Supplementary Material

Unravelling the Mechanism of the Ketene-Imine Staudinger Reaction. An ELF Quantum Topological Analysis

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*ELF topological analysis of bonding changes along the ketene-imine Staudinger reaction between MCK **18** and N-methyl imine **19**.*

The ELF topological analysis of the bonding changes along the Staudinger reaction between MCK **18** and *N*-methyl imine **19** has been divided into the two elementary steps of the stepwise reaction: i) the nucleophilic attack of imine **19** on the carbonyl carbon atom of ketene **18**, yielding ZW intermediate **ZW-6n**; and ii) the ring-closure process at the ZW intermediate **ZW-6n** yielding β-lactam *trans*-**20**. The attractor positions of the ELF for the most relevant points associated with the N1-C4 and C2-C3 bond formation along this two-step Staudinger reaction are given in Figure S1, while a graphical representation of the basin-population changes along both steps is graphically represented in Figure S2.

ELF topological analysis along the reaction path associated with the nucleophilic attack of imine **19** on the carbonyl carbon atom of ketene **18** indicates that this reaction step is topologically very simple; only four differentiated phases are characterised. The population of the more significant valence basins of the selected points of the IRC are gathered in Table S1.

Phase I, 3.11 Å ≤ d(N1-C4) < 2.26 Å, begins at **MC-6n**, d(N1-C4)= 3.110 Å and d(C2-C3) = 3.468 Å, which is a minimum over the PES connecting the separated reagents **18** and **19** with **TS1-6n**. The ELF picture of **MC-6n** recovers the topological characteristics of the separated reagents. ELF of **MC-6n** shows the presence of two disynaptic basins, V(C3,C4) and V'(C3,C4), with a population of 1.98e and 1.94e, respectively, and two disynaptic basins, V(C4,O5) and V'(C4,O5), with a population of 1.51e and 1.48e, respectively. Both pairs of disynaptic basins are associated with the C3-C4 and C4-O5 double bond regions, and are those in which the most relevant changes in electron density in ketene **18** will take place along the reaction. On the other hand, ELF topology of **MC-6n** also shows the presence of two disynaptic basins, V(N1,C2) and V'(N1,C2), integrating 1.52e each one, belonging to the imine N1-C2 double bond region, and one V(N1) monosynaptic basin, integrating 2.62e, associated with the lone pair in the N1 nitrogen atom. The integration of these valence basins indicates that the N1-C2 double bond is very polarized.

Phase II, 2.26 Å ≤ d(N1-C4) < 1.71 Å, begins at **P1-1**. At this point, the two V(C4,O5) and V'(C4,O5) disynaptic basins present at **MC-6n** have merged in a new V(C4,O5) disynaptic basin, integrating 2.77e. This bonding change is a consequence of

the loss of electron density observed in the C4-O5 bonding region, *ca.* 0.25e; this electron density is mainly collected at the V(O5) and V'(O5) monosynaptic basins, which have increased their integration. At the imine framework, only a slight depopulation of the V(N1) basin is observed, 0.1e. In this phase, the TS of the first step, **TS1-6n** d(N1-C4) = 2.177 Å and d(C2-C3) = 3.575 Å, is found. At this TS only slight changes in electron density with respect to those found at **P1-1** are observed. The GEDT at **TS1-6n** is 0.17e. *Phase II* ends at **P1-2**. At this point, the V(C4,O5) disynaptic basin and the V(N1) monosynaptic basin have lost *ca.* 0.5e and 0.3e, respectively, while the population of the V(O5) and V'(O5) monosynaptic basins have been increased by *ca.* 0.4e. At the end of this phase the GEDT that takes place from the imine framework to the ketene one has reached a large value, 0.46e.

Phase III, 1.71 Å ≤ d(N1-C4) ≤ 1.69 begins at **P1-2**. At this phase the most significant topological change along the IRC associated with the first step of this stepwise reaction takes place. The V(N1) monosynaptic basin present at **P1-2** is converted into a new V(N1,C4) disynaptic basin with an initial population of 2.15e (see the V(N1,C4) disynaptic basin, integrating 2.15e, in structure **P1-3** in Figure S1, and the change from V(N1), in red in **P1-2**, to V(N1,C4), in blue in **P1-3**, in Figure S2). This relevant topological change indicates that the formation of the new N1-C4 single bond has already begun at a length of *ca.* 1.69 Å.

Finally, *Phase IV*, 1.69 Å ≤ d(N1-C4) ≤ 1.53 Å, begins at **P1-3** and ends at the ZW intermediate **ZW-6n**, d(N1-C4) = 1.533 Å and d(C2-C3) = 3.188 Å. From **P1-3** to **ZW-6n**, only changes in basin populations are observed. At ZW intermediate **ZW-6n**, the maximum of GEDT along the stepwise Staudinger reaction is observed, 0.54e.

ELF topological analysis along the reaction path associated with the ring-closure process in the ZW intermediate **ZW-6n** indicates that this step is topologically characterised by seven differentiated phases (see Figure S2). The population of the more significant valence basins of the selected points of the IRC are gathered in Table S1.

Phase I, 3.18 Å ≤ d(C2-C3) < 2.96 Å, begins at ZW intermediate **ZW-6n**. In this phase, only small changes in the basin populations are observed. *Phase II*, 2.96 Å ≤ d(C2-C3) < 2.81 Å and *Phase III*, 2.81 Å ≤ d(C2-C3) < 2.73 Å, are two short phases in which the V(N1,C2) and V'(N1,C2) and the V(C3,C4) and V'(C3,C4) pairs of disynaptic basins associated with the N1-C2 and C3-C4 double bonds have merged

into the V(N1,C2) and the V(C3,C4) disynaptic basins, integrating 3.46e (**P2-2**) and 3.71e (**P2-1**), respectively (see Table S1). These topological changes are a consequence of the depopulation of the N1-C2 and C3-C4 bonding regions. From ZW intermediate **ZWn-25** to **P2-2**, GEDT has decreased only by 0.03e.

Phase IV, 2.73 Å ≤ d(C2-C3) < 2.47 Å, begins at **P2-3**. At this point, together with the decrease of the electron density of the V(N1,C2) disynaptic basin by 0.34e, a new V(N1) monosynaptic basin, integrating 0.43e, is created at the N1 nitrogen atom. This basin is associated to the lone pair present in the β-lactam nitrogen atom.

Phase V, 2.47 Å ≤ d(C2-C3) < 2.17 Å, begins at **P2-4**. At this point, the V(N1,C2) and V(C3,C4) disynaptic basins experience a strong depopulation; 0.44e and 0.82e, respectively. The first significant success occurs with the creation of a new V(C2) monosynaptic basin, integrating 0.56e (see Figure S2). These changes indicate that the electron density of the new V(C2) monosynaptic basin is mainly reached through the depopulation of the V(N1,C2) disynaptic basin, and the retro-donation that takes place along the ring-closure process. Note that at **P2-4**, GEDT has decreased by 0.20e. On the other hand, the V(N1) monosynaptic basin created in the previous phase has reached a population of 1.23e. At *Phase V*, the TS of the second step, **TS2-6n**, d(N1-C4) = 1.439 Å and d(C2-C3) = 2.202 Å, is found. At this TS, GEDT has decreased to 0.25e.

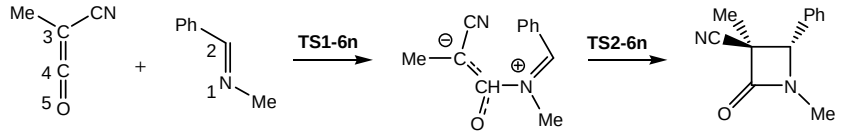
Phase VI, 2.17 Å ≤ d(C2-C3) < 2.08 Å, begins at **P2-5**. At this point, the population of the V(C3,C4) and the V(N1,C2) disynaptic basins continue their decrease to reach 2.44e and 2.26e, respectively. The second significant success occurs with the creation of a new V(C3) monosynaptic basin, integrating 0.23e. The V(C2) monosynaptic basin created in *phase V* has reached 0.68e. The two V(C2) and V(C3) monosynaptic basins are responsible of the formation of the second C2-C3 single bond in the next phase. On the other hand, the V(N1) monosynaptic basin has increased its population to 1.67e.

Phase VII, 2.08 Å ≤ d(C2-C3) < 1.57 Å, is the longest phase of the IRC that begins at **P2-6** and ends in β-lactam *trans*-**27**, d(N1-C4) = 1.350 Å and d(C2-C3) = 1570 Å. At **P2-6** the most remarkable success along the second step occurs. The two V(C2) and V(C3) monosynaptic basins have merged into the new V(C2,C3) disynaptic basin, which presents a population of 1.08e (see the V(C2) and V(C3) monosynaptic basins, integrating 0.68e and 0.23e, respectively, in structure **P2-5** in Figure S1, yielding the V(C2,C3) disynaptic basin, integrating 1.08e, in structure **P2-6**, and the

merger of V(C2) and V(C3), in green in **P2-5**, into the new V(C2,C3), in blue in **P2-6**, in Figure S2). This topological change indicates that the formation of the second C2-C3 single bond has already begun at a length of 2.08 Å. With the start of the C-C bond formation, GEDT has decreased to 0.10e. On going from **P2-6** to β-lactam *trans*-**20**, only changes in basin populations are observed. Along the end of this phase, the new V(C2,C3) disynaptic basin has reached 1.81e.

