Electronic Supplementary Material (ESI) for RSC Advances.

A Computational Study for the Reaction Mechanism of Metal-Free Cyanomethylation and Cyclization of Aryl Alkynoates with Acetonitrile

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Table of contents

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

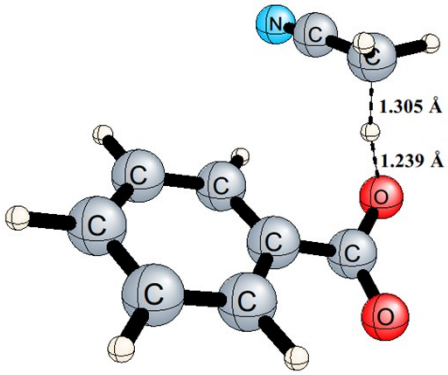

Figure S1. Computed structure of **2**/**5** at the B3LYP/6-311G(d,p) level (im. freq.= 1800i).

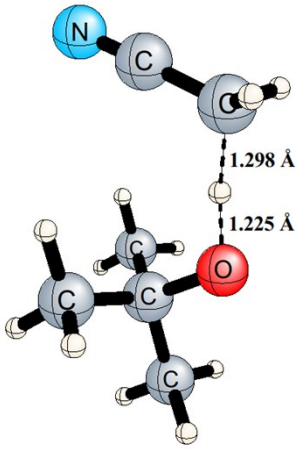

Figure S2. Computed structure of **3**/**5** at the B3LYP/6-311G(d,p) level (im. freq.= 1781i).

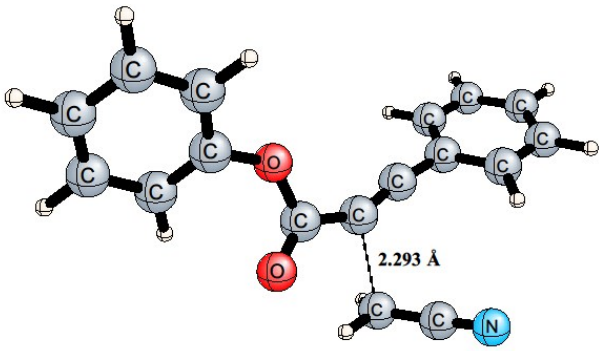

Figure S3. Computed structure of **8a**/**9a** at the B3LYP/6-311G(d,p) level (im. freq.= 422i).

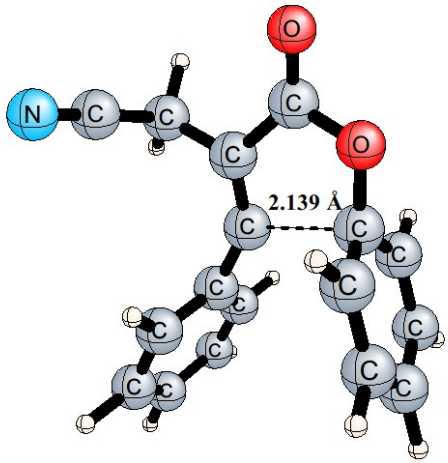

Figure S4. Computed structure of **9a**/**10a** at the B3LYP/6-311G(d,p) level (im. freq.= 436i).

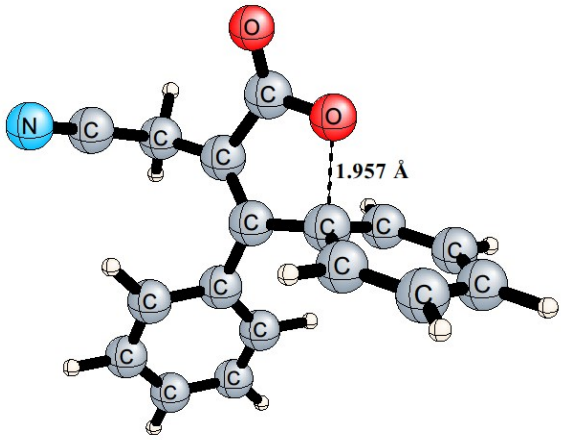

Figure S5. Computed structure of **10a**/**11a** at the B3LYP/6-311G(d,p) level (im. freq.= 328i).

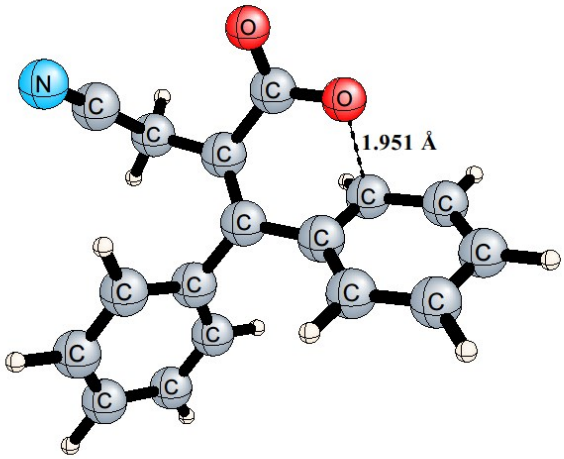

Figure S6. Computed structure of **11a**/**12a** at the B3LYP/6-311G(d,p) level (im. freq.= 326i).

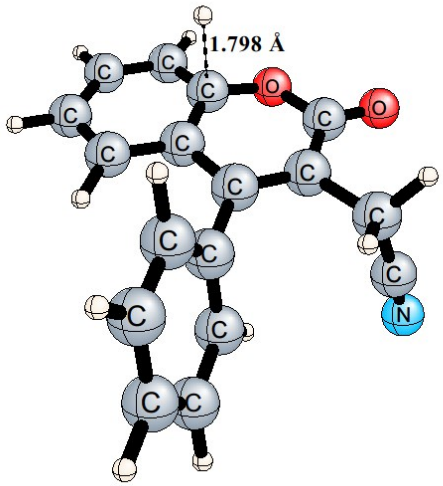

Figure S7. Computed structure of **12a**/**13a** at the B3LYP/6-311G(d,p) level (im. freq.= 924i).

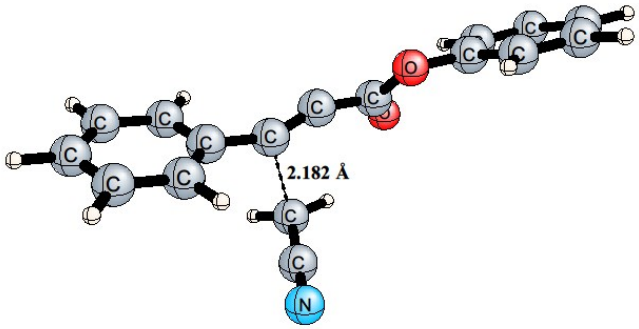

Figure S8. Computed structure of **8a**/**14a** at the B3LYP/6-311G(d,p) level (im. freq.= 575i).

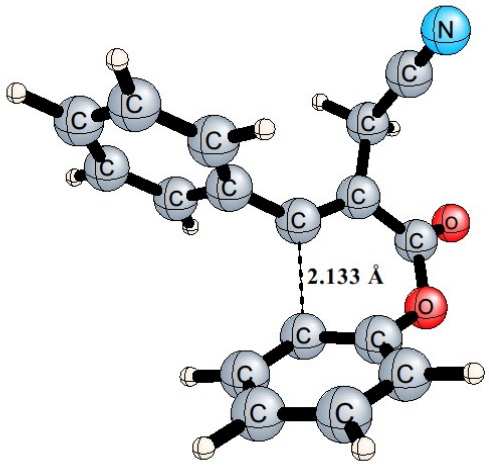

Figure S9. Computed structure of **9a**/**12a** at the B3LYP/6-311G(d,p) level (im. freq.= 426i).

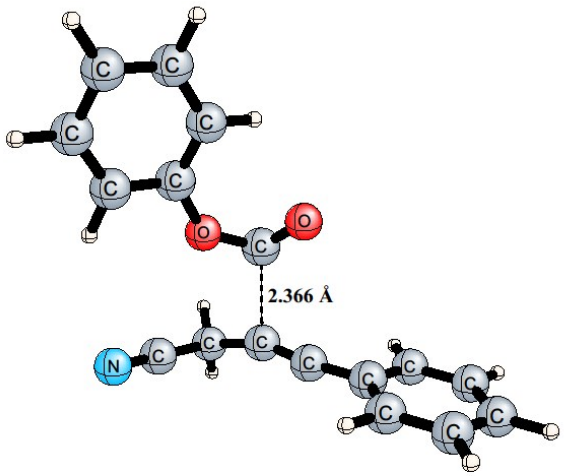

Figure S10. Computed structure of **9a**/**17a** at the B3LYP/6-311G(d,p) level (im. freq.= 333i).

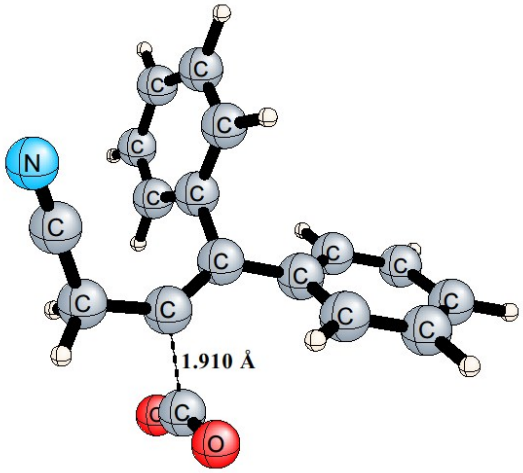

Figure S11. Computed structure of **11a**/**20a** at the B3LYP/6-311G(d,p) level (im. freq.= 423i).

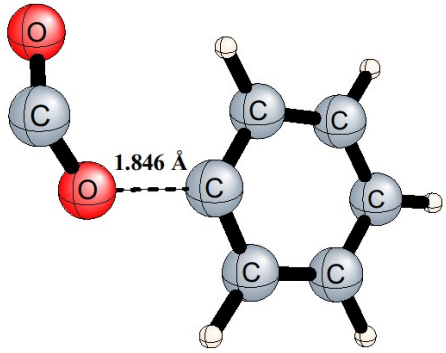

Figure S12. Computed structure of **17a**/**19a** at the B3LYP/6-311G(d,p) level (im. freq.= 668i).

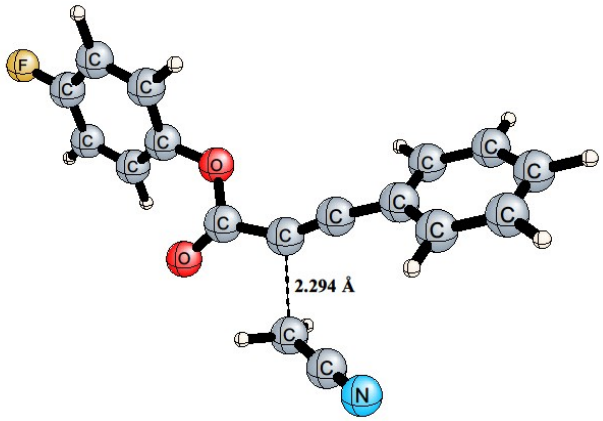

Figure S13. Computed structure of **8b**/**9b** at the B3LYP/6-311G(d,p) level (im. freq.= 420i).

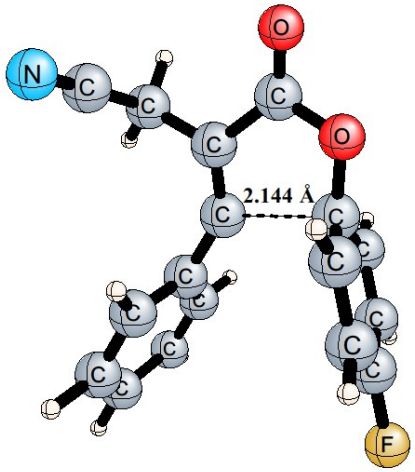

Figure S14. Computed structure of **9b**/**10b** at the B3LYP/6-311G(d,p) level (im. freq.= 432i).

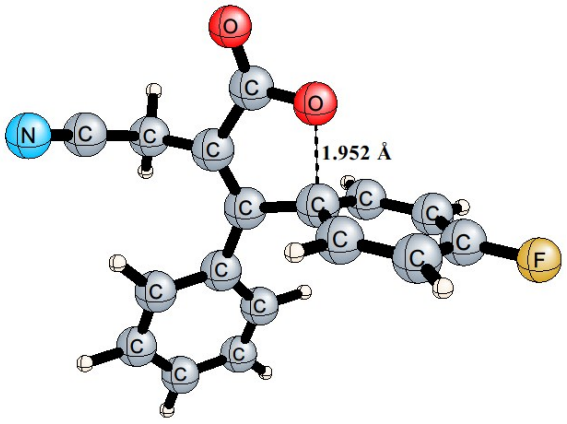

Figure S15. Computed structure of **10b**/**11b** at the B3LYP/6-311G(d,p) level (im. freq.= 315i).

