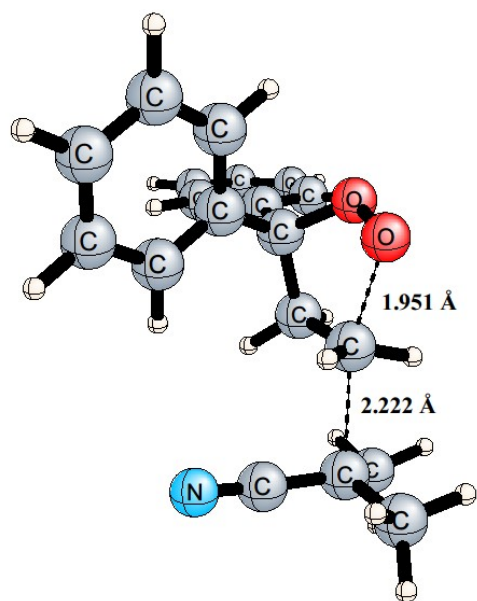


Figure S18. Computed structure of TS19-20 at the B3LYP/6-311G(d,p) level (im. freq. = 985*i*).

2. Solvent Corrected Relative Free Energy Profiles

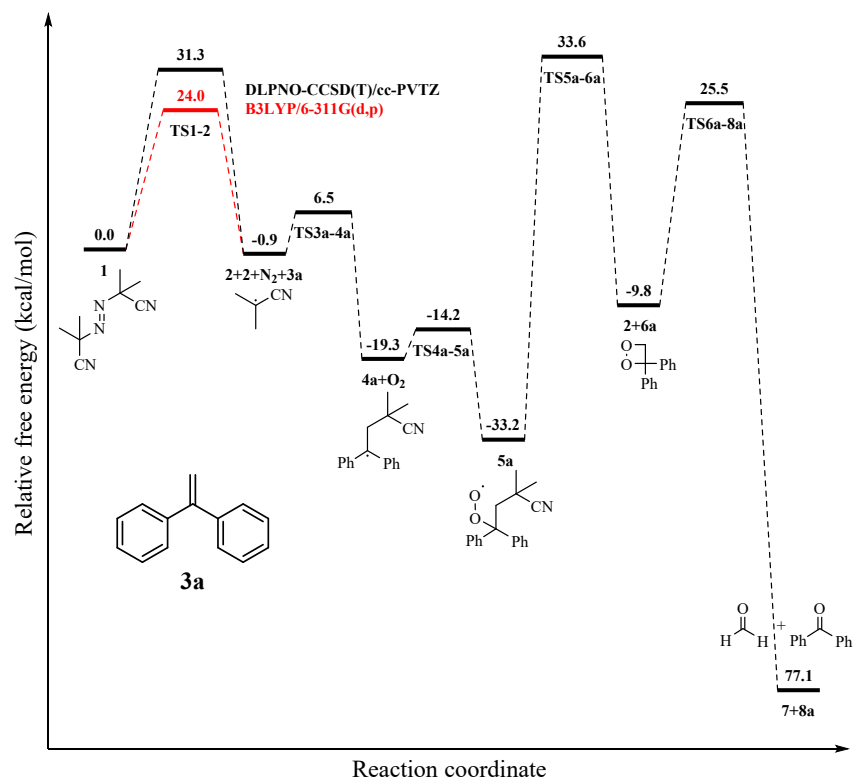


Figure S19. Solvent corrected (using PCM model) relative free energy profile (at 333.15 K) for reaction mechanism of **3a** shown in Scheme 1 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

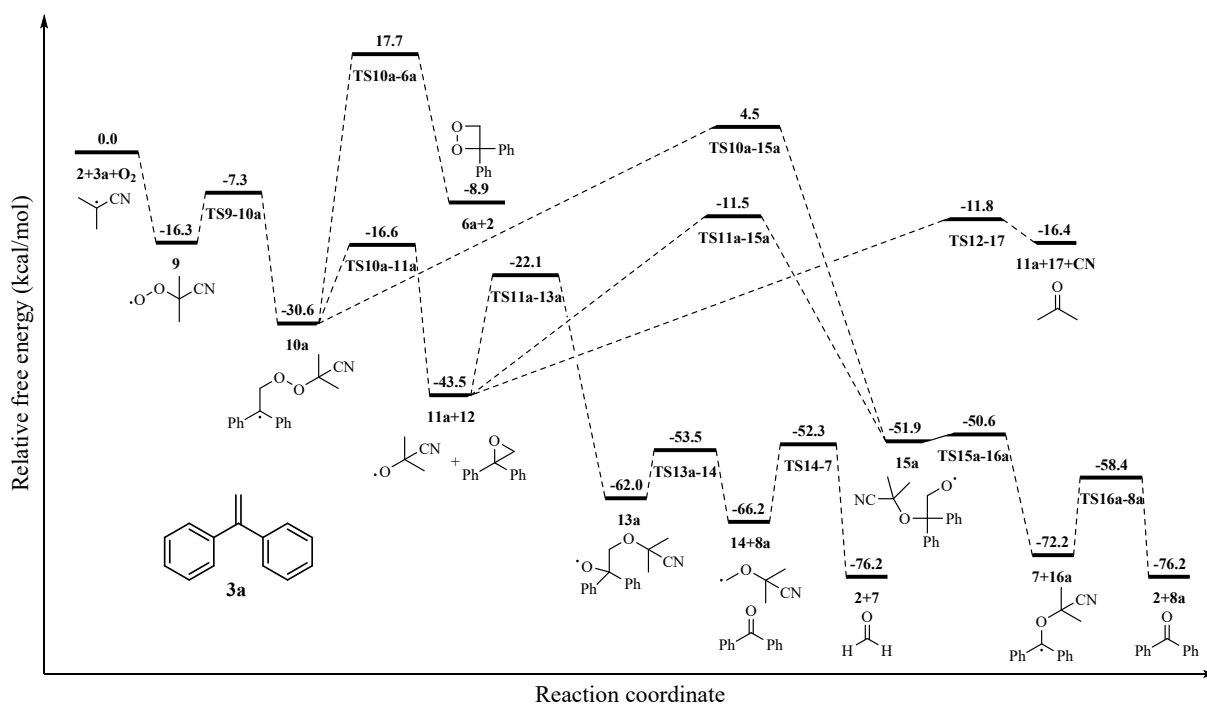


Figure S20. Solvent corrected (using PCM model) relative free energy profile (at 333.15 K) for reaction mechanism of **3a** shown in Scheme 2 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

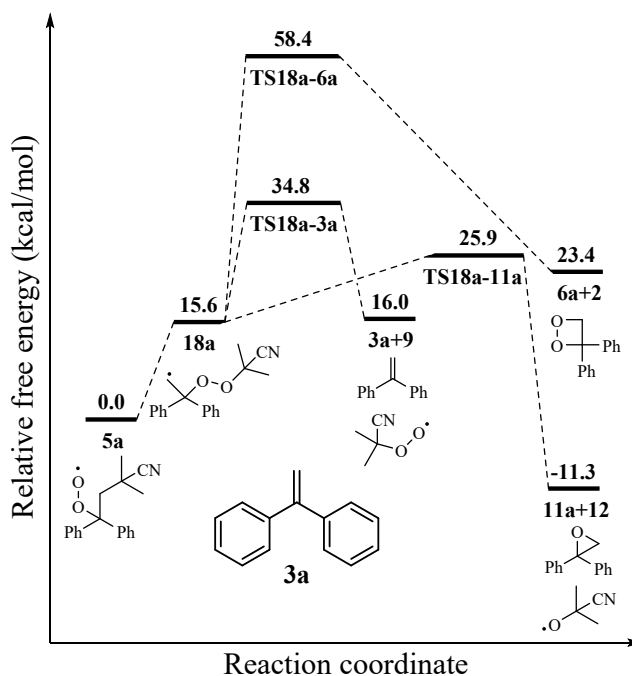


Figure S21. Solvent corrected (using PCM model) relative free energy profile (at 333.15 K) for reaction mechanism for converting of **5a** to **10a** shown in Scheme 3 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

3. Relative Energy Profiles

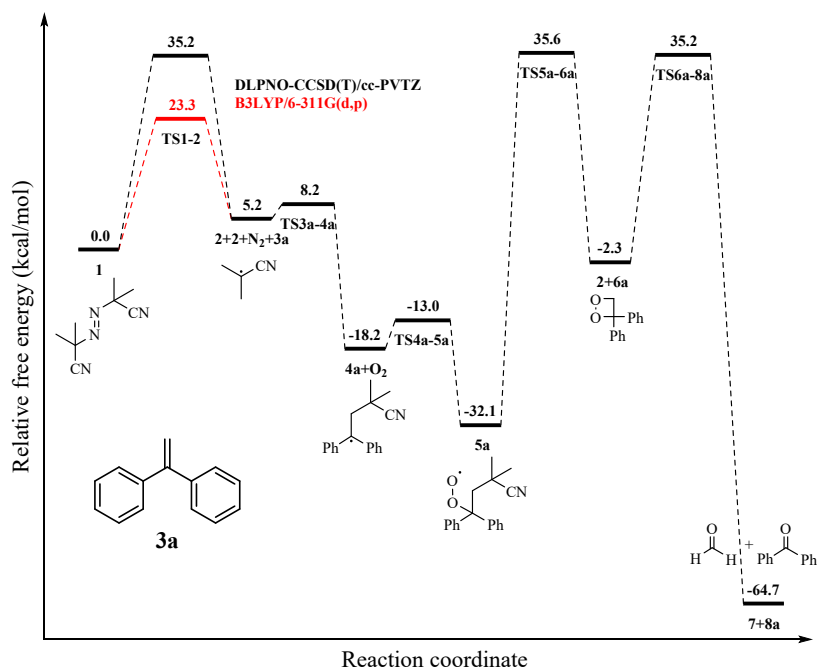


Figure S22. Relative energy profile for reaction mechanism of **3a** shown in Scheme 1 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

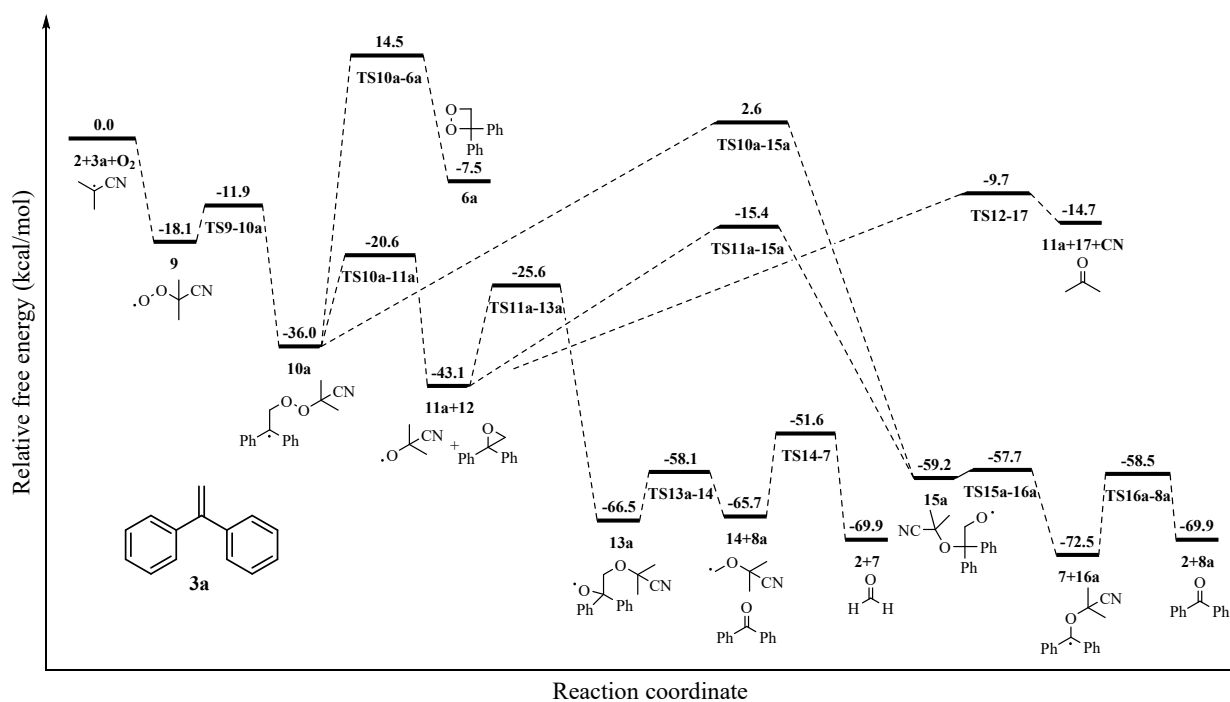


Figure S23. Relative energy profile for reaction mechanism of **3a** shown in Scheme 2 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

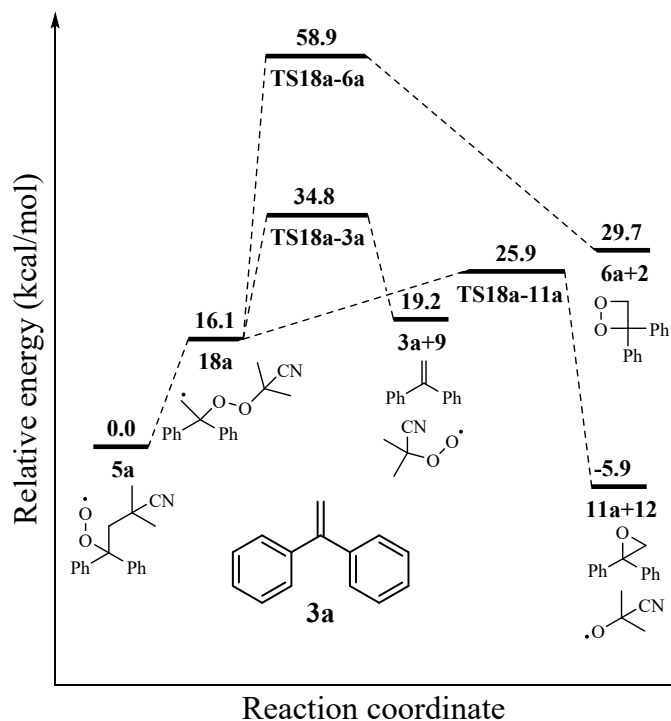


Figure S24. Relative energy profile for reaction mechanism for converting of **5a** to **10a** shown in Scheme 3 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

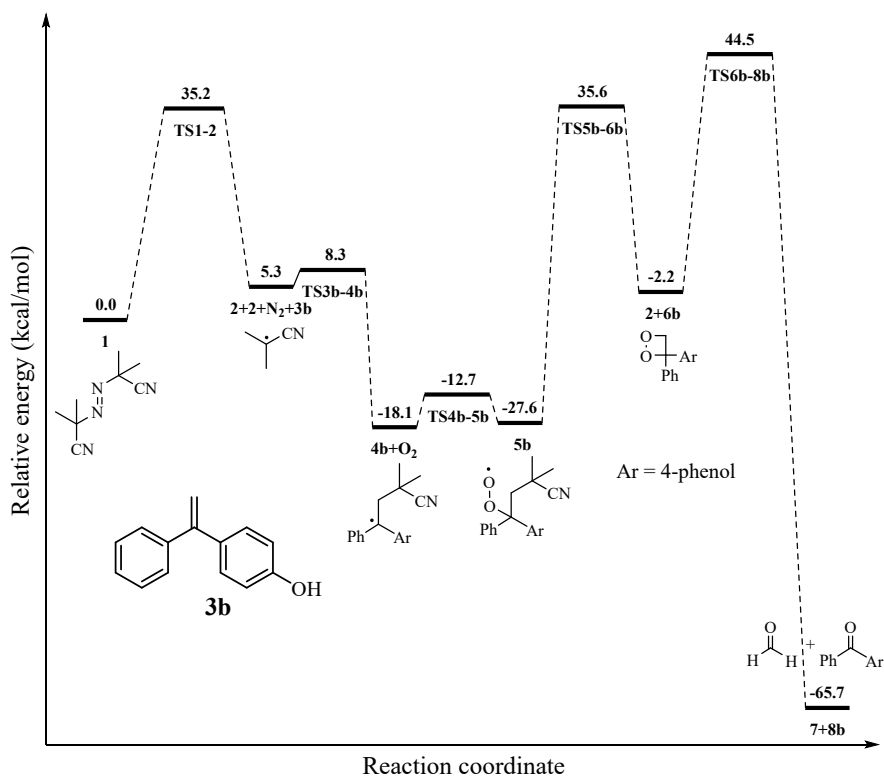


Figure S25. Relative energy profile for reaction mechanism of **3b** shown in Scheme 1 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

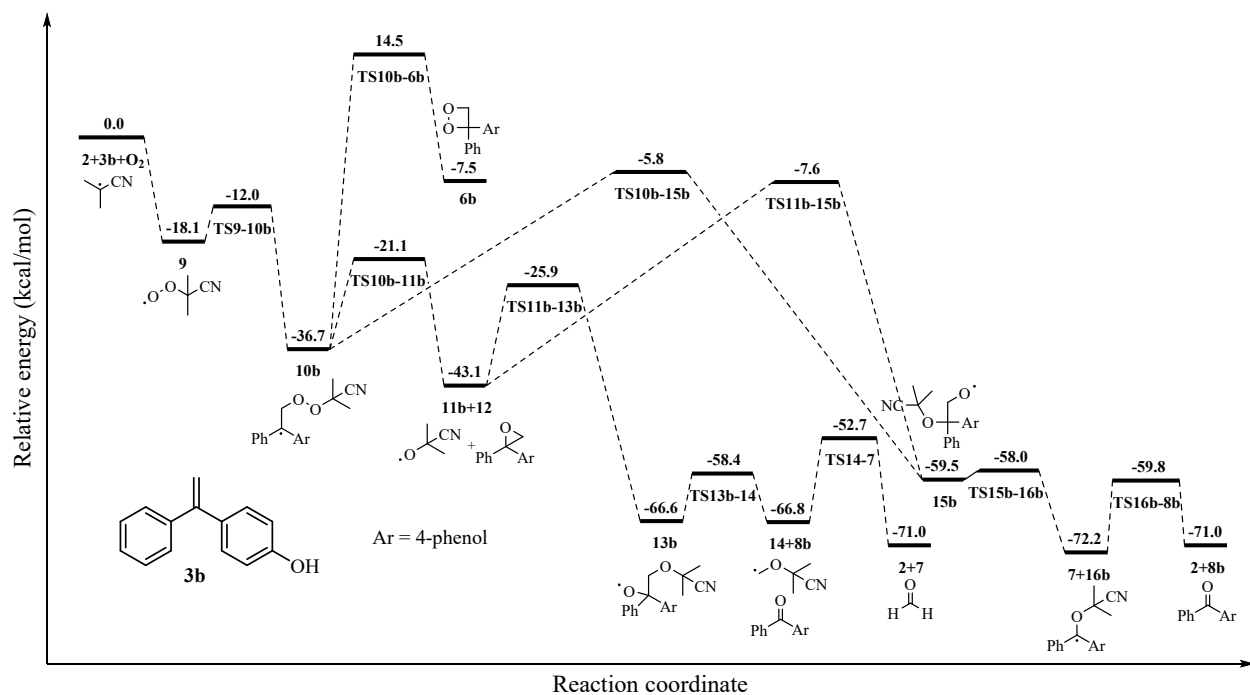


Figure S26. Relative energy profile for reaction mechanism of **3b** shown in Scheme 2 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

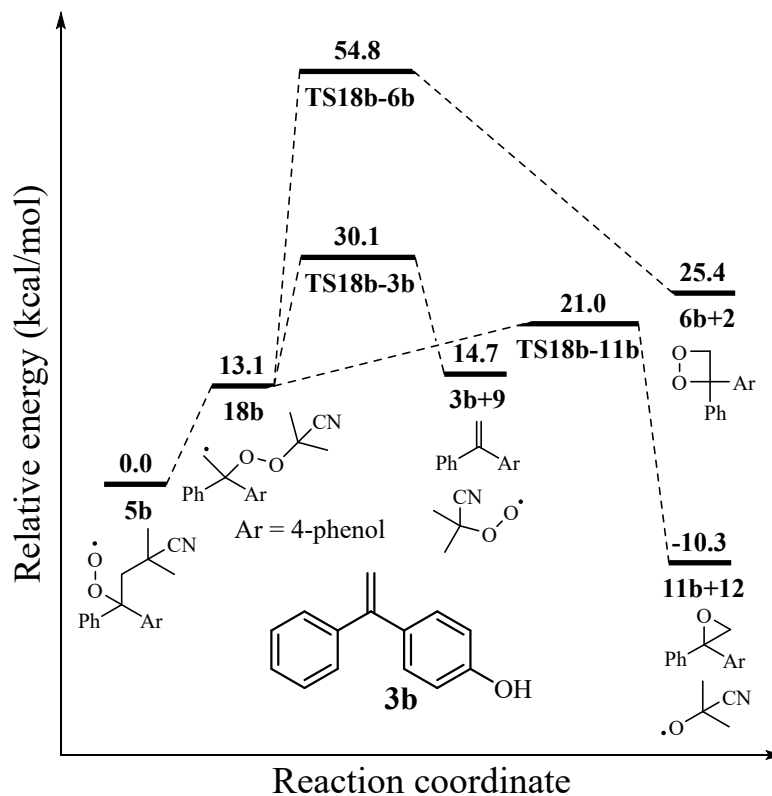


Figure S27. Relative energy profile for reaction mechanism for converting of **5b** to **10b** shown in Scheme 3 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

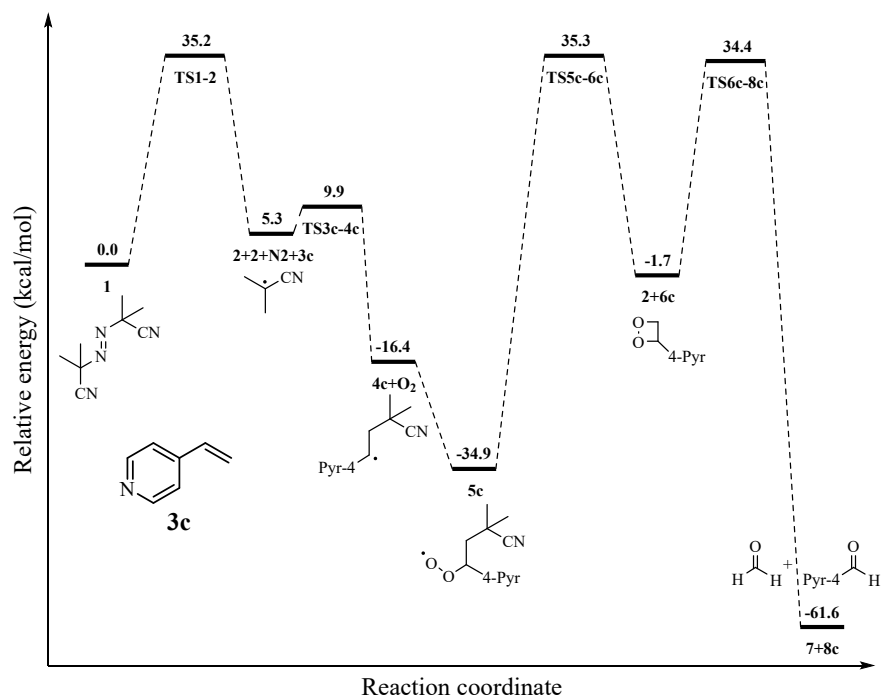


Figure S28. Relative energy profile for reaction mechanism of **3c** shown in Scheme 1 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

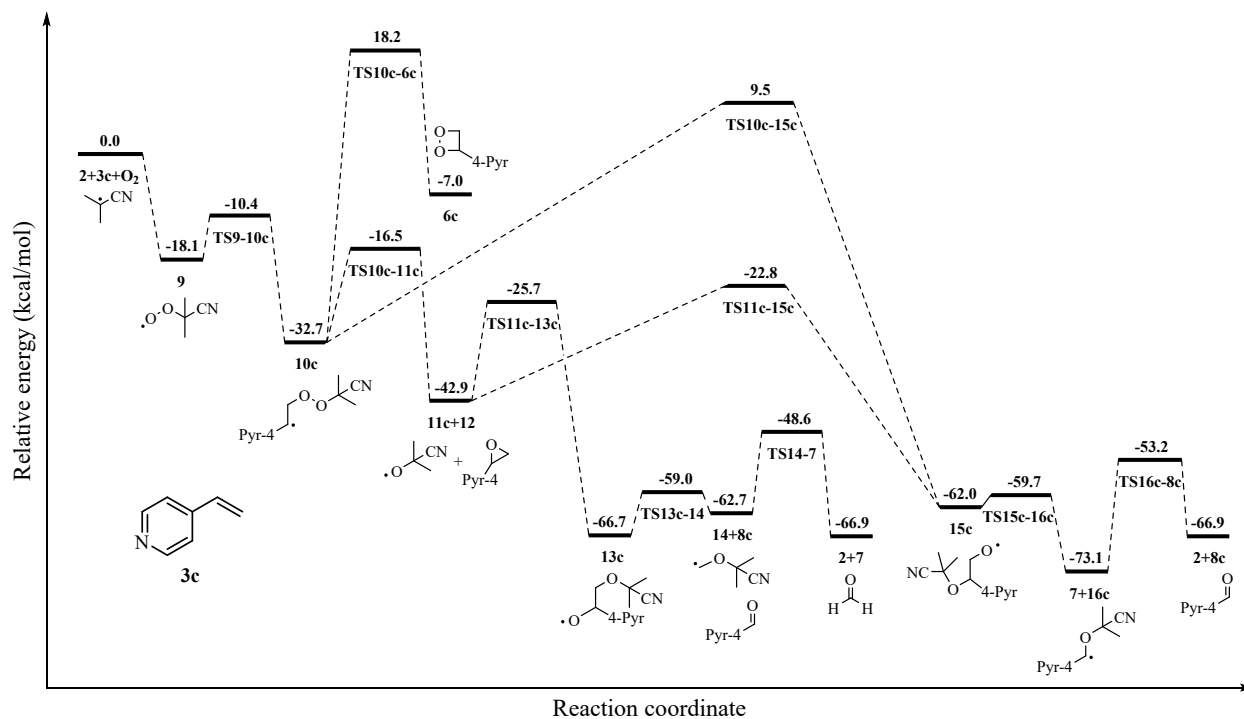


Figure S29. Relative energy profile for reaction mechanism of **3c** shown in Scheme 2 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