Finally, some topological behaviours in β-lactam *trans*-**20** are noteworthy; the V(N1,C2) disynaptic basin and the V(N1) monosynaptic basins have been depopulated to 1.68e and 1.14e, respectively, while the new V(N1,C4) disynaptic basin has reached 2.97e.

Table S1. Valence basin populations *N* calculated from the ELF at some selected points of the two-steps ketene-imine Staudinger reaction of MCK **18** with *N*-methyl imine **19**. Distances are given in Angstroms. The GEDT obtained by NBO analysis is given in e.



18 **19** **ZW-6n** *trans*-**20**

	Step-I						*Step-II*							
	MC-6n	**P1-1**	**TS1-6n**	**P1-2**	**P1-3**	**ZW-6n**	**P2-1**	**P2-2**	**P2-3**	**P2-4**	**TS2-6n**	**P2-5**	**P2-6**	*trans-**20***
d(N1-C4)	3.110	2.258	2.177	1.713	1.687	1.533	1.545	1.531	1.517	1.461	1.439	1.417	1.408	1.350
d(C2-C3)	3.468	3.621	3.575	3.320	3.305	3.184	2.957	2.808	2.727	2.466	2.202	2.172	2.079	1.570
GEDT	0.00	0.13	0.17	0.44	0.46	0.54	0.53	0.51	0.49	0.34	0.25	0.15	0.10	-0.01
V(C3,C4)	1.98	2.08	2.01	1.94	1.94	1.91	3.71	3.65	3.60	2.78	2.63	2.44	2.37	2.06
V'(C3,C4)	1.94	1.92	1.98	1.89	1.88	1.86								
V(C4,O5)	1.51	2.77	2.78	2.30	2.28	2.12	2.18	2.22	2.23	2.35	2.41	2.43	2.45	2.51
V'(C4,O5)	1.48													
V(C3,C6)	2.35	2.42	2.43	2.48	2.48	2.48	2.50	2.51	2.52	2.51	2.46	2.42	2.39	2.26
V(O5)	2.35	2.51	2.52	2.92	2.88	2.83	2.74	2.79	2.76	2.72	2.71	2.69	2.67	2.70
V'(O5)	2.32	2.42	2.41	2.49	2.53	2.71	2.70	2.74	2.74	2.68	2.67	2.65	2.62	2.60
V(N1,C2)	1.52	1.53	1.58	1.66	1.70	1.79	1.74	3.46	3.12	2.68	2.52	2.26	2.05	1.68
V'(N1,C2)	1.52	1.53	1.55	1.67	1.70	1.73	1.74							
V(N1)	2.62	2.51	2.43	2.19					0.43	1.23	1.47	1.67	1.75	1.14
V(N1,C4)					2.15	2.07	2.13	2.10	2.09	1.89	1.90	1.95	2.02	2.97
V(C2)										0.56	0.60	0.68		
V(C3)												0.23		
V(C2,C3)													1.08	1.81

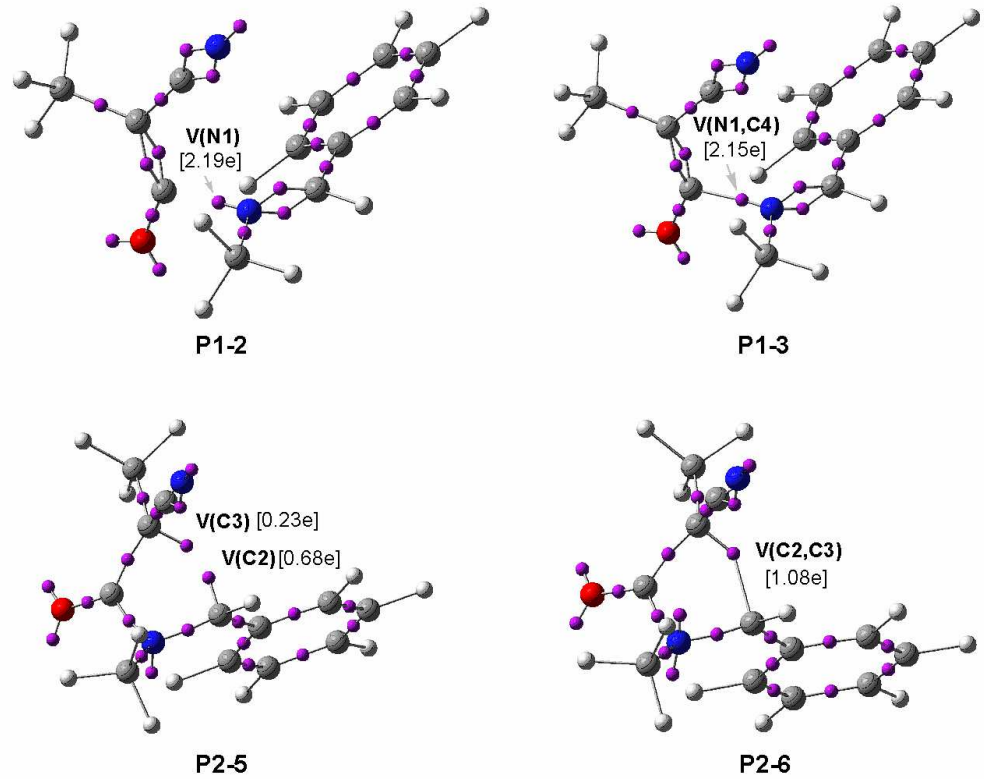


Figure S1. ELF attractor positions of the most relevant points associated with the N1-C4 and C2-C3 bond formation along the two-steps ketene-imine Staudinger reaction between MCK **18** and *N*-methyl imine **19**. The electron populations in e are given in brackets.

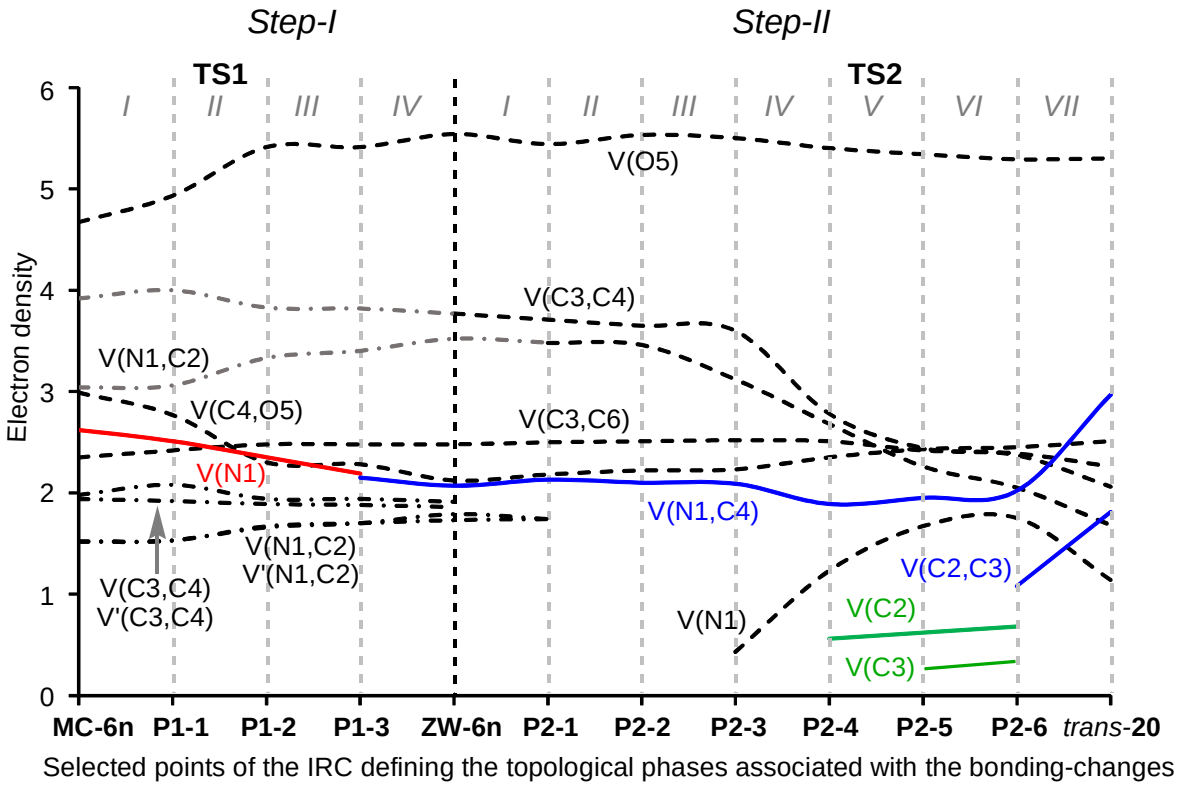


Figure S2. Graphical representation of the basin-population changes along the two-steps ketene-imine Staudinger reaction between MCK **18** and *N*-methyl imine **19**. Point-dotted curves in grey represent the sum of the V(Cx,Cy) and V'(Cx,Cy) disynaptic basins describing a C-C double bond region.