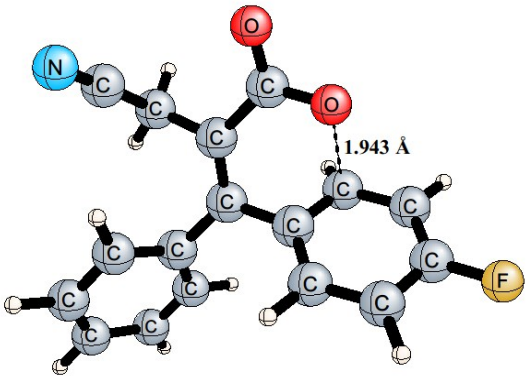

Figure S16. Computed structure of **11b**/**12b** at the B3LYP/6-311G(d,p) level (im. freq.= 337i).

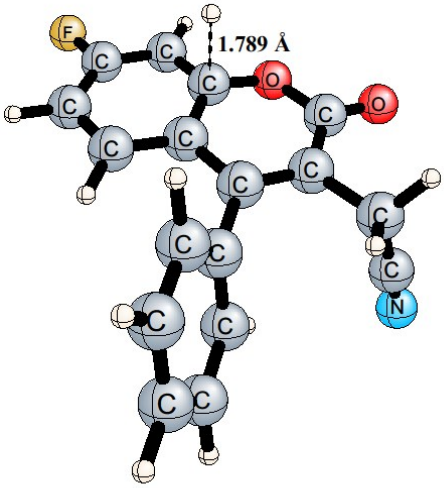

Figure S17. Computed structure of **12b**/**13b** at the B3LYP/6-311G(d,p) level (im. freq.= 945i).

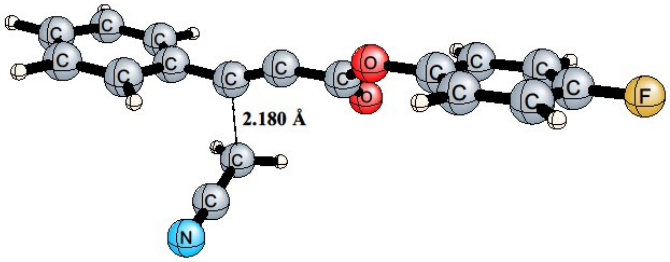

Figure S18. Computed structure of **8b**/**14b** at the B3LYP/6-311G(d,p) level (im. freq.= 573i).

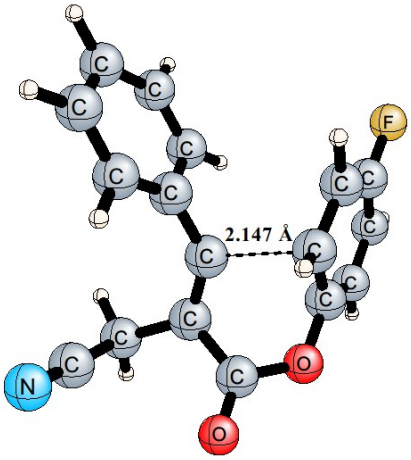

Figure S19. Computed structure of **9b**/**15b** at the B3LYP/6-311G(d,p) level (im. freq.= 402i).

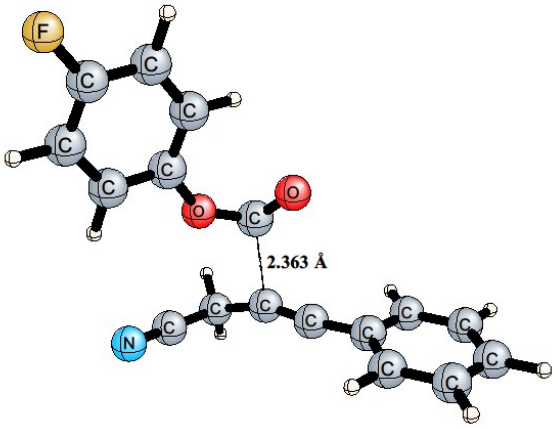

Figure S20. Computed structure of **9b**/**17b** at the B3LYP/6-311G(d,p) level (im. freq.= 335i).

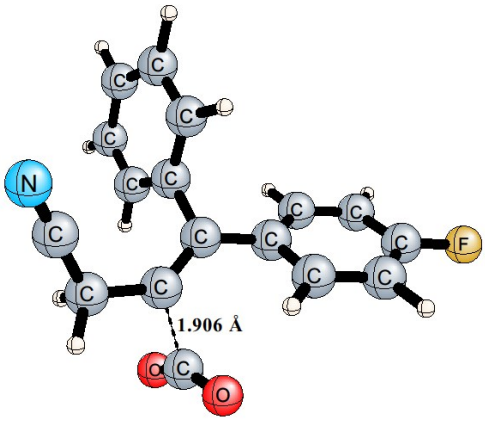

Figure S21. Computed structure of **11b**/**20b** at the B3LYP/6-311G(d,p) level (im. freq.= 423i).

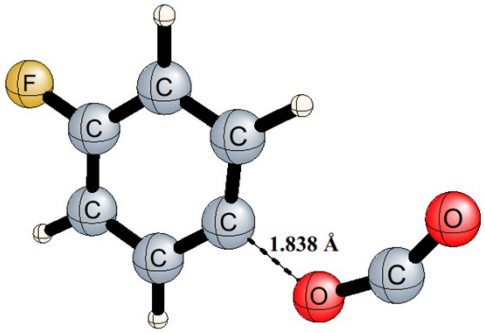

Figure S22. Computed structure of **17b**/**19b** at the B3LYP/6-311G(d,p) level (im. freq.= 677i).

2. Relative Free Energy Profile

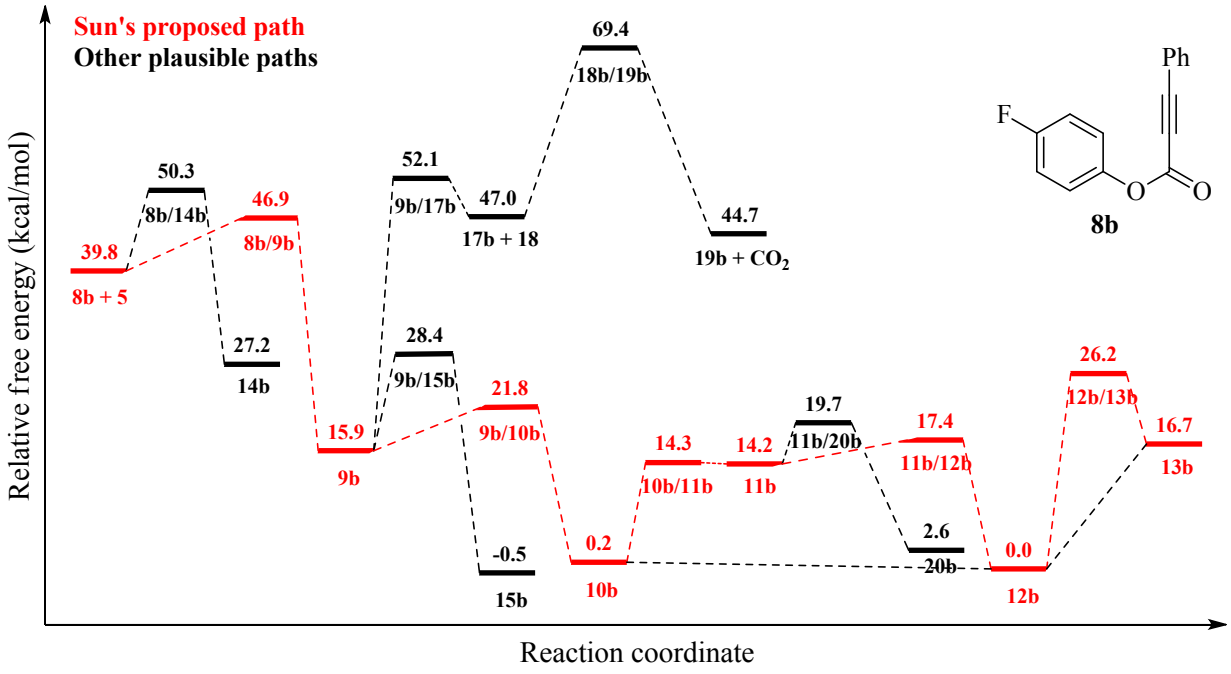

Figure S23. Relative free energy profile (at 403.15 K) for reaction mechanism of **8b** shown in Scheme 1 and Scheme 2 at the DLPNO-CCSD(T)/cc-PVTZ//B3LYP-6-311G(d,p) level.

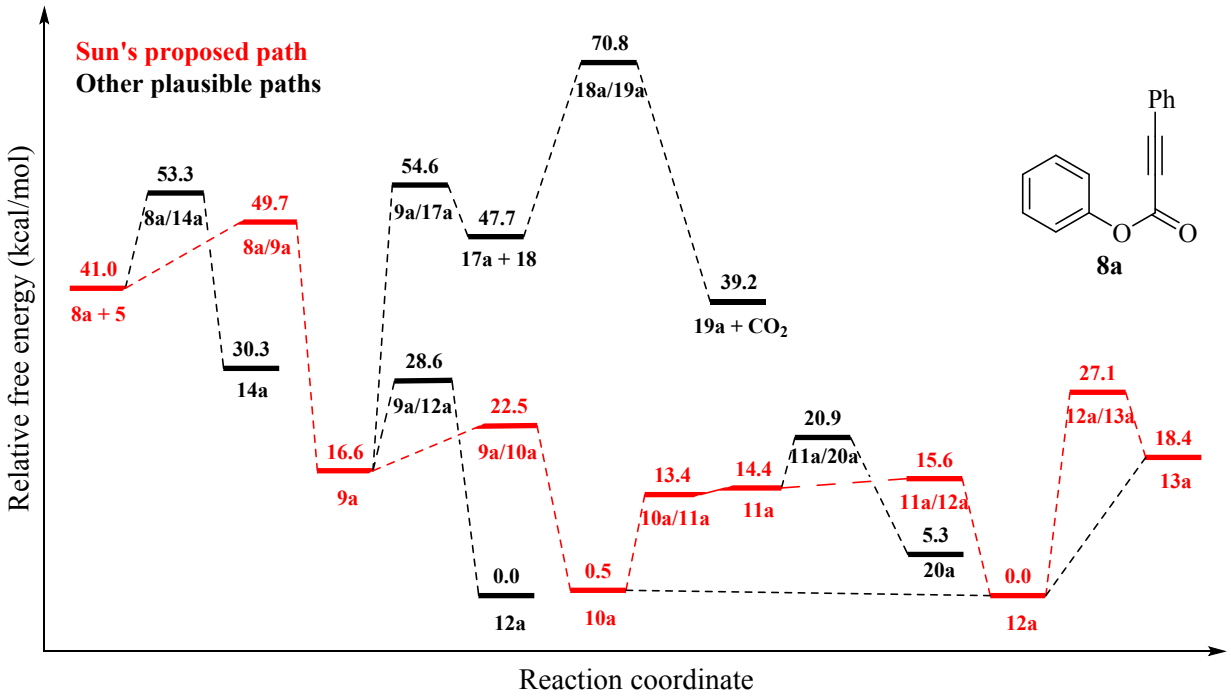

Figure S24. Solvent corrected relative free energy profile (at 403.15 K) for reaction mechanism of **8a** shown in Scheme 1 and Scheme 2 at the DLPNO-CCSD(T)/cc-PVTZ//B3LYP-6-311G(d,p) level.

3. Single Point Energy Computations

Table 1. Single point energies (**E**) for **a** using DLPNO-CCSD(T)/cc-PVTZ level in a.u.

Molecule	E	TS	E
TBPB (1)	-652.10120961	2-TS-5	-551.93690777
Acetonitrile (4)	-132.52638630	3-TS-5	-365.11525645
Benzoyloxy radical (2)	-419.43595843	8a-TS-9a	-858.56742562
t-Butoxy radical (3)	-232.60660617	9a-TS-10a	-858.61643941
Cyanomethyl radical (5)	-131.86284120	10a-TS-11a	-858.63089107
Benzoic acid (6)	-420.12251047	11a-TS-12a	-858.62854711
t-Butanol (7)	-233.28468445	12a-TS-13a	-858.60886867
Carbon dioxide	-188.32494069	8a-TS-14a	-858.56132587
8a	-726.71193923	9a-TS-12a	-858.60812417
9a	-858.62182698	9a-TS-17a	-858.55866571
10a	-858.65529310	17a-TS-19a	-419.38884985
11a	-858.62808683	11a-TS-20a	-858.61620934
12a	-858.65776696		
13a	-858.11949462		
14a	-858.60564183		

17a	-419.42884684		
18	-439.13653423		
19a	-231.11493779		
20a	-670.31694238		

Table 2. Single point energies (**E**) for **b** using DLPNO-CCSD(T)/cc-PVTZ level in a.u.