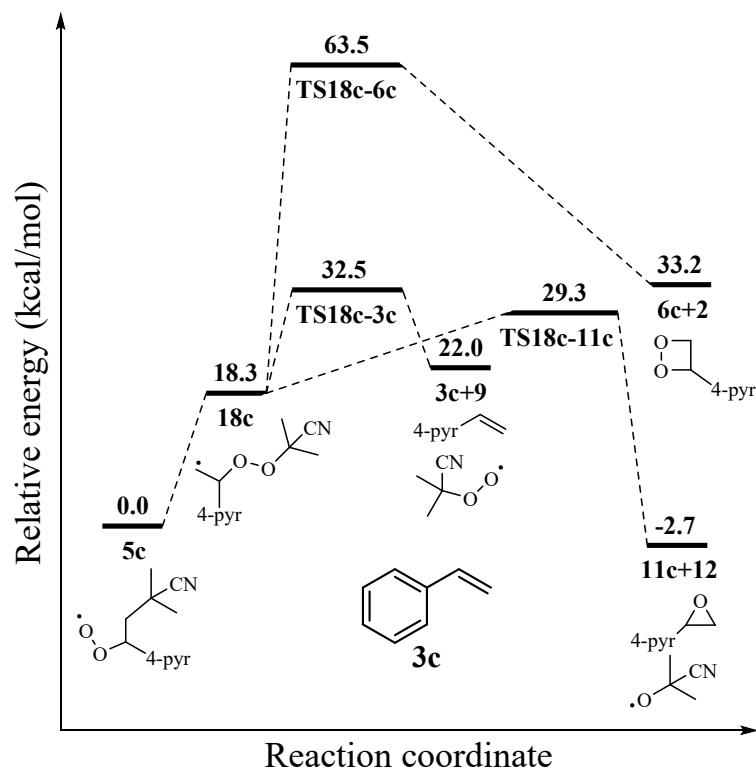


Figure S30. Relative energy profile for reaction mechanism for converting of **5c** to **10c** shown in Scheme 3 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

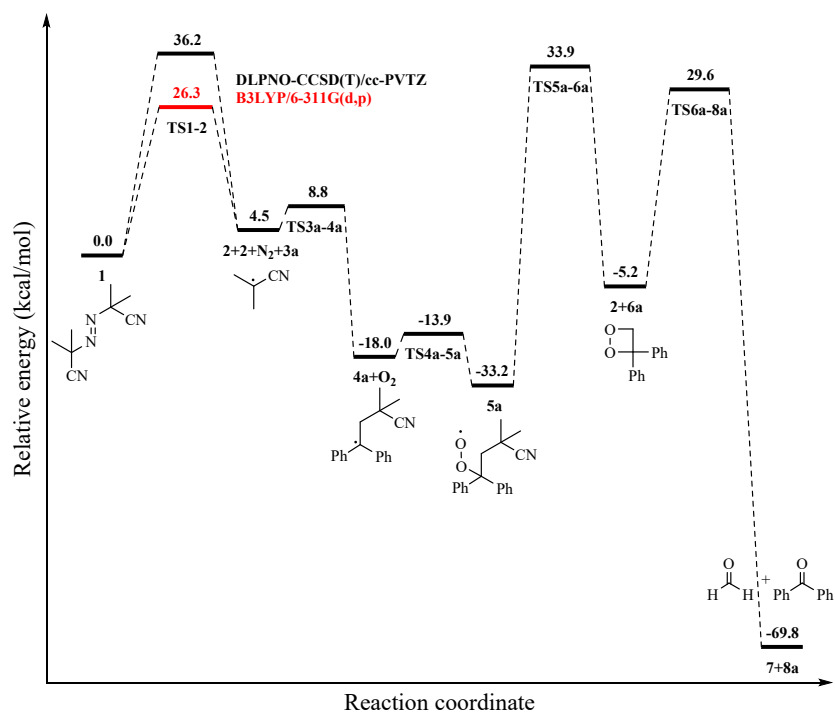


Figure S31. Solvent corrected (using PCM model) relative energy profile for reaction mechanism of **3a** shown in Scheme 1 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

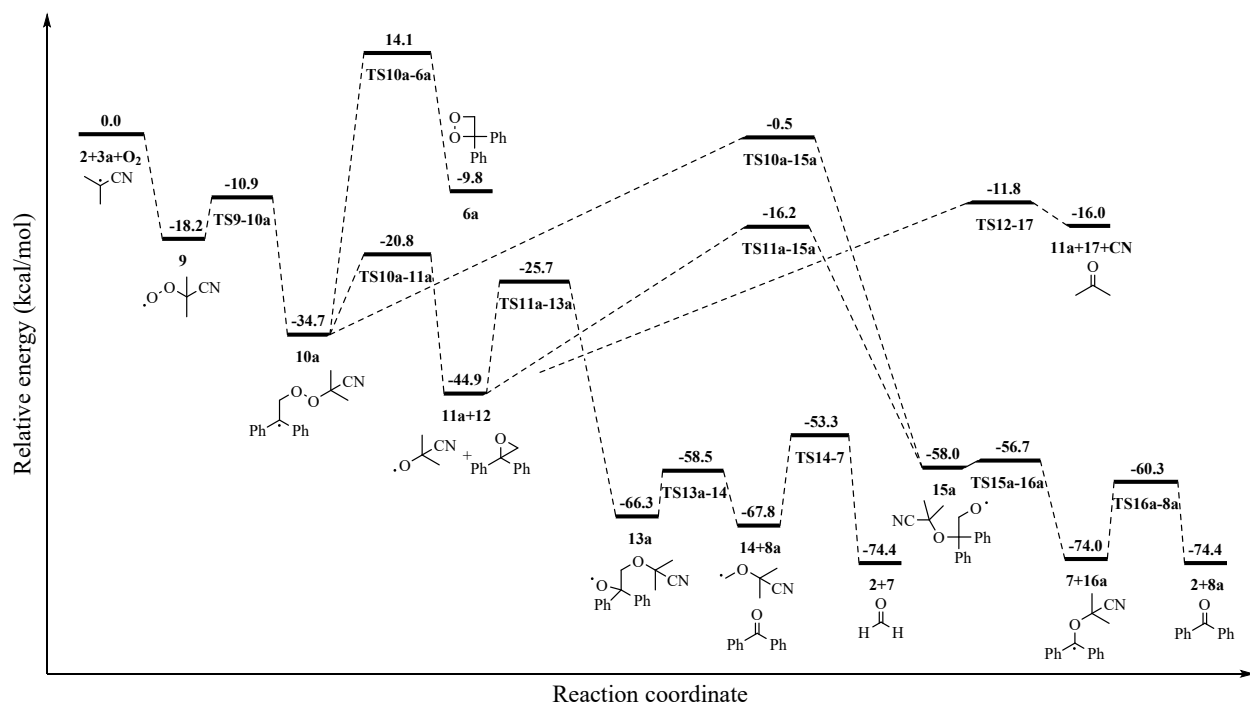


Figure S32. Solvent corrected (using PCM model) relative energy profile for reaction mechanism of **3a** shown in Scheme 2 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

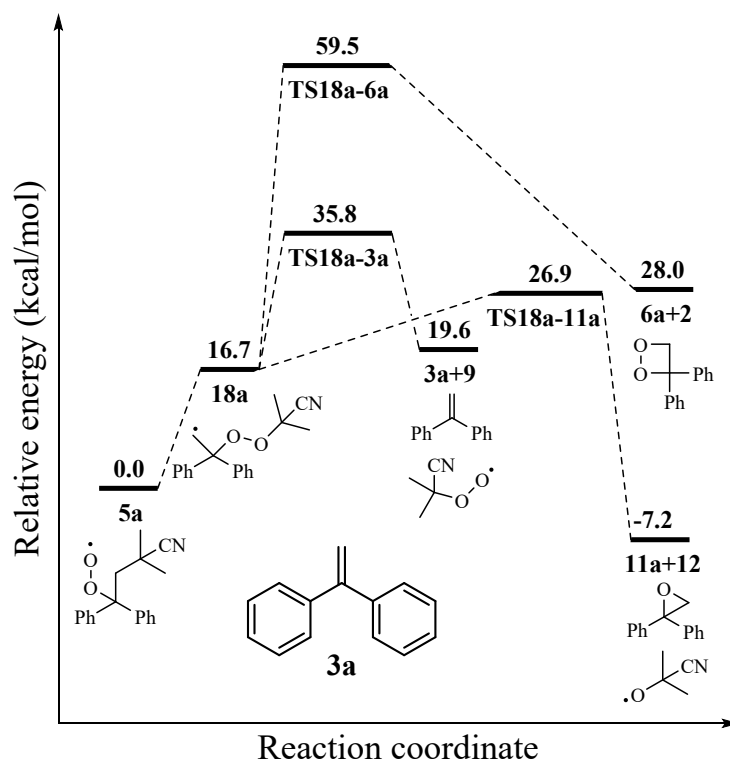


Figure S33. Solvent corrected (using PCM model) relative energy profile for reaction mechanism for converting of **5a** to **10a** shown in Scheme 3 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

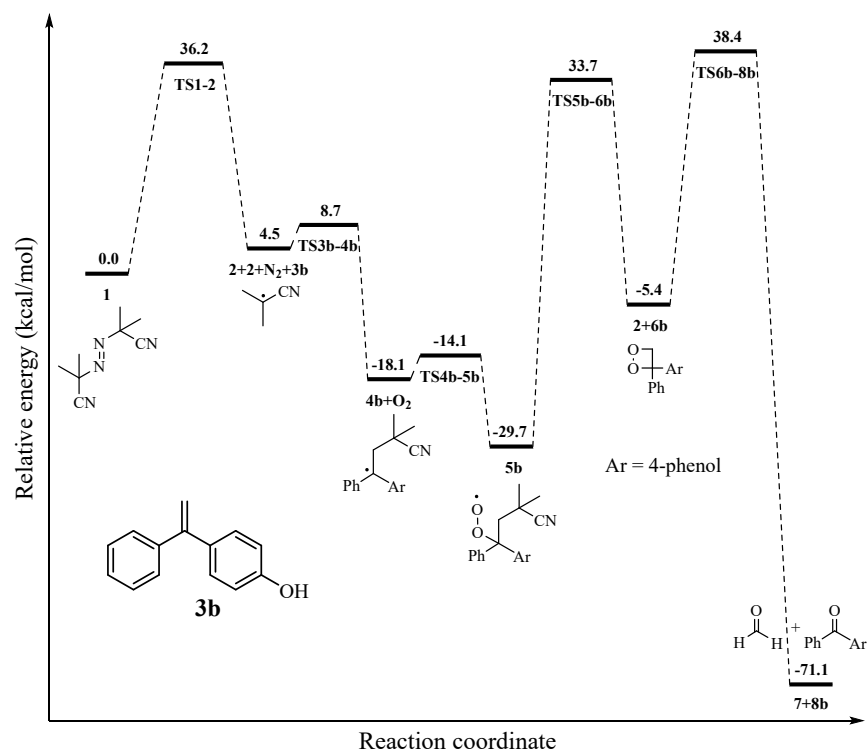


Figure S34. Solvent corrected (using PCM model) relative energy profile for reaction mechanism of **3b** shown in Scheme 1 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

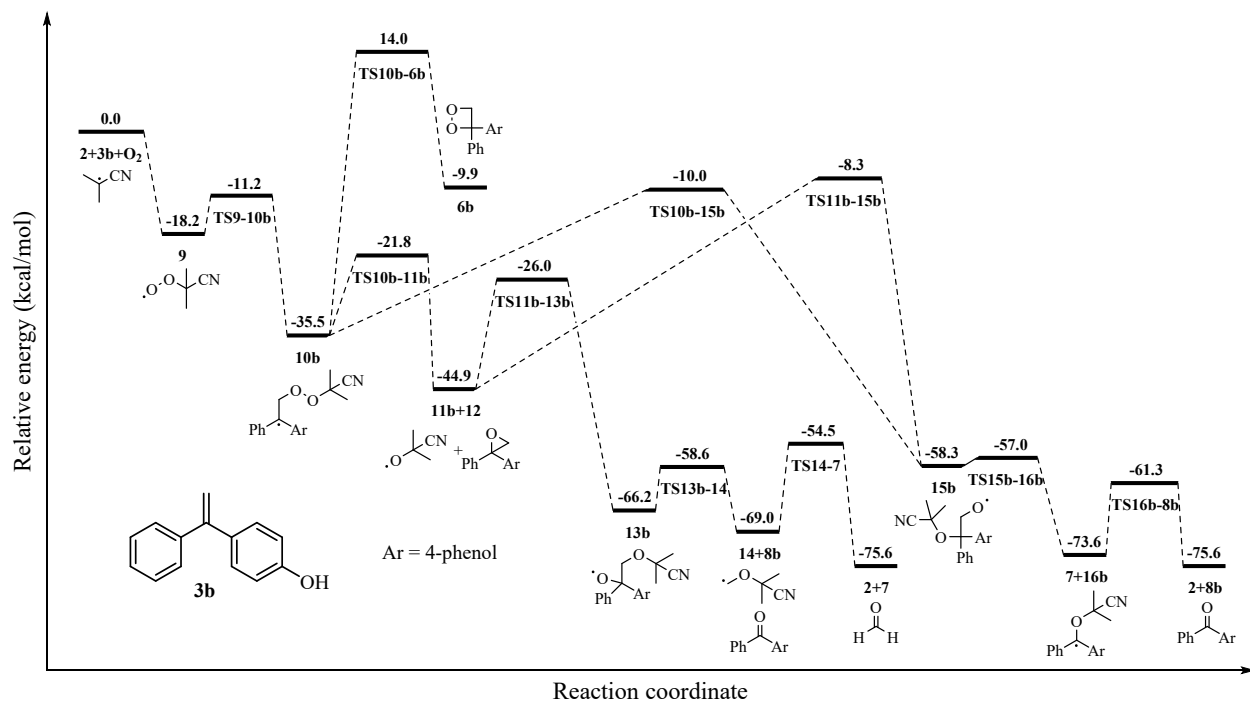


Figure S35. Solvent corrected (using PCM model) relative energy profile for reaction mechanism of **3b** shown in Scheme 2 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

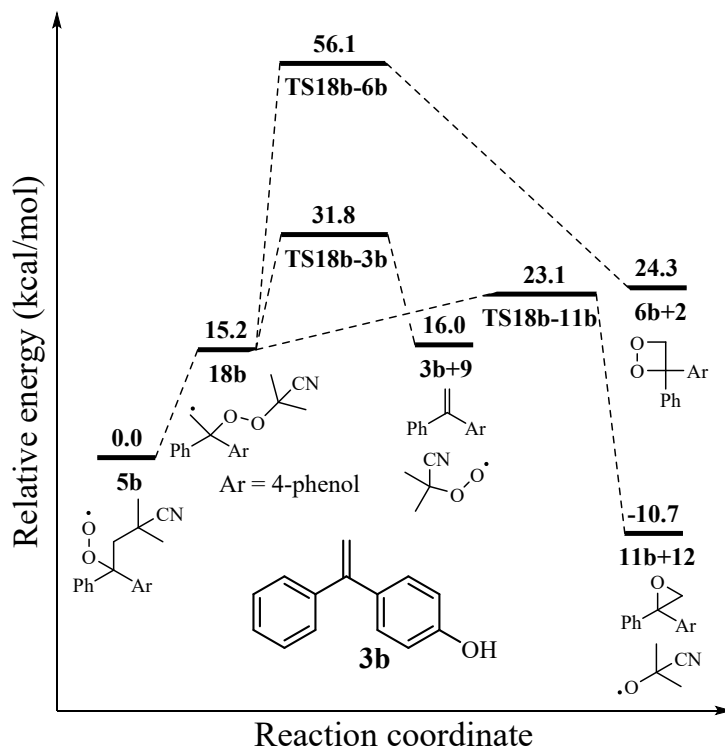


Figure S36. Solvent corrected (using PCM model) relative energy profile for reaction mechanism for converting of **5b** to **10b** shown in Scheme 3 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

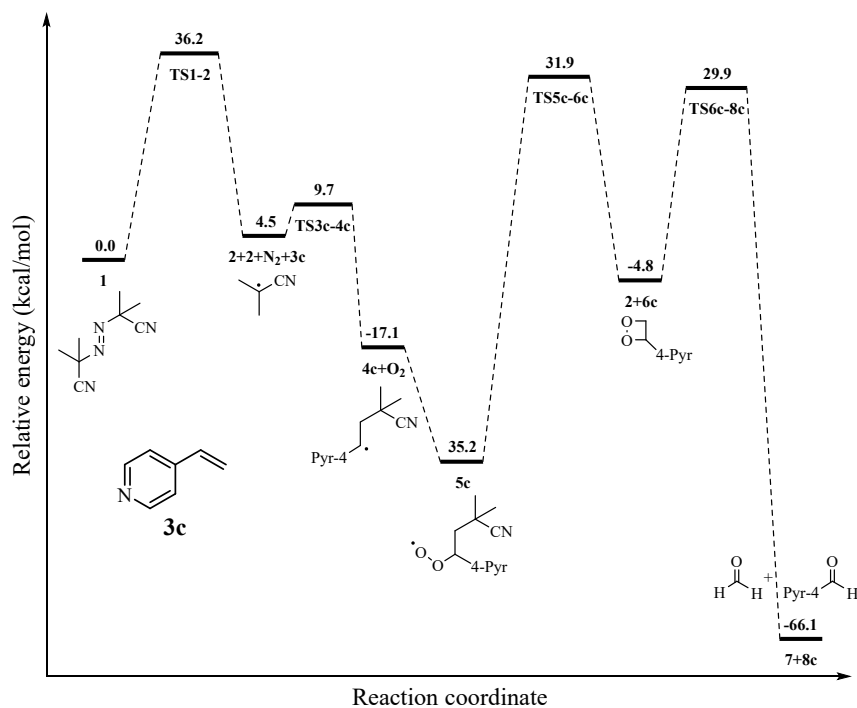


Figure S37. Solvent corrected (using PCM model) relative energy profile for reaction mechanism of **3c** shown in Scheme 1 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

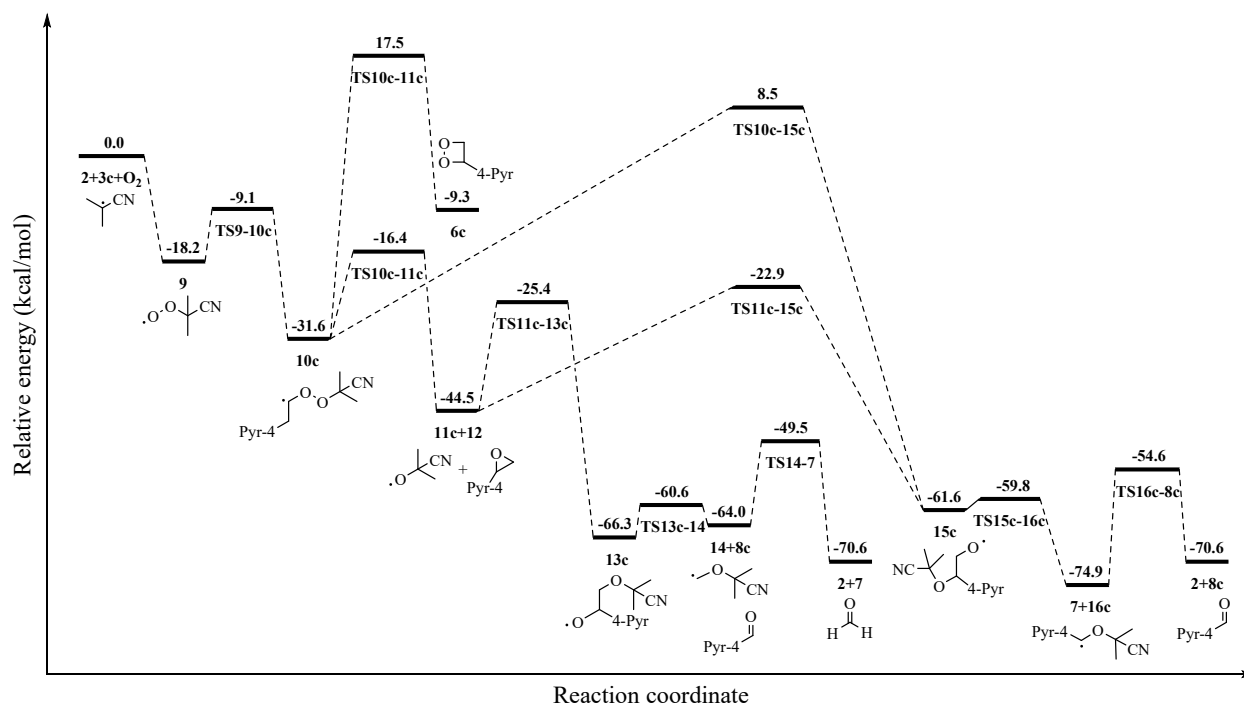


Figure S38. Solvent corrected (using PCM model) relative energy profile for reaction mechanism of **3c** shown in Scheme 2 at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

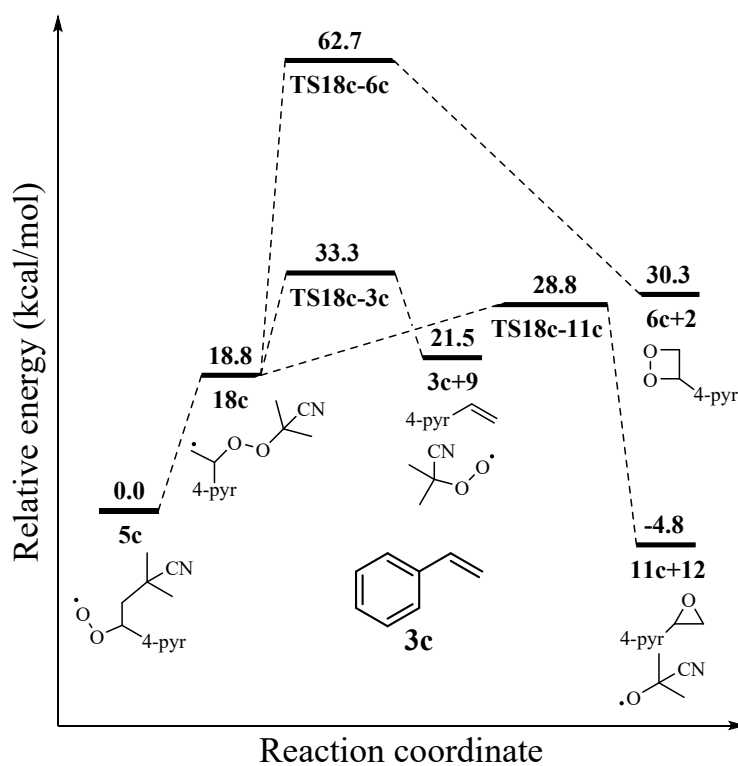


Figure S39. Solvent corrected (using PCM model) relative energy profile for reaction mechanism for converting of **5c** to **10c** shown in Scheme 3 computed at the DLPNO-CCSD(T)/cc-pVTZ//B3LYP/6-311G(d,p).

4. Single Point Energy Computations

Table S1. Single point energies (**E**) and free energies (**G(333.15 K, 1 atm)**) for **a** using DLPNO-CCSD(T)/cc-PVTZ level in a.u.

Molecule	E	G(333.15 K, 1 atm)	TS	E	G(333.15 K, 1 atm)
AIBN (1)	-530.09768247	-529.93249634	TS1-2	-530.03502899	-529.87992124
Nitrogen	-109.37281006	-109.37139554	TS14-7	-324.65836162	-324.56119613
Oxygen	-150.12809596	-150.12886174	TS12-17	-285.39308522	-285.32256184
Formaldehyde (7)	-114.33285618	-114.31402731	TS3a-4a	-750.02224605	-749.75322057
Acetone (17)	-192.83458594	-192.76570154	TS4a-5a	-900.18922756	-899.91261462
CN radical	-92.56556998	-92.56560707	TS5a-6a	-900.10993707	-899.83519059
2	-210.35242102	-210.28074286	TS6a-8a	-689.75338886	-689.56121295
9	-360.51493419	-360.43533719	TS9-10a	-900.17824380	-899.90496216
12	-285.44921633	-285.37356388	TS10a-11a	-900.19246026	-899.91809159
14	-324.68399965	-324.58251949	TS10a-15a	-900.15525750	-899.87985186
3a	-539.67218522	-539.48236115	TS10a-6a	-900.13543429	-899.86305083
4a	-750.06755364	-749.79366155	TS11a-13a	-900.19973514	-899.92681469
5a	-900.22222782	-899.94245880	TS11a-15a	-900.18326525	-899.90896747
6a	-689.81771201	-689.62163547	TS13a-14	-900.25304975	-899.97641434
8a	-575.57854583	-575.41139180	TS15a-16a	-900.25212963	-899.97403484
10a	-900.21921067	-899.94266270	TS16a-8a	-785.91416996	-787.5531399
11a	-614.77730468	-614.58483712	TS18a-3a	-900.16185090	-899.88850406
13a	-900.26845372	-899.99095480	TS18a-6a	-900.123125003	-899.85049312
15a	-900.25568542	-899.97653188	TS18a-11a	-900.175624875	-899.90277497
16a	-785.93887864	-785.69061879	TS19-20	-939.378801716	-939.07767028
18a	-900.19248012	-899.91858973			
19	-939.466367244	-939.16269194			
20	-729.086263628	-728.86163171			

Table S2. Single point energies (**E**) for **b** using DLPNO-CCSD(T)/cc-PVTZ level in a.u.

Molecule	E	TS	E
3b	-614.80161876	TS3b-4b	-825.15167607
4b	-825.19699113	TS4b-5b	-975.31831986
5b	-975.34441286	TS5b-6b	-975.23950268
6b	-764.94693780	TS6b-8b	-764.88226137
8b	-650.70984700	TS9-10b	-975.30787967
10b	-975.34968060	TS10b-11b	-975.32277724
11b	-689.90675387	TS10b-15b	-975.29829612
13b	-975.39800025	TS11b-13b	-975.32975821
15b	-975.38549071	TS11b-15b	-975.30024119
16b	-861.06804140	TS13b-14	-975.38306566
18b	-975.31958563	TS15b-16b	-975.38210791
		TS16b-8b	-861.04574751
		TS18b-3b	-975.29176009
		TS18b-6b	-975.25152250
		TS18b-11b	-975.30568830

Table S3. Single point energies (**E**) for **c** using DLPNO-CCSD(T)/cc-PVTZ level in a.u.