*ELF topological analysis of the stationary points involved in the endo stereoisomeric path of the ketene-imine Staudinger reaction of TBCK **11** with N-phenyl imine **12a**.*

Finally, an ELF topological analysis of the stationary points involved in the *endo* stereoisomeric path of the ketene-imine Staudinger reaction of TBCK **11** with *N*-phenyl imine **12a** was performed. The population of the most significant valence basins of the corresponding stationary points are gathered in Table S2.

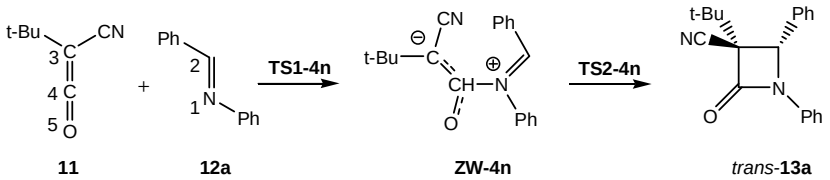
At **TS1-4n**, d(N1-C4) = 2.074 Å and d(C2-C3) = 3.432 Å, similar to **TS1-6n**, no significant topological behaviour associated with the formation of the N1-C4 bond is found. The V(N1) monosynaptic basin has a population of 2.44e, while the two V(C4,O5) and V'(C4,O5) disynaptic basins present in TBCK **11** have merged into the V(C4,O5) disynaptic basin, with an integration of 2.80e.

At **ZW-4n**, d(N1-C4) = 1.543 Å and d(C2-C3) = 3.101 Å, the population of the V(N1,C4) disynaptic basin has decreased to 2.06e. At this ZW intermediate, the V(C3,C4) and V'(C3,C4) disynaptic basins present in **TS1-4n**, have merged into one V(C3,C4) disynaptic basin, integrating 3.72e, while the N1-C2 bonding region remains characterised by the presence of two V(N1,C2) and V'(N1,C2) disynaptic basins, with a total integration of 3.48e.

At **TS2-4n**, d(N1-C4) = 1.444 Å and d(C2-C3) = 2.403 Å, no significant topological behaviour associated with the C2-C3 bond formation is found. The integration of the V(C3,C4) disynaptic basin has decreased to 3.21e, while the two V(N1,C2) and V'(N1,C2) disynaptic basins present in **ZW-4n** have merged into one V(N1,C2) disynaptic basin, integrating 2.39e.

Finally, at β-lactam *trans*-**13a**, while the V(C2,C3) disynaptic basin has reached 1.85e, the V(N1,C4) one has increased its population to 2.78e. On the other hand, the V(N1) monosynaptic basin has decreased its population to 1.17e. These behaviours are similar to those found in β-lactam *trans*-**20**.

Table S2. Valence basin populations *N* calculated from the ELF at some selected points of the two-steps ketene-imine Staudinger reaction of TBCK **11** with *N*-phenyl imine **12a**. Distances are given in Angstroms. The GEDT obtained by NBO analysis is given in e.



11 **12a** **ZW-4n** *trans*-**13a**

	MC-4n	**TS1-4n**	**ZW-4n**	**TS2-4n**	*trans*-**13a**
d(N1-C4)	3.326	2.074	1.543	1.444	1.359
d(C2-C3)	3.799	3.432	3.101	2.403	1.580
GEDT	0.00	0.21	0.53	0.26	-0.04
V(C3,C4)	1.98	1.98	3.70	3.21	2.05
V'(C3,C4)	2.01	2.01			
V(C3,C6)	2.40	2.47	2.53	2.50	2.24
V(O5)	2.45	2.52	2.74	2.77	2.65
V'(O5)	2.43	2.42	2.82	2.67	2.63
V(C4,O5)	1.50	2.80	2.19	2.33	2.46
V'(C4,O5)	1.49				
V(N1)	2.63	2.44		0.99	1.17
V'(N1)				0.38	
V(N1,C2)	2.94	1.58	1.66	2.39	1.74
V'(N1,C2)		1.44	1.82		
V(N1,C4)			2.06	1.98	2.78
V(C2,C3)					1.85

Table S3. MPWB1K/6-311G(d) gas phase total (E, in au) and relative[a] (ΔE, in kcal/mol) energies of the stationary structures involved in the reaction of TBCK **11** with *N*-phenyl imine **12a**.

	E	ΔE
11	-401.976421	
12a	-556.567558	
TS1-4n	-958.540690	2.1
TS1-4x	-958.519639	15.3
ZW-4n	-958.548612	-2.9
ZW-4x	-958.530419	8.51
TS2-4n	-958.524294	12.4
TS2-4x	-958.509654	21.5
trans-**13a**	-958.599293	-34.7
cis-**14a**	-958.605038	-38.3

[a] relative to TBCK **11** and *N*-phenyl imine **12a**.

Table S4. MPW1K/6-311G(d) total electronic energies (E, in au) in benzene, and enthalpies (H, in au), entropies (S, in cal/mol·K) and Gibbs free energies (G, in au), computed at 80 ºC and 1 atm in benzene, of the stationary structures involved in the reaction of TBCK **11** with *N*-phenyl imine **12a.**

	E	H	S	G
11	-401.979838	-401.816565	102.5	-401.874225
12a	-556.570691	-556.346391	112.6	-556.409747
TS1-4n	-958.546996	-958.157971	172.0	-958.254740
TS1-4x	-958.528462	-958.139235	171.4	-958.235660
ZW-4n	-958.558246	-958.166983	168.3	-958.261663
ZW-4x	-958.543396	-958.151979	163.3	-958.243863
TS2-4n	-958.531611	-958.142134	161.9	-958.233238
TS2-4x	-958.518700	-958.129547	162.7	-958.221096
trans-**13a**	-958.604871	-958.211756	161.0	-958.302330
cis-**14a**	-958.611046	-958.218468	163.9	-958.310681

Table S5. M062X/6-311G(d) Gibbs free energies (G, in au) and relative[a] Gibbs free energies (ΔG, in kcal/mol), computed at 80 ºC and 1 atm in benzene, of the most relevant stationary structures involved in the reaction of TBCK **11** with *N*-phenyl imine **12a.**

	G	ΔG
11	-401.927119	
12a	-556.473424	
TS2-4n	-958.353280	29.7
TS2-4x	-958.341073	37.3
trans-**13a**	-958.420143	-12.3
cis-**14a**	-958.427104	-16.7

[a] relative to TBCK **11** and *N*-phenyl imine **12a**.

Table S6. MPWB1K/6-311G(d) total (E, in au) and relative[a] (ΔE, in kcal/mol) energies, in benzene, of the stationary points along the *endo* and *exo* stereoisomeric channels associated with the Staudinger reactions of *N*-phenyl imine **12a** with the monosubtituted ketenes **15a-c**.

CN	E	ΔE	Me	E	ΔE	*t*-Bu	E (au)	ΔE
TS1-5an	-801.358362	-1.2	**TS1-5bn**	-748.414766	7.8	**TS1-5cn**	-866.307544	9.9
TS1-5ax	-801.356006	0.2	**TS1-5bx**	-748.414454	8.0	**TS1-5cx**	-866.296682	16.7
ZW-5an	-801.366762	-6.5	**ZW-5bn**	-748.417147	6.3	**ZW-5cn**	-866.310499	8.0
ZW-5ax	-801.363738	-4.6	**ZW-5bx**	-748.414436	8.0	**ZW-5cx**	-866.300264	14.4
TS2-5an	-801.333799	14.2	**TS2-5bn**	-748.404686	14.1	**TS2-5cn**	-866.297831	16.0
TS2-5ax	-801.337808	11.7	**TS2-5bx**	-748.393000	21.4	**TS2-5cx**	-866.280138	27.1
trans-**16a**	-801.417569	-38.4	*trans*-**16b**	-748.498093	-44.5	*trans*-**16c**	-866.386444	-39.6
cis-**17a**	-801.415918	-37.4	*cis*-**17b**	-748.498349	-44.7	*cis*-**17c**	-866.392612	-43.5

[a] relative to ketenes **15a-c** and *N*-phenyl imine **12a**.

Table S7. MPWB1K/6-311G(d) gas phase total (E, in au) and relative[a] (ΔE, in kcal/mol) energies of the stationary structures involved in the reaction of MCK **18** with *N*-methyl imine **19**.

	E	ΔE
18	-284.0803863	
19	-364.8784705	
TS1-6n	-648.9630930	-2.7
ZW-6n	-648.9741149	-9.6
TS2-6n	-648.9435846	9.6
trans-**20**	-649.0221015	-39.7

[a] relative to MCK **18** and *N*-methyl imine **19**.

MPWB1K/6-311G(d,p) computed total electronic energies and cartesian coordinates of the KI-S reactions of ketenes **11** and **15a-b** with *N*-phenyl imine **12a**, in benzene, and those of the KI-S reaction of ketene **18** with *N*-methyl imine **19**, in gas phase.