Molecule	**E**	**TS**	**E**
8b	-825.84206215	8b-TS-9b	-957.69731796
9b	-957.75234527	9b-TS-10b	-957.74579114
10b	-957.78536048	10b-TS-11b	-957.76257294
11b	-957.75909622	11b-TS-12b	-957.75869674
12b	-957.78761822	12b-TS-13b	-957.73846888
13b	-957.24983067	8b-TS-14b	-957.69107853
14b	-957.73608087	9b-TS-15b	-957.73826133
15b	-957.78840884	9b-TS-17b	-957.68863807
17b	-518.55820144	17b-TS-19b	-518.51866408
19b	-330.24314434	11b-TS-20b	-957.74668228
20b	-769.44804201		

4. Cartesian coordinates for optimized structures

TBPB (1)

E= -653.3736766 a.u., number of negative frequencies = 0

0 1

C	0.30939800	1.44206500	-0.38267400
O	-0.95521000	1.04519700	-0.76178400
O	0.46268400	2.63003800	-0.27799000
O	-1.24312000	-0.37219600	-0.53262700
C	-2.47761100	-0.46462900	0.24032300
C	-3.63209300	0.15852700	-0.54648900
C	-2.63409400	-1.98382800	0.35869300
C	-2.29368300	0.18843700	1.61111500
C	1.39679000	0.44262300	-0.18147300
C	2.42432700	0.81186600	0.69580700

C	3.51781900	-0.02393500	0.88720800
C	3.61022300	-1.22145100	0.17933300
C	2.60452500	-1.57993200	-0.71637000
C	1.49554700	-0.75850800	-0.89365700
H	-4.57275100	0.02269200	-0.00629400
H	-3.46863700	1.22690000	-0.69084200
H	-3.72263600	-0.31435600	-1.52693000
H	-3.54833600	-2.21329500	0.91074000
H	-1.78711900	-2.42149000	0.89088900
H	-2.70237600	-2.44270000	-0.62971100
H	-2.14583100	1.26514200	1.51462900
H	-3.18086000	0.02220900	2.22750200
H	-1.43103000	-0.24070900	2.12628200
H	2.35207500	1.75965800	1.21458300
H	4.30152300	0.26229700	1.57906600
H	4.46710500	-1.87064800	0.32070700
H	2.68249800	-2.50314900	-1.27903600
H	0.71464600	-1.04427000	-1.58327400

Acetonitrile (4)

E= -132.7933298 a.u., number of negative frequencies = 0

0 1

C	1.17569200	0.00000200	-0.00000300
C	-0.28079500	-0.00000300	0.00001100
N	-1.43280100	0.00000000	-0.00000600
H	1.55338100	1.02079100	0.08619700
H	1.55342100	-0.58504200	0.84092300
H	1.55342100	-0.43573800	-0.92712900

Benzoyloxy radical (2)

E= -420.260907 a.u., number of negative frequencies = 0

0 2

C	1.71995000	0.00000000	0.00000000
O	2.43270100	1.03983300	-0.00000100
O	2.43270100	-1.03983300	0.00000100
C	0.24730100	-0.00000100	0.00000000
C	-0.44637600	-1.21376200	0.00000000
C	-1.83630700	-1.21079600	-0.00000100
C	-2.52947500	0.00000000	0.00000000
C	-1.83630600	1.21079600	0.00000100
C	-0.44637700	1.21376200	0.00000100
H	0.10801800	-2.14502600	-0.00000100
H	-2.38004100	-2.14806900	-0.00000100
H	-3.61363600	0.00000100	0.00000000
H	-2.38004100	2.14806900	0.00000100
H	0.10801900	2.14502500	0.00000100

***t*-Butoxy radical (3)**

E= -233.0734125 a.u., number of negative frequencies = 0

0 2

C	-1.27729400	-0.79209100	-0.31533100
C	0.00000000	-0.02726800	0.08075000
C	1.27730400	-0.79207600	-0.31533100
C	-0.00000800	1.38913000	-0.57752000
O	-0.00000100	0.26102700	1.42838200
H	-1.31474900	-0.97073800	-1.39364000
H	-2.16158900	-0.22497700	-0.01828200
H	-1.30490300	-1.75933900	0.19251100
H	2.16159200	-0.22494800	-0.01829000
H	1.30492700	-1.75932000	0.19251800
H	1.31475600	-0.97073000	-1.39363900
H	0.88868900	1.94698700	-0.28035000

H	-0.88871700	1.94697400	-0.28035700
H	-0.00000300	1.26171100	-1.66292700

Cyanomethyl radical (5)

E= -132.1319245 a.u., number of negative frequencies = 0

0 2

C	-1.19098500	0.00000000	-0.00000100
C	0.18740100	-0.00000200	0.00000200
N	1.35581400	0.00000100	-0.00000100
H	-1.73460100	-0.93498100	0.00000100
H	-1.73459600	0.93498900	0.00000100

Benzoic acid (6)

E= -420.9394630 a.u., number of negative frequencies = 0

0 1

C	1.70337200	0.12419200	-0.00000100
O	2.33215300	1.15557700	-0.00001800
C	0.21927100	0.02927400	-0.00000100
C	-0.51352500	1.22085600	0.00000700
C	-1.90254900	1.18337900	0.00000700
C	-2.56638000	-0.04353400	0.00000100
C	-1.83913100	-1.23296500	-0.00000700
C	-0.44828600	-1.20043400	-0.00000800
H	0.02457600	2.16058100	0.00001000
H	-2.46865700	2.10768400	0.00001300
H	-3.65031900	-0.07251200	0.00000200
H	-2.35631100	-2.18555800	-0.00001400
H	0.12420800	-2.11853500	-0.00001300
O	2.31121400	-1.08867100	0.00001500
H	3.26293800	-0.91151300	0.00003000

_t_-Butanol (7)

E= -233.7466102 a.u., number of negative frequencies = 0

0 1

C	0.69027800	-1.26460200	-0.51005900
C	-0.00583100	0.00000000	0.01129300
C	0.69027200	1.26460500	-0.51005800
C	-1.48967300	-0.00000300	-0.35681500
H	0.65292700	-1.32316900	-1.60172900
H	0.21075100	-2.15446200	-0.09612500
H	1.74439500	-1.27584700	-0.21218300
H	0.21074100	2.15446300	-0.09612400
H	1.74438900	1.27585400	-0.21218200
H	0.65292200	1.32317300	-1.60172900
H	-1.97890000	0.88434400	0.05759300
H	-1.97889600	-0.88435200	0.05759200
H	-1.62489000	-0.00000300	-1.44116700
O	0.01498200	0.00000000	1.45113100
H	0.93642500	0.00000100	1.73083900

Carbondioxide

E= -188.6411388 a.u., number of negative frequencies = 0

0 1

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16043900
O	0.00000000	0.00000000	-1.16043900

Phenyl radical (19a)

E= -231.6194243 a.u., number of negative frequencies = 0

0 2

C	-1.22372300	-0.77066900	0.00000000
C	-1.21183000	0.63143700	0.00000000

C	0.00000000	1.32199300	0.00000000
C	1.21183000	0.63143600	0.00000000
C	1.22372300	-0.77066900	0.00000000
C	-0.00000100	-1.39605100	0.00000000
H	-2.15769400	-1.32152000	0.00000000
H	-2.15030400	1.17607600	0.00000000
H	0.00000100	2.40602700	0.00000000
H	2.15030400	1.17607500	0.00000000
H	2.15769300	-1.32152200	0.00000000

8a

E= -728.1911337 a.u., number of negative frequencies = 0

0 1

C	1.81463300	-0.26830700	0.05547000
C	0.62549400	-0.47896200	0.09557600
C	-0.76895500	-0.82414300	0.17162700
O	-1.53188300	0.27974100	-0.08150900
O	-1.18954100	-1.92270600	0.42236100
C	3.21415800	-0.01974000	0.00311400
C	3.69947200	1.26519200	-0.29799600
C	5.06767400	1.49964200	-0.34916200
C	5.96681100	0.46265900	-0.10179200
C	5.49419300	-0.81467900	0.19818500
C	4.12792300	-1.05942600	0.25133200
C	-2.92874700	0.23185400	-0.06000700
C	-3.55077100	1.35719700	0.47245900
C	-4.93982800	1.43720300	0.47037900
C	-5.70005200	0.39704700	-0.06076900
C	-5.06170600	-0.72057700	-0.59342000
C	-3.67136000	-0.81466900	-0.60064100
H	2.99480200	2.06518400	-0.48911500

H	5.43437800	2.49257700	-0.58223500
H	7.03378700	0.64968200	-0.14253600
H	6.19233000	-1.62105700	0.39066600
H	3.75270900	-2.04862300	0.48308600
H	-2.93715700	2.15316400	0.87586900
H	-5.42569800	2.31293300	0.88500700
H	-6.78207800	0.45756700	-0.06073600
H	-5.64672000	-1.53282300	-1.00945900
H	-3.17861300	-1.68663000	-1.00349500

9a

E= -860.3591019 a.u., number of negative frequencies = 0

0 2

C	0.61417400	0.99238500	-0.49144300
C	-0.45703300	0.00545200	-0.10921300
O	-0.27515600	-1.05637100	0.41380300
O	-1.68575800	0.49742600	-0.46377400
C	0.19742800	2.38164700	-0.98435900
C	1.86882900	0.63598200	-0.38804900
C	-2.83648700	-0.24324500	-0.16043800
C	-3.63906700	-0.64014800	-1.22163500
C	-4.83001300	-1.31266100	-0.95619300
C	-5.20295000	-1.58432200	0.35802700
C	-4.38381200	-1.17717900	1.41001700
C	-3.19363000	-0.50068900	1.15762700
C	3.02571600	-0.07031800	-0.15378000
C	3.64407900	-0.83605100	-1.18801500
C	4.82309700	-1.51365100	-0.94329300
C	5.43285200	-1.45528500	0.31541000
C	4.84241800	-0.70615500	1.34006300
C	3.66336500	-0.01956100	1.12296500

C	-0.34798800	3.21366600	0.08898300
N	-0.75985100	3.86642200	0.94478200
H	1.06633200	2.88839100	-1.40832600
H	-0.55835300	2.29086200	-1.76793700
H	-3.32949300	-0.41790300	-2.23549400
H	-5.46355400	-1.62397200	-1.77866600
H	-6.12907100	-2.10850900	0.56277300
H	-4.67126900	-1.38371700	2.43439800
H	-2.55213600	-0.17770700	1.96681600
H	3.17046100	-0.88345900	-2.16068500
H	5.27639000	-2.09812900	-1.73589100
H	6.35759200	-1.98990200	0.49649700
H	5.31052100	-0.66490500	2.31698600
H	3.20298800	0.55634300	1.91578700

10a

E= -860.3753179 a.u., number of negative frequencies = 0

0 2

C	3.39232900	-0.75087900	-0.74052000
C	2.08125600	-0.98696000	-1.02817600
C	1.02689900	-1.05908100	0.04171200
C	1.56785200	-0.81344500	1.42063700
C	2.88702400	-0.56343600	1.64792700
C	3.82352400	-0.52179500	0.58743200
C	-0.21731600	-0.19111600	-0.24529400
C	-1.26278900	-1.00627900	-0.46112800
C	-0.83269500	-2.41700200	-0.32963900
O	0.48876300	-2.43401300	-0.00143500
O	-1.48911500	-3.41011300	-0.48525400
C	-2.68995900	-0.70896800	-0.84018600
C	-0.19921300	1.28144300	-0.20577100

C	-1.25319600	1.97757700	0.41150200
C	-1.25632100	3.36778700	0.45742000
C	-0.21182000	4.09068000	-0.11387300
C	0.84324000	3.41290200	-0.72127200
C	0.85622100	2.02305300	-0.76069400
C	-3.58037500	-0.60909800	0.31847200
N	-4.26561200	-0.50355700	1.23920400
H	4.12102000	-0.74621000	-1.54401400
H	1.75045200	-1.18868700	-2.04063100
H	0.85353400	-0.86737000	2.23376000
H	3.23013700	-0.40460400	2.66433400
H	4.86973500	-0.33469300	0.79394200
H	-2.75661900	0.22442400	-1.40560700
H	-3.05307700	-1.52398800	-1.47381400
H	-2.05485900	1.43092800	0.89215700
H	-2.07382900	3.88386100	0.94741600
H	-0.21607000	5.17412300	-0.07975000
H	1.66212100	3.96797900	-1.16448100
H	1.68158400	1.50984100	-1.23552900