Molecule	E	TS	E
3c	-325.08118040	TS3c-4c	-535.42839814
4c	-535.47346875	TS5c-6c	-685.52050073
5c	-685.63665968	TS6c-8c	-475.16464667
6c	-475.22652105	TS9-10c	-685.58492201
8c	-360.98225885	TS10c-11c	-685.59460553
10c	-685.62237856	TS10c-15c	-685.55208676
11c	-400.18664743	TS11c-13c	-685.61002510
13c	-685.67744580	TS11c-15c	-685.60495685
15c	-685.66998252	TS13c-14	-685.66330759
16c	-571.34883153	TS15c-16c	-685.66495242
18c	-685.60313254	TS16c-8c	-571.31432189
		TS18c-3c	-685.58009977
		TS18c-6c	-685.53011433
		TS18c-11c	-685.58444980

5. Cartesian coordinates for optimized structures

AIBN (1)

E= -531.1441143 a.u., number of negative frequencies = 0

0 1

N	-0.34561800	0.23795900	-0.20919900
N	0.43368600	-0.65041600	0.12292700
C	-1.78916100	-0.20137800	-0.26838500
C	1.86850200	-0.23166800	0.18421200
C	-2.26065500	0.17022700	-1.68848200
C	-2.03521000	-1.68062400	0.05594700
C	2.24066200	-0.22604100	1.67975800
C	2.66403000	-1.29435500	-0.59506200
C	-2.47497900	0.64902500	0.72037200
N	-3.02705100	1.29059600	1.50243100
C	2.10712200	1.09977400	-0.40315600
N	2.35644900	2.12329200	-0.86978100
H	-3.33468600	0.00517000	-1.78573700
H	-2.03747700	1.21557700	-1.90182300
H	-1.73837400	-0.45726100	-2.41401700
H	-3.10449200	-1.89089200	-0.00369000
H	-1.68033400	-1.93223100	1.05486600
H	-1.50800900	-2.30926600	-0.66304700
H	3.30350000	-0.01077100	1.80131800
H	1.66414300	0.53032500	2.21430800
H	2.02311000	-1.20616300	2.10797600
H	3.73298000	-1.08374000	-0.53579900
H	2.36865900	-1.30304300	-1.64563600
H	2.46684900	-2.27749100	-0.16459200

Nitrogen

E= -109.5559302 a.u., number of negative frequencies = 0

0 1

N	0.00000000	0.00000000	0.54772100
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N	0.00000000	0.00000000	-0.54772100
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Oxygen

E= -150.3647909 a.u., number of negative frequencies = 0

0 3

O	0.00000000	0.00000000	0.60281300
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O	0.00000000	0.00000000	-0.60281300
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Formaldehyde (7)

E= -114.5363414 a.u., number of negative frequencies = 0

0 1

C	0.52592200	0.00000000	-0.00000800
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O	-0.67402300	0.00000100	0.00000200
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H	1.11831800	-0.93863600	0.00001500
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H	1.11833500	0.93862600	0.00001500
---	------------	------------	------------

Acetone (17)

E= -193.2130249 a.u., number of negative frequencies = 0

0 1

C	-1.29145900	-0.61343800	-0.00153700
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C	0.00000000	0.18640400	-0.00000400
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C	1.29146200	-0.61343400	0.00153600
---	------------	-------------	------------

O	-0.00000300	1.39551800	0.00000100
---	-------------	------------	------------

H	-1.30298200	-1.33200400	-0.82677700
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H	-1.37502200	-1.19084900	0.92512700
---	-------------	-------------	------------

H	-2.14147900	0.06217800	-0.08539800
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H	1.30299900	-1.33196200	0.82681100
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H	1.37501400	-1.19088600	-0.92510200
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H	2.14147900	0.06218900	0.08536000
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Radical 2

E= -210.7949653 a.u., number of negative frequencies = 0

0 2

C	0.30682500	0.00000000	-0.00000200
C	-1.08094500	0.00000300	-0.00000100
C	1.06166400	-1.29491900	-0.00000200
C	1.06167000	1.29491600	0.00000300
N	-2.24933300	0.00000100	0.00000100
H	0.39643900	2.15793300	0.00020000
H	1.71413700	-1.36050300	0.87983100
H	0.39642900	-2.15793300	-0.00020100
H	1.71444800	-1.36032000	-0.87961500
H	1.71445200	1.36031400	0.87961700
H	1.71414500	1.36049700	-0.87982900

CN radical

E= -92.7368676 a.u., number of negative frequencies = 0

Peroxyl radical 9

E= -361.1838283 a.u., number of negative frequencies = 0

0 2

C	-0.07362600	0.22871700	0.00000900
C	-1.44791500	-0.28681400	-0.00000700
C	0.22698500	1.00682200	-1.27992600
C	0.22701000	1.00665700	1.28003400
N	-2.53865200	-0.65696000	-0.00001500
O	0.75583100	-1.02798000	-0.00010100
O	2.03878900	-0.76183600	-0.00001700
H	1.28147300	1.28341200	-1.28204800

H	0.01097600	0.39850800	-2.15899700
H	-0.38304600	1.91086700	-1.31748700
H	1.28149600	1.28324800	1.28217900
H	0.01101200	0.39823600	2.15903500
H	-0.38302600	1.91069400	1.31771000

Alkoxy radical 12

E= -2860012447 a.u., number of negative frequencies = 0

0 2

C	-0.28950100	0.00000000	0.10550300
C	1.19839700	0.00000000	-0.00696200
C	-0.85993900	1.27738800	-0.57053200
C	-0.85993800	-1.27738900	-0.57053000
N	2.34763700	0.00000000	-0.09407400
O	-0.70094800	0.00000100	1.41118000
H	-1.94818700	1.25055800	-0.51453100
H	-0.49218200	2.16726800	-0.05958500
H	-0.53962400	1.30815200	-1.61378900
H	-1.94818600	-1.25056000	-0.51452800
H	-0.49218000	-2.16726900	-0.05958200
H	-0.53962500	-1.30815400	-1.61378800

14

E= -325.3183711 a.u., number of negative frequencies = 0

0 2

C	2.14139800	-0.72972700	0.00550200
O	0.79727700	-0.94083700	-0.06925000
C	-0.07704100	0.20586600	0.01274100
C	-1.43274000	-0.38166300	-0.02270700
C	0.09357700	1.12971100	-1.20539600
C	0.11347700	0.95126400	1.34384100

N	-2.50774700	-0.79414900	-0.04754300
H	2.70495700	-1.64847100	-0.06706900
H	2.55629300	0.20819800	-0.34537300
H	-0.67731000	1.90214900	-1.19870900
H	1.06780700	1.62017100	-1.18063900
H	0.00658100	0.55402800	-2.12771400
H	-0.62078900	1.75352400	1.43593500
H	-0.00853100	0.26173600	2.17986900
H	1.11497600	1.38169400	1.38660800

3a

E= -540.8340590 a.u., number of negative frequencies = 0

0 1

C	1.27997600	0.39046600	-0.03971800
C	0.00000000	1.15338400	0.00000000
C	-1.27997600	0.39046600	0.03971800
C	0.00000000	2.49538100	0.00000000
C	1.41234600	-0.74841200	-0.84834400
C	2.62175400	-1.43203600	-0.92546500
C	3.72122800	-1.00092400	-0.18526600
C	3.60019500	0.11923300	0.63411000
C	2.39170400	0.80620800	0.70710800
C	-2.39170500	0.80620900	-0.70710800
C	-3.60019600	0.11923300	-0.63411000
C	-3.72122800	-1.00092500	0.18526700
C	-2.62175300	-1.43203600	0.92546500
C	-1.41234500	-0.74841200	0.84834400
H	-0.92082900	3.06076500	0.07798000
H	0.92082900	3.06076500	-0.07797800
H	0.56336700	-1.09051900	-1.42863700
H	2.70610200	-2.30316600	-1.56579000

H	4.66139400	-1.53802000	-0.24082700
H	4.44520600	0.45408000	1.22561000
H	2.29681600	1.66336100	1.36370400
H	-2.29681700	1.66336100	-1.36370400
H	-4.44520700	0.45408000	-1.22561000
H	-4.66139400	-1.53802000	0.24082800
H	-2.70610200	-2.30316700	1.56579000
H	-0.56336600	-1.09051900	1.42863600

4a

E= -751.6499289 a.u., number of negative frequencies = 0

0 2

C	-1.38423200	0.60879700	-0.30578300
C	-0.06071500	0.05308600	-0.48137400
C	1.13756200	0.85672800	-0.20665400
C	0.11477600	-1.33787100	-1.04194200
C	-2.54085300	-0.20779000	-0.20440600
C	-3.80693600	0.34191900	-0.07220000
C	-3.98426500	1.72580500	-0.04872500
C	-2.86652000	2.55477200	-0.16277000
C	-1.59686900	2.01401300	-0.28799000
C	1.22520200	1.65250700	0.95692500
C	2.36695700	2.38981000	1.24451500
C	3.45852800	2.36967300	0.37658200
C	3.39314600	1.59599200	-0.78125500
C	2.25742200	0.84655800	-1.06432600
C	0.55025300	-2.49709100	-0.06961400
C	0.60665400	-3.81029500	-0.88612500
C	1.92227100	-2.23869100	0.58984300
C	-0.45014400	-2.66977000	0.99586300
N	-1.22854600	-2.83827700	1.83044700

H	-0.80370400	-1.65488700	-1.53923200
H	0.88614200	-1.32070000	-1.81961300
H	-2.44289600	-1.28408300	-0.18232800
H	-4.66339500	-0.31615000	0.02378400
H	-4.97602300	2.15102400	0.05288400
H	-2.98891000	3.63244200	-0.16669300
H	-0.75159700	2.67836300	-0.40958300
H	0.39325200	1.66168100	1.65058800
H	2.40802300	2.97774600	2.15485800
H	4.34777200	2.94777300	0.59987100
H	4.23009300	1.57985000	-1.47084800
H	2.22790800	0.26953900	-1.98103200
H	0.88697400	-4.65180400	-0.24965100
H	-0.35896500	-4.03434300	-1.34438100
H	1.35275800	-3.71416600	-1.67929500
H	2.20031900	-3.08611600	1.22059700
H	1.91292700	-1.34035000	1.20547900
H	2.68572200	-2.11679800	-0.18192400

5a

E= -902.0301403 a.u., number of negative frequencies = 0

0 2

C	1.77668200	-0.21331500	-0.05918600
C	0.28861800	-0.31381400	0.30293900
C	-0.40133000	1.04294800	0.18469100
C	-0.43383900	-1.44666700	-0.45393200
C	2.42551900	-1.11421400	-0.90592700
C	3.78952300	-0.98678400	-1.17074600
C	4.52659100	0.03394700	-0.58186400
C	3.89121600	0.93212200	0.27508800
C	2.53074200	0.81137300	0.52881500

C	-1.09326700	1.63496100	1.24461700
C	-1.72141300	2.86844900	1.07273900
C	-1.66984500	3.52115300	-0.15336200
C	-0.97416800	2.93942000	-1.21165400
C	-0.33978800	1.71560300	-1.04121800
C	-1.95966200	-1.70936200	-0.27189900
O	0.24784100	-0.64386600	1.77762300
O	0.75435500	-1.81926300	2.05602500
C	-2.27809200	-3.01419200	-1.05138000
C	-2.39794200	-1.89112200	1.19916500
C	-2.77659900	-0.64777100	-0.88754000
N	-3.47233600	0.11762100	-1.39767800
H	-0.25453000	-1.28754100	-1.51961000
H	0.07146400	-2.37398200	-0.17546800
H	1.88407300	-1.92667700	-1.37094300
H	4.27231600	-1.69354100	-1.83615000
H	5.58682600	0.13056100	-0.78629900
H	4.45577300	1.73064500	0.74295700
H	2.04435000	1.51842700	1.18987400
H	-1.13629900	1.14539900	2.20754600
H	-2.25512100	3.31415700	1.90451200
H	-2.16704600	4.47506000	-0.28609300
H	-0.92695400	3.43882100	-2.17239200
H	0.21063900	1.28082900	-1.86787000
H	-3.34678500	-3.23147900	-1.01250100
H	-1.98483800	-2.93098200	-2.10005200
H	-1.73688000	-3.85042500	-0.60187100
H	-3.44465900	-2.20018000	1.23535900
H	-2.29308700	-0.97216300	1.77266100
H	-1.78814600	-2.66164500	1.67482700

6a

E= -691.2013629 a.u., number of negative frequencies = 0

0 1

C	-1.26881400	0.11130800	0.02447300
C	0.05339000	0.85270000	0.12874100
C	-1.84765100	-0.48366400	1.14894100
C	-3.04469400	-1.18828600	1.03967400
C	-3.67737200	-1.30091900	-0.19615700
C	-3.10778100	-0.70356300	-1.31879300
C	-1.91034900	-0.00123900	-1.21006200
C	1.28680900	-0.03147100	0.02980400
C	2.51859000	0.56652300	-0.27063200
C	3.67766600	-0.19776100	-0.34592500
C	3.62721300	-1.57280500	-0.12044400
C	2.40791700	-2.17626900	0.17130800
C	1.24356300	-1.41270700	0.23991600
C	0.06994200	1.96204200	1.19756400
O	-0.16619900	2.94520900	0.16600200
O	0.12753700	1.92814900	-0.87512900
H	-1.36399400	-0.40253700	2.11725400
H	-3.48423400	-1.64301100	1.92038900
H	-4.61153000	-1.84426400	-0.28206100
H	-3.59960000	-0.77891900	-2.28213900
H	-1.47651200	0.48258000	-2.07611600
H	2.55511200	1.63059400	-0.46786900
H	4.62098400	0.27984800	-0.58596600
H	4.53104100	-2.16874000	-0.17924200
H	2.35642000	-3.24636300	0.33800400
H	0.30025500	-1.89936200	0.45095100
H	-0.73272300	1.95298600	1.93604700
H	1.04350500	2.10699300	1.67332000

8a

E= -576.7744054 a.u., number of negative frequencies = 0

0 1

C	1.30233100	0.33899500	-0.02229600
C	0.00000400	1.08603100	0.00002400
C	-1.30232800	0.33900000	0.02231000
O	0.00000400	2.30521700	0.00004800
C	1.45127000	-0.91112400	-0.63601500
C	2.70217400	-1.52126100	-0.69396100
C	3.81054000	-0.89722100	-0.12652700
C	3.67140400	0.35084100	0.48243500
C	2.42907500	0.97051300	0.52138100
C	-2.42904500	0.97049900	-0.52144200
C	-3.67137800	0.35083200	-0.48252400
C	-3.81054500	-0.89720100	0.12649000
C	-2.70220600	-1.52122100	0.69400000
C	-1.45129700	-0.91109200	0.63607800
H	0.59634600	-1.39568100	-1.09109200
H	2.81077600	-2.48197900	-1.18438700
H	4.78186600	-1.37767700	-0.16410500
H	4.53434400	0.84104800	0.91875000
H	2.30671900	1.95060600	0.96565400
H	-2.30666900	1.95057400	-0.96575000
H	-4.53429700	0.84102200	-0.91889800
H	-4.78187500	-1.37765100	0.16404900
H	-2.81083400	-2.48191500	1.18446600
H	-0.59639300	-1.39563200	1.09121000

10a

E= -902.0396536 a.u., number of negative frequencies = 0

0 2

C	-2.09143900	-0.82771600	0.22506000
C	-0.90065200	-0.00432200	0.42110400
C	-1.97553700	-2.14975600	-0.25929000
C	0.34350800	-0.71142400	0.87801400
O	1.15426000	-0.92755200	-0.30218400
O	2.31427300	-1.72104600	0.12333500
C	3.50960200	-1.02285300	-0.24490700
C	4.62925100	-1.97079200	0.20780600
C	3.59326100	0.24538200	0.52041400
C	3.56083500	-0.73931800	-1.75058000
C	-3.09426700	-2.95649800	-0.41900900
C	-4.36233900	-2.48022300	-0.08534200
C	-4.49782000	-1.18317500	0.40944400
C	-3.38374800	-0.36715700	0.55934200
N	3.66022300	1.22317100	1.12721200
C	-0.86562300	1.41414900	0.14633600
C	0.16898200	2.24997000	0.64185400
C	0.19817700	3.60717000	0.36143500
C	-0.79000200	4.19230100	-0.43187700
C	-1.80531000	3.38947100	-0.95504100
C	-1.84411500	2.03226200	-0.67742500
H	-0.99918600	-2.52255900	-0.54550700
H	0.10690700	-1.68043300	1.32061000
H	0.91615400	-0.12785400	1.60217700
H	5.60314500	-1.52562500	-0.00176000
H	4.53912500	-2.91071000	-0.33868900
H	4.55248000	-2.17046800	1.27697600
H	3.50363200	-1.68787100	-2.28803600
H	4.49409700	-0.23552100	-2.01101700
H	2.72273600	-0.11118300	-2.04734600

H	-2.97775800	-3.96140600	-0.80965300
H	-5.23359400	-3.11409300	-0.20430700
H	-5.47614300	-0.80923400	0.69070100
H	-3.50087200	0.62666400	0.97332600
H	0.96104000	1.83885000	1.25208400
H	1.00311400	4.21214500	0.76320400
H	-0.76143200	5.25354300	-0.65057300
H	-2.56385600	3.82391100	-1.59701300
H	-2.61600100	1.42360500	-1.12890500

11a

E= -616.0494443 a.u., number of negative frequencies = 0

0 1

C	1.28790100	0.15186300	-0.07963700
C	0.03562300	0.97974500	-0.23014800
C	1.31466300	-1.19898700	-0.44105200
O	0.10548700	2.28231300	0.37995100
C	2.48977600	-1.93813400	-0.32652200
C	3.65051200	-1.34213200	0.16035100
C	3.62715400	-0.00027300	0.53533500
C	2.45553500	0.74175700	0.41737900
C	-1.28674900	0.28182600	-0.05464600
C	-1.96744400	-0.26260600	-1.14619000
C	-3.18149600	-0.92342300	-0.96386300
C	-3.72755000	-1.03881300	0.31198800
C	-3.05675100	-0.48937200	1.40405300
C	-1.84222000	0.16524900	1.22206300
C	0.08154900	2.21279400	-1.04760700
H	0.41448300	-1.67873100	-0.80566100
H	2.49444900	-2.98408800	-0.61265400
H	4.56323200	-1.91982700	0.25350300

H	4.52217700	0.46994800	0.92768300
H	2.42732800	1.77983300	0.72471900
H	-1.54927800	-0.16561900	-2.14283300
H	-3.70220100	-1.34066500	-1.81856400
H	-4.67367300	-1.54868400	0.45470000
H	-3.48183900	-0.56935300	2.39834900
H	-1.32357500	0.60285000	2.06709000
H	-0.83054400	2.57735400	-1.51379700
H	1.01250800	2.48152500	-1.54116600

13a

E= -902.0838953 a.u., number of negative frequencies = 0

0 2

C	-1.54502100	-0.84341700	0.30887100
C	-0.56376300	0.14836200	0.94632000
C	-1.47893200	-1.16884800	-1.05001700
O	-0.94805500	0.55043700	2.20905100
C	-2.36536400	-2.09368800	-1.59499600
C	-3.32595600	-2.70670800	-0.79113400
C	-3.39632900	-2.38574700	0.56161500
C	-2.51085100	-1.45764900	1.10812100
C	-0.59885800	1.54848100	0.28151600
C	0.55349200	2.32393800	0.10239300
C	0.46008900	3.59017700	-0.46581700
C	-0.78167600	4.11084800	-0.82737300
C	-1.93656000	3.35841000	-0.61746300
C	-1.84801800	2.09010300	-0.05726600
C	0.85418400	-0.46065300	1.06270700
O	1.38900000	-0.71750500	-0.23216500
C	2.73236800	-1.19806900	-0.30961200
C	3.65039400	-0.17370800	0.25627400

C	2.92793800	-2.53047500	0.43296800
C	3.01549600	-1.35063600	-1.80912100
N	4.34338000	0.63665500	0.69542900
H	-0.73707500	-0.69310000	-1.67835100
H	-2.30954800	-2.33304300	-2.65139900
H	-4.01617600	-3.42550800	-1.21859100
H	-4.14285200	-2.85354000	1.19405900
H	-2.57230400	-1.19146000	2.15652700
H	1.52658100	1.94488900	0.38066400
H	1.36105500	4.17220900	-0.62213200
H	-0.84905300	5.10107600	-1.26370400
H	-2.90635400	3.76149500	-0.88573000
H	-2.74299200	1.50474900	0.10934600
H	1.48879200	0.23174700	1.62492200
H	0.75698400	-1.38591000	1.63989600
H	3.93466100	-2.91410600	0.25703600
H	2.79335700	-2.42202900	1.50956200
H	2.20106400	-3.25195500	0.05407400
H	4.04741300	-1.66207600	-1.97900600
H	2.83947300	-0.40379900	-2.32024000
H	2.33997300	-2.10400900	-2.21793600

15a

E= -902.0704362 a.u., number of negative frequencies = 0

0 2

O	-0.52076000	-1.19609700	-0.16517800
C	0.17645200	-0.15256400	0.47586600
C	1.65277200	-0.36446400	0.10449000
C	0.18360800	-0.35922200	2.12448700
C	-1.93539200	-1.53445400	-0.05326500
C	-2.22713600	-2.09562200	-1.39269200

C	-2.91202500	-0.37727600	0.20695200
C	-2.09425500	-2.64866800	0.99575700
N	-2.48416000	-2.53902100	-2.42477000
O	-1.02687300	-0.15977200	2.64110400
C	-0.30214900	1.23974500	0.05519100
C	2.11085200	-1.60662700	-0.34494800
C	3.45903700	-1.79529700	-0.64090900
C	4.36832900	-0.75314100	-0.48208100
C	3.91945800	0.48586000	-0.02913000
C	2.57252700	0.67935300	0.26068900
C	-0.37997800	1.49667900	-1.32023600
C	-0.76676600	2.74766200	-1.78658800
C	-1.07369100	3.76712700	-0.88521000
C	-0.99329100	3.52092900	0.48135000
C	-0.61026900	2.26373000	0.95122000
H	0.55328300	-1.38992500	2.22695900
H	0.93499100	0.36719800	2.46883900
H	-2.85259500	0.38586800	-0.56654000
H	-3.92433400	-0.78799900	0.20982400
H	-2.71885000	0.06762500	1.18144800
H	-1.39022800	-3.45673000	0.79332900
H	-1.91258800	-2.23301300	1.98632100
H	-3.10832900	-3.05291800	0.96007100
H	1.40734000	-2.41590800	-0.47859300
H	3.79609600	-2.76153400	-0.99902700
H	5.41704800	-0.90273600	-0.71239800
H	4.61657600	1.30714500	0.09247000
H	2.23443700	1.65313000	0.59420300
H	-0.13846200	0.70726700	-2.02220900
H	-0.82685900	2.92734200	-2.85407700
H	-1.37519400	4.74337500	-1.24758400

H	-1.23650000	4.30386400	1.19080600
H	-0.59414800	2.07555000	2.01647700

16a

E= -787.5569616 a.u., number of negative frequencies = 0

0 2

O	0.10120000	-1.18918600	-0.75333800
C	0.04316600	0.10595400	-0.27519300
C	1.29102700	0.81519400	-0.19747500
C	-0.20680700	-2.35270900	0.07793000
C	1.09118400	-2.97794100	0.42832200
C	-0.96237500	-2.03962400	1.37456200
C	-0.98668100	-3.31433100	-0.82620000
N	2.09263500	-3.48097100	0.69938200
C	-1.28566800	0.68873100	-0.12800200
C	1.35316900	2.23296600	-0.14316300
C	2.56916700	2.89378400	-0.07613900
C	3.76947500	2.17935400	-0.07362100
C	3.73244800	0.78615400	-0.15979400
C	2.52326100	0.11288800	-0.22892400
C	-1.58078000	1.65780800	0.85451500
C	-2.86261300	2.17856500	0.98136100
C	-3.88741200	1.75353100	0.13564700
C	-3.61515000	0.79227900	-0.83888500
C	-2.33819200	0.26244000	-0.96675600
H	-1.07855000	-2.96400200	1.94402700
H	-1.94904700	-1.63435400	1.15444400
H	-0.41345000	-1.32598200	1.98990800
H	-1.11584100	-4.28209000	-0.33763400
H	-1.96811400	-2.88929100	-1.04129100
H	-0.44790500	-3.46067900	-1.76287400

H	0.44083700	2.81179100	-0.18812000
H	2.58411400	3.97766000	-0.04175400
H	4.71788600	2.70115700	-0.01980600
H	4.65636400	0.21882000	-0.17495800
H	2.51915300	-0.96428800	-0.30769700
H	-0.80614800	1.97268400	1.54245300
H	-3.06663200	2.91217600	1.75349200
H	-4.88556900	2.16358700	0.23654300
H	-4.40183600	0.46151700	-1.50818300
H	-2.12662000	-0.46867500	-1.73663600

18a

E= -902.0033217 a.u., number of negative frequencies = 0

C	0.30022200	-0.05675900	0.49092300
O	-0.81919400	-0.10007000	-0.46909000
C	-0.21230800	-0.13129300	1.89380900
O	-1.74825800	0.99056500	-0.13234600
C	-3.07314900	0.48701500	-0.31380400
C	-3.96511100	1.67032200	0.09316400
C	-3.31829100	0.04984000	-1.76568500
C	1.03421400	-1.35931900	0.11457300
C	0.31961700	-2.56857000	0.13384800
C	0.95108700	-3.76877300	-0.18444100
C	2.30625000	-3.78254500	-0.52210500
C	3.02113500	-2.58614700	-0.54421300
C	2.38903600	-1.38042900	-0.23306900
C	1.13355900	1.20302500	0.24330300
C	1.11838400	1.83278900	-1.00708300
C	1.90364500	2.96090600	-1.24233500
C	2.72429200	3.47165300	-0.23513300
C	2.75407400	2.84426700	1.01032100

C	1.96327200	1.71853200	1.24700400
C	-3.31096000	-0.65968500	0.60453400
N	-3.51560200	-1.55710600	1.31185500
H	-0.36485700	0.77173600	2.47194700
H	-0.60408100	-1.06604300	2.27395300
H	-5.01801600	1.39397500	0.00108100
H	-3.76358600	1.96586300	1.12469800
H	-3.75817800	2.51584600	-0.56714300
H	-4.34796100	-0.29567500	-1.89223500
H	-2.63774500	-0.75566300	-2.04332300
H	-3.14492500	0.90525100	-2.42408100
H	-0.73527600	-2.56574900	0.38772200
H	0.38325800	-4.69451300	-0.16803800
H	2.79906600	-4.71900300	-0.76686600
H	4.07487300	-2.58502700	-0.80773600
H	2.95521000	-0.45685300	-0.25900700
H	0.47846300	1.43790100	-1.78739900
H	1.87362200	3.44231800	-2.21573800
H	3.33532100	4.35044600	-0.41962500
H	3.39110200	3.22968700	1.80121800
H	1.99873400	1.23232000	2.21741900

AIBN-TS-1

E= -531.1005048 a.u., im. freq.= 549.81*i*

0 1

N	-0.39381600	0.41428600	0.08879700
N	0.39381900	-0.41427900	0.08883100
C	-2.28633600	-0.36580100	0.15084000
C	2.28633900	0.36580400	0.15083300
C	-2.13803800	-1.72802800	-0.46599900
C	-2.51574800	-0.28885000	1.63862400