11
E(RmPW+HF-B95) = -401.979838 au

C	0.56694900	0.04842000	0.00005300
C	1.32733100	-1.02556500	-0.00004200
O	1.96411600	-1.97338900	-0.00012800
C	1.20573900	1.30334800	-0.00000900
N	1.68002600	2.34743800	-0.00006100
C	-0.95848100	-0.05460200	0.00004600
C	-1.48930400	0.63477400	-1.24542700
H	-2.57576500	0.60256700	-1.25332200
H	-1.18641200	1.67781500	-1.27761900
H	-1.12749200	0.14882900	-2.14670500
C	-1.48931300	0.63471400	1.24554800
H	-2.57577500	0.60250300	1.25343400
H	-1.12750600	0.14872700	2.14680500
H	-1.18642600	1.67775400	1.27779100
C	-1.36891100	-1.51480300	0.00001000
H	-2.45155500	-1.59174200	0.00000200
H	-1.00311500	-2.03454200	-0.88254900
H	-1.00312600	-2.03458200	0.88254900

12a
E(RmPW+HF-B95) = -556.570691 au

N	-0.44971400	-0.52636500	0.13708900
C	0.38510600	0.37279300	-0.16103500
H	0.06183900	1.35551500	-0.51042100
C	1.82651200	0.16861200	-0.08112400
C	2.36216900	-1.03452200	0.36159400
C	2.67809900	1.19751000	-0.45346400
C	3.72692900	-1.19898500	0.42828800
H	1.68911400	-1.82599100	0.64768800
C	4.04711500	1.03208700	-0.38551600
H	2.26367200	2.13302400	-0.79848300
C	4.57219100	-0.16620300	0.05553700
H	4.13937200	-2.13384900	0.77269400
H	4.70292900	1.83670800	-0.67664700
H	5.64099500	-0.29895400	0.11019300
C	-1.81246900	-0.23331500	0.08149400
C	-2.67228600	-1.20867800	-0.40536600
C	-2.34119100	0.96987200	0.53197300
C	-4.02676100	-0.96667200	-0.48532000
H	-2.25420800	-2.14834200	-0.72821700
C	-3.70061500	1.20008200	0.46555800
H	-1.68722400	1.70963300	0.96676600

C	-4.54762800	0.23890000	-0.05114400
H	-4.68204700	-1.72726300	-0.87931100
H	-4.10044300	2.13391700	0.82823600
H	-5.60901500	0.42127300	-0.10096700

TS1-4n

E(RmPW+HF-B95) = -958.546996 au

C	0.64450400	1.50527000	0.21274300
C	-0.02162200	1.06261500	-0.86163300
O	-0.36476700	1.16055300	-1.96279100
N	-0.94041200	-0.72925600	-0.18523600
C	-0.40270700	-1.83969800	0.10299300
H	-1.02067400	-2.63258200	0.51987700
C	0.62663700	0.83984400	1.44363900
N	0.63902700	0.33923000	2.47782100
C	1.45682500	2.79563000	0.01366900
C	1.01459300	-2.13175200	-0.04064100
C	1.79142400	-1.55685600	-1.03813100
C	1.59211900	-3.03055900	0.84556300
C	3.13276900	-1.86019900	-1.12591300
H	1.33538400	-0.90532400	-1.76506100
C	2.93804900	-3.31705900	0.76728800
H	0.98586400	-3.48641300	1.61276400
C	3.70913300	-2.73025800	-0.21769200
H	3.73033500	-1.42226900	-1.90890600
H	3.38495200	-4.00000700	1.47105400
H	4.76025600	-2.96034000	-0.28671900
C	2.16257100	3.14013600	1.31261600
H	2.73632200	4.05340300	1.18052200
H	1.45535500	3.29882600	2.12148200
H	2.84526600	2.35205300	1.61645300
C	0.52835500	3.93597800	-0.37321800
H	1.09594100	4.85172500	-0.52218400
H	-0.00014700	3.71967800	-1.29806200
H	-0.20899600	4.11734900	0.40376600
C	2.49288500	2.58399800	-1.07921400
H	3.08170700	3.48706100	-1.22211900
H	3.16899100	1.77405300	-0.81964100
H	2.02188800	2.34381700	-2.02920300
C	-2.33474700	-0.59447200	-0.08364400
C	-2.85810700	0.53102500	0.53259500
C	-3.18637100	-1.54997200	-0.61555000
C	-4.22402900	0.67660100	0.64572200
H	-2.18863700	1.27083000	0.94115800
C	-4.55334200	-1.39093700	-0.50768400
H	-2.77453100	-2.39770500	-1.14033100
C	-5.07579600	-0.28159900	0.12677200
H	-4.62620100	1.54601600	1.14018700
H	-5.21068000	-2.13336100	-0.93091800

H	-6.14342400	-0.15745400	0.20842600

TS1-4x
E(RmPW+HF-B95) = -958.528462 au

C	-0.08161200	1.96217700	0.38305500
C	0.26619100	0.92620300	1.17994500
O	0.51924400	0.54720500	2.25024000
N	0.59482300	-0.75833600	0.07682900
C	-0.22440500	-1.66944000	-0.26761100
H	0.16279800	-2.54195000	-0.78771900
C	-0.22944500	3.09894800	1.21546500
N	-0.34974800	4.02446500	1.88586800
C	-0.41735200	2.11901300	-1.10354500
C	-1.65602300	-1.68297300	-0.03304400
C	-2.25687300	-0.99467600	1.01518100
C	-2.43956200	-2.45582700	-0.88231400
C	-3.62263100	-1.05580500	1.18183300
H	-1.65576000	-0.44913600	1.72099300
C	-3.80757900	-2.49901900	-0.72336400
H	-1.97139900	-3.01134900	-1.68063700
C	-4.39996800	-1.79497900	0.30778200
H	-4.08319600	-0.52912300	2.00139300
H	-4.41027700	-3.08692300	-1.39598100
H	-5.46907100	-1.83399100	0.44116600
C	-0.64286800	3.60256600	-1.37521400
H	-0.85475300	3.74098900	-2.43156300
H	-1.48251900	3.99399100	-0.80929800
H	0.23243200	4.19548800	-1.12577900
C	-1.70107100	1.38925200	-1.46706400
H	-2.01599800	1.67513800	-2.46869100
H	-1.57107900	0.31512200	-1.46192600
H	-2.50362600	1.63339400	-0.77695100
C	0.69817800	1.66600200	-2.03187100
H	0.39264200	1.83653500	-3.06181000
H	1.60796000	2.23535100	-1.86338000
H	0.92817600	0.61197500	-1.93220200
C	1.98063900	-1.02316100	0.01276600
C	2.86606300	0.03657700	-0.10979500
C	2.48413600	-2.31103900	0.15025400
C	4.22414100	-0.19424900	-0.16345100
H	2.48833800	1.04288200	-0.15852800
C	3.84347300	-2.53511100	0.09508700
H	1.82145400	-3.13701700	0.35025700
C	4.71901700	-1.48042200	-0.07363400
H	4.89859200	0.64026600	-0.26542600
H	4.21946900	-3.53892100	0.20965400
H	5.78165400	-1.65747000	-0.10714200

ZW-4n
E(RmPW+HF-B95) = -958.558246 au

C	0.37966300	1.40826700	0.28289000
C	-0.19780300	0.66654300	-0.71882600
O	-0.32327500	0.83706300	-1.91399900
N	-0.81079100	-0.63831600	-0.20688200
C	-0.10801400	-1.65993700	0.11525100
H	-0.65591400	-2.47851100	0.56274300
C	0.37730800	0.91260000	1.59304800
N	0.37154600	0.49559000	2.66775800
C	1.04806100	2.73612300	-0.03806100
C	1.31524600	-1.82721600	-0.02418000
C	2.07767100	-1.18309300	-0.99778100
C	1.92178900	-2.72241000	0.85187200
C	3.43014000	-1.42395800	-1.06511500
H	1.60928500	-0.52894300	-1.71379700
C	3.28055800	-2.93659500	0.79374600
H	1.32571200	-3.22870700	1.59456700
C	4.03326200	-2.28664700	-0.16550900
H	4.01947700	-0.93696600	-1.82425200
H	3.75002100	-3.61259700	1.48867500
H	5.09571400	-2.46096100	-0.22161300
C	1.58259400	3.37086600	1.23325900
H	2.05569300	4.32150500	1.00020800
H	0.78733300	3.55786000	1.95033100
H	2.32077700	2.73627600	1.71686700
C	0.04077900	3.68139200	-0.67763300
H	0.51760400	4.62507400	-0.93635200
H	-0.37484100	3.24924500	-1.58170800
H	-0.77526500	3.89458900	0.00862200
C	2.20685700	2.50493600	-0.99851800
H	2.69841200	3.44647700	-1.23637400
H	2.94587600	1.83935300	-0.55858800
H	1.85497700	2.06538100	-1.92673400
C	-2.22962000	-0.68013300	-0.12773300
C	-2.90167800	0.38280300	0.44501500
C	-2.91157900	-1.77575800	-0.62105400
C	-4.27546700	0.32942200	0.54202900
H	-2.34788300	1.22701500	0.82042400
C	-4.28693700	-1.81749800	-0.51700800
H	-2.37403200	-2.56919000	-1.11544300
C	-4.96900100	-0.76791200	0.06594900
H	-4.80647600	1.14990900	0.99567600
H	-4.82488800	-2.66520000	-0.90831600
H	-6.04364300	-0.79979800	0.14108300