11a

E= -860.3641743 a.u., number of negative frequencies = 0

0 2

C	1.28310300	-0.58487900	0.00223200
C	1.57637900	-1.63484400	-0.88275700
C	2.74742500	-2.36361800	-0.74120500
C	3.63189200	-2.08407400	0.30796400
C	3.33856700	-1.07246700	1.21209400
C	2.17292300	-0.32098000	1.06280000
O	2.45441000	1.73964700	-0.39196200
C	1.29956800	2.29631000	-0.50193900

O	1.29586200	3.47613300	-0.87018800
C	0.03740900	1.54318400	-0.24786200
C	-1.19375500	2.43909900	-0.21946300
C	0.02371700	0.19283600	-0.14407500
C	-1.23104000	-0.60974500	-0.16861300
C	-1.50207200	-1.52499100	0.85808700
C	-2.66862400	-2.28097800	0.84077800
C	-3.56817600	-2.15785900	-0.21655500
C	-3.29576600	-1.27244900	-1.25673400
C	-2.13882000	-0.49944700	-1.23067000
C	-2.01566500	2.26284400	0.97626400
N	-2.65597000	2.14103400	1.92668600
H	0.88832800	-1.86059100	-1.68862100
H	2.97670100	-3.15623100	-1.44408200
H	4.53970100	-2.66599800	0.41797900
H	4.00990900	-0.86186800	2.03590800
H	1.92469600	0.44321200	1.78757300
H	-1.82297400	2.30134800	-1.10208200
H	-0.84779800	3.47635200	-0.25784500
H	-0.80452300	-1.62774500	1.68095600
H	-2.87540500	-2.96791800	1.65318400
H	-4.47457300	-2.75200200	-0.23170400
H	-3.98316000	-1.18322300	-2.09012800
H	-1.92367900	0.17352400	-2.05281300

12a

E= -860.3809100 a.u., number of negative frequencies = 0

0 2

C	-1.17375200	-0.77468600	-0.02504100
C	-2.44819100	-0.10516200	-0.46418800
C	-3.69869800	-0.75492800	0.02984800

C	-3.67561600	-1.99929300	0.56342600
C	-2.44052600	-2.68644600	0.77002300
C	-1.22446000	-2.05969800	0.50296700
O	-2.49473800	1.29924000	-0.10712900
C	-1.37555000	2.04466600	-0.31045000
O	-1.45788800	3.24856200	-0.30459100
C	-0.08448500	1.33334700	-0.46509600
C	1.08850900	2.23955100	-0.78497200
C	0.02878900	-0.01405300	-0.22563800
C	1.35432200	-0.69852800	-0.15960600
C	1.68402900	-1.68088000	-1.10365200
C	2.92114100	-2.31712400	-1.05931500
C	3.83901000	-1.99208500	-0.06190700
C	3.51567500	-1.02561300	0.88738200
C	2.28273500	-0.37882500	0.83883500
C	1.65010900	2.89703000	0.39825600
N	2.10726800	3.38487800	1.33714300
H	-2.46557900	-0.12832200	-1.57144100
H	-4.61834400	-0.19859200	-0.10452300
H	-4.60103500	-2.47570700	0.86679400
H	-2.44804100	-3.68008800	1.20087400
H	-0.29899400	-2.56271300	0.75542700
H	1.88731600	1.67299500	-1.26844600
H	0.75411700	3.02254200	-1.46995300
H	0.97102900	-1.93737300	-1.87931900
H	3.16776400	-3.06650500	-1.80287600
H	4.80115300	-2.49011600	-0.02538400
H	4.22299000	-0.76935300	1.66758700
H	2.03951700	0.37303100	1.57978000

13a

E= -859.8404632 a.u., number of negative frequencies = 0

0 1

C	1.20966400	-0.74306600	0.05120000
C	2.43982300	-0.06633500	0.00455000
C	3.64755700	-0.72616700	0.22229800
C	3.63555100	-2.08515100	0.49791100
C	2.42430400	-2.78367300	0.56256800
C	1.22857000	-2.12018400	0.34468900
O	2.50838300	1.27047500	-0.25287200
C	1.38366300	2.04712600	-0.46315400
O	1.53791500	3.21909900	-0.68705300
C	0.08717700	1.36131000	-0.41792800
C	-1.10419300	2.26131900	-0.68754900
C	-0.00591000	0.02432500	-0.17987300
C	-1.32661000	-0.67204300	-0.14969900
C	-2.21483800	-0.47081000	0.91281700
C	-3.44574200	-1.12330700	0.93243500
C	-3.80425000	-1.97651900	-0.10828300
C	-2.92545900	-2.17998200	-1.17078900
C	-1.69058600	-1.53731600	-1.18972200
C	-1.60614600	2.90514800	0.52858300
N	-2.00704800	3.38529800	1.49667000
H	4.56716400	-0.15704100	0.17339000
H	4.57147700	-2.60403400	0.66893600
H	2.42045900	-3.84313500	0.78814500
H	0.29082700	-2.65682400	0.40411000
H	-0.80326300	3.04659600	-1.38479200
H	-1.92169700	1.69185200	-1.13436400
H	-1.94406100	0.19706800	1.72198800
H	-4.12449000	-0.95873300	1.76119900
H	-4.76425700	-2.47956900	-0.09307300

H	-3.20019600	-2.83965100	-1.98597300
H	-1.00846200	-1.69826700	-2.01718300

14a

E= -860.3441893 a.u., number of negative frequencies = 0

0 2

C	2.44792200	-2.01229100	-1.17120200
C	1.73816000	-0.72501100	-0.71822100
C	0.43543800	-0.66010800	-0.87931500
C	-0.79848300	0.07329000	-0.83746000
O	-1.73901100	-0.63685200	-0.16342500
O	-0.96212900	1.15320800	-1.36434400
C	2.56117100	0.37498900	-0.13800800
C	2.17115800	1.71293000	-0.30776900
C	2.93903700	2.74234700	0.22412600
C	4.10496600	2.45844800	0.93342300
C	4.50097500	1.13463200	1.10485900
C	3.73993000	0.09868700	0.57082500
C	2.71947700	-2.94581000	-0.07828200
N	2.93495200	-3.68396200	0.78037700
C	-3.05113600	-0.21289500	0.05846000
C	-3.68915200	-0.89477900	1.09401900
C	-5.01480000	-0.60531900	1.39249700
C	-5.70298700	0.36086100	0.65935000
C	-5.05325200	1.03032900	-0.37333200
C	-3.72265000	0.75422100	-0.68820800
H	1.82743900	-2.52551700	-1.90832600
H	3.39488300	-1.75718100	-1.65620200
H	1.27620800	1.94222900	-0.87292700
H	2.62796400	3.77039400	0.07767600
H	4.70181500	3.26338400	1.34683100

H	5.40381100	0.90277900	1.65817100
H	4.05827500	-0.92343200	0.73415200
H	-3.13338100	-1.64303100	1.64521600
H	-5.50891100	-1.13575300	2.19821300
H	-6.73650700	0.58877600	0.89199400
H	-5.58088700	1.78254000	-0.94857900
H	-3.22090100	1.28456300	-1.48127200

17a

E= -420.2481714 a.u., number of negative frequencies = 0

0 2

O	1.43699100	-0.58861600	-0.18033400
C	0.08556100	-0.22717900	-0.07706000
C	-0.80823400	-1.28808100	-0.00509000
C	-2.17204700	-1.01852800	0.06601300
C	-2.63017700	0.29763400	0.06822600
C	-1.71665500	1.34662700	-0.00664900
C	-0.34864400	1.09311900	-0.08565200
C	2.38699300	0.30236200	0.15211600
O	3.55211000	0.12938100	0.08610600
H	-0.42692900	-2.30141400	-0.00484200
H	-2.87520800	-1.84119000	0.12245400
H	-3.69213800	0.50445900	0.12551200
H	-2.06523100	2.37280700	-0.00990500
H	0.36592000	1.90349400	-0.15081500

18

E= -440.0612020 a.u., number of negative frequencies = 0

0 1

C	0.51924800	-0.43661600	0.00000400
C	1.70363200	-0.65629900	0.00000600

C	3.13891900	-0.93385500	0.00001100
C	3.96227000	0.28183500	-0.00000400
N	4.62007000	1.22690800	-0.00001600
C	-0.88227900	-0.16364500	0.00000200
C	-1.34603100	1.16270300	0.00000700
C	-2.71045100	1.42730600	0.00000500
C	-3.63011500	0.37955000	-0.00000300
C	-3.17856400	-0.93930200	-0.00000900
C	-1.81587600	-1.21346100	-0.00000600
H	3.41312500	-1.53075100	0.87795300
H	3.41312600	-1.53077300	-0.87791600
H	-0.62869200	1.97431100	0.00001400
H	-3.05692200	2.45445000	0.00000900
H	-4.69350300	0.58973300	-0.00000600
H	-3.89001900	-1.75722300	-0.00001400
H	-1.46213300	-2.23740300	-0.00001000

20a

E= -671.7355225 a.u., number of negative frequencies = 0

0 2

C	0.98658700	-0.69063400	0.06886600
C	1.07234200	-1.36678400	-1.15579800
C	2.05095100	-2.33407500	-1.36049200
C	2.95418100	-2.64647400	-0.34455300
C	2.87201500	-1.98634900	0.87836700
C	1.89476600	-1.01324100	1.08353200
C	0.33245000	1.61634200	0.53897900
C	1.57526900	2.39961900	0.71547500
C	-0.05081900	0.37920000	0.26920800
C	-1.49179300	0.02072600	0.14300900
C	-1.93291500	-1.28357900	0.40405800

C	-3.28459400	-1.60683100	0.31596600
C	-4.21727700	-0.63592100	-0.03936000
C	-3.78872600	0.66418700	-0.30793100
C	-2.44068300	0.98897700	-0.22013500
C	1.64645000	3.56178800	-0.17857700
N	1.70532800	4.47478300	-0.87846500
H	0.37188100	-1.12625500	-1.94728600
H	2.11045900	-2.84400700	-2.31548900
H	3.71436300	-3.40229400	-0.50573100
H	3.56402500	-2.23062700	1.67652900
H	1.81965300	-0.51436300	2.04352700
H	1.66315100	2.76170600	1.74716500
H	2.45594800	1.76646600	0.52914000
H	-1.21583700	-2.04590700	0.68387600
H	-3.60808900	-2.62013900	0.52642200
H	-5.26871800	-0.88972600	-0.11247500
H	-4.50645900	1.42429600	-0.59564800
H	-2.10689700	1.99566800	-0.44445900

2-TS-5

E= -553.0321936 a.u., im. freq.= 1800.78i

0 2

C	-0.17795100	1.75061000	-0.25900800
O	1.14888100	1.81333300	-0.24977400
O	-0.75708200	2.81100600	-0.41234600
C	2.55040700	0.14899400	1.04624700
C	-0.88224100	0.44760200	-0.12443500
C	-0.32792800	-0.74745200	-0.59589000
C	-1.04779100	-1.93430600	-0.49473900
C	-2.31639600	-1.93425200	0.08266600
C	-2.87599700	-0.74265900	0.54440500

C	-2.16774700	0.44750000	0.43061000
H	0.64506800	-0.74978100	-1.07074700
H	-0.61887600	-2.85542100	-0.87122100
H	-2.87258300	-2.86110700	0.16531000
H	-3.86559700	-0.74221700	0.98619100
H	-2.59469500	1.38425600	0.76759800
C	3.07173900	-0.88657800	0.22398900
N	3.46486100	-1.72089900	-0.47711200
H	1.78653900	0.91295300	0.31487100
H	3.29440900	0.86552600	1.39094300
H	1.88074400	-0.19937400	1.83072300

3-TS-5

E= -365.8528882 a.u., im. freq.= 1781.29i

0 2

C	0.87069800	0.85742800	1.27226800
C	1.21860200	0.07002800	0.00000000
C	0.87070100	0.85734300	-1.27232200
C	2.71947300	-0.30766500	0.00001300
H	1.44504600	1.78625600	1.32464400
H	1.09537900	0.25828100	2.15748900
H	-0.18935300	1.12147900	1.29002500
H	1.09538100	0.25813600	-2.15750200
H	-0.18935000	1.12139500	-1.29009800
H	1.44505100	1.78616600	-1.32475900
H	2.96437200	-0.89399000	-0.88707400
H	2.96437200	-0.89392500	0.88714400
H	3.31969800	0.60605900	-0.00002000
C	-1.92749700	-1.24890300	0.00001000
H	-2.10884100	-1.82149700	0.90823200
H	-2.10882100	-1.82150000	-0.90821400