C	2.13804000	1.72802300	-0.46602200
C	2.51576600	0.28887100	1.63861400
C	-2.93548100	0.62544000	-0.63638500
N	-3.44199100	1.44467800	-1.27964600
C	2.93547000	-0.62545000	-0.63638500
N	3.44196800	-1.44470000	-1.27963900
H	-3.03035100	-2.33238500	-0.26497800
H	-1.99877200	-1.67122300	-1.54591100
H	-1.27691900	-2.24183500	-0.02849600
H	-3.53240000	-0.61963800	1.88285600
H	-2.39672400	0.73102500	2.00802100
H	-1.81499100	-0.94349000	2.16200700
H	3.03035000	2.33238200	-0.26500700
H	1.99877600	1.67120400	-1.54593200
H	1.27691900	2.24183400	-0.02852800
H	3.53242700	0.61963700	1.88282900
H	2.39672300	-0.73099500	2.00802700
H	1.81503100	0.94353500	2.16199400

14-TS-7

E= -325.3032577 a.u., im. freq.= 609.39i

0 2

C	2.17248400	-0.09055700	-0.11177900
O	1.17047200	0.54931900	-0.58150200
C	-0.50551300	0.28043500	0.06049100
C	-0.62803600	-1.14725900	0.04420600
C	-1.28852300	1.01309800	-0.99699800
C	-0.44732300	0.89628800	1.43519700
N	-0.65639800	-2.30376600	0.03409600
H	2.28065000	-1.16499900	-0.28191500
H	2.88992800	0.42136300	0.53570800

H	-2.35476000	1.02396200	-0.74788700
H	-0.93265400	2.04301900	-1.05718000
H	-1.16235800	0.53927300	-1.97050200
H	-1.41044600	0.79106200	1.94692100
H	0.31262600	0.40783100	2.04957100
H	-0.21050900	1.95827000	1.35192000

12-TS-17

E= -285.9473261 a.u., im. freq.= 300.49*i*

0 2

C	0.71517900	-0.00000100	0.18802500
C	1.03828100	-1.29373100	-0.52975300
C	1.03830100	1.29371700	-0.52976500
O	0.47955600	0.00000700	1.41439000
C	-1.49879500	0.00001300	-0.02012600
N	-2.63840800	0.00000100	-0.25227400
H	2.13020400	-1.38944200	-0.55569400
H	0.62592800	-2.14038700	0.01621700
H	0.68113100	-1.29189300	-1.56025000
H	2.13022500	1.38942300	-0.55568200
H	0.62594100	2.14038300	0.01618500
H	0.68117300	1.29186600	-1.56027000

3a-TS-4a

E= -751.6153302 a.u., im. freq.= 451.90*i*

0 2

C	0.82517500	-1.24251800	-0.33383400
C	-0.10137900	-0.13754400	-0.64306700
C	-1.53937700	-0.26529500	-0.30089800
C	0.35331500	1.03563300	-1.22437100
C	2.19887600	-1.01266900	-0.11836000

C	3.07195500	-2.06570800	0.12748400
C	2.60519700	-3.37903800	0.15772500
C	1.25145900	-3.62791500	-0.06254700
C	0.37353000	-2.57725300	-0.30096200
C	-1.95307100	-0.83228100	0.91870400
C	-3.30040300	-0.90870300	1.25494600
C	-4.27329000	-0.43291300	0.37723800
C	-3.88388800	0.12086000	-0.84097400
C	-2.53616900	0.20514900	-1.17425000
C	0.89179200	2.61972900	0.31973000
C	0.13585000	3.81429300	-0.21888800
C	0.42453800	2.06272900	1.64285600
C	2.29527800	2.64304500	0.11741900
N	3.43987600	2.62251200	-0.07930100
H	1.32908200	1.06152800	-1.69113100
H	-0.37290000	1.73195100	-1.62038900
H	2.59021900	-0.00359900	-0.13205400
H	4.12187900	-1.85670100	0.29914300
H	3.28854000	-4.19868200	0.34857800
H	0.87766900	-4.64586000	-0.05475700
H	-0.67150800	-2.79050900	-0.48718900
H	-1.20679200	-1.20035100	1.61225200
H	-3.59150300	-1.33910800	2.20672600
H	-5.32361100	-0.49852200	0.63722700
H	-4.63245200	0.47954700	-1.53874700
H	-2.24972800	0.61303100	-2.13661500
H	0.30496700	4.69300400	0.41749000
H	0.45268500	4.07536900	-1.23050000
H	-0.93848300	3.61478700	-0.22480600
H	0.61121000	2.78705300	2.44695800
H	0.94354700	1.13846900	1.89988300

H	-0.64827200	1.86340400	1.61532600
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4a-TS-5a

E= -902.0136748 a.u., im. freq.= 161.10i

0 2

C	0.61515900	1.04965700	-0.03034800
C	-0.26053600	-0.09518500	0.29063700
C	-1.69016200	-0.02351600	-0.03313600
C	0.37139300	-1.41821400	0.62190500
C	1.75455800	1.33720700	0.74416400
C	2.58773600	2.39958700	0.42211100
C	2.32077800	3.19305400	-0.69228300
C	1.20596500	2.91674500	-1.48070800
C	0.35934600	1.86474600	-1.15117000
C	-2.38364900	1.19959700	0.10598000
C	-3.74478200	1.28938400	-0.14843800
C	-4.46276100	0.16452500	-0.55413700
C	-3.80261900	-1.05503500	-0.68721900
C	-2.44180700	-1.15077100	-0.42108900
C	1.32055900	-2.11437900	-0.41959900
O	-0.64236200	0.38431700	2.42968400
O	0.11332200	-0.17408700	3.23837300
C	1.51332900	-3.58294600	0.03532300
C	0.76008600	-2.08349800	-1.85800100
C	2.65684400	-1.49531100	-0.42838900
N	3.73253600	-1.07990400	-0.44999500
H	0.93327100	-1.30115400	1.56005500
H	-0.41597400	-2.13607600	0.85554900
H	1.97775600	0.73800500	1.61650900
H	3.45565000	2.60190300	1.03854500
H	2.98017200	4.01472800	-0.94737300

H	0.99591800	3.51882800	-2.35756600
H	-0.49842300	1.65616000	-1.77802100
H	-1.84614500	2.07428700	0.44724500
H	-4.25085700	2.23952000	-0.01982000
H	-5.52524600	0.23645900	-0.75616500
H	-4.34957400	-1.93770300	-0.99902300
H	-1.96032000	-2.11244300	-0.53524800
H	2.21816600	-4.10059600	-0.61803500
H	1.89434000	-3.63088600	1.05743700
H	0.55514900	-4.10742400	-0.00364800
H	1.44195300	-2.59512500	-2.54045400
H	0.62651500	-1.06097000	-2.21278600
H	-0.20439600	-2.59391100	-1.89530000

5a-TS-6a

E= -901.9268896 a.u., im. freq.= 1238.33*i*

0 2

C	-1.70203300	-0.03273700	0.22495100
C	-0.32093600	-0.16001600	0.87611200
C	0.57255600	-1.19528900	0.19549400
C	0.32338600	1.21133700	1.21042500
C	-1.99241800	0.90968100	-0.76236300
C	-3.25827600	0.95554100	-1.34740200
C	-4.24712900	0.06193100	-0.95014500
C	-3.96366700	-0.88042400	0.03763300
C	-2.70184600	-0.92781100	0.61964500
C	1.46396700	-1.95242900	0.96610100
C	2.29940400	-2.88946100	0.36290700
C	2.26412500	-3.07620400	-1.01718500
C	1.37771200	-2.32807400	-1.78871900
C	0.52922800	-1.40177400	-1.18682900

C	1.91309900	1.97930600	-0.14650000
O	-0.48573500	-0.56565700	2.25867200
O	-0.63646200	0.75507300	2.78763800
C	2.03328500	3.36603000	0.45436600
C	3.11340400	1.07769900	0.04499400
C	1.32702500	1.94912600	-1.43911100
N	0.83713000	1.94686600	-2.49146800
H	-0.20469000	2.12638500	1.00142200
H	1.19607500	1.20106600	1.84247100
H	-1.23866400	1.60596100	-1.10507600
H	-3.46396200	1.69287900	-2.11510900
H	-5.23156500	0.09959300	-1.40287500
H	-4.72890000	-1.57798700	0.35944600
H	-2.48839200	-1.64632800	1.40062000
H	1.48763800	-1.81411400	2.03889200
H	2.97671200	-3.47520000	0.97444800
H	2.91603300	-3.80422100	-1.48679900
H	1.33659100	-2.46950900	-2.86267600
H	-0.16209500	-0.83807700	-1.79894000
H	2.85956300	3.90806800	-0.02144200
H	1.12655000	3.95668600	0.31508000
H	2.25172500	3.30551100	1.52367000
H	3.97913800	1.50919500	-0.47468500
H	2.94693400	0.07728700	-0.34860700
H	3.37364200	1.00081300	1.10370200

6a-TS-8a

E= -691.1385074 a.u., im. freq.= 1434.12i

0 1

C	-0.18401100	2.00989000	1.25202100
C	0.08453700	0.83996600	-0.01527000

C	-1.22703200	0.06719300	-0.01578000
C	1.32348600	0.01434800	0.00007600
C	1.37209300	-1.38526500	0.14965800
C	2.58591900	-2.05243400	0.09682000
C	3.77268700	-1.34221800	-0.11625900
C	3.74219800	0.04094300	-0.27699700
C	2.52944200	0.71605900	-0.21105200
O	0.21497200	1.77226100	-1.01378900
O	-0.86132900	2.77750600	0.41637900
H	-0.77063500	1.52394600	2.03822800
H	0.78456800	2.40158800	1.59438400
C	-2.00694900	0.09955900	-1.17439700
C	-3.18724800	-0.63722200	-1.24369500
C	-3.59882600	-1.41102200	-0.16223100
H	0.45501000	-1.94389300	0.27948200
H	2.61475800	-3.13058200	0.20514100
H	4.71791600	-1.87213900	-0.15639000
H	4.66109600	0.59087900	-0.44308800
H	2.48675700	1.79195800	-0.31972400
C	-2.82431600	-1.44321400	0.99780400
C	-1.64872700	-0.70260100	1.07248400
H	-1.66924500	0.70171000	-2.00693600
H	-3.78705000	-0.60132300	-2.14633000
H	-4.51948900	-1.98087500	-0.21688200
H	-3.14043200	-2.03852400	1.84708800
H	-1.06191500	-0.72477500	1.98521500

9-TS-10a

E= -902.0117308 a.u., im. freq.= 364.59i

0 2

C	1.95723700	-1.00523400	-0.30463300
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C	0.91427700	0.00499700	-0.56655600
C	1.60508100	-2.30222500	0.11326900
C	-0.29959700	-0.39545300	-1.09954200
O	-1.39627700	-0.99364800	0.52408400
O	-2.57544600	-1.58135700	0.08952300
C	-3.71626600	-0.70058700	0.26744600
C	-4.90965000	-1.55734100	-0.16734800
C	-3.57865600	0.46129200	-0.63820800
C	-3.81833800	-0.23293100	1.72155800
C	2.58123800	-3.27054300	0.31886500
C	3.92628800	-2.97258200	0.10412700
C	4.29055400	-1.69171500	-0.30983000
C	3.31985800	-0.71603500	-0.50428600
N	-3.48351000	1.35940700	-1.35465300
C	1.13561600	1.41366600	-0.19170300
C	0.54795300	2.46535500	-0.92068400
C	0.73429000	3.78915200	-0.54417500
C	1.50844800	4.10083800	0.57319500
C	2.09643600	3.07371800	1.30946900
C	1.91762000	1.74852900	0.93062600
H	0.56299100	-2.52234200	0.31046600
H	-0.39287800	-1.37454600	-1.54730100
H	-1.02988300	0.34205800	-1.39602800
H	-5.83489200	-0.98377800	-0.09325500
H	-4.97462500	-2.42847800	0.48648300
H	-4.78271300	-1.89482300	-1.19656800
H	-3.94711600	-1.10584600	2.36468900
H	-4.67234400	0.43547000	1.84875600
H	-2.90663400	0.28888000	2.00762900
H	2.29168300	-4.26025000	0.65430900
H	4.68513100	-3.73094900	0.26085300

H	5.33377100	-1.45369400	-0.48546000
H	3.61121800	0.27319400	-0.83642900
H	-0.04383700	2.24381900	-1.80013100
H	0.27659100	4.58052800	-1.12678100
H	1.65169200	5.13460100	0.86666300
H	2.69155000	3.30503600	2.18586600
H	2.36430800	0.95791500	1.52040500

10a-TS-11a

E= -902.0234615 a.u., im. freq.= 469.33*i*

0 2

C	2.04852100	-0.77488100	-0.25524600
C	0.85641400	0.02044400	-0.56288200
C	1.94551900	-2.14396200	0.06773800
C	-0.28745300	-0.68559200	-1.21477900
O	-0.79745700	-0.94468500	0.05636900
O	-2.34833300	-1.91321300	-0.20357200
C	-3.37089000	-1.12447600	0.32328000
C	-4.66132200	-1.94212500	0.07537900
C	-3.46652600	0.15568800	-0.43727000
C	-3.18019600	-0.82725400	1.81991900
C	3.08381100	-2.90719700	0.28479700
C	4.35216400	-2.33633000	0.16936200
C	4.47183100	-0.98836600	-0.16169600
C	3.33627300	-0.21218300	-0.36442900
N	-3.51777200	1.13173400	-1.05012800
C	0.75027900	1.42879800	-0.20841500
C	-0.10852000	2.30210500	-0.91027800
C	-0.20045900	3.64231500	-0.56382100
C	0.54912300	4.14928200	0.49728500
C	1.38818600	3.29936900	1.21906200

C	1.48865300	1.95995800	0.87373300
H	0.96107400	-2.57728300	0.19030500
H	0.01116800	-1.58539800	-1.76164000
H	-0.94129000	-0.06678000	-1.83305900
H	-5.53304600	-1.38540100	0.42676000
H	-4.58869500	-2.88370900	0.62157800
H	-4.77609500	-2.15419700	-0.98781900
H	-3.12041600	-1.77724800	2.35483400
H	-4.01417000	-0.24218700	2.21578500
H	-2.25183300	-0.27885700	1.97037900
H	2.98208000	-3.95312700	0.55125400
H	5.23852300	-2.93804200	0.33488400
H	5.45258300	-0.53874600	-0.26800700
H	3.44337700	0.82775500	-0.64580500
H	-0.71566500	1.93176900	-1.72410500
H	-0.86834500	4.29078500	-1.11828100
H	0.46940500	5.19568600	0.76915600
H	1.95434000	3.68091300	2.06111400
H	2.11528100	1.30156200	1.46074600

10a-TS-15a

E= -902.0084098 a.u., im. freq.= 117.29i

0 2

C	0.34673800	-1.53836200	0.34965900
C	-0.47902900	-0.49789900	0.92528700
C	1.72534000	-1.64575900	0.65389700
C	-0.07108800	0.13352900	2.24188300
O	1.04540800	0.87663800	1.93227000
O	0.27035000	1.57525000	-0.09010600
C	1.38436300	2.31967100	-0.44833100
C	1.07015400	2.92645900	-1.84279000

C	2.58754900	1.44895100	-0.60025800
C	1.69320700	3.44272700	0.56060200
C	2.47391400	-2.70141400	0.16231700
C	1.87643100	-3.68590200	-0.62678900
C	0.51657300	-3.60902200	-0.92632900
C	-0.24007900	-2.54676600	-0.45510600
N	3.50903900	0.76739300	-0.73523700
C	-1.77458700	-0.17047300	0.34616400
C	-2.89328500	0.03513200	1.17608600
C	-4.14446900	0.28436900	0.62738900
C	-4.29257600	0.38433100	-0.75530300
C	-3.18652500	0.22067100	-1.59060300
C	-1.94148100	-0.06216500	-1.04952200
H	2.18747100	-0.85172700	1.22181200
H	0.17211500	-0.66049300	2.97092300
H	-0.89009200	0.73903100	2.65134900
H	1.90351700	3.53959500	-2.19502300
H	0.17690200	3.54726300	-1.75364000
H	0.88157600	2.13344800	-2.56771400
H	0.81492100	4.08931900	0.62553100
H	2.55573200	4.03821000	0.24786800
H	1.87923400	3.00763900	1.54022200
H	3.53507000	-2.74338600	0.37503700
H	2.46949200	-4.50915400	-1.00923700
H	0.04514200	-4.38062200	-1.52373900
H	-1.30080900	-2.51884500	-0.66250300
H	-2.79063700	-0.03582200	2.25115200
H	-5.00165500	0.41318700	1.27762200
H	-5.26572700	0.60157100	-1.18102200
H	-3.29672500	0.32359900	-2.66379800
H	-1.07175500	-0.14815000	-1.68500900

10a-TS-6a

E= -901.963386 a.u., im. freq.= 727.36i

0 2

C	-0.81357600	1.54188800	-0.28930100
C	-0.58167600	0.14841200	-0.73221100
C	0.26448100	2.43540900	-0.14924900
C	0.25037800	-0.05441800	-1.99279800
O	1.25446400	-0.91954300	-1.48426000
O	1.11675500	-0.44915400	-0.08852000
C	2.95741400	-0.94410200	0.70537900
C	2.60137300	-0.61876800	2.12824000
C	3.74560900	-0.00016700	0.00728200
C	3.07323200	-2.38752900	0.30876500
C	0.04651800	3.76064500	0.20679300
C	-1.24984800	4.23156100	0.41450700
C	-2.32812500	3.36240300	0.26737300
C	-2.11445000	2.03053400	-0.07486300
N	4.37722300	0.79455500	-0.55674700
C	-1.48764300	-0.92405200	-0.29537600
C	-1.77679400	-2.03371700	-1.10983900
C	-2.60115800	-3.05860000	-0.65861400
C	-3.14683900	-3.01245700	0.62212400
C	-2.85342800	-1.93067400	1.45338000
C	-2.03645500	-0.90294100	1.00344300
H	1.27363200	2.07262600	-0.29602200
H	0.67892900	0.89364200	-2.32875000
H	-0.26541600	-0.53299800	-2.83064400
H	3.42940000	-0.87818800	2.80047600
H	1.72546400	-1.19731200	2.42936200
H	2.38494200	0.44290600	2.25282100

H	2.20125400	-2.93953900	0.66472200
H	3.96885900	-2.83430700	0.76246600
H	3.14304800	-2.49831600	-0.77222600
H	0.89286400	4.42811900	0.32322500
H	-1.41717800	5.26754600	0.68661000
H	-3.34063000	3.72083700	0.41554000
H	-2.96231200	1.36904200	-0.20065400
H	-1.35573200	-2.10349400	-2.10360400
H	-2.81561200	-3.89803700	-1.31041200
H	-3.78756100	-3.81345300	0.97273100
H	-3.25888900	-1.89227600	2.45827800
H	-1.79945700	-0.07967300	1.66534200

11a-TS-13a

E= -902.0225726 a.u., im. freq.= 834.83*i*

0 2

C	-1.92354500	-0.38095500	0.30940000
C	-0.67961300	0.27895500	0.87063500
C	-1.89522100	-1.23950900	-0.79394800
O	-0.63295100	0.29508400	2.25048300
C	-3.07722200	-1.80471100	-1.26934300
C	-4.29272100	-1.51789400	-0.65239300
C	-4.32311100	-0.66814100	0.45223100
C	-3.14486200	-0.10675700	0.93374700
C	-0.19596600	1.53895200	0.18373400
C	0.42334500	2.53314000	0.94918900
C	0.88990300	3.69759000	0.34804900
C	0.74678300	3.88252800	-1.02572300
C	0.12868100	2.89744400	-1.79344900
C	-0.34213600	1.73317500	-1.19420100
C	0.41547200	-0.67763900	1.32817600

O	1.18820700	-1.17930300	-0.37300500
C	2.46602100	-1.74003000	-0.27441100
C	3.42454100	-0.77034800	0.32510100
C	2.49866600	-3.05168900	0.53451800
C	2.88412800	-1.99642600	-1.74526800
N	4.15309200	-0.02283200	0.81563200
H	-0.94706700	-1.47771500	-1.25754600
H	-3.04624500	-2.47408000	-2.12196800
H	-5.21060200	-1.95740000	-1.02640700
H	-5.26464800	-0.44531600	0.94157300
H	-3.16224800	0.54293700	1.80073400
H	0.52245600	2.38683400	2.01720000
H	1.36461700	4.46143600	0.95338700
H	1.11099700	4.78980600	-1.49443000
H	0.00821900	3.03723200	-2.86189400
H	-0.83191000	0.98094900	-1.79812100
H	1.35544400	-0.27358900	1.67336100
H	0.12421200	-1.67393600	1.61822500
H	3.49146300	-3.50584200	0.50220200
H	2.24237100	-2.87861600	1.58089300
H	1.77347400	-3.74465100	0.10319400
H	3.90148300	-2.39249800	-1.77962500
H	2.83776700	-1.06677100	-2.31145200
H	2.19767300	-2.72132400	-2.18484600

11a-TS-15a

E= -902.0092886 a.u., im. freq.= 552.38i

0 2

O	-0.56138500	-1.39203800	-0.08312500
C	0.44857200	0.33877700	0.76495000
C	1.75694200	-0.02403000	0.17454900

C	0.16435700	-0.09947300	2.19459200
C	-1.86285100	-1.90583600	0.07614300
C	-2.05705200	-2.68478300	-1.17439100
C	-2.94961800	-0.81096400	0.13841500
C	-1.96234400	-2.86638500	1.27862900
N	-2.20715900	-3.29378600	-2.14250300
O	0.93773500	0.97196400	2.52479900
C	-0.35305600	1.43223800	0.16718700
C	2.27253500	-1.32466200	0.28498400
C	3.51999600	-1.63597400	-0.24082000
C	4.27947100	-0.65510800	-0.87664500
C	3.78146600	0.64127000	-0.98751400
C	2.52874200	0.95372800	-0.47275100
C	-0.50299600	1.48070400	-1.22865500
C	-1.29488600	2.45827800	-1.82004300
C	-1.94479900	3.40757100	-1.03262300
C	-1.79519300	3.37221700	0.35255900
C	-1.00817100	2.39407200	0.95072600
H	-0.89480500	-0.02356900	2.46868900
H	0.57712100	-1.08179900	2.44071100
H	-2.88182300	-0.15028700	-0.72479700
H	-3.94130200	-1.26789500	0.16099700
H	-2.82075100	-0.21697700	1.04424500
H	-1.18733000	-3.63087300	1.21067700
H	-1.82462400	-2.30465200	2.20474600
H	-2.93827000	-3.35608000	1.31517800
H	1.67230000	-2.09575100	0.74507000
H	3.89841700	-2.64841800	-0.15954300
H	5.25439600	-0.90021700	-1.28267400
H	4.37066700	1.41201700	-1.47084900
H	2.15641900	1.96728100	-0.54362900

H	-0.02489500	0.72657400	-1.83925900
H	-1.40705900	2.47539700	-2.89809600
H	-2.55861000	4.17186800	-1.49560300
H	-2.28417400	4.11591300	0.97144000
H	-0.85305800	2.39471400	2.02107200

13a-TS-14

E= -902.0726696 a.u., im. freq.= 289.90i

0 2

C	2.09357600	-0.04177100	-0.34828000
C	0.77976600	0.35711800	-1.01933400
C	2.17688400	-0.67179800	0.90023000
O	0.81343900	0.48588200	-2.29574800
C	3.41479000	-1.01716600	1.43780600
C	4.58750900	-0.73617500	0.73964400
C	4.51317200	-0.11649000	-0.50599700
C	3.27623000	0.22209000	-1.04735600
C	-0.13173400	1.32960100	-0.27188300
C	-1.24641400	1.83141000	-0.95680300
C	-2.09283100	2.75835700	-0.35971400
C	-1.82996800	3.21863000	0.93125300
C	-0.71224500	2.74514400	1.61225400
C	0.13093800	1.80619700	1.01689100
C	-0.19842100	-1.31349200	-1.02594000
O	-0.74049000	-1.65342000	0.17767200
C	-2.17730300	-1.70153100	0.42190600
C	-2.96151800	-1.21628100	-0.72909600
C	-2.51250100	-3.18238700	0.66074200
C	-2.47020500	-0.84114400	1.65485500
N	-3.62090900	-0.87445200	-1.61036500
H	1.27273300	-0.91863100	1.44226600

H	3.46215300	-1.51142600	2.40207400
H	5.55030400	-1.00273500	1.16112800
H	5.41989000	0.10308200	-1.05897000
H	3.20584600	0.69016000	-2.02115600
H	-1.42806800	1.49599200	-1.96975000
H	-2.95362500	3.12823100	-0.90534000
H	-2.48424800	3.94838000	1.39515400
H	-0.48515700	3.11276100	2.60704300
H	1.00740200	1.46910100	1.55324400
H	-0.90258400	-1.13638600	-1.83274000
H	0.64190000	-1.95249300	-1.27281700
H	-3.57094500	-3.30237000	0.89962700
H	-2.28165800	-3.77561800	-0.22508000
H	-1.91276100	-3.54576900	1.49672600
H	-3.52516100	-0.92070500	1.92476500
H	-2.22743400	0.20337200	1.46752400
H	-1.86415900	-1.20536200	2.48639600

15a-TS-16a

E= -902.0691041 a.u., im. freq.= 304.54i

0 2

O	-0.43481300	-1.23797900	-0.19231800
C	0.21022100	-0.14632100	0.35385200
C	1.67839400	-0.26567500	0.02521800
C	0.28048800	-0.38693200	2.22531100
C	-1.83921100	-1.63710500	-0.05584600
C	-2.14763000	-2.16827800	-1.40235300
C	-2.85566000	-0.53952300	0.28545400
C	-1.89232100	-2.78257800	0.96760100
N	-2.41694300	-2.58922400	-2.44066500
O	-0.89816100	-0.28928400	2.70825500