ZW-4x
E(RmPW+HF-B95) = -958.543396 au

C	-0.35969000	1.57461400	0.39783400
C	0.25169300	0.55728600	1.08761300
O	0.44699400	0.38276000	2.27678000
N	0.76911800	-0.60016400	0.25367900
C	-0.00892200	-1.51822100	-0.18580900
H	0.46071300	-2.27912500	-0.79480700
C	-0.87939300	2.55301000	1.27600100
N	-1.33601400	3.36657700	1.94839000
C	-0.63189600	1.87303700	-1.07588700
C	-1.43486500	-1.62698300	-0.00886400
C	-2.12979500	-1.12527200	1.09106900
C	-2.12300700	-2.30344300	-1.01370000
C	-3.49632500	-1.27221400	1.14903900
H	-1.60247400	-0.65557500	1.90322200
C	-3.49364500	-2.41853900	-0.96110600
H	-1.57815800	-2.71776300	-1.84817500
C	-4.17956600	-1.89836000	0.12050600
H	-4.03364700	-0.89127500	2.00127200
H	-4.02417700	-2.92066000	-1.75285000
H	-5.25205400	-1.99492400	0.17159200
C	-0.07716100	3.26301500	-1.38069000
H	-0.32011200	3.55434500	-2.40039900
H	-0.49081000	4.01140400	-0.71183100
H	1.00514800	3.27955000	-1.27180800
C	-2.14052900	1.88864200	-1.30548900
H	-2.36821000	2.17601300	-2.33030800
H	-2.57294100	0.90697500	-1.12306600
H	-2.62783500	2.59808000	-0.64257600
C	-0.01924500	0.92406200	-2.09344600
H	-0.16397600	1.35193100	-3.08202100
H	1.04950800	0.78452900	-1.96018700
H	-0.50507100	-0.04641500	-2.10832700
C	2.18062200	-0.70250100	0.12968600
C	2.92025500	0.45214000	-0.05055300
C	2.79913500	-1.93647300	0.20541100
C	4.28753600	0.35800100	-0.19822100
H	2.42259100	1.40861500	-0.07153600
C	4.16714700	-2.01856700	0.05083100
H	2.22585600	-2.82144500	0.42960300
C	4.91204300	-0.87447000	-0.15800800
H	4.86700800	1.25479300	-0.34229900
H	4.65272700	-2.97809300	0.11770800
H	5.98187500	-0.94052400	-0.26923900

TS2-4n

E(RmPW+HF-B95) = -958.531611 au

C	-0.16683200	-0.86990000	0.73371900
N	-0.98141800	-0.26595200	-0.14468300
C	-0.19235700	0.73776300	-0.80769900

O	-0.19361900	0.91445300	-1.99768100
C	0.62386200	1.32402500	0.21544500
C	-0.01202200	1.64159300	1.43750500
N	-0.49795900	1.95148900	2.43385000
H	-0.56458600	-1.04928400	1.72611800
C	-2.37582100	-0.35289500	-0.12898800
C	-2.97824600	-1.50354500	0.35149200
C	-3.14469000	0.70937700	-0.57730900
C	-4.35501400	-1.57498500	0.41726300
H	-2.37266400	-2.34682700	0.64476400
C	-4.51716400	0.61535500	-0.52784400
H	-2.66585600	1.59623500	-0.95803700
C	-5.12759300	-0.51961000	-0.02320900
H	-4.82258400	-2.46919000	0.79600400
H	-5.11599200	1.44095300	-0.87617000
H	-6.20265800	-0.58232100	0.01689400
C	1.03294300	-1.56896600	0.34889800
C	1.94852100	-1.93233100	1.33292300
C	1.27754600	-1.90895600	-0.98087500
C	3.11571000	-2.57304300	0.98659100
H	1.75062900	-1.68163200	2.36355500
C	2.44299600	-2.56120300	-1.31591200
H	0.55461600	-1.65783500	-1.74002300
C	3.36879000	-2.88192600	-0.33933200
H	3.83058200	-2.83653300	1.74886100
H	2.63040100	-2.82354200	-2.34429000
H	4.28160600	-3.38807600	-0.60871900
C	1.88795000	2.07901100	-0.12711900
C	2.64438000	2.43098200	1.14362000
H	2.08226700	3.11252300	1.77490200
H	2.86858600	1.53963000	1.72549400
H	3.58570800	2.90921000	0.88665400
C	1.52872400	3.36009800	-0.87419700
H	1.01390900	3.13597500	-1.80189300
H	0.88981300	3.99760300	-0.26814800
H	2.43416000	3.91675800	-1.10773400
C	2.77915300	1.20144600	-0.99512600
H	3.65661100	1.76532200	-1.30252200
H	3.12054600	0.32594000	-0.44770900
H	2.26446900	0.86696500	-1.88981000

TS2-4x

E(RmPW+HF-B95) = -958.518700 au

C	-0.10294400	-0.73520700	-0.64600300
N	0.81169300	-0.28149800	0.21587500
C	0.22925000	0.65260900	1.12906400
O	0.45253700	0.62680100	2.31491400
C	-0.72178500	1.43032000	0.39267600
C	-1.85089000	1.79640100	1.15193400

N	-2.82491000	2.02658800	1.71925000
H	0.26240100	-0.92475400	-1.65023600
C	-1.37491000	-1.32935700	-0.33291100
C	-2.16467900	-1.75160700	-1.40014100
C	-1.80072800	-1.58583800	0.97370800
C	-3.36265300	-2.39363800	-1.17363600
H	-1.83438700	-1.56854100	-2.41142200
C	-2.98920600	-2.23684400	1.18911000
H	-1.19580600	-1.27886200	1.81158400
C	-3.77776500	-2.63736000	0.12014400
H	-3.96922900	-2.70794000	-2.00711100
H	-3.30979100	-2.43416700	2.19867900
H	-4.71242700	-3.14266800	0.30124000
C	-0.47410300	2.29156400	-0.84483700
C	-0.48081500	3.75278600	-0.38782300
H	-0.32445600	4.41075300	-1.23954900
H	-1.42712900	4.01980700	0.07266500
H	0.30877600	3.93797600	0.33539600
C	0.86244000	2.04903900	-1.52083200
H	1.69048600	2.11784200	-0.82096200
H	0.92564500	1.09163600	-2.02808400
H	1.01141400	2.81322300	-2.27845800
C	-1.59681400	2.09501800	-1.85271800
H	-1.49379400	2.79508300	-2.67846200
H	-1.58204100	1.08513200	-2.25601300
H	-2.57041200	2.25633600	-1.39740200
C	2.17110500	-0.60806000	0.13997400
C	3.11826000	0.23949600	0.69594600
C	2.56306000	-1.77104000	-0.50218500
C	4.45355900	-0.07274300	0.58052000
H	2.80307100	1.12393700	1.22362500
C	3.90673000	-2.06004900	-0.63163800
H	1.82142700	-2.46475500	-0.86463100
C	4.85421200	-1.21384800	-0.09314300
H	5.18923800	0.58332900	1.01618500
H	4.20910200	-2.96428400	-1.13409900
H	5.90219700	-1.44895900	-0.18138800

trans-**13a**
E(RmPW+HF-B95) = -958.604871 au

C	-0.27997700	0.06385100	0.74579100
N	0.73990500	-0.72552100	0.07466300
C	-0.05536400	-1.79128900	-0.19102600
O	0.14948100	-2.85511100	-0.68535400
C	-1.29927000	-1.08690900	0.37840600
C	-1.76454500	-1.71932900	1.59764300
N	-2.12348800	-2.18926500	2.57596000
H	-0.12027300	0.06145200	1.82309900
C	2.12701100	-0.57660200	0.06985500

C	2.70002100	0.49086400	0.74243500
C	2.92612400	-1.49473700	-0.59637000
C	4.07216100	0.63716900	0.74717100
H	2.07730400	1.20512600	1.25640000
C	4.29555200	-1.33438900	-0.57810200
H	2.47213800	-2.32448100	-1.10885800
C	4.87599000	-0.27153800	0.08838200
H	4.51177800	1.46986000	1.27215000
H	4.91442200	-2.05175700	-1.09271700
H	5.94728300	-0.15404300	0.09481900
C	-0.44760100	1.48200700	0.30061300
C	-1.16130300	2.35017500	1.11201000
C	0.14529800	1.97034000	-0.85086400
C	-1.31681300	3.67421800	0.75781400
H	-1.60330900	1.98322000	2.02657000
C	-0.00111400	3.29858400	-1.20153100
H	0.72661600	1.31047800	-1.47548700
C	-0.73747200	4.15138200	-0.40304200
H	-1.88223400	4.33639900	1.39343600
H	0.46714300	3.66716000	-2.09993000
H	-0.85029400	5.18772100	-0.67793400
C	-2.46098900	-0.93752200	-0.63386600
C	-3.51030200	0.02661000	-0.11261800
H	-3.86595000	-0.26756600	0.87216400
H	-3.13744200	1.04342400	-0.05682000
H	-4.36596500	0.02448600	-0.78279500
C	-3.08647300	-2.31635900	-0.80643300
H	-2.34797000	-3.04991100	-1.11460100
H	-3.55250300	-2.66443200	0.11085100
H	-3.85641800	-2.26759200	-1.57137100
C	-1.94564000	-0.47751200	-1.98587400
H	-2.77310000	-0.45641000	-2.68958200
H	-1.52397100	0.51893000	-1.95055800
H	-1.19978100	-1.16175600	-2.38273200

cis-**14a**
E(RmPW+HF-B95) = -958.611046 au

C	-0.37342300	0.13474800	0.51343000
N	0.64828700	-0.66504000	-0.14250200
C	-0.20708300	-1.45265600	-0.83928500
O	-0.05341500	-2.36835800	-1.58580700
C	-1.42965100	-0.74973900	-0.22926100
C	-2.22242800	-0.02614600	-1.19786000
N	-2.85990000	0.53477000	-1.96265100
H	-0.39822700	-0.04078800	1.58618200
C	2.03143200	-0.66837700	0.01862400
C	2.61437900	0.23771900	0.88968500
C	2.81727600	-1.57156200	-0.68345900
C	3.98378800	0.23566300	1.06025100