O	0.59076800	-1.20189500	0.00004200
H	-0.63295600	-1.14764000	0.00002700
C	-2.54477300	0.03595000	0.00000100
N	-3.00990800	1.09583600	-0.00000600

8a-TS-9a

E= -860.3121907 a.u., im. freq.= 422.92i

0 2

C	0.42015100	0.75524300	-0.23846100
C	-1.02614300	0.92268900	-0.09224800
O	-1.61485400	1.96016600	0.06207100
O	-1.61986600	-0.30261700	-0.16145400
C	1.09737200	2.90263000	-0.67258900
C	1.38408100	-0.01182900	-0.16433700
C	-3.00718800	-0.44152100	-0.01745900
C	-3.42349700	-1.48348400	0.80356700
C	-4.78448500	-1.74337000	0.93763700
C	-5.71658900	-0.96410200	0.25561300
C	-5.28087300	0.07388700	-0.56539600
C	-3.92198700	0.34396600	-0.71160400
C	2.60968200	-0.70720200	-0.10715300
C	2.87037200	-1.75980600	-1.00991600
C	4.07514900	-2.44447600	-0.94957000
C	5.03154200	-2.09978700	0.00702900
C	4.78168900	-1.06090400	0.90437100
C	3.58320000	-0.36314600	0.85487700
C	2.21069300	3.11526800	0.14867600
N	3.13086800	3.23800500	0.84832500
H	1.27072300	2.76958700	-1.73248900
H	0.14108500	3.29885300	-0.35857200
H	-2.67889900	-2.07647500	1.31998000

H	-5.11349400	-2.55467700	1.57656600
H	-6.77616700	-1.16486600	0.36194300
H	-6.00122200	0.68299700	-1.09920100
H	-3.58411800	1.15479100	-1.34040100
H	2.12008500	-2.02529100	-1.74451800
H	4.27032100	-3.25085800	-1.64689200
H	5.97105000	-2.63858800	0.05092600
H	5.52811200	-0.78762000	1.64084900
H	3.39518700	0.46137900	1.53038600

9a-TS-10a

E= -860.3455089 a.u., im. freq.= 436.52i

0 2

C	1.85971300	-2.64550300	-0.62919300
C	0.52917800	-2.41669700	-0.92119200
C	-0.33352000	-1.91585600	0.09434400
C	0.12381300	-1.90293400	1.44321800
C	1.45883900	-2.13483500	1.70922800
C	2.34138900	-2.48407000	0.67746800
C	-0.35793400	0.18106600	-0.32791200
C	-1.65917000	0.29649100	-0.49495700
C	-2.46392800	-0.95104200	-0.39902700
O	-1.71081700	-2.05855700	-0.11436000
O	-3.64732200	-1.03921200	-0.56404700
C	-2.42798800	1.58094700	-0.78213700
C	0.81893300	0.98607900	-0.28453700
C	1.13404800	1.72931400	0.87381800
C	2.29121800	2.49495900	0.92055100
C	3.15679300	2.53511300	-0.17304300
C	2.85813400	1.80078100	-1.32141400
C	1.70800200	1.02552600	-1.37970600

C	-2.75615200	2.30579700	0.44529300
N	-2.99058100	2.87013200	1.42266500
H	2.52909500	-2.98322700	-1.41216500
H	0.12414700	-2.57693700	-1.91282300
H	-0.58445900	-1.67208700	2.22933500
H	1.81886400	-2.07653900	2.72993100
H	3.38486100	-2.67332900	0.89754500
H	-1.83990300	2.23746800	-1.42747200
H	-3.35869800	1.32840200	-1.29665000
H	0.45697100	1.70769100	1.71896100
H	2.51586100	3.06900200	1.81223900
H	4.05722200	3.13688700	-0.13160500
H	3.52673100	1.83204500	-2.17424600
H	1.48028500	0.45103000	-2.26926900

10a-TS-11a

E= -860.3616738 a.u., im. freq.= 328.79i

0 2

C	3.49507400	0.88386200	-0.78466100
C	2.24077500	0.37330700	-1.03620400
C	1.37155200	-0.00432500	0.04558700
C	1.80456700	0.30268000	1.37963600
C	3.06411900	0.80744400	1.61012000
C	3.91995900	1.09502000	0.53531000
C	-0.10838000	-0.16824800	-0.20938100
C	-0.50642600	-1.43076400	-0.44180500
C	0.58788500	-2.44369700	-0.35194500
O	1.75006900	-1.92327900	-0.02331800
O	0.43368800	-3.63181300	-0.56397900
C	-1.87452000	-1.94184800	-0.82224300
C	-0.95657900	1.04576600	-0.16392300

C	-2.22816900	1.01653300	0.43298000
C	-3.02071700	2.15969500	0.47299900
C	-2.56328300	3.35285200	-0.08071500
C	-1.29810000	3.40018900	-0.66298700
C	-0.49870900	2.26320400	-0.69505900
C	-2.67208400	-2.36459500	0.33054300
N	-3.30366800	-2.66436100	1.24708700
H	4.15580500	1.12379600	-1.60937500
H	1.90555100	0.19603900	-2.05102600
H	1.13126200	0.09056400	2.20100200
H	3.39318400	0.99478200	2.62542000
H	4.91001200	1.49226600	0.72596300
H	-2.44002000	-1.18648400	-1.37421100
H	-1.73301900	-2.81582700	-1.46562500
H	-2.58684300	0.11035700	0.90389100
H	-3.99432300	2.11641800	0.94738200
H	-3.18306500	4.24159200	-0.04996500
H	-0.92991200	4.32622500	-1.08961800
H	0.48520900	2.31907400	-1.14457400

11a-TS-12a

E= -860.3603932 a.u., im. freq.= 326.29i

0 2

C	-1.19473500	-0.75079700	-0.01033500
C	-2.35300000	-0.37959500	-0.76746500
C	-3.60245900	-1.00087800	-0.48058300
C	-3.69586000	-1.92166400	0.53649900
C	-2.55005600	-2.28902000	1.27028600
C	-1.31310900	-1.71269100	0.99115900
O	-2.48467200	1.46913600	-0.15692900
C	-1.34085100	2.10638100	-0.24696400

O	-1.31400500	3.32217800	-0.14044300
C	-0.05389100	1.34808500	-0.44560800
C	1.12195400	2.24419800	-0.79452700
C	0.04625100	0.00994500	-0.23652400
C	1.33122100	-0.74143500	-0.19113500
C	1.48695700	-1.88983000	-0.98351300
C	2.67699800	-2.60879900	-0.96542500
C	3.72397600	-2.20727900	-0.13683400
C	3.57330400	-1.08267700	0.67044300
C	2.38788100	-0.35151900	0.64355500
C	1.72106400	2.90610700	0.36614200
N	2.22119800	3.39080900	1.28458200
H	-2.20289100	0.01546900	-1.76410200
H	-4.46793000	-0.73555100	-1.07478700
H	-4.64764100	-2.38879600	0.76130300
H	-2.63449800	-3.01711800	2.06841600
H	-0.44275500	-1.98457700	1.57581400
H	1.90358200	1.67006900	-1.29721300
H	0.77314300	3.02697700	-1.47333900
H	0.67373600	-2.21060300	-1.62484100
H	2.78633800	-3.48438400	-1.59518400
H	4.64936500	-2.77149500	-0.11729500
H	4.37746200	-0.77036000	1.32659900
H	2.27924800	0.51300600	1.28650400

12a-TS-13a

E= -860.3341476 a.u., im. freq.= 924.67i

0 2

C	1.18830100	-0.74057400	-0.05164600
C	2.43345900	-0.06593700	0.09025500
C	3.64591200	-0.70718600	-0.24980600

C	3.63411100	-2.05060900	-0.56152100
C	2.42205500	-2.75815200	-0.60759000
C	1.22132700	-2.10825200	-0.36878100
O	2.48770900	1.29790600	0.19322400
C	1.35738200	2.05929500	0.42146600
O	1.49587600	3.24124400	0.59615300
C	0.06719500	1.35779300	0.41989400
C	-1.12530500	2.25004900	0.70864700
C	-0.02504900	0.02012600	0.17249100
C	-1.34360500	-0.68009400	0.13988200
C	-1.69209000	-1.56736400	1.16689300
C	-2.92489500	-2.21379200	1.15015300
C	-3.81691000	-1.99258400	0.10219500
C	-3.47384800	-1.11781600	-0.92577200
C	-2.24517300	-0.46098900	-0.90775400
C	-1.64730000	2.89774000	-0.49711000
N	-2.06495800	3.37982200	-1.45710200
H	2.56643100	-0.42115200	1.84812900
H	4.55734900	-0.12421700	-0.22261200
H	4.56507000	-2.55605400	-0.78942400
H	2.42160700	-3.81148200	-0.86015400
H	0.28778300	-2.64955900	-0.44867600
H	-1.93351200	1.67352200	1.16326300
H	-0.82017700	3.03362300	1.40593100
H	-0.99931700	-1.74157700	1.98280300
H	-3.18783900	-2.89006300	1.95555300
H	-4.77530800	-2.49875700	0.08842200
H	-4.16292600	-0.93980800	-1.74314700
H	-1.98654300	0.22365800	-1.70676700

8a-TS-14a

E= -860.3042218 a.u., im. freq.= 575.67i

0 2

C	1.66981100	1.60018600	1.51654300
C	1.52587600	-0.20052800	0.29238200
C	0.31493600	-0.47095500	0.26347100
C	-1.06475600	-0.29391700	0.64287800
O	-1.88164400	-0.51387200	-0.41565600
O	-1.41232500	0.01119400	1.75834000
C	2.89755800	-0.49115000	-0.06946200
C	3.61277900	-1.46202700	0.64788600
C	4.92498700	-1.75966500	0.29717800
C	5.53799500	-1.08864100	-0.75972100
C	4.83270100	-0.11829800	-1.46908500
C	3.51811400	0.18420500	-1.12998400
C	1.89702500	2.64409000	0.60543100
N	2.08726100	3.47106200	-0.18838400
C	-3.27223900	-0.36538300	-0.33440500
C	-3.87343700	0.14857900	-1.47898700
C	-5.25849400	0.26959000	-1.52609600
C	-6.03280800	-0.12262300	-0.43569500
C	-5.41396000	-0.63981300	0.69982400
C	-4.02759800	-0.76860000	0.76309300
H	0.70229000	1.55645800	2.00149700
H	2.51773200	1.26935300	2.10402400
H	3.13149000	-1.98228000	1.46736100
H	5.46883500	-2.51676100	0.85030400
H	6.56185700	-1.32100000	-1.02905500
H	5.30586100	0.40674500	-2.29062400
H	2.97156600	0.94224100	-1.67627400
H	-3.24874800	0.44207500	-2.31337900
H	-5.73004800	0.67092100	-2.41553400

H	-7.11163000	-0.02694200	-0.47126100
H	-6.01070700	-0.94800500	1.55057700
H	-3.54851800	-1.15912100	1.64805800

9a-TS-12a

E= -860.3378689 a.u., im. freq.= 426.27i

0 2

C	0.86218100	1.60141600	-0.93236600
C	1.99733900	1.26108200	-0.15409000
C	2.30335400	1.91100300	1.02334900
C	1.49630900	2.97436700	1.44360100
C	0.39405300	3.36936900	0.67391300
C	0.09529500	2.72257000	-0.51195900
O	2.78830800	0.20647000	-0.57087500
C	2.24777500	-1.04014300	-0.77531900
O	2.97761500	-1.92957000	-1.11604000
C	0.78155600	-1.23653300	-0.53743700
C	0.38428700	-2.70664600	-0.36859000
C	-0.10952000	-0.25514300	-0.53363700
C	-1.52854100	-0.17635500	-0.32010600
C	-2.40799900	0.09958300	-1.38633600
C	-3.77414300	0.20794300	-1.16082700
C	-4.28950100	0.06607400	0.12830700
C	-3.42722600	-0.19111100	1.19354700
C	-2.05920700	-0.31015400	0.97885500
C	0.54810400	-3.16255300	1.01121000
N	0.66474900	-3.49650200	2.10847700
H	0.85370000	1.32064700	-1.97982700
H	3.15955400	1.58352100	1.59977600
H	1.73088800	3.49341900	2.36490000
H	-0.21157700	4.20854300	0.99613300

H	-0.73373500	3.05489600	-1.12451300
H	-0.65853800	-2.84689200	-0.65928800
H	1.01509300	-3.31946800	-1.01649500
H	-2.01174900	0.21259000	-2.38919600
H	-4.44073800	0.40529800	-1.99276300
H	-5.35570700	0.15600700	0.30047600
H	-3.82163800	-0.30442100	2.19690700
H	-1.39088000	-0.51243000	1.80717800