C	-0.38888300	1.21204100	0.02418800
C	2.22904200	-1.48897200	-0.38108300
C	3.59077400	-1.59595300	-0.64593000
C	4.42670100	-0.49127300	-0.49795500
C	3.88898300	0.72752400	-0.08778100
C	2.52752400	0.84128600	0.17056100
C	-0.53629900	1.51241500	-1.33804700
C	-1.03492700	2.74595800	-1.74117500
C	-1.38782800	3.70211200	-0.78938800
C	-1.24067300	3.41126900	0.56326600
C	-0.74476200	2.17288700	0.97152800
H	0.75135800	-1.38260500	2.19097900
H	0.99739800	0.42169900	2.44611500
H	-2.87366900	0.24893700	-0.46370000
H	-3.84283400	-1.00642600	0.31764200
H	-2.63617800	-0.12129300	1.26561100
H	-1.16094500	-3.55032500	0.71279500
H	-1.68320500	-2.37528400	1.95680500
H	-2.88683900	-3.23400700	0.96781900
H	1.58287600	-2.34660500	-0.50356300
H	3.99853000	-2.54661000	-0.97042200
H	5.48761400	-0.57788300	-0.70310300
H	4.52952200	1.59471000	0.02534000
H	2.11972100	1.79776900	0.47339100
H	-0.25668900	0.77294800	-2.07963200
H	-1.14516900	2.96059400	-2.79812800
H	-1.77679300	4.66457500	-1.10186700
H	-1.52068400	4.14504800	1.31060400
H	-0.68521400	1.94012800	2.02594400

16a-TS-8a

E= -787.5427843 a.u., im. freq.= 573.15i

0 2

O	-0.08257600	1.10356100	-0.86992800
C	-0.03661400	-0.11531600	-0.43180700
C	-1.29239000	-0.84466200	-0.24729400
C	0.23119300	2.55706500	0.23463200
C	-1.08181500	3.12810800	0.26435400
C	0.70772900	2.02176400	1.55950400
C	1.22071500	3.31385600	-0.61420700
N	-2.14681500	3.58195300	0.28729500
C	1.29219100	-0.72273100	-0.20133400
C	-1.35321400	-2.25551500	-0.24468600
C	-2.56772400	-2.91595900	-0.11360800
C	-3.75406500	-2.19383500	0.01701500
C	-3.71437700	-0.79884300	-0.00712000
C	-2.50648300	-0.13110600	-0.14898700
C	1.54203600	-1.65584900	0.82131600
C	2.82093500	-2.16400900	1.02417100
C	3.87697900	-1.76181300	0.20764700
C	3.64501800	-0.83701600	-0.81146100
C	2.37171800	-0.31826100	-1.00894600
H	0.81343800	2.84604300	2.27376100
H	1.67597800	1.53407900	1.44990900
H	-0.00545000	1.30962600	1.97988300
H	1.41037100	4.30487400	-0.18596200
H	2.16382000	2.76912700	-0.66260100
H	0.83207100	3.44622300	-1.62454400
H	-0.44846300	-2.83349900	-0.37893000
H	-2.59052500	-4.00006900	-0.12371400
H	-4.70004900	-2.71246400	0.12353500
H	-4.63192700	-0.22772300	0.07908800

H	-2.49050100	0.94913000	-0.19006000
H	0.73645900	-1.95881900	1.47863300
H	2.99542800	-2.87096000	1.82766300
H	4.87152700	-2.16349800	0.36453300
H	4.45930700	-0.52494600	-1.45613300
H	2.18582600	0.39543300	-1.80182800

18a-TS-3a

E= -901.9863459 a.u., im. freq.= 304.26i

0 2

C	2.02174500	-0.25421200	-0.34382300
C	0.80351100	0.26460300	-1.04004600
O	-0.36584800	-1.25154600	-0.54116700
C	0.66348900	-0.01728700	-2.40549300
C	0.11355600	1.45873900	-0.47038400
O	-1.72715600	-0.92855900	-0.88101700
C	-2.60318900	-1.58757000	0.03588400
C	-2.35305900	-1.14086600	1.42902300
C	-2.44358300	-3.11320300	-0.04633000
C	-4.00065400	-1.12731500	-0.40194200
C	2.80228100	0.58111600	0.46589600
C	3.96663500	0.10449500	1.06243100
C	4.36378700	-1.21599000	0.87115100
C	3.59088300	-2.05854900	0.07334200
H	-0.17636800	0.37134100	-2.96516000
H	1.31470600	-0.73058300	-2.89121800
C	2.43525200	-1.58216700	-0.53469900
C	-0.25995500	1.49296800	0.87959400
C	-0.88990900	2.61166300	1.41150800
H	-3.14573000	-3.61096800	0.62596900
H	-1.42823600	-3.40084600	0.22332200

H	-2.64091900	-3.42999800	-1.07251500
H	-4.76286600	-1.57231600	0.23957800
H	-4.07542500	-0.04108000	-0.34547100
H	-4.16905100	-1.44381400	-1.43249700
C	-1.14338900	3.72386000	0.60890100
C	-0.76703700	3.70651300	-0.73142300
C	-0.14606200	2.58108800	-1.26770600
N	-2.20604100	-0.81517200	2.52484000
H	2.50418800	1.61003000	0.62052100
H	4.56217600	0.76816200	1.67908200
H	5.26691100	-1.58769500	1.34194400
H	3.88703100	-3.09131700	-0.07248700
H	1.82514100	-2.24574500	-1.13371200
H	-0.08571400	0.62542600	1.50059700
H	-1.19217400	2.60703400	2.45225100
H	-1.63149800	4.59744200	1.02646400
H	-0.95250600	4.56920600	-1.36143800
H	0.16083600	2.58545400	-2.30694400

18a-TS-6a

E= -901.9463987 a.u., im. freq.= 888.02i

0 2

C	-1.72846700	-0.87978300	0.08878500
C	-0.45707800	-0.12283800	0.48368600
O	0.64420800	-0.71637800	-0.26108900
C	0.06396600	-0.45336600	1.86762100
C	-0.52465000	1.38422800	0.24501200
O	1.61610100	-0.70835000	0.85910400
C	3.26286900	-1.06357400	-0.02924000
C	3.32084200	-0.03546600	-1.01178500
C	3.06721700	-2.46435700	-0.55018000

C	4.17152600	-0.88387900	1.16040300
C	-2.91696500	-0.23472600	-0.26122100
C	-4.05175200	-0.97249400	-0.59763700
C	-4.01201900	-2.36279200	-0.59880700
C	-2.82575300	-3.01616800	-0.26567600
H	0.26173300	0.34080600	2.57401500
H	-0.14798900	-1.43384600	2.27412000
C	-1.69556600	-2.28145500	0.07289300
C	0.06353300	1.95109800	-0.88590200
C	-0.01569100	3.32521400	-1.10535400
H	3.98786000	-2.82443600	-1.02698400
H	2.26302900	-2.50217600	-1.28410100
H	2.82647500	-3.13433900	0.27716200
H	5.20557300	-1.12903500	0.89124700
H	4.14671100	0.14371300	1.52375600
H	3.86214700	-1.55450300	1.96501400
C	-0.68703700	4.14612500	-0.20318000
C	-1.27697200	3.58639000	0.92864600
C	-1.19309000	2.21433400	1.15175600
N	3.37529900	0.80207500	-1.81175700
H	-2.96053600	0.84606300	-0.27880400
H	-4.96526800	-0.45409700	-0.86661700
H	-4.89418200	-2.93465400	-0.86387600
H	-2.78017700	-4.09952700	-0.27570800
H	-0.77070500	-2.79427200	0.30702700
H	0.60765200	1.32163400	-1.57670800
H	0.45951000	3.75174400	-1.98138200
H	-0.74480800	5.21505900	-0.37539400
H	-1.79817300	4.21677700	1.64061900
H	-1.65789900	1.78945500	2.03588100

18a-TS-11a

E= -901.9950399 a.u., im. freq.= 597.32i

0 2

C	0.54802200	0.14393100	0.85568800
O	-0.60754400	-0.69220000	0.90360000
C	0.47448100	0.17287800	2.34899800
O	-1.29875100	-0.91739000	-0.62338700
C	-2.53773800	-1.54114700	-0.38316500
C	-3.14179100	-1.70574600	-1.79505900
C	-2.39433300	-2.89592400	0.32871100
C	1.79548800	-0.56335100	0.33548300
C	3.03375200	-0.32493300	0.93994500
C	4.18803300	-0.94862900	0.47032200
C	4.11622400	-1.82262600	-0.61124800
C	2.88547900	-2.06482600	-1.21786900
C	1.73169100	-1.43900700	-0.75158800
C	0.27366000	1.50954000	0.21866500
C	-0.97810400	2.11081600	0.39956500
C	-1.24265900	3.36584300	-0.13718600
C	-0.26216800	4.04188400	-0.86278800
C	0.98175500	3.44859000	-1.05090200
C	1.24816400	2.18842500	-0.51584200
C	-3.41855100	-0.64551500	0.41262300
N	-4.11124900	0.04509600	1.02280200
H	-0.17759000	0.88594300	2.83322800
H	0.93995200	-0.61317300	2.92788800
H	-4.13788500	-2.14703700	-1.72182600
H	-3.21401100	-0.73807600	-2.29134000
H	-2.49975800	-2.36393700	-2.38219700
H	-1.92992200	-2.76388600	1.30429200
H	-1.76042400	-3.54552800	-0.27823600

H	-3.37067100	-3.36827700	0.45892800
H	3.10046900	0.35658300	1.78187500
H	5.13966300	-0.75281100	0.95173400
H	5.01172900	-2.31209700	-0.97730200
H	2.82141400	-2.74531000	-2.05985400
H	0.77635200	-1.62790800	-1.22103700
H	-1.75439400	1.58733300	0.94259900
H	-2.22033100	3.81211100	0.00630600
H	-0.47034100	5.01998800	-1.28193400
H	1.74946000	3.96079500	-1.62017800
H	2.21698400	1.73511700	-0.68037900

3b

E= -616.0776031 a.u., number of negative frequencies = 0

0 1

C	-1.70540100	0.36351100	0.02986400
C	-0.50381700	1.24583500	-0.01535000
C	0.84140000	0.60951100	-0.01990400
C	-0.64127400	2.58101400	-0.04685900
C	-1.74939100	-0.74923900	0.88336000
C	-2.88882400	-1.54386600	0.96207900
C	-4.00432300	-1.25273800	0.17854900
C	-3.96968500	-0.16020000	-0.68499200
C	-2.83163500	0.63822600	-0.75911400
C	1.91544800	1.16718500	0.69231300
C	3.18372700	0.60538000	0.65506700
C	3.41255600	-0.54460100	-0.10297200
C	2.35734400	-1.12364000	-0.81042900
C	1.08988800	-0.55381700	-0.76083100
O	4.67722200	-1.05921700	-0.10524500
H	0.21644400	3.23717400	-0.13315700

H	-1.61568800	3.04994800	0.01654600
H	-0.88745800	-0.98156600	1.49790000
H	-2.90650200	-2.39170700	1.63808500
H	-4.88944900	-1.87631300	0.23557300
H	-4.82683200	0.06657000	-1.30949200
H	-2.80254000	1.47419100	-1.44851800
H	1.74535200	2.04619300	1.30307900
H	4.00554400	1.03440500	1.21548900
H	2.52637000	-2.01914200	-1.40191100
H	0.28271100	-1.01424100	-1.31820600
H	4.69819200	-1.84714800	-0.65811400

4b

E= -826.8940426 a.u., number of negative frequencies = 0

0 2

C	1.16188100	-0.15504500	-0.31368000
C	-0.26199700	0.00551800	-0.48296600
C	-1.18689900	-1.10271500	-0.20768500
C	-0.82507500	1.29153200	-1.03934800
C	2.05368900	0.95060400	-0.24599500
C	3.42052600	0.78835800	-0.12455600
C	3.97700100	-0.49357900	-0.07393400
C	3.13407400	-1.60691600	-0.15232400
C	1.76489400	-1.44071600	-0.26957800
C	-1.05133300	-1.89171900	0.95614200
C	-1.93955500	-2.92156700	1.24033300
C	-2.99061300	-3.20969500	0.36972200
C	-3.14222100	-2.44775400	-0.78782100
C	-2.26189300	-1.40939200	-1.06838500
C	-1.54074800	2.29111900	-0.05565900
C	-0.60390300	2.73778400	0.98738800

C	-1.97700800	3.53447400	-0.86685000
C	-2.77252800	1.66387200	0.63206600
N	0.11642600	3.11807200	1.80434500
H	-0.04182000	1.84673800	-1.55928600
H	-1.58047000	1.05974900	-1.79763800
H	1.66451000	1.95886800	-0.24425900
H	4.07813200	1.64617500	-0.05308500
H	3.55593500	-2.60826300	-0.13810900
H	1.14351600	-2.32120400	-0.36327100
H	-0.25390300	-1.66470200	1.65341800
H	-1.81657700	-3.49682500	2.15152800
H	-3.68200300	-4.01451600	0.59120500
H	-3.94817500	-2.66713100	-1.47974100
H	-2.39236800	-0.84691300	-1.98544000
H	-2.46133100	4.26974700	-0.22135200
H	-2.68845000	3.23334900	-1.64023600
H	-1.12244600	4.01308300	-1.34990300
H	-3.48574700	1.33002800	-0.12519800
H	-2.49989200	0.80667300	1.24616200
H	-3.26427300	2.40243600	1.26928700
O	5.33135600	-0.59433000	0.04470900
H	5.57978500	-1.52414100	0.07661700

5b

E= -977.2678823 a.u., number of negative frequencies = 0

0 2

C	1.46313900	-0.21527200	0.10375800
C	-0.05972200	-0.21456300	0.29169500
C	-0.65040100	1.18059300	0.10739600
C	-0.64675000	-1.33780100	-0.60419400
C	2.10861400	0.74227900	-0.67953800

C	3.48594300	0.69676900	-0.88161800
C	4.24823100	-0.30774700	-0.28705200
C	3.61810100	-1.27005900	0.50602600
C	2.24434700	-1.22394400	0.68902900
C	-0.49417700	2.12853200	1.12744600
C	-0.95010400	3.43077200	0.96463000
C	-1.56251600	3.81781900	-0.22641100
C	-1.71222600	2.88928500	-1.24944000
C	-1.25906900	1.58102400	-1.08275300
O	-0.20669500	-0.61954800	1.73348400
O	-1.42265300	-0.46302500	2.20678700
C	-2.09160000	-1.92940200	-0.47140400
C	-3.14892700	-0.91853500	-0.31393900
C	-2.20383200	-2.95446400	0.68484300
C	-2.38123300	-2.67474300	-1.80297300
N	-4.04502800	-0.19678100	-0.23961100
H	-0.51496800	-0.98670200	-1.63034400
H	0.02269900	-2.19550800	-0.50880500
H	1.53933200	1.53985100	-1.13877200
H	3.96553800	1.45226200	-1.49716200
H	4.21974900	-2.04196100	0.97006300
H	1.77579700	-1.97400600	1.31369500
H	-0.01746300	1.84397600	2.05644500
H	-0.82819700	4.14471600	1.77131000
H	-1.92229300	4.83265300	-0.35189700
H	-2.19408000	3.17238600	-2.17806600
H	-1.39861200	0.88123800	-1.89615800
H	-3.18992700	-3.42334400	0.66963500
H	-1.45110900	-3.73581100	0.54798100
H	-2.06171200	-2.49693200	1.66076600
H	-1.61641900	-3.43771500	-1.97094600

H	-3.35516800	-3.16562000	-1.76291200
H	-2.37932800	-1.98745300	-2.65158900
O	5.59978300	-0.40324800	-0.43835400
H	5.91096300	0.31874500	-0.99431300

6b

E= -766.4444920 a.u., number of negative frequencies = 0

0 1

C	-1.61552800	-0.12288600	0.03186600
C	-0.52192000	0.92967900	0.12548300
C	-1.38331900	-1.47063500	0.32060300
C	-2.42240600	-2.39772200	0.25875300
C	-3.70310300	-1.99320200	-0.10562700
C	-3.94106900	-0.65328100	-0.40856100
C	-2.90745800	0.27454700	-0.33881100
C	0.89264200	0.38368700	0.05324400
C	1.53720000	0.27290400	-1.18274400
C	2.81798000	-0.25216000	-1.27812200
C	3.48315500	-0.68226200	-0.12735100
C	2.85385400	-0.57567100	1.11331200
C	1.56879600	-0.04290800	1.19612800
C	-0.71861300	2.04836700	1.16578400
O	-0.60515600	3.03245700	0.11479600
O	-0.73139000	1.96168500	-0.90585200
O	4.74165700	-1.18875400	-0.27877300
H	-0.38778900	-1.80207200	0.58642600
H	-2.22498300	-3.43923800	0.48656900
H	-4.50906200	-2.71634800	-0.16053400
H	-4.93294100	-0.33053300	-0.70470600
H	-3.08815600	1.31135700	-0.59336700
H	1.03278000	0.62441000	-2.07422400

H	3.32294200	-0.33054400	-2.23318000
H	3.36690900	-0.89917000	2.01439100
H	1.09786400	0.03151100	2.17100400
H	-1.71227000	2.06261900	1.62163200
H	0.06168200	2.17216600	1.91782500
H	5.09087500	-1.43801000	0.58304300

8b

E= -652.0197362 a.u., number of negative frequencies = 0

0 1

C	0.86677500	0.52173800	0.00427100
C	-0.48375200	1.16089200	0.02441600
C	-1.72647200	0.31528500	0.02508100
O	-0.58647900	2.37750000	0.04172200
C	1.11894100	-0.74706000	-0.53955600
C	2.40733700	-1.25883900	-0.59575500
C	3.47407200	-0.50910600	-0.09401000
C	3.24130300	0.76195400	0.44435800
C	1.95303300	1.27083200	0.47745300
C	-2.88070000	0.84822500	-0.56403300
C	-4.07469700	0.13855000	-0.54448400
C	-4.13958800	-1.10239800	0.09053400
C	-3.00519600	-1.62854900	0.70370600
C	-1.80159000	-0.92796500	0.66535800
O	4.71542200	-1.06138900	-0.16074600
H	0.30453100	-1.33150500	-0.94862400
H	2.60982000	-2.23090100	-1.02816500
H	4.07111000	1.34824700	0.82862900
H	1.76184100	2.26243600	0.86850700
H	-2.81928200	1.82540200	-1.02696400
H	-4.95824400	0.55374000	-1.01609900

H	-5.07353900	-1.65282700	0.11323700
H	-3.05682100	-2.58299000	1.21536000
H	-0.92839500	-1.33614700	1.15920800
H	5.36063300	-0.44569600	0.20307300

10b

E= -977.2837537 a.u., number of negative frequencies = 0

0 2

C	1.88892600	-0.28665200	-0.25823300
C	0.56662600	0.29562300	-0.44044100
C	2.03565800	-1.62857400	0.15866400
C	-0.52626300	-0.62946300	-0.89234600
O	-1.24219400	-1.03703900	0.30021800
O	-2.23506500	-2.03522300	-0.11939400
C	-3.53910400	-1.58084900	0.26142300
C	-4.45850400	-2.72925400	-0.17809600
C	-3.87774400	-0.35547600	-0.50377000
C	-3.62910600	-1.30721600	1.76711000
C	3.28459000	-2.21406100	0.30276800
C	4.44106800	-1.48198800	0.01973500
C	4.32730200	-0.15645600	-0.41072300
C	3.07846600	0.42528200	-0.54228400
N	-4.14296600	0.58805100	-1.11057000
C	0.26267900	1.68188600	-0.15287100
C	-0.89883500	2.31850400	-0.66143900
C	-1.18289500	3.64431000	-0.37171900
C	-0.33374400	4.39364500	0.44370400
C	0.80200600	3.78528600	0.98070400
C	1.09419600	2.46076700	0.69434100
H	1.15289000	-2.20342100	0.41144900
H	-0.11832200	-1.51983700	-1.37405700

H	-1.22591800	-0.15099100	-1.58016100
H	-5.49825800	-2.47984700	0.03947500
H	-4.18344500	-3.63178100	0.36970800
H	-4.35408300	-2.91489500	-1.24747400
H	-3.38435400	-2.22452400	2.30615600
H	-4.63929000	-0.99158700	2.03642100
H	-2.92493600	-0.52791500	2.05312600
H	3.36338300	-3.24249300	0.64416000
H	5.22930100	0.39326900	-0.65119400
H	3.01179900	1.44183000	-0.90884600
H	-1.59076500	1.77534300	-1.29004400
H	-2.07841400	4.09495800	-0.78460800
H	-0.56087000	5.42932600	0.66881500
H	1.45613800	4.34436400	1.64096400
H	1.95490100	1.99900500	1.15925500
O	5.69536900	-2.00299700	0.13756200
H	5.63418000	-2.91698100	0.43458000

11b

E= -691.2929612 a.u., number of negative frequencies = 0

0 1

C	-1.66826400	0.10928400	0.06385800
C	-0.51244900	1.07236200	0.17495500
C	-1.56232700	-1.20402100	0.53315500
O	-0.70479400	2.31486100	-0.53184400
C	-2.64927600	-2.07173500	0.45659900
C	-3.85256300	-1.64353100	-0.09914500
C	-3.96066900	-0.34050100	-0.58093200
C	-2.87744400	0.53004500	-0.50078800
C	0.87747500	0.50744900	0.07786300
C	1.62493600	0.20264700	1.21886800

C	2.90293500	-0.33625100	1.12001400
C	3.45796100	-0.57242700	-0.13831800
C	2.72456100	-0.26632700	-1.28769800
C	1.44497200	0.26550800	-1.17459900
C	-0.71094200	2.34943900	0.89637000
O	4.71746500	-1.09750600	-0.18418900
H	-0.62651700	-1.55236500	0.95357000
H	-2.55202400	-3.08646000	0.82652800
H	-4.69638700	-2.32138000	-0.16264400
H	-4.88937300	-0.00136500	-1.02666400
H	-2.95007500	1.53847300	-0.88891200
H	1.20452500	0.38941300	2.20151100
H	3.48577700	-0.57186200	2.00206700
H	3.15585000	-0.44122900	-2.26931500
H	0.88384200	0.50879600	-2.06940900
H	0.14439000	2.84319700	1.35120900
H	-1.67752500	2.55071300	1.35235000
H	4.98271900	-1.20642200	-1.10324900

13b

E= -977.3275019 a.u., number of negative frequencies = 0

0 2

C	-1.44705600	-0.00060500	0.47305500
C	-0.09852400	0.48971900	1.00852400
C	-1.62428500	-0.36202300	-0.86819000
O	-0.19054600	1.05431800	2.26447700
C	-2.84592600	-0.83643000	-1.32595700
C	-3.92159600	-0.96017100	-0.44271300
C	-3.75983300	-0.60068600	0.89491200
C	-2.52937600	-0.12402000	1.34317200
C	0.42725800	1.74827800	0.26969000

C	1.78279700	1.93668200	-0.02670200
C	2.20308100	3.10386200	-0.65645600
C	1.28662400	4.10833400	-0.96432300
C	-0.05917000	3.94132900	-0.64024900
C	-0.48536100	2.77387600	-0.01918000
C	0.92964200	-0.66373100	1.09367800
O	1.20887600	-1.17070800	-0.20805100
C	2.19635800	-2.19692100	-0.31944900
C	3.50690100	-1.66625800	0.14261100
C	1.83757900	-3.45535400	0.48888900
C	2.28112300	-2.50662400	-1.81916600
N	4.51359800	-1.23300900	0.50129000
H	-0.79842700	-0.26611800	-1.56110900
H	-2.98911200	-1.11091100	-2.36418900
H	-4.59279500	-0.68891600	1.58695400
H	-2.40991900	0.16929800	2.37923200
H	2.51319900	1.17529700	0.20735700
H	3.25116600	3.22857600	-0.90336900
H	1.62099500	5.01865200	-1.44907900
H	-0.77574900	4.72220800	-0.86780200
H	-1.52887000	2.64129700	0.23527700
H	1.83834300	-0.29350600	1.57901800
H	0.48819700	-1.43651100	1.73098400
H	2.55976000	-4.24880900	0.28748100
H	1.83765200	-3.26632500	1.56276400
H	0.84429700	-3.79366400	0.18649900
H	3.05782800	-3.24642000	-2.01939500
H	2.50278000	-1.59599800	-2.37622100
H	1.31730600	-2.89741300	-2.14988800
O	-5.10033400	-1.43319600	-0.94679900
H	-5.75723000	-1.45853200	-0.24343700

15b

E= -977.3142440 a.u., number of negative frequencies = 0

0 2

O	-0.91486600	1.20107000	-0.22711200
C	-0.52661400	0.05403900	0.49462100
C	-1.52604900	-1.03782000	0.08250300
C	-0.84098700	0.23746800	2.12186200
C	-0.37415600	2.55185200	-0.13178500
C	-0.55936400	3.05889800	-1.51133200
C	1.11190800	2.68499100	0.23446700
C	-1.26151800	3.37303400	0.81967800
N	-0.69319300	3.48303400	-2.57437100
O	-0.02221600	1.12924000	2.67110300
C	0.91346700	-0.37829200	0.22283000
C	-2.75449600	-0.71145100	-0.50024200
C	-3.66276900	-1.71267400	-0.83710200
C	-3.36434800	-3.04910900	-0.58609200
C	-2.14491300	-3.38117000	0.00107200
C	-1.23291400	-2.38405400	0.33168300
C	1.28963600	-0.55813900	-1.11728400
C	2.56382100	-0.98231600	-1.45786000
C	3.49892300	-1.25053800	-0.45299000
C	3.13853000	-1.08154600	0.88297300
C	1.85514400	-0.64817500	1.21396300
H	-1.89942700	0.53623100	2.11842800
H	-0.71632700	-0.78177800	2.51776300
H	1.75016200	2.14525100	-0.46224700
H	1.37323300	3.74499700	0.19291100
H	1.28450400	2.32666800	1.24770700
H	-2.31005500	3.26798200	0.53837100

H	-1.10976900	3.01979800	1.83895800
H	-0.99023900	4.42965700	0.76448600
H	-2.98699600	0.32360800	-0.70563400
H	-4.60564300	-1.44352700	-1.29974300
H	-4.07328300	-3.82615700	-0.84852500
H	-1.89828400	-4.41874200	0.19585500
H	-0.28060200	-2.65688700	0.77042100
H	0.57006300	-0.35811300	-1.90260200
H	2.85354300	-1.11544300	-2.49298700
H	3.86005600	-1.27891600	1.67052500
H	1.61073700	-0.48325600	2.25492100
O	4.73670200	-1.66875500	-0.84160700
H	5.28390000	-1.81503300	-0.06287100

16b

E= -862.8010180 a.u., number of negative frequencies = 0

0 2

O	0.61394500	1.22155600	-0.75507700
C	0.25163900	-0.02361600	-0.27065700
C	-1.15645100	-0.29176400	-0.19153000
C	1.27104100	2.22752400	0.07760400
C	0.23926400	3.23551000	0.42175500
C	1.88155000	1.69232200	1.37806700
C	2.32141400	2.88925100	-0.82226400
N	-0.55193100	4.03126500	0.68703700
C	1.32031400	-1.00323300	-0.12737200
C	-1.67838100	-1.61023600	-0.14960300
C	-3.04077700	-1.84857000	-0.08572700
C	-3.94644300	-0.78237200	-0.07541000
C	-3.46229800	0.52833500	-0.15169000
C	-2.10360700	0.76686700	-0.21561400