H	2.00100300	0.94555100	1.42289900
C	4.18376300	-1.55922800	-0.49992600
H	2.35447500	-2.26973700	-1.35845500
C	4.77438300	-0.66020000	0.36845400
H	4.43232600	0.94379700	1.73822700
H	4.79261700	-2.26275600	-1.04471700
H	5.84363700	-0.65780800	0.50339400
C	-0.35446100	1.60194300	0.23436700
C	-0.97156300	2.46665300	1.12228900
C	0.23967400	2.11022100	-0.90753300
C	-1.00506200	3.82278000	0.86792300
H	-1.42989600	2.07745600	2.01932000
C	0.21264400	3.46723600	-1.15838600
H	0.73085300	1.44400800	-1.59948600
C	-0.41127600	4.32537200	-0.27351200
H	-1.49108900	4.48751100	1.56380700
H	0.68081200	3.85491200	-2.04864500
H	-0.43252800	5.38483200	-0.47215600
C	-2.30453400	-1.67486900	0.64520600
C	-3.13177400	-2.56503200	-0.26827800
H	-3.83175400	-1.98578700	-0.86359100
H	-2.49465500	-3.12755200	-0.94419900
H	-3.70427700	-3.27079400	0.32712100
C	-3.21700500	-0.82660600	1.51201200
H	-2.65503100	-0.21791000	2.21686300
H	-3.83546700	-0.16471000	0.91112100
H	-3.87874200	-1.46608700	2.08945200
C	-1.42136300	-2.55431100	1.51523100
H	-2.04791500	-3.17956800	2.14432300
H	-0.79998300	-3.21375800	0.91520200
H	-0.77384400	-1.98371400	2.17603500

15a

E(RmPW+HF-B95) = -244.785686 au

C	-0.03000500	0.73680700	0.00000000
C	1.11345600	0.08442700	0.00000000
O	2.11290000	-0.45814100	0.00000000
C	-1.25672100	0.05373600	0.00000000
N	-2.26733200	-0.48539200	0.00000000
H	0.00774200	1.81305000	0.00000000

TS1-5an

E(RmPW+HF-B95) = -801.358362 au

C	-0.00470200	1.83299300	1.60903200
C	-0.19716800	2.05125500	0.30252300
O	-0.30962200	2.74370400	-0.61639500
N	-0.44734100	0.09321000	-0.38579400
C	0.41967100	-0.81489300	-0.55377700

H	0.08129900	-1.83516500	-0.72443600
C	0.04160500	0.59458100	2.25279600
N	0.08761400	-0.40302900	2.81897800
C	1.85815000	-0.61740400	-0.52051100
C	2.45284900	0.61711300	-0.75438800
C	2.65652400	-1.72249800	-0.25706600
C	3.82311800	0.74064000	-0.69944800
H	1.84608900	1.46700500	-1.01723700
C	4.02699300	-1.59210600	-0.18769200
H	2.19691800	-2.68403000	-0.08816900
C	4.61047400	-0.35936600	-0.40704200
H	4.28177400	1.69695500	-0.89101800
H	4.63931300	-2.45102900	0.03281300
H	5.68265600	-0.25560700	-0.36114600
C	-1.81296300	-0.24661400	-0.39131300
C	-2.28833700	-1.29212800	0.38433700
C	-2.68813900	0.51334700	-1.15041900
C	-3.63575600	-1.59198600	0.37414200
H	-1.60714400	-1.83140600	1.02306500
C	-4.03105500	0.19956200	-1.15949200
H	-2.30620000	1.33141200	-1.73830900
C	-4.50829100	-0.85308300	-0.40028800
H	-4.00468200	-2.39958000	0.98565300
H	-4.70904400	0.78294600	-1.76140800
H	-5.56016500	-1.08884700	-0.40423800
H	0.11642500	2.72997700	2.19493900

TS1-5ax
E(RmPW+HF-B95) = -801.356006 au

C	-0.38727000	2.08989300	-0.53313500
C	0.11330600	1.63057500	0.62500800
O	0.43102700	1.74052400	1.73210100
N	0.55641900	-0.27382600	0.06619100
C	-0.24902200	-1.21229200	-0.22151800
H	0.15799500	-2.13784500	-0.62331400
C	-0.82114000	3.42394700	-0.59332100
N	-1.18179900	4.51145100	-0.66578700
C	-1.69431500	-1.16630600	-0.09062900
C	-2.34785300	-0.35335300	0.82844100
C	-2.43712800	-2.01319400	-0.90446400
C	-3.72264300	-0.37084700	0.90368600
H	-1.78065200	0.26156500	1.50675000
C	-3.81369000	-2.01517400	-0.83877500
H	-1.92958500	-2.66371800	-1.60035300
C	-4.45653200	-1.19125700	0.06457000
H	-4.22537100	0.25461000	1.62277700
H	-4.38360900	-2.66320700	-1.48406800
H	-5.53282100	-1.19621000	0.12635800
C	1.94172400	-0.50928300	-0.00399300

C	2.49126700	-1.68564000	0.48234500
C	2.76457300	0.46699100	-0.54325300
C	3.85220700	-1.89609100	0.39627500
H	1.85680600	-2.41583600	0.95933800
C	4.12216700	0.24501800	-0.63199600
H	2.33174500	1.38549700	-0.90531300
C	4.66990600	-0.93595700	-0.16654500
H	4.27495000	-2.80903900	0.78348000
H	4.75635100	1.00214600	-1.06364700
H	5.73320500	-1.10067700	-0.22948300
H	-0.48292100	1.45297500	-1.38834400

ZW-5an
E(RmPW+HF-B95) = -801.366762 au

C	-0.23107900	2.28349200	0.21307700
C	0.19019400	1.27146400	1.03722400
O	0.36226700	1.17608500	2.22786400
N	0.52338100	-0.00239000	0.24110400
C	-0.36848200	-0.77664500	-0.25507300
H	0.00693900	-1.57120800	-0.88638300
C	-0.37702700	2.13087600	-1.16686000
N	-0.49646400	1.99026400	-2.30389300
C	-1.79639600	-0.70080400	-0.08678000
C	-2.41413500	-0.15402500	1.03694200
C	-2.56948800	-1.26735900	-1.09598700
C	-3.78660800	-0.16069000	1.12400700
H	-1.82495500	0.23807200	1.84823200
C	-3.94328400	-1.24465200	-1.01270600
H	-2.08727600	-1.70454500	-1.95603300
C	-4.55036600	-0.69163500	0.09857000
H	-4.26579800	0.24949600	1.99729500
H	-4.53844200	-1.66378500	-1.80666200
H	-5.62582500	-0.68399500	0.17351300
C	1.90380000	-0.30920800	0.09570300
C	2.78087300	0.68427700	-0.29626900
C	2.34338300	-1.59470900	0.34538600
C	4.11295500	0.36955400	-0.46205000
H	2.41593800	1.68063200	-0.48264000
C	3.67896200	-1.89671400	0.17546700
H	1.65301300	-2.34072700	0.70539800
C	4.56306500	-0.91702400	-0.23099600
H	4.80204200	1.13547200	-0.77741400
H	4.02919900	-2.89561300	0.37693400
H	5.60686700	-1.15295900	-0.35866300
H	-0.47646800	3.22817000	0.66510400