9a-TS-17a

E= -860.3007207 a.u., im. freq.= 333.66i

0 2

C	1.04575200	1.48325700	-0.64874000
C	-0.51448700	-0.28706600	-0.81589400
O	-0.20614200	-1.42598300	-0.71166200
O	-1.70076400	0.31206800	-0.67740800
C	0.18165500	2.64060300	-0.96278200
C	2.09568900	0.93494000	-0.34271000
C	-2.86751700	-0.37389900	-0.24285700
C	-3.74092700	0.39068200	0.52052500
C	-4.93473000	-0.18325700	0.94813700
C	-5.24061400	-1.50158200	0.61344300
C	-4.34775300	-2.24669100	-0.15252500
C	-3.14768700	-1.68846500	-0.59312900
C	3.20785900	0.12906900	-0.00517300
C	4.05072500	-0.38650200	-1.01033100
C	5.14439900	-1.17118300	-0.67187900
C	5.41961100	-1.45662200	0.66584000
C	4.59129800	-0.95179500	1.66871000
C	3.49529100	-0.16482900	1.34313400
C	-0.64251400	3.07334800	0.17083100

N	-1.29745300	3.42800400	1.04941100
H	0.80733700	3.48539700	-1.27069700
H	-0.48958300	2.41245600	-1.79519400
H	-3.47312700	1.40906600	0.77389200
H	-5.62287100	0.40240600	1.54652500
H	-6.17009300	-1.94620100	0.94924500
H	-4.58005600	-3.27222700	-0.41537800
H	-2.44939500	-2.26627000	-1.18064500
H	3.83086400	-0.16682800	-2.04785300
H	5.78403000	-1.56499900	-1.45346800
H	6.27418900	-2.07076500	0.92535800
H	4.80080100	-1.17440100	2.70870800
H	2.84901400	0.22760300	2.11858700

17a-TS-19a

E= -420.2179641 a.u., im. freq.= 668.35i

0 2

C	-2.68361200	-0.27553500	0.00000100
O	-1.70755700	-1.00954900	0.00001100
O	-3.15106000	0.80720600	-0.00001300
C	0.00828300	-0.32731600	0.00000400
C	0.96264000	-1.31364000	-0.00000300
C	2.29766500	-0.89614000	-0.00000600
C	2.60514000	0.46468800	-0.00000300
C	1.59069400	1.42110400	0.00000400
C	0.24633200	1.02717300	0.00000700
H	0.69123700	-2.36280900	-0.00000500
H	3.09172100	-1.63490700	-0.00001200
H	3.64152100	0.78159100	-0.00000600
H	1.83608300	2.47754000	0.00000600
H	-0.55447900	1.75532700	0.00001200

11a-TS-20a

E= -860.3502216 a.u., im. freq.= 423.28i

0 2

C	1.35445700	-0.61652500	0.10789100
C	1.52152400	-1.77812900	-0.66404900
C	2.69984200	-2.51159200	-0.59108000
C	3.72001500	-2.11283400	0.27122400
C	3.55666000	-0.97366700	1.05704900
C	2.38533900	-0.22880400	0.97746300
O	2.16614000	2.65823500	0.06123800
C	1.37484400	2.51776000	-0.83367600
O	1.01702200	2.75763200	-1.94200000
C	0.01164200	1.49270800	0.02629700
C	-1.08048900	2.47829500	0.31606000
C	0.09051700	0.15432900	0.01779600
C	-1.18288400	-0.61987800	-0.15393500
C	-1.52001800	-1.63310300	0.75346200
C	-2.71316500	-2.33165000	0.60780700
C	-3.57190400	-2.04405800	-0.45265400
C	-3.23381500	-1.05176200	-1.36894400
C	-2.04717600	-0.33868500	-1.21824200
C	-2.06558100	2.03714300	1.30464500
N	-2.83553700	1.71816600	2.10006400
H	0.72943300	-2.09489400	-1.33141900
H	2.82087300	-3.39637500	-1.20545600
H	4.63526400	-2.69041200	0.33454900
H	4.34213600	-0.66447200	1.73691700
H	2.26260800	0.65499600	1.58792700
H	-1.59089900	2.76536200	-0.61043800
H	-0.62366100	3.39980600	0.69660500

H	-0.85426800	-1.85831700	1.57781900
H	-2.97408000	-3.10191400	1.32441000
H	-4.49912600	-2.59417000	-0.56437600
H	-3.89118000	-0.83233200	-2.20238500
H	-1.77248600	0.42133700	-1.94119300

8b

E= -827.454306 a.u., number of negative frequencies = 0

0 1

C	-2.27233400	-0.27113100	-0.05022400
C	-1.08566900	-0.49620300	-0.08738600
C	0.30373100	-0.85694200	-0.16114100
O	1.08018000	0.23839900	0.09515300
O	0.71526100	-1.95944400	-0.40994100
C	-3.66879700	-0.00626800	-0.00158100
C	-4.13977400	1.28399700	0.29965400
C	-5.50524800	1.53427900	0.34695400
C	-6.41555600	0.50804800	0.09550500
C	-5.95710400	-0.77442800	-0.20460900
C	-4.59369400	-1.03513600	-0.25383300
C	2.47481300	0.17253100	0.06103300
C	3.10878500	1.29390900	-0.46629800
C	4.49779200	1.36399500	-0.47925300
C	5.22248200	0.30135400	0.03864600
C	4.60237500	-0.81908500	0.56906800
C	3.21149300	-0.88772000	0.58474000
H	-3.42646100	2.07552400	0.49391000
H	-5.86113900	2.53108100	0.58015600
H	-7.48038000	0.70745800	0.13321900
H	-6.66406300	-1.57228800	-0.40021500
H	-4.22937100	-2.02837600	-0.48562400

H	2.50528900	2.10294500	-0.85778000
H	5.01705200	2.22355800	-0.88338400
H	5.20530600	-1.62668900	0.96442800
H	2.71432100	-1.75829300	0.98430300
F	6.57290400	0.36069300	0.02684900

9b

E= -959.6231437 a.u., number of negative frequencies = 0

0 2

C	1.05460600	1.00706900	-0.54304500
C	-0.05554300	0.03329900	-0.25004600
O	0.08264500	-1.07601700	0.18194100
O	-1.25663100	0.60956700	-0.55991700
C	0.69473300	2.41225400	-1.03712700
C	2.29443800	0.62727600	-0.36650200
C	-2.46694600	-0.02958800	-0.26739800
C	-2.72834500	-1.34595800	-0.63453300
C	-3.98466200	-1.88483600	-0.36946600
C	-4.94272600	-1.09573400	0.24868500
C	-4.68969900	0.21790800	0.61395900
C	-3.43323400	0.75547700	0.35249200
C	3.42190800	-0.10342700	-0.07202900
C	4.09392400	-0.85851300	-1.08037800
C	5.24339200	-1.56132000	-0.77430600
C	5.77063100	-1.53908300	0.52228300
C	5.12684100	-0.80086500	1.52241600
C	3.97569200	-0.08944400	1.24420000
C	0.02664200	3.22030000	-0.01625400
N	-0.49545400	3.85349000	0.79295500
H	1.60609600	2.92677000	-1.34710200
H	0.03358900	2.34609800	-1.90513400

H	-1.96374600	-1.94661500	-1.10487400
H	-4.22420000	-2.90623000	-0.63648000
H	-5.46407800	0.80105300	1.09565700
H	-3.19233200	1.77560200	0.62432900
H	3.68416500	-0.87758800	-2.08254500
H	5.73816500	-2.13708500	-1.54822500
H	6.67303300	-2.09306700	0.75139600
H	5.53093800	-0.78766400	2.52822800
H	3.47427800	0.47837400	2.01775300
F	-6.16063900	-1.62348600	0.50249000

10b

E= -959.6391352 a.u., number of negative frequencies = 0

0 2

C	3.12131700	-0.54594900	-0.93152200
C	1.80866400	-0.83232400	-1.16039400
C	0.80979900	-0.97605400	-0.04469100
C	1.39281700	-0.70337100	1.31285500
C	2.70836200	-0.40447700	1.49415700
C	3.56809000	-0.32286000	0.38297500
C	-0.50280200	-0.19709300	-0.27113500
C	-1.49843800	-1.08175200	-0.44405900
C	-0.96697800	-2.46024400	-0.34005200
O	0.36684100	-2.38727300	-0.07227800
O	-1.55997900	-3.49540300	-0.47149900
C	-2.95815300	-0.88175000	-0.75710500
C	-0.58196500	1.27325300	-0.22603000
C	-1.64879900	1.89680500	0.44436700
C	-1.74178400	3.28369100	0.49650800
C	-0.77672600	4.07533000	-0.12147600
C	0.29011200	3.47022300	-0.78273600

C	0.39342400	2.08438000	-0.82846600
C	-3.79852800	-0.83751900	0.44160500
N	-4.44500100	-0.77481600	1.39371800
H	3.83644800	-0.49030500	-1.74376200
H	1.44545800	-1.03168300	-2.16143800
H	0.71715500	-0.78620300	2.15524300
H	3.11549400	-0.23148400	2.48319200
H	-3.11258400	0.04323300	-1.31921900
H	-3.29461800	-1.72124400	-1.37318400
H	-2.38871500	1.29762600	0.96017500
H	-2.56710100	3.74354900	1.02760500
H	-0.85129200	5.15599000	-0.08233800
H	1.04742800	4.07901200	-1.26319800
H	1.22665700	1.62871600	-1.34655300
F	4.86392400	-0.02709000	0.58542900

11b

E= -959.628267 a.u., number of negative frequencies = 0

0 2

C	1.09664100	-0.13146700	-0.05522600
C	1.64488200	-1.03182100	-0.98581300
C	2.96236900	-1.44368300	-0.88065000
C	3.72826200	-0.98048900	0.18866800
C	3.21710500	-0.12448900	1.14751700
C	1.89971200	0.30377100	1.01932400
O	1.61475700	2.37472100	-0.45524300
C	0.35670200	2.64526700	-0.49450800
O	0.04902500	3.80108100	-0.80260800
C	-0.66813800	1.59414800	-0.23011200
C	-2.08192600	2.15024400	-0.14288400
C	-0.32768500	0.28522400	-0.16056800

C	-1.32402100	-0.82043300	-0.17945300
C	-1.28870100	-1.81754900	0.80591700
C	-2.21392400	-2.85498000	0.79507000
C	-3.16984500	-2.93076200	-0.21623600
C	-3.19682700	-1.96196200	-1.21685900
C	-2.28471300	-0.91132800	-1.19612800
C	-2.81707300	1.70566200	1.03937200
N	-3.39409100	1.37589100	1.98082300
H	1.03277600	-1.39448900	-1.80244900
H	3.40886100	-2.11714300	-1.60126500
H	3.84121400	0.19808200	1.97069600
H	1.47415900	0.95367200	1.77246500
H	-2.67187600	1.91858700	-1.03350200
H	-2.00231000	3.24150100	-0.11710100
H	-0.54632500	-1.76508200	1.59353300
H	-2.18852400	-3.60575500	1.57626500
H	-3.88716600	-3.74319200	-0.22686100
H	-3.92723500	-2.02397100	-2.01532400
H	-2.29823300	-0.17235700	-1.98878600
F	5.00179100	-1.39773700	0.29386700

12b

E= -959.6432717 a.u., number of negative frequencies = 0

0 2

C	-1.03035700	-0.38711200	-0.12818300
C	-2.08625400	0.58103500	-0.59342100
C	-3.48012400	0.24523800	-0.18004900
C	-3.74764000	-0.97592600	0.32408800
C	-2.74385000	-1.94957200	0.58550000
C	-1.40659900	-1.62927000	0.37160000
O	-1.80770300	1.94332600	-0.18265800

C	-0.53476800	2.40131400	-0.32716400
O	-0.32454300	3.58797800	-0.28240000
C	0.55226200	1.40221400	-0.46624500
C	1.92024600	2.00418400	-0.72149600
C	0.32766900	0.06283900	-0.26621500
C	1.44392000	-0.92433000	-0.17402600
C	1.56674000	-1.93742500	-1.13500900
C	2.60854500	-2.85758800	-1.06260300
C	3.53213700	-2.78741400	-0.02095300
C	3.41160200	-1.79081600	0.94441500
C	2.37687500	-0.86120000	0.86840700
C	2.58080300	2.47492600	0.49885100
N	3.10746500	2.81297200	1.46668600
H	-2.05002500	0.59406500	-1.69956000
H	-4.25895400	0.97709200	-0.34733900
H	-3.03911000	-2.90423200	1.00067300
H	-0.64104300	-2.34504800	0.64381300
H	2.57460300	1.27309700	-1.20120900
H	1.80946400	2.86236400	-1.38895000
H	0.84923400	-1.99573500	-1.94603300
H	2.69846700	-3.62871900	-1.81921400
H	4.34141900	-3.50620400	0.03711300
H	4.12428700	-1.73123800	1.75874500
H	2.29208900	-0.08828900	1.62271800
F	-5.01577400	-1.31944200	0.63199100