C	1.28390200	-2.02547400	0.84610900
C	2.32967600	-2.93134300	0.97197100
C	3.44318400	-2.85091900	0.13530900
C	3.49969000	-1.84388800	-0.82956600
C	2.46107500	-0.93166300	-0.95749300
H	2.28428700	2.53193700	1.94827500
H	2.68810500	0.99321700	1.16149800
H	1.13096300	1.19111900	1.99016400
H	2.75210800	3.76484600	-0.33249400
H	3.11555000	2.17192600	-1.03393800
H	1.86163400	3.19981200	-1.76100400
H	-1.00680700	-2.45603700	-0.20232500
H	-3.40742700	-2.87115300	-0.06381300
H	-4.17110900	1.34743300	-0.16098700
H	-1.75730200	1.78748900	-0.28599300
H	0.44680700	-2.07986800	1.53095500
H	2.28210800	-3.69778300	1.73784400
H	4.25648300	-3.56016800	0.23578700
H	4.35583500	-1.77621100	-1.49206300
H	2.50142000	-0.16449200	-1.72034200
O	-5.29676500	-0.95692900	-0.00928400
H	-5.49533600	-1.89833200	0.03072600

18b

E= -977.247068 a.u., number of negative frequencies = 0

0 2

C	1.56453700	-0.19864200	-0.37865500
C	0.14878600	0.15254800	-0.86300100
O	-0.63760700	-0.90810800	-0.20630100
C	0.04724300	-0.00486300	-2.34720800
C	-0.32344100	1.52521000	-0.37963600

O	-2.01857900	-0.80614100	-0.72019900
C	-2.81130800	-1.74339800	0.00370500
C	-2.85780700	-1.36968800	1.43984100
C	-2.29085500	-3.17981600	-0.14580500
C	-4.20805600	-1.56921600	-0.61255800
C	2.40359500	0.73781300	0.23323300
C	3.69076500	0.39896000	0.63239000
C	4.16404300	-0.89816900	0.43695800
C	3.33602600	-1.84900900	-0.16470400
H	-0.70368900	0.53338500	-2.90887500
H	0.59222900	-0.80203900	-2.83452600
C	2.05413400	-1.49673900	-0.56859500
C	-0.87303200	1.67121100	0.89733200
C	-1.27043900	2.92326500	1.35720000
H	-2.95862800	-3.87782700	0.36342500
H	-1.29281800	-3.27319500	0.27855400
H	-2.25302600	-3.43046300	-1.20782700
H	-4.92268000	-2.21805600	-0.10408400
H	-4.53726500	-0.53421800	-0.51878300
H	-4.16652700	-1.83786000	-1.66917200
C	-1.11505400	4.05128500	0.55331200
C	-0.55713200	3.91693100	-0.71487000
C	-0.16566900	2.66132000	-1.17798100
N	-2.92182600	-1.09272800	2.55673000
H	2.05295000	1.74719700	0.40165200
H	4.33938900	1.12740100	1.10331400
H	3.69293100	-2.86384000	-0.31588500
H	1.42117000	-2.24717300	-1.02541600
H	-0.99546900	0.80112900	1.52817500
H	-1.70437200	3.01439500	2.34664400
H	-1.42569000	5.02591800	0.91291700

H	-0.42667000	4.78731700	-1.34840700
H	0.27499300	2.57132300	-2.16439200
O	5.43339600	-1.17881600	0.85026700
H	5.63025900	-2.10379100	0.66968800

3b-TS-4b

E= -826.8594459 a.u., im. freq.= 445.37i

0 2

C	1.09430800	-0.36329100	-0.37615400
C	-0.32488000	-0.09834100	-0.65609800
C	-1.34781600	-1.11520500	-0.30298300
C	-0.73722100	1.09952400	-1.21876800
C	1.59530500	-1.67846900	-0.32345900
C	2.94396200	-1.93701500	-0.11922300
C	3.84298300	-0.88115300	0.04772600
C	3.37286800	0.43435400	-0.00005500
C	2.02740200	0.68392200	-0.21146700
C	-2.41311600	-1.39910900	-1.17548700
C	-3.39684100	-2.32205000	-0.83539200
C	-3.34449100	-2.98535600	0.38910700
C	-2.29306000	-2.72166700	1.26570100
C	-1.30492500	-1.80466800	0.92261200
C	-1.26919500	2.66893300	0.34957100
C	-2.62707000	3.11703900	-0.14401300
C	-1.23502000	1.93816100	1.67023200
C	-0.20206400	3.57125000	0.11198400
N	0.69439600	4.27403900	-0.11665800
H	-0.01652700	1.74298800	-1.70554300
H	-1.75279400	1.17777400	-1.58131700
H	0.92159200	-2.51318700	-0.46933700
H	3.30065800	-2.96300600	-0.09838500

H	4.07552900	1.24753100	0.13481400
H	1.69765400	1.71474000	-0.23616100
H	-2.45153900	-0.90869700	-2.14123600
H	-4.20135100	-2.53008000	-1.53211400
H	-4.11126800	-3.70389500	0.65533200
H	-2.24392500	-3.22938800	2.22270500
H	-0.49776600	-1.60254000	1.61646100
H	-2.57957900	3.52065300	-1.15739000
H	-3.33256200	2.28255100	-0.12927000
H	-3.03237800	3.90356900	0.50639000
H	-1.52099300	2.61368900	2.48763500
H	-0.24040300	1.54916300	1.89227900
H	-1.94050900	1.10524200	1.66287500
O	5.17625200	-1.06922200	0.25779200
H	5.36861500	-2.01275700	0.26352100

4b-TS-5b

E= -977.2586094 a.u., im. freq.= 141.75i

0 2

C	0.89236900	1.05448900	-0.02348000
C	0.05402500	-0.11186800	0.32321400
C	-1.38237900	-0.07020900	0.06126600
C	0.73142600	-1.41993900	0.62358400
C	2.04319300	1.37621500	0.71967600
C	2.84056900	2.45733900	0.37025200
C	2.52568500	3.23731200	-0.74113800
C	1.39886600	2.92751900	-1.49914700
C	0.58865000	1.85560900	-1.14226200
C	-2.09649500	1.14021900	0.20846400
C	-3.46728700	1.20639500	0.02210100
C	-4.18594300	0.05764100	-0.32324800

C	-3.51024800	-1.15726900	-0.46410000
C	-2.14159900	-1.21572800	-0.26370800
C	1.64490300	-2.09117500	-0.46433900
O	-0.23748500	0.34526900	2.50001400
O	0.56613900	-0.20181300	3.27206100
C	1.91057900	-3.55023600	-0.01575600
C	1.00391700	-2.08512500	-1.86892000
C	2.95774800	-1.42919700	-0.54943800
N	4.01663400	-0.97984300	-0.63318900
H	1.33386400	-1.29080600	1.53455400
H	-0.02634200	-2.15745800	0.89228000
H	2.30409400	0.78869600	1.58958400
H	3.71859500	2.68532700	0.96307600
H	3.15752900	4.07352500	-1.01786700
H	1.15172100	3.51764300	-2.37457800
H	-0.27717100	1.61918600	-1.74820500
H	-1.56471800	2.03422100	0.50530300
H	-3.98661900	2.15044600	0.15976100
H	-4.07604900	-2.04203500	-0.72889900
H	-1.65360300	-2.17346700	-0.38280700
H	2.59370200	-4.04882700	-0.70604200
H	2.35056000	-3.58004000	0.98315000
H	0.96956900	-4.10590900	0.00247400
H	1.66087400	-2.57966800	-2.58747100
H	0.81955100	-1.06877600	-2.21872000
H	0.05432400	-2.62419000	-1.84958200
O	-5.53095600	0.05919700	-0.52629500
H	-5.87577200	0.94785600	-0.38805900

5b-TS-6b

E= -977.1706558 a.u., im. freq.= 1250.18i

0 2

C	-1.37303500	-0.05989000	0.44848300
C	0.06507400	-0.17373900	0.95424600
C	0.90201600	-1.19039200	0.18051500
C	0.72589900	1.20057700	1.23853800
C	-1.79804200	0.91527700	-0.45109500
C	-3.11615400	0.94805400	-0.90499400
C	-4.03221100	-0.00202200	-0.45830600
C	-3.61932500	-0.98455400	0.44598400
C	-2.30623800	-1.00814800	0.88794300
C	1.88713300	-1.92933300	0.84782000
C	2.66987200	-2.84961200	0.15492800
C	2.48813200	-3.03672000	-1.21361400
C	1.50819000	-2.30678700	-1.88256300
C	0.71191900	-1.39815600	-1.18908500
C	2.14220600	2.00804100	-0.28323600
O	0.04554600	-0.59560500	2.34444300
O	-0.05663100	0.71663600	2.90083600
C	3.37342700	1.12979000	-0.23478100
C	2.30403400	3.39336200	0.31122400
C	1.41194100	1.97416100	-1.49986100
N	0.80110400	1.97027900	-2.48708100
H	0.17055800	2.11273200	1.10101300
H	1.66406100	1.19320800	1.76881400
H	-1.11044600	1.65598600	-0.83657300
H	-4.34146400	-1.71393300	0.79217100
H	-1.99735700	-1.76071300	1.60243900
H	2.02439500	-1.79169400	1.91222500
H	3.42084300	-3.42267300	0.68739800
H	3.09930900	-3.75181600	-1.75277000
H	1.35282800	-2.44951900	-2.94585600

H	-0.05493400	-0.84843400	-1.71849300
H	4.16922400	1.58435400	-0.83977800
H	3.18543100	0.13001300	-0.62011000
H	3.74881400	1.04767700	0.78834900
H	3.06177300	3.95402100	-0.24959800
H	1.37688300	3.96776100	0.27963900
H	2.64230800	3.33061100	1.34881300
H	-3.42369900	1.71533900	-1.60948900
O	-5.33598000	-0.02386700	-0.86173700
H	-5.48876100	0.69836200	-1.47984600

6b-TS-8b

E= -766.3822359 a.u., im. freq.= 1431.14i

0 1

C	-1.65762300	-0.08275200	-0.00735200
C	-0.53764400	0.89845300	-0.01616000
C	-1.52096000	-1.47607400	0.14082500
C	-2.63500100	-2.29945900	0.08391700
C	-3.90453000	-1.75401600	-0.13486800
C	-4.05638300	-0.37910900	-0.29832200
C	-2.94440600	0.45138100	-0.22701800
C	0.86335400	0.32357200	0.00147700
C	1.66957300	0.50197100	-1.12934200
C	2.94502700	-0.04114200	-1.18829300
C	3.44347500	-0.77016800	-0.10729100
C	2.65195000	-0.94794400	1.03274500
C	1.37744600	-0.39601500	1.08360000
C	-0.45784100	2.10101700	1.25786600
O	0.09857800	2.95991800	0.42164900
O	-0.77768100	1.80970400	-1.01938500
O	4.70261300	-1.28065400	-0.21460900

H	-0.53802100	-1.90881300	0.26976900
H	-2.51994100	-3.37203600	0.19110300
H	-4.77064100	-2.40493200	-0.18025800
H	-5.03895900	0.04380200	-0.47217800
H	-3.04334700	1.52295100	-0.34135000
H	1.26847300	1.06558800	-1.96058300
H	3.57052000	0.09119300	-2.06268400
H	3.03769500	-1.50564300	1.88126200
H	0.78577400	-0.52681900	1.98375100
H	-1.47648000	2.34217700	1.59419400
H	0.18989000	1.71268300	2.04986700
H	4.92833000	-1.75019500	0.59515400

9-TS-10b

E= -977.2564860 a.u., im. freq.= 339.20i

0 2

C	1.82258600	-0.38809300	-0.35501000
C	0.59459200	0.38294000	-0.59546900
C	1.75863400	-1.75288700	-0.01615900
C	-0.51949200	-0.24547900	-1.12479100
O	-1.42121300	-1.13595000	0.50312600
O	-2.43824700	-1.97662700	0.06961700
C	-3.74888900	-1.39245500	0.28438600
C	-4.71769600	-2.49654700	-0.15160000
C	-3.90608700	-0.21453300	-0.59733900
C	-3.92956000	-0.98759200	1.74980900
C	2.91184000	-2.50054900	0.17540000
C	4.16759900	-1.90569000	0.02377900
C	4.25572000	-0.55134500	-0.31218100
C	3.10056500	0.19169600	-0.48971500
N	-4.04053100	0.69263800	-1.29583800

C	0.52059700	1.80363000	-0.19924800
C	-0.24545900	2.72576300	-0.93647800
C	-0.34004600	4.05481000	-0.54302900
C	0.32507900	4.49932600	0.59905200
C	1.08730900	3.60050800	1.34340300
C	1.18856800	2.27166400	0.94794600
H	0.78864400	-2.20784100	0.14182000
H	-0.42091100	-1.20888600	-1.60415300
H	-1.39598200	0.33189200	-1.37709600
H	-5.74982500	-2.15720100	-0.05100100
H	-4.56448500	-3.37103000	0.48281400
H	-4.53567100	-2.77564100	-1.19003600
H	-3.83608700	-1.87722000	2.37597000
H	-4.91418000	-0.54164500	1.90459100
H	-3.16035300	-0.27098700	2.03267300
H	2.83848500	-3.54766900	0.45567700
H	5.23549700	-0.10596200	-0.43445100
H	3.18398100	1.23670800	-0.76225400
H	-0.75527900	2.40033300	-1.83512300
H	-0.93161600	4.74664500	-1.13185500
H	0.24966300	5.53645600	0.90566600
H	1.59948000	3.93394200	2.23913100
H	1.76793900	1.57736400	1.54381700
O	5.33358500	-2.58918000	0.19462100
H	5.13625400	-3.50467500	0.41922600

10b-TS-11b

E= -977.2688650 a.u., im. freq.= 428.32i

0 2

C	1.84551400	-0.24752500	-0.30275700
C	0.52288900	0.29568400	-0.58103700

C	2.03255900	-1.62791800	-0.07122800
C	-0.48346200	-0.61327700	-1.20673300
O	-0.89754400	-0.99915300	0.06701500
O	-2.24405200	-2.24668100	-0.20020900
C	-3.39493100	-1.67292600	0.33726300
C	-4.50864400	-2.71886200	0.09059500
C	-3.74046400	-0.42825600	-0.41125600
C	-3.25533100	-1.35336900	1.83514000
C	3.29630700	-2.15794600	0.12117100
C	4.42420200	-1.33004000	0.06796000
C	4.26662100	0.03796800	-0.17195900
C	2.99920700	0.56744100	-0.34358600
N	-3.98179900	0.52494500	-1.01480900
C	0.14973900	1.65825500	-0.21487200
C	-0.82798500	2.37159500	-0.93871900
C	-1.17502900	3.66758000	-0.58332800
C	-0.56808100	4.28522700	0.50924500
C	0.38668500	3.59036600	1.25246200
C	0.74159100	2.29712900	0.89737100
H	1.16171300	-2.26499400	0.01284000
H	-0.03646200	-1.42538900	-1.79004100
H	-1.26539700	-0.12136200	-1.78973100
H	-5.46798400	-2.34216700	0.45288600
H	-4.25287200	-3.63382500	0.62693800
H	-4.58938800	-2.94057200	-0.97383200
H	-3.01155500	-2.27743800	2.36343900
H	-4.18271700	-0.94009500	2.23993000
H	-2.44689400	-0.63939900	1.98315000
H	3.41208300	-3.21888000	0.32326100
H	5.14836000	0.66421700	-0.22862800
H	2.89810600	1.62396700	-0.55539500

H	-1.32488400	1.91105000	-1.78119800
H	-1.92996600	4.19282300	-1.15631300
H	-0.84703900	5.29486300	0.78862100
H	0.84409600	4.05402100	2.11911400
H	1.45518800	1.75340500	1.50277600
O	5.68867000	-1.79704000	0.24100700
H	5.66329900	-2.74860800	0.38894600

10b-TS-15b

E= -977.2560594 a.u., im. freq.= 90.05*i*

0 2

C	-0.80253600	1.52788700	0.36379100
C	0.06234000	0.54326100	0.99108600
C	-2.21121400	1.46215100	0.46922500
C	-0.41163500	-0.15450700	2.25731300
O	-1.47884600	-0.94193700	1.90140000
O	-0.42184100	-1.61359000	0.04381900
C	-1.39649400	-2.44941000	-0.47707500
C	-0.82232200	-3.04442700	-1.79014000
C	-2.63148000	-1.68843300	-0.83415900
C	-1.77183800	-3.58033400	0.50154600
C	-3.00395800	2.46565800	-0.06414700
C	-2.42471000	3.56678700	-0.69551800
C	-1.03686800	3.66232800	-0.79281000
C	-0.23345300	2.65482500	-0.27967800
N	-3.57564300	-1.09166700	-1.12515500
C	1.41287800	0.35131200	0.52041300
C	2.47044200	0.08625300	1.41464500
C	3.77089400	-0.05684100	0.96558500
C	4.04451300	0.00080500	-0.40708700
C	3.00364000	0.21568300	-1.32159300

C	1.71660900	0.39460700	-0.86198700
H	-2.64768400	0.58777700	0.92766700
H	-0.72435500	0.61455600	2.98852700
H	0.40942700	-0.73082400	2.70399600
H	-1.53569600	-3.72922700	-2.25603200
H	0.09406500	-3.58604400	-1.54835500
H	-0.58487600	-2.24586300	-2.49460000
H	-0.86807300	-4.15595100	0.71551100
H	-2.53024100	-4.24545400	0.07837100
H	-2.13560600	-3.14497600	1.43018300
H	-4.08180800	2.37545600	-0.00570600
H	-3.05206200	4.34763400	-1.11091100
H	-0.58070400	4.52551600	-1.26348100
H	0.84188600	2.76182900	-0.32456400
H	2.27969100	0.03137400	2.47783700
H	4.57645100	-0.22802200	1.67286800
H	3.23208500	0.21857500	-2.37995000
H	0.90743500	0.51675000	-1.56834700
O	5.28883500	-0.15657900	-0.91100200
H	5.91553600	-0.32022400	-0.19712300

11b-TS-13b

E= -977.2080855 a.u., im. freq.= 704.91*i*

0 2

C	-0.50857600	1.78530400	0.29513900
C	0.08266800	0.51812400	0.78301300
C	-1.89392300	1.88832500	0.07026200
C	-0.55051400	-0.11760300	2.01554400
O	-0.84991000	-1.40768000	1.50684600
O	-0.95065800	-0.96084600	0.10081400
C	-2.17135700	-2.41713100	-0.73247300

C	-1.96542400	-1.98301700	-2.15596200
C	-3.38584100	-2.04414600	-0.11340900
C	-1.49905300	-3.67507700	-0.26379000
C	-2.46065700	3.09161200	-0.33193300
C	-1.66531200	4.22444600	-0.50379100
C	-0.29459000	4.14219800	-0.27138700
C	0.27982600	2.93625700	0.11918300
N	-4.37968400	-1.71141000	0.38745500
C	1.45578500	0.15805800	0.42702000
C	2.26580700	-0.62595700	1.26853500
C	3.54807000	-1.00476000	0.89550400
C	4.05892400	-0.62385300	-0.34710200
C	3.26484600	0.13370800	-1.21493000
C	1.99131800	0.51197600	-0.83172000
H	-2.51484400	1.00983200	0.18896100
H	-1.46127400	0.41649900	2.29978500
H	0.10258100	-0.20367000	2.89000100
H	-2.47841300	-2.66597900	-2.84553700
H	-0.89976400	-1.99721600	-2.39393500
H	-2.35232600	-0.97760200	-2.32668100
H	-0.44455900	-3.65706500	-0.54640600
H	-1.96357200	-4.55256000	-0.73506400
H	-1.57165600	-3.78582100	0.81705600
H	-3.52833800	3.14396500	-0.51288100
H	-2.11123000	5.16304800	-0.81284400
H	0.33151100	5.01954100	-0.38943800
H	1.34404600	2.89058500	0.31337100
H	1.89528100	-0.95459900	2.22975700
H	4.15356300	-1.60156700	1.57154600
H	3.66346000	0.40527300	-2.18478200
H	1.38327400	1.07783000	-1.52566300

O	5.30729500	-0.96301000	-0.77056400
H	5.74424500	-1.48913000	-0.09241200

11b-TS-13b

E= 977.2668060 a.u., im. freq.= 821.75i

0 2

C	1.64887900	0.08055000	-0.44927400
C	0.27458100	0.47943000	-0.93517300
C	1.85922700	-0.71917500	0.68220500
O	0.15784000	0.51772000	-2.31019400
C	3.14456300	-1.05149900	1.08831800
C	4.24727600	-0.58490800	0.36832200
C	4.04965200	0.20469800	-0.76717000
C	2.75955800	0.52596400	-1.17160900
C	-0.44722100	1.58401100	-0.18944300
C	-1.34209800	2.39905500	-0.89182800
C	-2.03438700	3.41412700	-0.23972000
C	-1.84449700	3.62771600	1.12395900
C	-0.95162000	2.82334200	1.82888700
C	-0.25504600	1.80965600	1.17773800
C	-0.60409300	-0.68554700	-1.38655200
O	-1.13877800	-1.40319100	0.32657900
C	-2.32258900	-2.14663000	0.28766200
C	-3.46678300	-1.30087500	-0.15432900
C	-2.23257000	-3.38903200	-0.62090200
C	-2.56434300	-2.56576500	1.76007600
N	-4.34233400	-0.64786400	-0.52489400
H	1.00692100	-1.10402200	1.22592700
H	3.31508300	-1.67451900	1.95789000
H	4.90296200	0.56587000	-1.33406700
H	2.60707900	1.12557100	-2.06075700

H	-1.47887600	2.23490800	-1.95299700
H	-2.72321600	4.03818200	-0.79764500
H	-2.38564700	4.41741500	1.63292600
H	-0.79218700	2.98771600	2.88873700
H	0.44536800	1.20218000	1.73478400
H	-1.62707900	-0.49267900	-1.67344200
H	-0.11450900	-1.58437300	-1.72348900
H	-3.14118600	-3.99132100	-0.55235100
H	-2.09441900	-3.10623900	-1.66576200
H	-1.37872400	-3.99094400	-0.30305600
H	-3.49893400	-3.12538200	1.84155500
H	-2.61604000	-1.68127800	2.39426400
H	-1.73512000	-3.19512100	2.08616100
O	5.48581700	-0.93553500	0.81724700
H	6.15491300	-0.55357700	0.23952600

11b-TS-15b

E= -977.2600559 a.u., im. freq.= 376.90i

0 2

O	-0.70002000	1.87115100	0.81157900
C	-0.45883000	-0.50028000	0.95644300
C	-1.66189300	-0.90884400	0.20656300
C	-0.62163800	-0.14189300	2.42315900
C	0.01141000	2.73329200	0.00680700
C	-0.15564200	2.38214600	-1.43665300
C	1.51597000	2.77979200	0.35253300
C	-0.62823200	4.13608700	0.23189200
N	-0.28824800	2.09006900	-2.54477800
O	-0.57041100	-1.47596500	2.70871700
C	0.87402200	-0.79294600	0.43802800
C	-2.83730900	-0.14157200	0.24387300

C	-3.97404900	-0.55948400	-0.43641900
C	-3.96677700	-1.75694300	-1.15013300
C	-2.81142000	-2.53514200	-1.18421400
C	-1.66732600	-2.11352700	-0.51776500
C	1.12366100	-0.77164400	-0.95074300
C	2.39748200	-0.96735500	-1.45630700
C	3.46279800	-1.21461600	-0.58562900
C	3.23511200	-1.25518200	0.79608200
C	1.96373100	-1.03828000	1.29768400
H	0.20059500	0.46795800	2.81370500
H	-1.58408000	0.34559100	2.61201600
H	1.97180100	1.80004100	0.21698200
H	2.04019400	3.49960900	-0.28086100
H	1.62129400	3.07693400	1.39791800
H	-1.68688700	4.11106700	-0.02533300
H	-0.51925400	4.40030400	1.28429700
H	-0.12210200	4.87914300	-0.38907300
H	-2.83147000	0.80271000	0.76826600
H	-4.86809400	0.05301500	-0.41314500
H	-2.80249300	-3.47424100	-1.72542700
H	-0.78138800	-2.73520500	-0.52415400
H	0.31829600	-0.55056600	-1.63777900
H	2.58748400	-0.92499800	-2.52136200
H	4.05540800	-1.46946400	1.47488300
H	1.78623000	-1.12065800	2.36112900
O	4.68912900	-1.41262500	-1.13281000
H	5.33380400	-1.57087100	-0.43458500
H	-4.85759900	-2.08299500	-1.67513400

13b-TS-14

E= -977.3167674 a.u., im. freq.= 285.68i

0 2

C	-1.74115800	0.17251200	0.51980100
C	-0.37249600	0.50598300	1.10281600
C	-1.94185800	-0.48092900	-0.70454300
O	-0.32937400	0.70325700	2.37255100
C	-3.21966500	-0.76897700	-1.16634800
C	-4.33332600	-0.40274700	-0.40725700
C	-4.15096600	0.24104600	0.81800400
C	-2.86659700	0.51708600	1.27374400
C	0.56335500	1.37930800	0.26570300
C	1.76566200	1.79500900	0.85320500
C	2.64083400	2.63254100	0.17141600
C	2.32099200	3.08910000	-1.10813700
C	1.11759300	2.70359600	-1.69140600
C	0.24469900	1.85365600	-1.01093000
C	0.48270200	-1.21334600	1.15255100
O	0.88012500	-1.69317300	-0.06237600
C	2.27781200	-1.85291800	-0.44446000
C	3.20451000	-1.43444700	0.62416100
C	2.46408700	-3.35680200	-0.70133400
C	2.52741900	-1.02279500	-1.70765600
N	3.96769300	-1.14392600	1.43750000
H	-1.08961100	-0.79420800	-1.29359800
H	-3.37510600	-1.28079100	-2.10844900
H	-5.01250700	0.52742700	1.41499300
H	-2.71829500	1.00367100	2.22945400
H	1.99419600	1.46674500	1.85908800
H	3.56936400	2.93600200	0.64180700
H	2.99902600	3.74872000	-1.63821200
H	0.84764200	3.07100000	-2.67550500
H	-0.69660300	1.58509800	-1.47058400

H	1.27582700	-1.03369600	1.87159100
H	-0.36615100	-1.77176500	1.53045800
H	3.48020700	-3.56472800	-1.04194300
H	2.27212600	-3.92770500	0.20795300
H	1.75688500	-3.66925400	-1.47130000
H	3.54238300	-1.19284200	-2.07255100
H	2.39298500	0.03889300	-1.50985000
H	1.81852800	-1.33573800	-2.47638900
O	-5.56633300	-0.70228100	-0.91050100
H	-6.24168500	-0.40303100	-0.29284100