ZW-5ax
E(RmPW+HF-B95) = -801.363738 au

C	-0.24854200	1.97627000	-0.63565400
C	0.16128700	1.26763600	0.46033300
O	0.28466500	1.48790900	1.63993800
N	0.55862500	-0.16196300	0.03726100
C	-0.29905900	-1.08099100	-0.21185900
H	0.11413800	-2.01368100	-0.57371400
C	-0.65887400	3.30906300	-0.51151000
N	-1.00412400	4.40295100	-0.43444900
C	-1.73326700	-1.02778500	-0.09031400
C	-2.42151600	-0.16627600	0.76359700
C	-2.44201400	-1.95365300	-0.85314900
C	-3.79426800	-0.22253500	0.81854900
H	-1.88778400	0.51361500	1.40406900
C	-3.81729600	-1.98547300	-0.81059900
H	-1.90756400	-2.63808700	-1.49363600
C	-4.49283000	-1.11736600	0.02561700
H	-4.32469100	0.43700800	1.48476000
H	-4.36003400	-2.69056400	-1.41772900
H	-5.56952100	-1.14520500	0.07146900
C	1.95235600	-0.44133200	0.00387800
C	2.80967800	0.48696900	-0.55706400
C	2.43136900	-1.62552200	0.53238000
C	4.15736900	0.20348500	-0.61570400
H	2.41714800	1.41205300	-0.94546100
C	3.78217200	-1.89801200	0.46624800
H	1.76004300	-2.30759600	1.02899100
C	4.64512800	-0.98782200	-0.11195400
H	4.82987200	0.91995500	-1.05762100
H	4.16067900	-2.81532900	0.88618100
H	5.70078500	-1.19993700	-0.15640600
H	-0.28205700	1.51763600	-1.60685100

TS2-5an

E(RmPW+HF-B95) = -801.333799 au

C	-0.49619300	0.05913600	-0.64440100
N	0.50113700	0.17498400	0.25733500
C	0.15723200	1.27380500	1.11176600
O	0.32214400	1.29334000	2.29846600
C	-0.49260600	2.21638400	0.25046800
C	0.09661800	2.59583900	-0.97092800
N	0.55161000	2.93759500	-1.97051400
H	-0.20094600	-0.02757900	-1.68422600
C	1.77081900	-0.38862400	0.10309200
C	1.91167300	-1.55025800	-0.63796300
C	2.87861100	0.21670500	0.67671900
C	3.16920200	-2.08238800	-0.84017100
H	1.03967700	-2.04981100	-1.02993100
C	4.12370000	-0.33877000	0.48652500
H	2.76003000	1.11011000	1.26644100

C	4.27729600	-1.48135800	-0.27898000
H	3.27629100	-2.98296400	-1.42255300
H	4.98453800	0.13196900	0.93259100
H	5.25673200	-1.90580600	-0.42662000
C	-1.83492000	-0.34649900	-0.30353200
C	-2.79101500	-0.41190800	-1.31321700
C	-2.17376600	-0.73273400	0.99335700
C	-4.07363700	-0.82215300	-1.02612700
H	-2.52451400	-0.12591400	-2.31887000
C	-3.45563200	-1.14357700	1.27037200
H	-1.42810800	-0.71344400	1.77186200
C	-4.40901400	-1.18354800	0.26548000
H	-4.81254000	-0.86352400	-1.80937700
H	-3.71508900	-1.44468700	2.27203500
H	-5.41172300	-1.50978700	0.48939100
H	-1.12093700	2.96636200	0.70902100

TS2-5ax

E(RmPW+HF-B95) = -801.337808 au

C	-0.26962200	-0.42635500	-0.76993800
N	0.67623100	0.17122900	-0.02451800
C	0.15732000	1.45610700	0.37270100
O	0.30775900	1.94386300	1.45771500
C	-0.58309000	1.87294100	-0.77033900
C	-1.55487700	2.88255600	-0.68755200
N	-2.38990900	3.66930500	-0.63431000
H	0.06750800	-0.89198700	-1.69098400
C	-1.55855800	-0.83658200	-0.27296400
C	-2.45243900	-1.43700900	-1.15428000
C	-1.90231800	-0.70790200	1.07293200
C	-3.68038800	-1.87277900	-0.70813300
H	-2.18354900	-1.54863800	-2.19341200
C	-3.12863300	-1.14728600	1.51017900
H	-1.20568300	-0.26753100	1.76788700
C	-4.02246900	-1.72458000	0.62270500
H	-4.37121200	-2.32952900	-1.39762800
H	-3.39079800	-1.04642300	2.55047900
H	-4.98236300	-2.06728100	0.97342300
C	2.02296200	-0.20327900	-0.00841400
C	3.00544000	0.74138900	0.24920200
C	2.36718800	-1.52253100	-0.25420100
C	4.32781800	0.35941000	0.23722700
H	2.73014500	1.75999900	0.46464800
C	3.69855300	-1.88648400	-0.28482200
H	1.59634200	-2.26525500	-0.38786600
C	4.68182700	-0.94976100	-0.03909700
H	5.09043900	1.09341700	0.44036200
H	3.96300400	-2.91308600	-0.47936100
H	5.71983100	-1.23907400	-0.04819600

H	-0.15227600	1.69362400	-1.74051300

trans-**16a**
E(RmPW+HF-B95) = -801.417569 au

C	-0.75307400	0.68944200	-0.49138800
N	0.58934600	0.78374900	0.06340600
C	0.39899600	1.96441000	0.70526100
O	1.10475000	2.67577600	1.34357300
C	-1.07629900	1.99693600	0.28294200
C	-1.50227700	3.13073400	-0.49380200
N	-1.83751100	4.02153300	-1.12526900
H	-0.75737300	0.84093400	-1.56778300
C	1.70245900	-0.03265100	-0.12266700
C	1.59633700	-1.14742100	-0.93844700
C	2.90328800	0.26627400	0.50476500
C	2.69496100	-1.96071000	-1.12720100
H	0.65827500	-1.37950300	-1.41632100
C	3.99035800	-0.55779200	0.30434900
H	2.97679500	1.13601000	1.13330500
C	3.89474400	-1.67220000	-0.50798500
H	2.60706100	-2.82699900	-1.76279800
H	4.92338800	-0.32272900	0.79077000
H	4.75024300	-2.31044100	-0.65703400
C	-1.54983400	-0.51656000	-0.11544400
C	-2.62244600	-0.89745900	-0.90379100
C	-1.25113700	-1.24206500	1.02537600
C	-3.39733700	-1.98345100	-0.54870100
H	-2.85241500	-0.34152500	-1.80045100
C	-2.02232200	-2.33212400	1.37599900
H	-0.40477500	-0.96505200	1.63466900
C	-3.09780400	-2.70298500	0.59212500
H	-4.23157200	-2.27164300	-1.16777500
H	-1.77869300	-2.89656600	2.26156900
H	-3.69805800	-3.55558100	0.86608800
H	-1.74539600	1.83565100	1.12186500

cis-**17a**
E(RmPW+HF-B95) = -801.415918 au

C	-0.57812300	0.55614900	-1.02105300
N	0.68342500	0.85419700	-0.35923400
C	0.40751400	2.15527600	-0.09041500
O	1.01183800	3.02982100	0.44078300
C	-0.96174500	2.04534700	-0.77512300
C	-2.11391600	2.31859500	0.04288700
N	-3.02515600	2.54500100	0.69289900
H	-0.44509000	0.35506600	-2.08108700
C	1.81349600	0.06078600	-0.17782900
C	1.80995700	-1.24100800	-0.65185600

C	2.93086700	0.56863800	0.46942400
C	2.92737200	-2.03233800	-0.47961200
H	0.93616900	-1.63570500	-1.14435000
C	4.03841300	-0.23674700	0.63178400
H	2.92377200	1.58035500	0.83492400
C	4.04490700	-1.53651900	0.16144000
H	2.91845500	-3.04514500	-0.84887700
H	4.90600800	0.15992300	1.13412000
H	4.91504800	-2.15812700	0.29528800
C	-1.41984000	-0.50112600	-0.38619900
C	-2.29853600	-1.23501200	-1.16388900
C	-1.35095600	-0.74100200	0.97561200
C	-3.10723600	-2.19352600	-0.58642700
H	-2.35051500	-1.05688400	-2.22771500
C	-2.15574300	-1.70195700	1.55180000
H	-0.65766400	-0.18260800	1.58538600
C	-3.03594900	-2.42855600	0.77271400
H	-3.78935200	-2.76011600	-1.19957100
H	-2.09412500	-1.88511100	2.61224400
H	-3.66349200	-3.17982700	1.22448000
H	-1.00469800	2.63322500	-1.68630100

15b

E(RmPW+HF-B95) = -191.856479 au

C	0.46116500	0.55997000	-0.00004300
C	-0.76372400	0.12146300	0.00001200
O	-1.84963000	-0.26634900	0.00000400
H	0.55871800	1.63313800	0.00011300
C	1.67397600	-0.32645500	0.00001800
H	1.72207600	-0.96397900	-0.87755200
H	2.56306600	0.29212700	-0.00259500
H	1.72467900	-0.96035900	0.88007600

TS1-5bn

E(RmPW+HF-B95) = -748.414766 au

C	-0.15817100	2.05867000	1.17441900
C	-0.17740100	1.63600200	-0.09891000
O	-0.04131800	2.13586400	-1.21572400
N	-0.44228900	0.08851900	-0.18867600
C	0.47444300	-0.79014500	-0.31363700
H	0.13619700	-1.81198900	-0.43578200
C	1.90520300	-0.60268200	-0.27520100
C	2.55567600	0.60439300	-0.52798700
C	2.65528800	-1.74015800	0.01841700
C	3.92954500	0.65993700	-0.44697400
H	1.99384100	1.46807800	-0.83706400
C	4.02643600	-1.66927400	0.11516600
H	2.15332600	-2.68077800	0.18707600