13b

E= -959.1037020 a.u., number of negative frequencies = 0

0 1

C	1.06349000	-0.31857300	-0.03080300
C	2.07194100	0.65977100	-0.09597100

C	3.41746500	0.34312800	0.07374300
C	3.74405600	-0.97642400	0.31935500
C	2.78421700	-1.98288700	0.40693900
C	1.45362700	-1.64521500	0.23406300
O	1.78075600	1.96711800	-0.32472400
C	0.48018000	2.42618400	-0.48312700
O	0.31999500	3.60071900	-0.68164000
C	-0.58687100	1.42337300	-0.41801100
C	-1.98197500	1.98121700	-0.62936700
C	-0.31612300	0.10514500	-0.21002000
C	-1.40405100	-0.91656200	-0.16108900
C	-2.27512200	-0.97816000	0.93259500
C	-3.28625700	-1.93589200	0.97142100
C	-3.44140500	-2.83558200	-0.08027600
C	-2.57892600	-2.77846600	-1.17363100
C	-1.56125200	-1.82901700	-1.21250000
C	-2.59650300	2.43893300	0.61901300
N	-3.07707700	2.77179800	1.61232600
H	4.17502700	1.11282100	0.01822500
H	3.09324700	-2.99931300	0.61217200
H	0.69386700	-2.41162400	0.30869800
H	-1.92302700	2.83446700	-1.30894400
H	-2.63356600	1.22633600	-1.07419900
H	-2.16379000	-0.27657000	1.75080900
H	-3.95434200	-1.97324900	1.82397000
H	-4.23162900	-3.57684000	-0.04988700
H	-2.69726000	-3.47281500	-1.99762300
H	-0.89153200	-1.78676300	-2.06436000
F	5.03862100	-1.30083900	0.48575100

14b

E= -959.6072045 a.u., number of negative frequencies = 0

0 2

C	2.93233800	2.01252000	1.07202700
C	2.16418700	0.73743500	0.68479900
C	0.86375200	0.73111500	0.87317600
C	-0.40078700	0.05413500	0.89028800
O	-1.32825300	0.77151000	0.19963500
O	-0.60712900	-0.98958700	1.47097300
C	2.93048600	-0.41581700	0.13150900
C	2.48309500	-1.72917700	0.34638100
C	3.19703500	-2.80752800	-0.16299900
C	4.36528100	-2.59762100	-0.89401000
C	4.81868000	-1.29884600	-1.10904500
C	4.11195200	-0.21414100	-0.59758800
C	3.21461300	2.89091500	-0.06302200
N	3.43833600	3.58536700	-0.95532900
C	-2.65070200	0.35357200	0.03676600
C	-3.24836700	0.77747100	-1.14805000
C	-4.58380600	0.48255500	-1.39542300
C	-5.29470600	-0.23390900	-0.44387600
C	-4.71170100	-0.65760800	0.73982000
C	-3.37347100	-0.36213200	0.98984400
H	2.34864900	2.57793400	1.80094000
H	3.87930900	1.73954200	1.54710500
H	1.58681800	-1.90153100	0.92948700
H	2.84226400	-3.81567600	0.01813300
H	4.91989600	-3.44058900	-1.29000600
H	5.72429400	-1.12471900	-1.67868900
H	4.47466600	0.78716400	-0.79395900
H	-2.65852900	1.33897400	-1.86127500
H	-5.07276600	0.79875600	-2.30789900

H	-5.30190800	-1.21418400	1.45669100
H	-2.90393500	-0.69642000	1.90155400
F	-6.59236900	-0.52664900	-0.67813700

15b

E= -959.6447169 a.u., number of negative frequencies = 0

0 2

C	-1.15910000	-0.14586000	-0.16022700
C	-2.09462400	0.95926300	-0.58189200
C	-3.51597500	0.77496300	-0.15384900
C	-3.96480200	-0.41910800	0.29198000
C	-3.04620600	-1.49371000	0.45934200
C	-1.68102000	-1.35978700	0.27426200
O	-1.65781200	2.26112300	-0.12587800
C	-0.33794000	2.57144400	-0.26401300
O	0.00779000	3.72417000	-0.18210900
C	0.62072400	1.45710600	-0.44039000
C	2.05178500	1.89859900	-0.67730500
C	0.23957000	0.14567100	-0.28188500
C	1.23206300	-0.96824400	-0.22222300
C	1.23922900	-1.95582800	-1.21707500
C	2.16321500	-2.99581300	-1.17415400
C	3.08236700	-3.07142000	-0.12901000
C	3.07592200	-2.10044000	0.86949400
C	2.15942000	-1.05229100	0.82371600
C	2.76041700	2.24646400	0.55750600
N	3.32042700	2.48757800	1.53561100
H	-2.07159100	1.00714600	-1.68779700
H	-4.17038200	1.63085100	-0.26103600
H	-5.00251900	-0.57947300	0.55806400
H	-1.03237700	-2.19042800	0.52088800

H	2.61542700	1.11002700	-1.18069400
H	2.04806300	2.78477900	-1.31669900
H	0.52428900	-1.90071400	-2.03053900
H	2.16458200	-3.74683000	-1.95590900
H	3.79938300	-3.88357700	-0.09346000
H	3.78567000	-2.15381100	1.68682300
H	2.16217400	-0.30017300	1.60328500
F	-3.53508900	-2.66880500	0.89178000

17b

E= -519.5104027 a.u., number of negative frequencies = 0

0 2

O	1.91399800	0.54647300	0.22048800
C	0.54600500	0.25975200	0.11028600
C	-0.29375800	1.36293800	0.02139900
C	-1.66981900	1.17089400	-0.05048200
C	-2.16733200	-0.12383600	-0.03582400
C	-1.33452200	-1.22874400	0.05469000
C	0.04227400	-1.03570000	0.13589300
C	2.81073700	-0.36207300	-0.20397400
O	3.98382500	-0.25824000	-0.14357100
H	0.13521100	2.35659100	0.00848600
H	-2.35263700	2.00778000	-0.12092900
H	-1.76273900	-2.22278500	0.06903900
H	0.71176800	-1.88216900	0.21570700
F	-3.50174400	-0.31385100	-0.10884100

17b

E= -330.8820953 a.u., number of negative frequencies = 0

0 2

C	-1.20497500	-1.22285400	0.00000000

C	0.19588900	-1.21947900	0.00000000
C	0.86031100	0.00000000	0.00000000
C	0.19588900	1.21947900	0.00000000
C	-1.20497500	1.22285400	0.00000000
C	-1.83323500	0.00000000	0.00000000
H	-1.75335400	-2.15776300	0.00000000
H	0.76698500	-2.14016000	0.00000000
H	0.76698500	2.14016000	0.00000000
H	-1.75335400	2.15776300	0.00000000
F	2.21325700	0.00000000	0.00000000

20b

E= -770.9997428 a.u., number of negative frequencies = 0

0 2

C	-1.27830400	-0.75475800	-0.07002400
C	-1.30599000	-1.42527200	1.16040400
C	-2.18731500	-2.48140400	1.36811000
C	-3.04890100	-2.88894600	0.34969600
C	-3.02322900	-2.23442700	-0.87874000
C	-2.14391000	-1.17267800	-1.08709700
C	-0.85223500	1.60370000	-0.54353100
C	-2.16676000	2.26195000	-0.70995000
C	-0.34924400	0.40979800	-0.27528800
C	1.11875800	0.19064300	-0.15582000
C	1.68215100	-1.06814600	-0.40593600
C	3.05750400	-1.26760800	-0.32936700
C	3.86926100	-0.19579800	0.00502000
C	3.34888600	1.06411600	0.26725400
C	1.97510000	1.24893400	0.18721600
C	-2.34515700	3.40895300	0.18861600
N	-2.48686600	4.30985400	0.89227000

H	-0.63915600	-1.11005000	1.95479500
H	-2.20384800	-2.98613600	2.32752800
H	-3.73300700	-3.71368700	0.51342100
H	-3.68311800	-2.55131900	-1.67852500
H	-2.11238500	-0.67562000	-2.05045300
H	-2.29672700	2.61616300	-1.73989100
H	-2.97914400	1.54430300	-0.51984800
H	1.04170700	-1.90025100	-0.67079500
H	3.50210100	-2.23525600	-0.52573100
H	4.01608200	1.87288200	0.53816200
H	1.55134800	2.22274700	0.40269600
F	5.20450200	-0.38300900	0.08659700

8b-TS-9b

E= -959.5751436 a.u., im. freq.= 420.97i

0 2

C	-0.84313300	0.79662800	0.24765400
C	0.59625900	1.01790400	0.11924500
O	1.14932700	2.07427400	-0.03876200
O	1.23726700	-0.18344200	0.21379700
C	-1.60905400	2.92186000	0.64820200
C	-1.77463900	-0.00920400	0.16904300
C	2.62801100	-0.26864100	0.07634600
C	3.09058800	-1.31340600	-0.71654600
C	4.45898400	-1.52895300	-0.84634000
C	5.33228900	-0.68586000	-0.17631900
C	4.88116000	0.35725100	0.61818800
C	3.51162600	0.56979900	0.75026300
C	-2.96916800	-0.75557300	0.10360500
C	-3.19885000	-1.80602100	1.01734600
C	-4.37238900	-2.54205100	0.94880900

C	-5.32748200	-2.25150600	-0.02690600
C	-5.10820600	-1.21502100	-0.93501300
C	-3.94152100	-0.46597000	-0.87743000
C	-2.72290500	3.07718500	-0.18509700
N	-3.64084900	3.15171300	-0.89433600
H	-1.78602800	2.79473300	1.70823900
H	-0.66757600	3.35426800	0.33729700
H	2.37475700	-1.95054100	-1.22015200
H	4.84938800	-2.33370200	-1.45598900
H	5.59741900	0.99177500	1.12442200
H	3.14341900	1.38344300	1.35736900
H	-2.44952000	-2.02949000	1.76676500
H	-4.54408500	-3.34642400	1.65454600
H	-6.24247700	-2.83040000	-0.07721100
H	-5.85413700	-0.98368800	-1.68619300
H	-3.77836100	0.35695300	-1.56129200
F	6.66233000	-0.88734600	-0.29978200

9b-TS-10b

E= -959.6086324 a.u., im. freq.= 432.92i

0 2

C	2.41562300	-1.70872200	-0.85491200
C	1.07823100	-1.97214100	-1.07097600
C	0.14727100	-1.83337900	-0.00222700
C	0.64396400	-1.69027000	1.32573400
C	1.98239000	-1.42556300	1.53233400
C	2.84734500	-1.41159200	0.43800800
C	-0.65758400	0.12380300	-0.34425600
C	-1.91750800	-0.24101800	-0.46102800
C	-2.20898300	-1.69748600	-0.38100400
O	-1.09276100	-2.46243200	-0.15761500

O	-3.28453900	-2.20845200	-0.50813900
C	-3.11389400	0.67983600	-0.67148600
C	0.14855400	1.29955400	-0.31296100
C	0.25292000	2.06234300	0.87115300
C	1.05940500	3.19164400	0.90718700
C	1.77905700	3.58290200	-0.22241800
C	1.68680300	2.83525200	-1.39701600
C	0.88913500	1.70020300	-1.44612000
C	-3.65370700	1.16828600	0.59727600
N	-4.05309700	1.55548600	1.60679800
H	3.14101900	-1.76074300	-1.65709100
H	0.70810900	-2.24979400	-2.04973000
H	-0.05312300	-1.75084000	2.15180700
H	2.38104100	-1.26207900	2.52563700
H	-2.82584300	1.53897100	-1.28142900
H	-3.89935900	0.12790300	-1.19409800
H	-0.31368800	1.76611300	1.74552700
H	1.12310200	3.77333400	1.81965400
H	2.40634900	4.46594100	-0.18819100
H	2.24180500	3.13821400	-2.27757700
H	0.82206800	1.11827300	-2.35737100
F	4.15383000	-1.15650300	0.64417500

10b-TS-11b

E= -959.6266042 a.u., im. freq.= 315.13i

0 2

C	3.27285900	0.16009700	-0.96223600
C	1.93546600	-0.09823900	-1.15291600
C	1.05135000	-0.29674300	-0.03552400
C	1.58434400	-0.06227400	1.27759500
C	2.92265400	0.18984500	1.46433400