15b-TS-16b

E= -977.3139655 a.u., im. freq.= 272.81*i*

0 2

O	-0.64286200	-1.25146000	-0.18205900
C	-0.09817900	-0.11580000	0.39424200
C	1.38249700	-0.13822200	0.13591000
C	-0.11941200	-0.33941500	2.25669600
C	-2.01917800	-1.74684300	-0.10453000
C	-2.22041600	-2.32113300	-1.45414600
C	-3.12522600	-0.71686300	0.16159400
C	-2.04989700	-2.87763800	0.93642100
N	-2.40455900	-2.77866900	-2.49562000
O	-1.32760800	-0.31266500	2.67763800
C	-0.76742600	1.19885900	0.01939800
C	2.03872200	-1.32112500	-0.22928800
C	3.41313700	-1.34360300	-0.42813900
C	4.16731200	-0.18104800	-0.25009800
C	3.52873400	1.00558500	0.12308500
C	2.15671500	1.02107800	0.31156600
C	-0.86150700	1.48193500	-1.35112300

C	-1.41792200	2.67761000	-1.79093600
C	-1.88191500	3.61423400	-0.86767100
C	-1.78853600	3.34067500	0.49323800
C	-1.23602600	2.13911800	0.93773800
H	0.41330900	-1.30428900	2.26389900
H	0.53333700	0.51112400	2.51676800
H	-3.15375200	0.05882900	-0.60062200
H	-4.07959100	-1.24848800	0.14745500
H	-2.98849200	-0.27188600	1.14501100
H	-1.25475400	-3.59657300	0.73560500
H	-1.92418900	-2.44179600	1.92746800
H	-3.00941900	-3.39752100	0.89159200
H	1.46245400	-2.22359100	-0.37620900
H	3.90090200	-2.26752500	-0.72498900
H	4.12309100	1.90167200	0.25150300
H	1.67575500	1.95199100	0.58556300
H	-0.49545400	0.75807100	-2.07009900
H	-1.48593600	2.87878800	-2.85412900
H	-2.31509800	4.54763600	-1.20888400
H	-2.15458300	4.05864800	1.21846200
H	-1.21869700	1.91520400	1.99552900
O	5.51564800	-0.13994200	-0.42700600
H	5.83275200	-1.01150900	-0.68690900

16b-TS-8b

E= -862.7879134 a.u., im. freq.= 583.10i

0 2

O	0.61276500	1.13593600	-0.86940500
C	0.26107600	-0.03780000	-0.43634700
C	-1.15853300	-0.32643200	-0.26453100
C	1.33593500	2.40807800	0.24664700

C	0.26346700	3.35758300	0.27435500
C	1.61310000	1.74689700	1.57206700
C	2.52044200	2.83416200	-0.58429200
N	-0.61263200	4.11479100	0.29254500
C	1.32654300	-1.03600600	-0.20282500
C	-1.67759700	-1.64208800	-0.24407700
C	-3.03499200	-1.88398200	-0.12659100
C	-3.93056900	-0.81433200	-0.02797400
C	-3.44565400	0.49689200	-0.07415200
C	-2.08739500	0.73492000	-0.20172400
C	1.26072200	-2.01042200	0.81009800
C	2.31074900	-2.90026100	1.01239900
C	3.44698800	-2.84560500	0.20657000
C	3.52876200	-1.88347800	-0.80111400
C	2.48685500	-0.98649800	-0.99869100
H	1.95058600	2.49638700	2.29658400
H	2.39215300	0.99195400	1.46841000
H	0.71391900	1.27706100	1.97626800
H	3.00073600	3.71478200	-0.14259800
H	3.25083400	2.02621300	-0.63281500
H	2.20245000	3.08840500	-1.59609300
H	-1.00904300	-2.48535700	-0.35498900
H	-3.42574000	-2.89427300	-0.12296800
H	-4.13592600	1.33373700	-0.01558900
H	-1.73244100	1.75432500	-0.25846200
H	0.39774400	-2.04808700	1.46332500
H	2.24520500	-3.63396200	1.80823300
H	4.26151400	-3.54353900	0.36318700
H	4.40597600	-1.83770000	-1.43717100
H	2.54401000	-0.24197600	-1.78293500
O	-5.25443000	-1.10862400	0.09682000

H	-5.75962400	-0.28978400	0.14157100
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18b-TS-3b

E= -977.2306214 a.u., im. freq.= 297.94i

0 2

C	1.70584700	0.10782900	-0.54784500
C	0.38025500	0.45865600	-1.13295700
O	-0.51843500	-1.21924700	-0.60189200
C	0.16822900	0.19287700	-2.49460500
C	-0.42725000	1.52644100	-0.47272600
O	-1.93501200	-1.10232200	-0.84405200
C	-2.63409500	-1.91308200	0.10072200
C	-2.36277500	-1.46627500	1.49034500
C	-2.24663300	-3.39260700	-0.04332900
C	-4.11291900	-1.66841700	-0.23130300
C	2.41767900	1.01352900	0.25330100
C	3.67504300	0.70310800	0.75075700
C	4.24867400	-0.53794400	0.46942600
C	3.55175200	-1.45748300	-0.31929300
H	-0.76662900	0.46034000	-2.96794400
H	0.87487700	-0.40005500	-3.05836800
C	2.30092500	-1.13199400	-0.82560500
C	-0.70597000	1.46761000	0.89908600
C	-1.45044900	2.46749900	1.51347800
H	-2.81354600	-4.00985300	0.65700500
H	-1.18238100	-3.52265300	0.14812300
H	-2.46511500	-3.71260900	-1.06423200
H	-4.35300200	-0.60967600	-0.13111600
H	-4.29889700	-1.98078700	-1.26015700
H	-4.75117800	-2.24495800	0.44015400
C	-1.91510100	3.55397600	0.77249100

C	-1.63438400	3.63001400	-0.58909300
C	-0.89860700	2.62199100	-1.20760300
N	-2.19393200	-1.14673400	2.58487100
H	1.98806300	1.98061200	0.48031200
H	4.22611200	1.40831400	1.36063700
H	3.98600700	-2.43020500	-0.53180600
H	1.75801800	-1.86100400	-1.41299500
H	-0.36781000	0.61583800	1.47251500
H	-1.67637700	2.38873700	2.57049200
H	-2.49282000	4.33506600	1.25408400
H	-1.98473400	4.47440000	-1.17208800
H	-0.66976000	2.69948300	-2.26399400
O	5.48185800	-0.79549300	0.98859500
H	5.75807800	-1.68173400	0.73259700

18b-TS-6b

E= -977.1896337 a.u., im. freq.= 895.05*i*

0 2

C	0.05655700	1.74414500	0.14189800
C	0.09100300	0.25953200	0.50122200
O	-0.91236100	-0.46382000	-0.27243100
C	-0.47658100	-0.03950700	1.87208500
C	1.44556500	-0.39525700	0.23256200
O	-1.91329900	-0.57832800	0.81591400
C	-3.43841600	-1.24443300	-0.09824700
C	-2.95686900	-2.49010100	-0.59550700
C	-3.74287500	-0.18533800	-1.12511600
C	-4.35704500	-1.33219100	1.09490800
C	0.37161800	2.73372400	1.07673300
C	0.37400700	4.08035800	0.71440000
C	0.05999500	4.45380800	-0.58923300

C	-0.25137900	3.47210700	-1.52872500
H	-0.16606900	-0.95488200	2.35796800
H	-0.82253200	0.76262200	2.50908900
C	-0.24976500	2.12830900	-1.16647000
C	1.50965400	-1.78592000	0.05398200
C	2.72191200	-2.42777000	-0.14875700
H	-2.97024800	-0.14141000	-1.89057100
H	-3.81528800	0.78895500	-0.63852400
H	-4.70306300	-0.39899900	-1.61283800
H	-5.34718200	-1.68853200	0.78796800
H	-3.96517500	-2.02063400	1.84441000
H	-4.47420000	-0.34389600	1.54406200
C	3.90728200	-1.68841800	-0.17207700
C	3.85929400	-0.30499500	-0.00056300
C	2.63630700	0.33220000	0.19322400
N	-2.56410600	-3.50871700	-0.98497400
H	0.62549200	2.45907400	2.09486900
H	0.61824200	4.83529900	1.45347000
H	-0.49619800	3.75333100	-2.54698900
H	-0.49330800	1.36658400	-1.89635000
H	0.59377600	-2.36327400	0.04665500
H	2.76942300	-3.49939500	-0.29911400
H	4.77516300	0.27873000	-0.02648600
H	2.62052300	1.40851900	0.30774000
H	0.05678000	5.50060900	-0.87126800
O	5.07243500	-2.36984800	-0.37163300
H	5.80682200	-1.74721700	-0.38197600

18b-TS-11b

E= -977.239128 a.u., im. freq.= 593.73i

0 2

C	-0.18073100	1.20825900	0.40840700
C	0.64063300	0.02289700	0.91291500
O	-0.08381300	-1.20840300	0.88805200
C	0.63688400	-0.11237600	2.40256800
C	2.04344400	-0.07966600	0.32264400
O	-0.69496100	-1.55861600	-0.65180100
C	-1.62895900	-2.59319800	-0.45892700
C	-2.75315200	-2.12090300	0.39282200
C	-1.00368100	-3.85375400	0.15986500
C	-2.16576300	-2.86878400	-1.88080100
C	0.37684200	2.23891100	-0.35381100
C	-0.39185300	3.31590100	-0.78170600
C	-1.74613600	3.37668500	-0.45707400
C	-2.32068500	2.34840900	0.29497500
H	1.41079600	-0.68524400	2.89513000
H	-0.21937600	0.23227500	2.96505700
C	-1.54310500	1.27978200	0.72027100
C	2.31116700	-0.89664000	-0.77785500
C	3.60037400	-0.96841200	-1.30186600
H	-1.74917500	-4.64613400	0.25856700
H	-0.59150400	-3.62847200	1.14186400
H	-0.19738200	-4.20036100	-0.48974800
H	-2.94103300	-3.63674800	-1.84180100
H	-2.58387900	-1.95871300	-2.31081800
H	-1.34488900	-3.21835300	-2.50856100
C	4.63543200	-0.22627000	-0.73760500
C	4.37532900	0.59079500	0.36003700
C	3.08734600	0.66157900	0.88615100
N	-3.63229600	-1.76040700	1.04580200
H	1.42308300	2.20504000	-0.62787700
H	0.04182100	4.11229600	-1.37407800

H	-3.37884900	2.37567700	0.53902800
H	-2.01409400	0.47949400	1.27648500
H	1.50667400	-1.47199000	-1.21423200
H	3.79569300	-1.60873600	-2.15507700
H	5.63728500	-0.28565300	-1.14784600
H	5.17340800	1.17099800	0.80968000
H	2.89330900	1.30186700	1.74070000
O	-2.45892500	4.45224300	-0.90198900
H	-3.37453100	4.36452100	-0.61724700

3c

E= -325.7661208 a.u., number of negative frequencies = 0

0 1

C	1.94423300	-0.53673900	-0.00028500
C	0.50686700	-0.22317800	-0.00016400
C	2.95552200	0.33406600	0.00036100
C	-0.00922400	1.08089900	-0.00023400
C	-1.38484500	1.26907900	-0.00006900
N	-2.27946300	0.27260500	0.00014100
C	-1.78961700	-0.96923900	0.00017600
C	-0.42933800	-1.26450900	0.00001900
H	2.17690100	-1.59894900	-0.00091100
H	3.98329700	-0.00794400	0.00021500
H	2.80500500	1.40773600	0.00108900
H	0.64575100	1.94365500	-0.00046700
H	-1.79501400	2.27532900	-0.00012600
H	-2.52167600	-1.77243900	0.00033200
H	-0.09961600	-2.29789800	0.00005500

4c

E= -536.5820648 a.u., number of negative frequencies = 0

0 2

C	-1.22862200	-0.54828700	0.21463600
C	0.04019200	-1.16142300	0.34626200
C	1.24731300	-0.57634900	1.00272000
C	-1.52760400	0.77352900	0.63583400
C	-2.81081100	1.26893400	0.47165200
N	-3.82673900	0.57989000	-0.06879900
C	-3.55254900	-0.66889400	-0.47791100
C	-2.30956000	-1.26504100	-0.36601900
C	2.38625900	-0.07578700	0.04393000
C	2.85159700	-1.19771200	-0.90840400
C	3.57403300	0.42184500	0.89757600
C	1.88080500	1.05410500	-0.75204300
N	1.49702800	1.95296500	-1.36435700
H	0.13297600	-2.17057600	-0.04341300
H	0.97417100	0.25157600	1.66101800
H	1.71161100	-1.34177500	1.63682300
H	-0.76499000	1.41050200	1.06442200
H	-3.04235700	2.28206300	0.78851100
H	-4.38135700	-1.21614300	-0.91873000
H	-2.15955900	-2.28040500	-0.71658800
H	3.67051700	-0.84946100	-1.54097400
H	2.04157700	-1.53369700	-1.55712100
H	3.20819600	-2.04978100	-0.32287600
H	4.37464400	0.80693500	0.26310700
H	3.26541700	1.21789700	1.57849200
H	3.97081000	-0.40664200	1.49001900

5c

E= -686.9749054 a.u., number of negative frequencies = 0

0 2

C	-1.15175200	0.30744200	0.15960700
C	0.15629800	1.03564700	0.32365400
C	1.29930900	0.65748900	-0.62696900
C	-1.62712100	-0.53903600	1.16091500
C	-2.83946800	-1.19837500	0.96486700
N	-3.59193900	-1.05588700	-0.12896500
C	-3.13862300	-0.22755900	-1.07526300
C	-1.93652800	0.46776800	-0.98441800
O	-0.16155400	2.46701000	0.07578500
O	0.81064500	3.26196700	0.46149700
C	1.96614500	-0.73827700	-0.43656400
C	2.16274700	-0.99979600	0.99960200
C	3.35310600	-0.71110100	-1.12315400
N	2.29900600	-1.20280500	2.12697800
C	1.12217400	-1.88567700	-1.04007900
H	0.49616000	0.98549300	1.35881700
H	0.95288500	0.72532300	-1.66233800
H	2.06207800	1.42639900	-0.48228700
H	-1.06323600	-0.69182800	2.07419100
H	-3.22473600	-1.86913500	1.72754200
H	-3.76943200	-0.11415800	-1.95238700
H	-1.63143600	1.13240800	-1.78367900
H	3.84835400	-1.67971000	-1.03274900
H	3.22824300	-0.48577800	-2.18538700
H	3.99860400	0.04975000	-0.68066700
H	0.98278200	-1.70645900	-2.10913000
H	1.63815800	-2.83983600	-0.91619300
H	0.14166600	-1.96458600	-0.57328400

6c

E= -476.1348498 a.u., number of negative frequencies = 0

0 1

C	1.24384200	0.54078700	-0.34214300
C	-0.21617400	0.23454800	-0.18499900
C	-1.16602800	1.25672900	-0.20906900
C	-2.50623900	0.93393200	-0.01301300
N	-2.94720000	-0.31188200	0.18254900
C	-2.03191500	-1.28595700	0.18814200
C	-0.66714600	-1.07055100	0.01531100
C	2.14793900	0.53790800	0.89165000
O	3.04921900	-0.35905600	0.19897100
O	2.02463200	-0.57512500	-0.85675700
H	1.39002000	1.42317200	-0.97396900
H	-0.87444700	2.28756500	-0.38071000
H	-3.26305600	1.71341700	-0.02172000
H	-2.40941700	-2.29358700	0.33810500
H	0.03221600	-1.89687500	0.01712800
H	2.63531200	1.47674600	1.16001100
H	1.70329300	0.06180700	1.77031900

8c

E= -361.6978305 a.u., number of negative frequencies = 0

0 1

C	0.52297100	0.21448300	0.00000100
C	1.98875400	0.47154300	0.00000100
O	2.83020600	-0.39336600	-0.00000300
C	0.02375000	-1.08999800	0.00000100
C	-1.35412900	-1.26902400	0.00000100
N	-2.23333600	-0.25819900	-0.00000100
C	-1.74652800	0.98478100	-0.00000200
C	-0.38309100	1.27433500	0.00000000
H	2.26983100	1.54621400	0.00001300

H	0.70821400	-1.92935400	0.00000200
H	-1.77936300	-2.26830200	0.00000100
H	-2.47981100	1.78607400	-0.00000300
H	-0.03753200	2.30297500	0.00000000

10c

E= -686.9663065 a.u., number of negative frequencies = 0

0 2

C	2.24969800	0.55072400	-0.16524500
C	2.36122700	-0.83363000	-0.45425100
C	-0.16856000	0.74593500	-1.01286100
O	-0.75911800	-0.13185200	-0.02696500
O	-1.94226100	-0.72247500	-0.65465900
C	-3.07978600	-0.44268000	0.17401100
C	-4.24287500	-1.09436400	-0.58610900
C	-3.28461800	1.02414600	0.24436000
C	-2.90532600	-1.02259500	1.58219600
C	3.55956800	-1.48340100	-0.20823400
C	4.55160200	0.41731900	0.58039700
C	3.40597000	1.16751000	0.37737600
N	-3.44955700	2.16394500	0.29004000
H	1.51368200	-1.38652900	-0.83827600
H	0.04692800	0.15813200	-1.91278600
H	-0.87429700	1.54009900	-1.26344000
H	-5.17785200	-0.92927600	-0.04860700
H	-4.05895600	-2.16699800	-0.66363000
H	-4.32974400	-0.67314400	-1.58799600
H	-2.76366800	-2.10218100	1.50333000
H	-3.79013300	-0.82052000	2.18942700
H	-2.03474200	-0.58450300	2.06757600
H	3.65521600	-2.54398700	-0.42395500

H	5.44254400	0.88305100	0.99240300
H	3.39245900	2.22262400	0.62723900
C	1.07213100	1.30123600	-0.39898400
H	1.05895400	2.34063000	-0.09170100
N	4.65190800	-0.89022800	0.29674000

11c

E= -400.9823696 a.u., number of negative frequencies = 0

0 1

C	-1.59527300	0.55263200	0.26563100
O	-2.47376000	-0.54382200	0.52772500
C	-0.14160600	0.25199200	0.14088200
C	0.79648900	1.28360600	0.07377700
C	2.14345600	0.96009500	-0.06227500
C	1.69916500	-1.27357800	-0.04781400
C	0.33029700	-1.05990900	0.08500500
C	-2.56973600	0.09589200	-0.74547400
H	0.48901000	2.32265300	0.12705200
H	2.89025000	1.74736400	-0.12008800
H	2.09030700	-2.28652300	-0.08953000
H	-0.36100300	-1.88981300	0.16255600
H	-2.21249200	-0.48866400	-1.58957700
H	-3.47723000	0.67084000	-0.91316400
H	-1.83610800	1.45905200	0.81806300
N	2.60437000	-0.29267200	-0.12507200

13c

E= -687.0196792 a.u., number of negative frequencies = 0

0 2

C	-1.75838700	0.45073400	-0.26426500
C	-0.60922800	1.42154200	-0.50441900

C	-1.74221800	-0.85209100	-0.76603800
O	-0.91130500	2.72753800	-0.26401300
C	-2.82604100	-1.68576800	-0.50138400
C	-3.90235100	-0.06554200	0.68182000
C	-2.87342100	0.84891600	0.47180900
C	0.71328700	1.05162000	0.21887000
O	1.21235800	-0.15192100	-0.35330200
C	2.45965600	-0.65202400	0.14455500
C	3.51547300	0.37506200	-0.04670600
C	2.38186000	-1.03864000	1.63092400
C	2.77576800	-1.86964900	-0.73195200
N	4.32923500	1.17836700	-0.19291500
H	-0.90360100	-1.21271600	-1.34739200
H	-2.83725000	-2.70251300	-0.88503200
H	-4.77926500	0.22309100	1.25496700
H	-2.94061100	1.85791700	0.85889100
H	1.41290200	1.88038800	0.07168400
H	0.51031200	0.93347400	1.28863100
H	3.31439400	-1.51123400	1.94476600
H	2.21540500	-0.17182700	2.27128600
H	1.56141900	-1.74600100	1.76780300
H	3.74126800	-2.29950600	-0.46143800
H	2.79702700	-1.57837900	-1.78239500
H	1.99592600	-2.61940300	-0.58710500
H	-0.34843000	1.40361400	-1.58618600
N	-3.89413500	-1.31648100	0.21159400

15c

E= -687.0144300 a.u., number of negative frequencies = 0

0 2

O	-0.85043700	-0.26642000	0.29997800
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C	0.04089200	0.67107600	-0.21638400
C	1.44887800	0.12640300	-0.11009800
C	-0.00380600	2.07283200	0.62077900
C	-2.25643400	-0.30952400	-0.07599000
C	-2.52437700	-1.75347300	-0.26195200
C	-2.59190800	0.42374700	-1.38203500
C	-3.08540600	0.21576600	1.10519900
N	-2.76052000	-2.87122000	-0.41196400
O	-1.16339300	2.67723400	0.34217100
C	1.77649700	-0.90049000	0.77310300
C	3.09745200	-1.34175800	0.82145700
C	3.75586700	0.14359200	-0.77449700
C	2.46895100	0.65776600	-0.90154500
H	0.10389800	1.75521300	1.66976800
H	0.87879500	2.63449400	0.27911800
H	-2.00935600	0.03752200	-2.22057300
H	-3.64736200	0.26402600	-1.60854900
H	-2.42344300	1.49549000	-1.26890800
H	-2.82450100	-0.33080300	2.01218200
H	-2.86972700	1.27545000	1.24162900
H	-4.15164100	0.08229000	0.90978400
H	1.01702600	-1.35706400	1.39272700
H	3.37632700	-2.14411400	1.49865100
H	4.56343900	0.53773200	-1.38495000
H	2.27153600	1.45187600	-1.61393100
N	4.08116200	-0.83786500	0.07173300
H	-0.17847300	0.93934600	-1.25073700

16c

E= -572.4925512 a.u., number of negative frequencies = 0

0 2

O	-0.94896900	0.50070000	-0.24662400
C	-0.07349000	-0.49900400	0.03302300
C	-2.33744100	0.33492300	0.11728900
C	-2.84817400	-0.95229100	-0.40914900
C	-2.49235600	0.37148900	1.64410300
C	-3.06798800	1.49352800	-0.56685400
N	-3.26123700	-1.95347300	-0.80309100
C	1.30842500	-0.23673300	-0.00572500
C	2.24534700	-1.27928000	0.21181700
C	3.59788900	-0.99180400	0.17631800
C	3.22018500	1.21519100	-0.26666200
C	1.84564100	1.05178000	-0.25450800
H	-3.54355100	0.27885300	1.92302700
H	-2.10632400	1.32314700	2.01387800
H	-1.93540500	-0.44058000	2.11345400
H	-4.13778800	1.44561800	-0.35887300
H	-2.66980100	2.43529200	-0.18572600
H	-2.91162200	1.45309300	-1.64497700
H	1.90765700	-2.29201100	0.40282900
H	4.32378500	-1.78318200	0.34277400
H	3.64444600	2.19772600	-0.45655200
H	1.18821500	1.89238800	-0.43331900
H	-0.47361200	-1.49289600	0.19782500
N	4.10659800	0.22920900	-0.05680400

18c

E= -686.9442157 a.u., number of negative frequencies = 0

0 2

C	0.53784200	1.60789400	-0.03421000
O	-0.76558200	1.13127400	-0.41787600
C	0.87075300	2.64966400	-1.04767200

C	1.57732500	0.50694700	0.04591400
O	-1.28708300	0.40355200	0.76002400
C	-2.49099100	-0.25079400	0.35888000
C	-2.93432700	-0.98295500	1.63437600
C	-3.54663700	0.74764800	-0.13410800
C	-2.19090400	-1.24196900	-0.70354200
C	2.67232700	0.63859100	0.89938300
C	3.63916300	-0.36336500	0.91539900
N	3.57942800	-1.46263400	0.15875800
C	2.52213800	-1.58192600	-0.65098500
C	1.50450200	-0.63578800	-0.74838400
N	-1.97436500	-2.02249300	-1.52319700
H	0.42666600	2.07402400	0.95465300
H	1.60563000	2.45926200	-1.81752700
H	0.30087600	3.56974400	-1.06978300
H	-3.84471800	-1.55109700	1.43786900
H	-2.15430400	-1.66583300	1.97147800
H	-3.13140600	-0.24844800	2.41668900
H	-4.46837600	0.22503100	-0.39767200
H	-3.18476300	1.28788400	-1.00717600
H	-3.75596100	1.46125900	0.66528200
H	2.77510500	1.50369200	1.54627200
H	4.50071200	-0.28081100	1.57264700
H	2.48255400	-2.48437800	-1.25453100
H	0.66672600	-0.79672600	-1.41460700

3c-TS-4c

E= -536.5475244 a.u., im. freq.= 459.86i

0 2

C	1.38287300	-0.35622600	-0.50288600
C	0.13617000	-0.91355700	-0.99505000

C	-1.00528100	-0.22012900	-1.31694600
C	2.43752300	-1.21293100	-0.13623200
C	3.63430600	-0.67772700	0.32315800
C	2.86708300	1.45352900	0.09298000
C	1.63441100	1.02419000	-0.37755800
C	-2.37299600	-0.13452000	0.48447400
C	-2.70582200	-1.58883000	0.71738800
C	-1.54227000	0.55063800	1.54095800
C	-3.38157300	0.64952600	-0.13014600
N	-4.17806200	1.29321500	-0.67704000
H	-0.99419500	0.85873800	-1.41225100
H	-1.78470900	-0.72165600	-1.87599100
H	2.31875900	-2.28842000	-0.21187000
H	4.45109600	-1.33530600	0.60828700
H	3.06897000	2.51666000	0.19145400
H	0.88503100	1.75725300	-0.64930000
H	-3.36948300	-1.69090400	1.58572700
H	-3.21247900	-2.03540200	-0.13979800
H	-1.79677200	-2.15691200	0.92780700
H	-2.09787400	0.59421000	2.48705000
H	-1.28531600	1.57326000	1.26149500
H	-0.62069400	-0.00606500	1.72323400
H	0.11400100	-1.99705400	-1.07788700
N	3.86622300	0.63361600	0.44578300

5c-TS-6c

E= -686.8657162 a.u., im. freq.= 1250.71*i*

0 2

C	-1.33708000	0.22052100	0.30341500
C	-0.09908400	0.92687600	0.81328100
C	1.07970900	1.00879400	-0.16287000

C	-1.95226600	-0.77818900	1.05684200
C	-3.10740900	-1.38542100	0.56495500
N	-3.67240100	-1.06139300	-0.59903700
C	-3.08651300	-0.08979000	-1.30914200
C	-1.93316900	0.57719900	-0.90930000
O	-0.31632400	2.33666800	0.96900200
O	0.27654500	2.70179300	-0.29759200
C	2.17701700	-0.86764600	0.07994500
C	3.30154800	-0.50758700	-0.72254600
C	1.29483200	-1.94059000	-0.52113000
N	4.19810200	-0.18677400	-1.38208200
C	2.46906900	-0.97457200	1.56014600
H	0.17832800	0.52873900	1.79288000
H	0.97406900	0.74303600	-1.20204000
H	1.99133100	1.47270000	0.17984600
H	-1.55034400	-1.07931100	2.01885600
H	-3.60091900	-2.16646300	1.13699800
H	-3.56798300	0.16962800	-2.24770100
H	-1.51596400	1.37407800	-1.51201300
H	1.05301700	-1.73409700	-1.56473200
H	1.81808300	-2.90554300	-0.48902700
H	0.36594000	-2.04789100	0.03946400
H	1.55151100	-1.11864800	2.13358500
H	3.10718300	-1.84765600	1.74830100
H	2.99413400	-0.09664800	1.94056000

6c-TS-8c

E= -476.0714369 a.u., im. freq.= 1479.15i

0 1

C	1.22911200	0.21659900	-0.35157500
C	-0.23680000	0.13086100	-0.15849600

C	-0.81769700	-1.10734400	0.13904700
C	-2.20133300	-1.17685200	0.28239700
C	-2.44374600	1.06923500	-0.09086000
C	-1.07795500	1.24477600	-0.27289500
C	2.36447700	0.51674800	0.87579400
O	3.32117600	0.03733000	0.08002700
O	1.77745200	-0.93734900	-0.80346400
H	1.50328900	1.10446400	-0.93183100
H	-0.19354200	-1.98544600	0.25113700
H	-2.68512000	-2.12435200	0.50027300
H	-3.12397800	1.91195100	-0.17091600
H	-0.67535300	2.22518500	-0.50385300
H	2.39414800	1.59671600	1.05872400
H	2.13877500	-0.08408200	1.76666600
N	-3.00622800	-0.11548800	0.18240400

9-TS-10c

E= -686.9414674 a.u., im. freq.= 436.02i

0 2

C	2.05813800	0.13516500	-0.47245800
C	2.64138100	-1.10317000	-0.14122600
C	0.00013300	-0.76155400	-1.61171700
O	-1.11589900	-1.27698200	-0.05777000
O	-2.45747300	-1.11216800	-0.34657600
C	-3.03991400	-0.00233800	0.39433800
C	-4.52555000	-0.06235300	0.02705400
C	-2.44700200	1.25710300	-0.10328500
C	-2.79083300	-0.15901000	1.89608300
C	3.87089900	-1.12504300	0.50155700
C	4.00971300	1.14960200	0.53038600
C	2.78336400	1.28462700	-0.10761800

N	-1.99240400	2.23858200	-0.50146800
H	2.14063800	-2.03655100	-0.36645700
H	0.39604600	-1.76346700	-1.70684000
H	-0.85569300	-0.53799100	-2.23401300
H	-5.06810800	0.74783100	0.51650800
H	-4.93285400	-1.01836700	0.35971400
H	-4.65771800	0.02387300	-1.05198300
H	-3.26264600	-1.08215200	2.23828600
H	-3.21790400	0.68477400	2.44164500
H	-1.72164100	-0.21048800	2.09426600
H	4.32899600	-2.07451700	0.76457700
H	4.57825500	2.03172900	0.81174300
H	2.38744000	2.27023500	-0.32539100
C	0.78579000	0.27441800	-1.15011700
H	0.40026900	1.28403100	-1.24296800
N	4.56314400	-0.02864400	0.83828200

10c-TS-11c

E= -686.9475610 a.u., im. freq.= 625.27i

0 2

C	2.15904200	0.39767100	-0.23084600
C	2.58427600	-0.89779100	-0.59299500
C	-0.13213600	0.25556600	-1.42318500
O	-0.60246800	-0.25758400	-0.20848400
O	-2.19684600	-1.01794300	-0.54388500
C	-3.10096300	-0.37017200	0.30643700
C	-4.47549500	-0.96979700	-0.07163000
C	-3.10893000	1.08886900	0.01044800
C	-2.77797800	-0.60037000	1.79116400
C	3.84861000	-1.32164600	-0.21265100
C	4.31208500	0.65609200	0.83300500

C	3.06603000	1.17828400	0.51545100
N	-3.09158300	2.21576600	-0.23456500
H	1.92769600	-1.56820500	-1.13188100
H	0.23178700	-0.50636400	-2.11790000
H	-0.83621100	0.93304400	-1.91215000
H	-5.26065800	-0.50815600	0.53084800
H	-4.45621400	-2.04320600	0.12184800
H	-4.68668700	-0.79992800	-1.12743000
H	-2.78486600	-1.67476600	1.98497800
H	-3.51477800	-0.11332700	2.43444600
H	-1.78834400	-0.20808200	2.02085800
H	4.19046000	-2.31809300	-0.47688500
H	5.02439700	1.24806600	1.40037800
H	2.79536400	2.17927100	0.83160900
C	0.88969600	0.94423500	-0.60535300
H	0.60660700	1.90653200	-0.19654400
N	4.71451600	-0.57122800	0.48281000

10c-TS-15c

E= -686.9273195 a.u., im. freq.= 566.30i

0 2

C	-1.69471500	0.61122900	-0.05412300
C	-1.95598000	-0.36274100	0.93664300
C	0.41716200	1.63588200	1.03862100
O	1.68429700	1.87883700	0.60865800
O	1.64423400	0.57356100	-0.84798300
C	2.46000200	-0.48075300	-0.43847700
C	2.49892600	-1.46761300	-1.63000200
C	1.84268600	-1.17810500	0.72841900
C	3.87205000	0.00091800	-0.06586400
C	-3.13471300	-1.09217000	0.86154100

C	-3.79671000	-0.03316500	-1.05720400
C	-2.65371800	0.75084800	-1.08355900
N	1.31082400	-1.68124400	1.62044500
H	-1.23728800	-0.57979400	1.71545600
H	0.33820700	0.86422200	1.81880500
H	0.05579400	2.58227200	1.51246200
H	1.48993300	-1.79078000	-1.88810100
H	3.10246900	-2.34397100	-1.38096700
H	2.93940200	-0.95652400	-2.48724500
H	4.30808800	0.49284300	-0.93734200
H	4.50741300	-0.83672100	0.23268700
H	3.80774600	0.72091700	0.74806900
H	-3.35410200	-1.84781600	1.60949500
H	-4.54817600	0.06446600	-1.83499700
H	-2.49914800	1.47037000	-1.87934000
C	-0.52421300	1.42298500	-0.06738500
H	-0.35153500	2.04930800	-0.93578300
N	-4.04964000	-0.94045300	-0.10476800

10c-TS-6c

E= -686.8919679 a.u., im. freq.= 813.80i

0 2

C	1.71303800	0.62730700	0.11523200
C	1.87299700	-0.24559900	-0.97640900
C	-0.10647600	2.09117900	-1.02082800
O	-1.14363300	1.11171700	-1.11570400
O	-0.97349100	0.61422300	0.27152000
C	-2.63690800	-0.47543200	0.50990800
C	-2.30490900	-0.99591500	1.88123700
C	-2.49781200	-1.39166600	-0.56382300
C	-3.70628300	0.57246900	0.38059600

C	2.94392100	-1.12881500	-0.97968600
C	3.69402700	-0.38810800	1.04346200
C	2.65637100	0.52979200	1.15195600
N	-2.38245600	-2.15161400	-1.43247200
H	1.15490800	-0.25635900	-1.78702100
H	0.48257900	2.09029700	-1.94234000
H	-0.52357300	3.08896500	-0.84740300
H	-3.12830600	-1.61121900	2.26455100
H	-2.15793600	-0.16129500	2.56992500
H	-1.40284400	-1.60803000	1.86336000
H	-4.69562600	0.12697500	0.55071100
H	-3.69814100	1.02174200	-0.61156600
H	-3.55269000	1.35339500	1.12754600
H	3.08008800	-1.81358400	-1.81177800
H	4.43659300	-0.46826300	1.83271000
H	2.58493100	1.17048500	2.02428000
C	0.61482700	1.57059800	0.20102300
H	0.60268000	2.19601100	1.08652000
N	3.85353900	-1.21002900	0.00075400

11c-TS-13c

E= -686.9572308 a.u., im. freq.= 836.19i

0 2

C	-1.58655000	0.33722400	-0.31930500
C	-0.44729200	1.22177300	-0.72911800
C	-1.56099900	-1.03316200	-0.58125900
O	-0.61247800	2.57772600	-0.63463900
C	-2.64564000	-1.80745100	-0.17788500
C	-3.73666200	0.00034000	0.68271600
C	-2.70625500	0.86432300	0.32388500
C	0.46722200	1.71925900	0.37812300

O	1.33344600	0.10635900	0.97567900
C	2.51542800	-0.33405800	0.36967700
C	2.23379100	-0.86332300	-0.99229400
C	3.62017200	0.73577200	0.28770300
C	2.96924800	-1.51260400	1.27195500
N	1.98409800	-1.25267400	-2.04902000
H	-0.72215500	-1.48787400	-1.09458600
H	-2.65257000	-2.87696400	-0.36882700
H	-4.62261000	0.38428500	1.18099900
H	-2.77234500	1.92725400	0.52044700
H	1.38230900	2.23378800	0.13886600
H	0.03735300	1.85617800	1.35561500
H	4.55754900	0.29571800	-0.05879500
H	3.35384500	1.53545000	-0.40523400
H	3.77181800	1.16026100	1.28207100
H	3.86387500	-1.97842000	0.85315300
H	2.17434500	-2.25395500	1.34444900
H	3.19005400	-1.12505500	2.26706700
H	0.08816400	0.86539900	-1.61324900
N	-3.72012000	-1.31551000	0.44680700

11c-TS-15c

E= -686.9528220 a.u., im. freq.= 783.90*i*

0 2

O	-1.10325000	0.09634900	0.82679300
C	0.12998100	1.00470100	-0.46826300
C	1.35577900	0.23347700	-0.17922200
C	-0.09615300	2.39459100	0.05233300
C	-2.36112500	-0.32608000	0.39527000
C	-2.23812600	-1.18289400	-0.81734300
C	-3.32713300	0.83756300	0.09991100

C	-2.89453100	-1.19319500	1.56674100
N	-2.10440300	-1.82392200	-1.76698200
O	0.65705000	2.60203000	-1.07045300
C	2.43690500	0.76136400	0.53073500
C	3.53991100	-0.05015300	0.77257900
C	2.60255100	-1.81428100	-0.32136800
C	1.45314700	-1.08905700	-0.61997800
H	-1.12709100	2.75317200	0.02296400
H	0.38368700	2.58236700	1.01796600
H	-4.32311100	0.46043300	-0.14225400
H	-3.39055800	1.47404400	0.98439700
H	-2.97608900	1.43352300	-0.74394200
H	-2.19811500	-2.00353800	1.77939600
H	-2.99251100	-0.56245200	2.45076300
H	-3.86858200	-1.61156200	1.30382200
H	2.44415800	1.79198600	0.85988000
H	4.39281600	0.34214100	1.31918500
H	2.69685400	-2.84403000	-0.65393200
H	0.64908700	-1.54867600	-1.18168700
N	3.63631100	-1.31972500	0.36536100
H	-0.45153400	0.69486900	-1.32431700

13c-TS-14

E= -687.0106759 a.u., im. freq.= 311.78i

0 2

C	-1.64494900	0.47576600	-0.28798400
C	-0.61959100	1.54379500	-0.54145400
C	-1.53982600	-0.78647200	-0.87256000
O	-0.84885400	2.74713900	-0.25549400
C	-2.53124500	-1.73055500	-0.61548000
C	-3.68402300	-0.28324200	0.71828300

C	-2.75268900	0.73029400	0.52227800
C	0.76395800	1.15244100	0.87767400
O	1.19074100	-0.13512500	0.92687400
C	2.45409700	-0.51000800	0.31757600
C	2.50747700	-0.04431800	-1.08441400
C	3.62195400	0.08756400	1.11488400
C	2.46250200	-2.04109900	0.35282200
N	2.56729300	0.30537100	-2.18103700
H	-0.71278400	-1.02644800	-1.53232800
H	-2.47611100	-2.71910500	-1.06383100
H	-4.55612900	-0.11243500	1.34362400
H	-2.87809700	1.70945400	0.96856000
H	1.48416900	1.91006600	0.58237400
H	0.13115200	1.38861800	1.72406400
H	4.57301700	-0.23285200	0.68598200
H	3.59630700	1.17796900	1.10792600
H	3.55951700	-0.26367100	2.14634400
H	3.38149200	-2.42759400	-0.09001900
H	1.60699100	-2.43756500	-0.19372100
H	2.39783500	-2.36748800	1.39190500
H	0.07534800	1.30655900	-1.36715400
N	-3.58783500	-1.50060300	0.16896300

15c-TS-16c

E= -687.0118965 a.u., im. freq.= 381.90i

0 2

O	0.85107400	-0.32342700	-0.25756700
C	-0.05007400	0.51400600	0.31617200
C	-1.44503600	0.03944800	0.16522800
C	-0.02347100	2.17906900	-0.60413300
C	2.28295900	-0.29604500	0.05939600

C	2.61723600	-1.72177900	0.26256900
C	2.63540300	0.48952500	1.32727500
C	3.01298100	0.24208200	-1.17744500
N	2.90618800	-2.82493000	0.42700400
O	1.11754700	2.69075000	-0.37446600
C	-1.80769400	-0.90829800	-0.79642900
C	-3.14393400	-1.28559800	-0.88887100
C	-3.76041000	0.11265200	0.80309500
C	-2.45577900	0.55973800	0.98177000
H	-0.23293600	1.75950300	-1.60419300
H	-0.90880700	2.62923400	-0.12250400
H	2.12566200	0.08790200	2.20523300
H	3.70944800	0.39927900	1.49783600
H	2.39181100	1.54388300	1.19277800
H	2.73319600	-0.33864300	-2.05716900
H	2.73205900	1.28625900	-1.31675600
H	4.09320400	0.16637200	-1.03645900
H	-1.06138500	-1.35010300	-1.44274100
H	-3.44946300	-2.02476000	-1.62383600
H	-4.55955000	0.49835700	1.42961800
H	-2.23297900	1.29244200	1.74975600
N	-4.11559900	-0.79180400	-0.11478400
H	0.20356200	0.88003600	1.30740800

16c-TS-8c

E= -572.4696250 a.u., im. freq.= 573.62i

0 2

O	0.96564100	-0.22790900	-0.94682600
C	0.06662800	0.64519000	-0.70922300
C	2.46904500	-0.37775300	0.17547600
C	2.85901900	0.98879600	0.31732900

C	1.90067800	-1.01599000	1.41449900
C	3.32298200	-1.22240700	-0.72814900
N	3.10691500	2.11504300	0.41862900
C	-1.28693000	0.30013500	-0.33825800
C	-2.24352900	1.30780400	-0.11583900
C	-3.54247000	0.94432900	0.21422300
C	-3.04354200	-1.28180100	0.11321200
C	-1.72155800	-1.03440000	-0.22289900
H	1.11207200	-0.40055000	1.85204400
H	2.68519200	-1.13815300	2.17112400
H	1.49673500	-2.00083100	1.17621300
H	4.25225200	-1.50360600	-0.22022100
H	2.78170500	-2.13309800	-0.99003500
H	3.57479600	-0.68525900	-1.64230200
H	-1.97110600	2.35457500	-0.19633100
H	-4.29344200	1.70850500	0.39466300
H	-3.39910600	-2.30405300	0.20969500
H	-1.03015800	-1.84737300	-0.40414800
H	0.32576000	1.70864700	-0.76727900
N	-3.95573700	-0.32346500	0.33407900

18c-TS-3c

E= -686.9295755 a.u., im. freq.= 491.88*i*

0 2

C	0.58788600	1.77438200	0.19063600
O	-0.78114700	1.01940300	1.14975900
C	-0.04826700	2.36379700	-0.91137000
C	1.58785200	0.69072800	0.03436700
O	-0.95869400	-0.34348000	0.88027000
C	-2.25389700	-0.61896200	0.29144800
C	-2.32458000	-2.15104400	0.30189000

C	-3.38524200	0.02529200	1.09658100
C	-2.26860900	-0.13342500	-1.10571300
C	2.59073300	0.52700500	0.99340200
C	3.52176800	-0.49508400	0.83805800
N	3.51532700	-1.35364200	-0.18570500
C	2.54817700	-1.20023700	-1.09597100
C	1.57311900	-0.20974000	-1.03528300
N	-2.26880600	0.22424600	-2.20180600
H	0.79607100	2.43728400	1.02474300
H	-0.11986100	1.87263200	-1.87121200
H	-0.58792300	3.29361500	-0.78740000
H	-3.25388600	-2.48859700	-0.15959400
H	-1.48185800	-2.57675800	-0.24348200
H	-2.28924100	-2.49736000	1.33573500
H	-4.35092000	-0.21012100	0.64457600
H	-3.25836400	1.10569800	1.13021100
H	-3.36113100	-0.36735200	2.11494500
H	2.64509500	1.18655500	1.85221500
H	4.31103200	-0.63168700	1.57220400
H	2.55275400	-1.90822200	-1.92013700
H	0.81767200	-0.15358300	-1.80871500

18c-TS-6c

E= -686.8816329 a.u., im. freq.= 875.97i

0 2

C	0.51986400	-0.80203600	0.34649800
O	-0.46706900	0.04091200	-0.27534500
C	0.03897300	-0.66916800	1.76782200
C	1.91774200	-0.31291500	0.06233700
O	-1.45939600	-0.08181500	0.82047200
C	-3.10316100	0.36603100	-0.08463400

C	-4.02399400	0.21988500	1.09900200
C	-2.84858700	1.75717600	-0.60143400
C	-3.16994400	-0.67201800	-1.05598700
C	2.97538600	-1.21378000	-0.06363500
C	4.25993700	-0.71963700	-0.27532200
N	4.54593600	0.58107900	-0.38043500
C	3.52427600	1.43647200	-0.27289100
C	2.20610100	1.04805000	-0.05086500
N	-3.23390400	-1.52643500	-1.83651500
H	0.39812600	-1.83092800	-0.01003400
H	0.35711400	0.19942300	2.33170600
H	-0.23269700	-1.54895200	2.33641800
H	-5.04935900	0.48889600	0.81895400
H	-4.03151500	-0.80526900	1.47048600
H	-3.70424200	0.88873300	1.90075400
H	-3.76160300	2.16140400	-1.05812600
H	-2.05877500	1.76365700	-1.35114600
H	-2.56318000	2.41163600	0.22423600
H	2.80681900	-2.28355700	-0.00235800
H	5.09881800	-1.40324400	-0.37270100
H	3.77273000	2.48969300	-0.37103400
H	1.41570300	1.78484900	0.01513200

18c-TS-11c

E= -686.9324121 a.u., im. freq.= 663.05*i*

0 2

C	0.61631000	1.60316600	0.05206500
O	-0.66290400	1.22015800	-0.37228000
C	0.64702300	2.49864300	-1.13236900
C	1.66581800	0.51810000	0.08893900
O	-1.36558200	0.27167500	0.89832800

C	-2.55156900	-0.26522900	0.37598600
C	-3.11403700	-1.10679400	1.54525300
C	-3.54754600	0.81889700	-0.06468800
C	-2.24810300	-1.16988700	-0.76524900
C	2.83260400	0.69726900	0.83182000
C	3.80260800	-0.30125600	0.81114200
N	3.67947700	-1.43869000	0.12141900
C	2.55267600	-1.60327300	-0.57944400
C	1.52411500	-0.66553300	-0.63296200
N	-2.00810300	-1.87323300	-1.64662800
H	0.58015000	2.15045100	1.00033600
H	0.96023600	2.10636600	-2.09027800
H	0.21714000	3.48914100	-1.07435100
H	-4.03638600	-1.60068400	1.23299200
H	-2.38988200	-1.86135100	1.85204600
H	-3.32408400	-0.44590600	2.38719800
H	-4.47758000	0.36929500	-0.41964800
H	-3.11784900	1.42293200	-0.86228500
H	-3.76273700	1.46278300	0.79037600
H	2.98796600	1.59450100	1.42214900
H	4.72057900	-0.18362600	1.38069600
H	2.46328800	-2.53744400	-1.12664500
H	0.62804100	-0.86227600	-1.20745100

19

E= -941.3619615 a.u., number of negative frequencies = 0

0 2

C	0.51352400	-0.09434800	0.41589600
C	0.69919400	1.39559000	0.12808000
C	1.74052600	-0.90785100	0.00157500
C	0.51077500	2.38089900	1.10185700

C	0.65710400	3.73020800	0.77786600
C	0.98282500	4.11403600	-0.51872000
C	1.16936800	3.13691400	-1.49543600
C	1.03381800	1.79079600	-1.17294000
C	3.00280600	-0.48113300	0.43602000
C	4.14701300	-1.20197100	0.11794700
C	4.05278100	-2.36178900	-0.65093600
C	2.80589700	-2.79431700	-1.08782400
C	1.65611800	-2.07581500	-0.75839400
O	0.42448200	-0.18292600	1.91825300
O	0.16863100	-1.39675100	2.34440600
C	-2.06036900	0.12093700	0.33492500
C	-0.81479100	-0.62376500	-0.15729200
C	-3.40131400	-0.34956500	-0.29859600
C	-4.57237300	0.34648100	0.43274100
C	-3.46474800	-0.01709100	-1.80729700
C	-3.54940400	-1.80604900	-0.13165500
N	-3.66786600	-2.94711600	-0.01122300
H	0.25690900	2.09862800	2.11421200
H	0.51417000	4.48062300	1.54738900
H	1.09497200	5.16325100	-0.76714100
H	1.43035600	3.42208300	-2.50840700
H	1.20527800	1.03967100	-1.93588700
H	3.08544100	0.42094500	1.03063800
H	5.11368900	-0.85799800	0.46812800
H	4.94515700	-2.92320600	-0.90352200
H	2.71908900	-3.69737500	-1.68126100
H	0.69801400	-2.44444100	-1.09922300
H	-2.13705500	0.01043200	1.41947400
H	-1.97445300	1.19134900	0.12844500
H	-0.73894200	-0.56565600	-1.24591700

H	-0.89975000	-1.67757400	0.11365800
H	-5.53306900	0.03705200	0.01624100
H	-4.56660100	0.10817400	1.49811900
H	-4.47921000	1.42971400	0.31933000
H	-4.42884700	-0.31247300	-2.22617500
H	-2.68460000	-0.52931200	-2.37206900
H	-3.34289700	1.06035000	-1.94564500

20

E= -730.553553 a.u., number of negative frequencies = 0

0 1

C	0.06320400	0.68815400	0.10522400
C	-1.24007000	-0.11504200	0.04429600
C	1.32462700	-0.18082100	0.01774100
C	-1.91713700	-0.25746100	-1.16885400
C	-3.08597400	-1.01121200	-1.24441600
C	-3.59247500	-1.64247000	-0.11098600
C	-2.92105500	-1.51245100	1.10229100
C	-1.75594300	-0.75228900	1.17806200
C	1.28790000	-1.57322200	0.10831500
C	2.46391400	-2.32148500	0.04387500
C	3.69098800	-1.69008900	-0.12411400
C	3.73683900	-0.30020700	-0.23074100
C	2.56624700	0.44570000	-0.16000900
O	0.15629500	1.57212300	-1.04039600
O	-0.65873000	2.71950800	-0.66993200
C	-0.14966800	3.04414100	0.62201300
C	0.08603400	1.68925600	1.31061400
H	-1.52758500	0.23952100	-2.04724200
H	-3.60280200	-1.10271400	-2.19335200
H	-4.50286500	-2.22817900	-0.17125600

H	-3.30395100	-1.99927700	1.99242700
H	-1.24337700	-0.66919900	2.13049900
H	0.34105300	-2.08300200	0.22570000
H	2.41314300	-3.40202000	0.11862100
H	4.60377600	-2.27263200	-0.17842400
H	4.68635100	0.20343900	-0.37438700
H	2.60986300	1.52262100	-0.26527600
H	0.77784500	3.61984300	0.52899100
H	-0.91643000	3.65501100	1.10179300
H	-0.70254700	1.45681200	2.02317100
H	1.04240600	1.66372000	1.83149600

19-TS-20

E= -941.286267 a.u., im. freq.= 985.40i

0 2

C	-0.61559700	-0.14235900	0.52130900
C	-1.79302700	-0.98797900	0.03862200
C	-0.77059000	1.34644100	0.20091400
C	-2.12379100	-2.17173100	0.71095100
C	-3.16432300	-2.97601000	0.25565500
C	-3.88078100	-2.62031200	-0.88525600
C	-3.55390100	-1.44877100	-1.56184800
C	-2.52183900	-0.63416100	-1.09981900
C	-1.60724000	2.11629300	1.01781000
C	-1.81810600	3.46354700	0.75070600
C	-1.19887200	4.06810600	-0.34329900
C	-0.36708000	3.31223800	-1.16140800
C	-0.15351100	1.95892900	-0.89193300
O	-0.53025800	-0.33244600	1.95185500
O	0.64006300	0.27848900	2.34718700
C	1.85641700	-0.25794100	0.91937500

C	0.74350800	-0.75593300	0.04303900
C	3.65740300	-0.86819200	-0.23097200
C	4.74926700	-0.28067800	0.63608500
C	3.59404900	-2.37808100	-0.29872300
C	3.40187400	-0.18154200	-1.44617100
N	3.13062100	0.39214400	-2.41847200
H	-1.57461300	-2.45139000	1.60083300
H	-3.41527400	-3.88288600	0.79462500
H	-4.68851800	-3.24972800	-1.24142400
H	-4.10673100	-1.15961000	-2.44858300
H	-2.29031200	0.28381600	-1.62518200
H	-2.07979100	1.65230100	1.87457900
H	-2.46540500	4.04402500	1.39869400
H	-1.36252800	5.11939600	-0.55197700
H	0.12506800	3.76896900	-2.01264200
H	0.50445100	1.40291300	-1.54887500
H	2.19712600	0.76122700	0.83671900
H	2.30635000	-0.89559300	1.66325100
H	0.65351100	-1.83951600	0.12403300
H	0.90475800	-0.51375900	-1.00626900
H	4.70906800	-0.70287600	1.64355100
H	5.73625700	-0.51724800	0.21868600
H	4.67225100	0.80523200	0.71000100
H	4.50949900	-2.77653500	-0.75537100
H	2.75019800	-2.72942700	-0.89342300
H	3.51868900	-2.80384700	0.70552200