C	3.75210400	0.28874500	0.34364400
C	-0.44103000	-0.17501300	-0.23580700
C	-1.07942000	-1.34018300	-0.43709200
C	-0.19430300	-2.54343300	-0.37064200
O	1.05584600	-2.24793500	-0.08753600
O	-0.58135900	-3.68030000	-0.56222900
C	-2.53343800	-1.58173600	-0.76042800
C	-1.04257800	1.17790600	-0.17389900
C	-2.26419700	1.39391500	0.48538700
C	-2.82722000	2.66542200	0.53941600
C	-2.18548300	3.74503500	-0.06235200
C	-0.96592600	3.54800400	-0.70728800
C	-0.39475800	2.28134600	-0.75385800
C	-3.34794200	-1.84790200	0.42666200
N	-3.98561500	-2.02313200	1.37080300
H	3.95927600	0.26592400	-1.79266900
H	1.53648900	-0.21336200	-2.15304400
H	0.91524500	-0.13039500	2.12592800
H	3.34691400	0.32526600	2.45111900
H	-2.96722000	-0.73089200	-1.29233400
H	-2.58675700	-2.46492000	-1.40454300
H	-2.76003700	0.57535700	0.99123300
H	-3.76580600	2.81046900	1.06169600
H	-2.62664700	4.73421500	-0.02087000
H	-0.45541200	4.38357300	-1.17233700
H	0.55622600	2.14729500	-1.25490200
F	5.05513900	0.53961500	0.52813800

11b-TS-12b

E= -959.6235041 a.u., im. freq.= 337.46i

0 2

C	-1.04640900	-0.35964000	-0.10759500
C	-2.05327300	0.30565800	-0.88453200
C	-3.42525900	0.00355800	-0.66597000
C	-3.74874200	-0.88131100	0.32583700
C	-2.77737700	-1.54604700	1.09554300
C	-1.43312900	-1.28567000	0.86362200
O	-1.74018200	2.10073900	-0.21001400
C	-0.47373800	2.44410300	-0.25633100
O	-0.15646400	3.61355000	-0.11180100
C	0.59238700	1.39876000	-0.44884000
C	1.96234100	1.98233500	-0.74631600
C	0.34978800	0.07335400	-0.27237300
C	1.40613700	-0.97367800	-0.20217400
C	1.30456700	-2.11400400	-1.01498800
C	2.27697000	-3.10692800	-0.96890700
C	3.35554000	-2.98932300	-0.09330100
C	3.45620800	-1.87269600	0.73277600
C	2.49149300	-0.86945500	0.67917800
C	2.67348700	2.45091900	0.44483200
N	3.25105600	2.77799500	1.38713200
H	-1.77594200	0.67359000	-1.86366300
H	-4.19778200	0.46098600	-1.26915100
H	-3.09862500	-2.23791100	1.86371600
H	-0.67857900	-1.77812300	1.46400400
H	2.59166700	1.24374300	-1.24802100
H	1.83655100	2.84154500	-1.41078100
H	0.46519700	-2.21338500	-1.69407500
H	2.19160900	-3.97383500	-1.61411100
H	4.11012700	-3.76644800	-0.05268600
H	4.28535900	-1.77861100	1.42436800
H	2.57444000	-0.01383900	1.33769300

F	-5.03935400	-1.17528900	0.56050300

12b-TS-13b

E= -959.5967464 a.u., im. freq.= 945.18i

0 2

C	-1.04280800	-0.33609200	-0.04639600
C	-2.07179200	0.63698300	-0.20704100
C	-3.41855800	0.32565300	0.08300300
C	-3.73193300	-0.98563000	0.34939900
C	-2.76369300	-1.99137000	0.41990200
C	-1.43327500	-1.65556100	0.23310000
O	-1.77578900	1.96897700	-0.27080000
C	-0.47793800	2.42336800	-0.44371800
O	-0.31062000	3.60436500	-0.59027000
C	0.59034100	1.41752500	-0.42072200
C	1.98072100	1.98269000	-0.64221300
C	0.33010400	0.09548300	-0.21061400
C	1.42489800	-0.91829700	-0.15373500
C	1.57810700	-1.84633900	-1.19222400
C	2.60286600	-2.78780600	-1.14861300
C	3.47641000	-2.82160100	-0.06296500
C	3.32528000	-1.90663100	0.97605100
C	2.30724600	-0.95648400	0.93201000
C	2.60303300	2.44529900	0.60060800
N	3.09076400	2.78072600	1.58953800
H	-2.19940800	0.35850500	-1.96934600
H	-4.17277900	1.09947800	0.04990100
H	-3.06773700	-3.00558000	0.64312500
H	-0.67281900	-2.41925200	0.32644600
H	2.63253000	1.23066500	-1.09144900
H	1.91239300	2.83512600	-1.32192300

H	0.89994100	-1.82152300	-2.03813300
H	2.71837900	-3.49395200	-1.96291500
H	4.27211200	-3.55682000	-0.02878200
H	4.00168000	-1.92622400	1.82260400
H	2.19896300	-0.24316800	1.74040100
F	-5.01570900	-1.31513500	0.57743000

8b-TS-14b

E= -959.5671715 a.u., im. freq.= 573.55i

0 2

C	-2.07943100	1.41534200	-1.68446800
C	-1.93566200	-0.26702900	-0.30630400
C	-0.72726700	-0.54625100	-0.26903800
C	0.65008800	-0.43577300	-0.67111500
O	1.46689500	-0.48460500	0.41244400
O	1.00407300	-0.31609300	-1.81937400
C	-3.30217000	-0.48031500	0.12045800
C	-4.13481900	-1.35182700	-0.59755100
C	-5.44248900	-1.56735700	-0.17749200
C	-5.93485000	-0.90902700	0.94864600
C	-5.11357000	-0.03509500	1.65822100
C	-3.80164100	0.18245600	1.25057900
C	-2.27598000	2.53134600	-0.85501000
N	-2.43859200	3.42073700	-0.12543500
C	2.85403900	-0.33805100	0.30485100
C	3.45422600	0.36565000	1.34468600
C	4.83694700	0.50950300	1.37467600
C	5.58760100	-0.05903800	0.35649900
C	4.99978600	-0.76537200	-0.68137500
C	3.61506700	-0.91139300	-0.71094300
H	-1.12355100	1.32203900	-2.18520900

H	-2.94260900	1.04932400	-2.22699900
H	-3.74731800	-1.86302600	-1.47087200
H	-6.07771500	-2.25002800	-0.72997500
H	-6.95602600	-1.07635300	1.27111600
H	-5.49379600	0.48048300	2.53227500
H	-3.16258400	0.86553200	1.79545000
H	2.83125400	0.79054900	2.12135700
H	5.33169400	1.05244700	2.16971000
H	5.62261600	-1.19437400	-1.45594800
H	3.14175000	-1.44938000	-1.51795500
F	6.93104900	0.07850900	0.37762500

9b-TS-15b

E= -959.6008279 a.u., im. freq.= 402.92i

0 2

C	1.27401400	-0.60974200	-1.04788900
C	1.53265000	-1.74596100	-0.24036500
C	2.63875900	-1.82150400	0.58325500
C	3.56261800	-0.77229700	0.59465200
C	3.33626100	0.32974500	-0.23024700
C	2.24524500	0.42464700	-1.06616200
O	0.62624400	-2.78563500	-0.24357200
C	-0.70388100	-2.57863200	0.05129500
O	-1.43009400	-3.53174100	0.09432500
C	-1.17000700	-1.19132200	0.35213900
C	-2.54473800	-1.14914400	1.03253900
C	-0.50742200	-0.08859400	0.03068000
C	-0.76827100	1.32104900	0.10013400
C	-1.80889500	1.89523200	-0.66092600
C	-2.03078300	3.26632600	-0.62060800
C	-1.22690300	4.08853700	0.16875300

C	-0.19049800	3.53203900	0.91951900
C	0.04901600	2.16478000	0.87990800
C	-3.63747400	-1.14459600	0.06083200
N	-4.48461000	-1.10520500	-0.71998800
H	0.61863700	-0.72089500	-1.90389400
H	2.77421000	-2.69526000	1.20785700
H	4.44425200	-0.79938400	1.22137500
H	2.13953800	1.27869800	-1.72145400
H	-2.66302700	-2.01951500	1.68107500
H	-2.62245500	-0.24641700	1.64236200
H	-2.43928600	1.25947600	-1.27123300
H	-2.83806900	3.69329100	-1.20449500
H	-1.40542800	5.15713000	0.19769600
H	0.43661400	4.16790900	1.53390300
H	0.85823200	1.73567100	1.45820400
F	4.24685500	1.32681800	-0.22806300

9b-TS-17b

E= -959.5636712 a.u., im. freq.= 335.75i

0 2

C	1.51167400	1.53863500	-0.58623300
C	-0.14644100	-0.11082400	-0.92074300
O	0.07591200	-1.27237300	-0.85759000
O	-1.29687700	0.56087900	-0.79066900
C	0.73481000	2.76761700	-0.85259800
C	2.51247200	0.90544600	-0.27917800
C	-2.50664100	-0.07005500	-0.39826200
C	-3.32055800	0.68495400	0.43766000
C	-4.55166600	0.17046000	0.83144600
C	-4.92837000	-1.08517600	0.37727000
C	-4.11741200	-1.84064200	-0.45534500

C	-2.88508800	-1.32664700	-0.85486700
C	3.56056700	0.01330300	0.04571700
C	4.39690300	-0.50758300	-0.96215900
C	5.42895300	-1.37599300	-0.63490300
C	5.64788900	-1.74066600	0.69391500
C	4.82526400	-1.23141700	1.69927500
C	3.79051900	-0.36141600	1.38496400
C	-0.12298100	3.16423600	0.26927000
N	-0.80427200	3.48831300	1.13956700
H	1.42401600	3.59255100	-1.06316900
H	0.09709500	2.64363700	-1.73217700
H	-2.98237800	1.65673800	0.77523200
H	-5.21230500	0.72713900	1.48369800
H	-4.45001700	-2.81645000	-0.78549200
H	-2.23463700	-1.90194700	-1.49721500
H	4.22064200	-0.22550700	-1.99287000
H	6.06437000	-1.77292300	-1.41830300
H	6.45459000	-2.41974400	0.94463800
H	4.99126800	-1.51554700	2.73206900
H	3.14878500	0.03507200	2.16211700
F	-6.12257500	-1.58829500	0.75880100

17b-TS-19b

E= =-519.4803723 a.u., im. freq.= 677.90i

0 2

C	3.13767700	0.12716500	-0.00002800
O	2.22217200	0.93588800	0.00023700
O	3.51927900	-0.98795400	-0.00032500
C	0.46687400	0.39022100	0.00011600
C	-0.41275800	1.44510600	-0.00003500
C	-1.77675500	1.14159700	-0.00012500

C	-2.16246100	-0.19292900	-0.00003700
C	-1.24857400	-1.23816600	0.00013100
C	0.11899700	-0.94133100	0.00021500
H	-0.06425000	2.47099300	-0.00007400
H	-2.53253500	1.91749800	-0.00023600
H	-1.60441200	-2.26117400	0.00022000
H	0.85761400	-1.73230800	0.00036900
F	-3.48066900	-0.48538400	-0.00011100

11b-TS-20b

E= -959.6146637 a.u., im. freq.= 423.53i

0 2

C	1.17702900	-0.15934200	0.06596900
C	1.62084000	-1.24548100	-0.70851100
C	2.94670300	-1.65522100	-0.67229600
C	3.82744300	-0.98462300	0.16500600
C	3.42411100	0.07921300	0.95910200
C	2.09870800	0.48864800	0.90526500
O	1.18542700	3.14202800	-0.10520100
C	0.29345300	2.87948300	-0.86718100
O	-0.29278100	3.09883400	-1.87993500
C	-0.66821100	1.52946000	0.07474100
C	-1.97071800	2.17053400	0.45096600
C	-0.24128600	0.25606100	0.01522800
C	-1.27518200	-0.81401200	-0.17005200
C	-1.31831200	-1.91486100	0.69639200
C	-2.29762400	-2.88905000	0.53902400
C	-3.22988000	-2.78891000	-0.49308200
C	-3.18094700	-1.70788600	-1.36937500
C	-2.21194700	-0.72141100	-1.20636400
C	-2.74407500	1.44996100	1.46294900

N	-3.35259500	0.90793400	2.27735000
H	0.92363500	-1.76210200	-1.35591800
H	3.30410000	-2.47942200	-1.27644500
H	4.14180900	0.56704300	1.60630700
H	1.77143800	1.31624500	1.51815300
H	-2.58549400	2.33124600	-0.44186500
H	-1.76448800	3.17332000	0.84462600
H	-0.59685300	-1.99413200	1.50060000
H	-2.33440900	-3.72749200	1.22492700
H	-3.98920100	-3.55283600	-0.61411900
H	-3.89507300	-1.63127700	-2.18114800
H	-2.16127000	0.11240200	-1.89780900
F	5.11246400	-1.38564600	0.21396100