C	4.66354900	-0.46426100	-0.11442100
H	4.43306400	1.59032900	-0.65181700
H	4.59673800	-2.55038200	0.35882100
H	5.73821900	-0.40442700	-0.04955200
C	-1.81275300	-0.27745900	-0.19973800
C	-2.25553400	-1.36865100	0.52414700
C	-2.69517500	0.50243500	-0.92592400
C	-3.59588400	-1.69904900	0.49796300
H	-1.56596700	-1.93322100	1.13172000
C	-4.02997700	0.16008900	-0.94485500
H	-2.31480500	1.35055800	-1.47083900
C	-4.48291200	-0.93971600	-0.23864400
H	-3.94705000	-2.54287400	1.06917300
H	-4.72125500	0.75864200	-1.51527600
H	-5.52947200	-1.19719500	-0.25364500
H	-0.00988100	3.12288700	1.28177100
C	-0.37715500	1.26043000	2.41349000
H	0.28746300	1.59301300	3.20777800
H	-1.39340400	1.34754700	2.80228800
H	-0.18151800	0.19990800	2.27800600

TS1-5bx

E(RmPW+HF-B95) = -748.414454 au

C	-0.19940200	2.21454200	-0.68533200
C	0.11480400	1.65464300	0.48247600
O	0.24133700	1.79875800	1.65685800
N	0.51590800	-0.08897400	0.04157100
C	-0.34045300	-0.99777100	-0.19323800
H	0.02940300	-1.96321300	-0.52947800
C	-1.78369000	-0.88830400	-0.08565800
C	-2.42626900	-0.00134600	0.77212000
C	-2.53832800	-1.76670400	-0.85437500
C	-3.80224800	0.01609100	0.82754600
H	-1.85015200	0.64272400	1.41414500
C	-3.91550100	-1.73010700	-0.81064000
H	-2.03891900	-2.47315400	-1.49989000
C	-4.54766300	-0.83578200	0.03065200
H	-4.29787100	0.69703400	1.49997100
H	-4.49317400	-2.40329200	-1.42255400
H	-5.62458700	-0.80982000	0.07776400
C	1.88939200	-0.40366100	0.00740500
C	2.36203500	-1.57907900	0.56919400
C	2.77074200	0.48875800	-0.58001800
C	3.70862000	-1.87552100	0.51069000
H	1.68128100	-2.23857400	1.08379500
C	4.11307900	0.18063000	-0.63924200
H	2.38881700	1.40856800	-0.99036100
C	4.58621000	-1.00112800	-0.09956100
H	4.07266100	-2.78649400	0.95764600

H	4.79545900	0.87161700	-1.10719200
H	5.63820600	-1.23250200	-0.14137200
H	-0.19917800	1.61352200	-1.57571200
C	-0.58667700	3.65474100	-0.75299500
H	-0.51706000	4.12161900	0.22428500
H	0.05527000	4.21921500	-1.42775000
H	-1.61011400	3.78549100	-1.10329300

ZW-5bn
E(RmPW+HF-B95) = -748.417147 au

C	0.19653300	2.30089600	0.41560600
C	-0.14179200	1.53956000	-0.64143500
O	-0.23908000	1.65954500	-1.85323300
N	-0.50643000	0.06786800	-0.16783300
C	0.38235100	-0.80456400	0.11170800
H	0.02192200	-1.75108300	0.49668600
C	1.81707000	-0.66743900	0.01057600
C	2.45850800	0.18641800	-0.88442600
C	2.57114600	-1.49686400	0.83552400
C	3.83454400	0.21811000	-0.91679900
H	1.88172300	0.78498800	-1.56913400
C	3.94716700	-1.44077200	0.81286900
H	2.07102800	-2.17752200	1.50741600
C	4.57812100	-0.58019600	-0.06429300
H	4.33237000	0.87021400	-1.61537900
H	4.52469700	-2.07215000	1.46760900
H	5.65516500	-0.53980500	-0.09598700
C	-1.88205000	-0.26278000	-0.10495900
C	-2.76719500	0.66595600	0.41185000
C	-2.32849200	-1.49626700	-0.54486800
C	-4.10141800	0.33543700	0.52092500
H	-2.39968300	1.63128000	0.71936900
C	-3.66589700	-1.81514100	-0.43170100
H	-1.64130300	-2.18485600	-1.00999400
C	-4.55284900	-0.90396500	0.10773100
H	-4.79304600	1.05348700	0.93028400
H	-4.01642400	-2.77169100	-0.78348200
H	-5.59812100	-1.15342700	0.19098700
C	0.31094500	1.87631500	1.84125700
H	1.29539700	1.47344200	2.09457000
H	0.14516300	2.72111600	2.50423900
H	-0.42034600	1.11915500	2.12211000
H	0.45896300	3.31719700	0.16401300

ZW-5bx
E(RmPW+HF-B95) = -748.414436 au

C	-0.17969500	2.13338300	-0.72577400
C	0.14891700	1.44172700	0.38179300

O	0.23168100	1.66017800	1.58546800
N	0.52134400	-0.02470800	0.00549200
C	-0.36019600	-0.92007400	-0.23090600
H	0.01600700	-1.87719500	-0.57123000
C	-1.79576900	-0.81311200	-0.10697200
C	-2.43965900	0.07440400	0.75427800
C	-2.54564300	-1.71810500	-0.85159600
C	-3.81311800	0.05994100	0.83331900
H	-1.86320000	0.74017800	1.37515100
C	-3.92193400	-1.70794300	-0.78449900
H	-2.04395800	-2.42224700	-1.49761000
C	-4.55521700	-0.81694500	0.05890900
H	-4.31143900	0.73791200	1.50652900
H	-4.49669800	-2.39934400	-1.37824600
H	-5.63137400	-0.81203600	0.12583200
C	1.90059300	-0.35822500	0.00296800
C	2.80528400	0.53056000	-0.54744700
C	2.32780300	-1.55608700	0.54739800
C	4.14204300	0.19605800	-0.57964500
H	2.44596400	1.46478100	-0.94581600
C	3.66823800	-1.88125300	0.50788700
H	1.62252100	-2.20863800	1.03674600
C	4.57618000	-1.00958000	-0.06020000
H	4.84972600	0.88315100	-1.01399400
H	4.00337600	-2.80982500	0.94032500
H	5.62366000	-1.26257500	-0.08498900
H	-0.19234600	1.62697500	-1.67713600
C	-0.55249500	3.57110100	-0.64662200
H	0.04455200	4.19297400	-1.31281500
H	-1.59755700	3.74573800	-0.90693600
H	-0.40409000	3.93658700	0.36464500

TS2-5bn

E(RmPW+HF-B95) = -748.404686 au

C	0.47683200	-0.29836700	0.63196000
N	-0.46078600	0.11211900	-0.22515400
C	-0.04499500	1.49861100	-0.53346200
O	0.19678300	1.84988900	-1.66674300
C	0.15172600	2.16223900	0.68329500
H	0.15444900	-0.75774000	1.56079400
C	1.85842400	-0.43496600	0.25869200
C	2.81015900	-0.70979000	1.23964700
C	2.25341600	-0.35980100	-1.07767200
C	4.13302100	-0.86802400	0.89814300
H	2.50428300	-0.78312800	2.27216100
C	3.58118200	-0.51554400	-1.40838000
H	1.51390800	-0.18516100	-1.84034000
C	4.52278900	-0.76472200	-0.42660600
H	4.86447500	-1.07478000	1.66250400

H	3.88261900	-0.45489000	-2.44150900
H	5.55929700	-0.89337500	-0.69399800
C	-1.78650900	-0.31214300	-0.19506900
C	-2.79988700	0.54673100	-0.59798900
C	-2.09651100	-1.59411400	0.23288100
C	-4.10927500	0.12412400	-0.55535500
H	-2.55150500	1.53697000	-0.94400700
C	-3.41603700	-1.99732800	0.29082900
H	-1.30709200	-2.28418300	0.48567500
C	-4.42730400	-1.14390200	-0.10110000
H	-4.89069000	0.79599400	-0.87205800
H	-3.64901400	-2.99495300	0.62698200
H	-5.45504200	-1.46607500	-0.06495900
H	0.59860000	3.14256300	0.56354000
C	-0.62065400	1.99004900	1.94635500
H	0.02830900	2.02589100	2.81902400
H	-1.33435000	2.80640600	2.06607200
H	-1.18528600	1.06419400	1.99311700

TS2-5bx
E(RmPW+HF-B95) = -748.393000 au

C	-0.37111200	-0.46023300	-0.72702300
N	0.59670100	0.14481900	-0.04537300
C	0.13958600	1.49101400	0.26948500
O	0.20735000	1.96588700	1.38682200
C	-0.41974200	1.98841700	-0.90987000
H	-0.06559300	-1.05982200	-1.57914500
C	1.92929800	-0.26808000	0.00247300
C	2.25540400	-1.60121800	-0.18781200
C	2.92689600	0.66540100	0.24521500
C	3.58090200	-1.98896400	-0.17917100
H	1.47500800	-2.33558600	-0.30949500
C	4.24187800	0.26162300	0.27279300
H	2.66210300	1.69470200	0.42017800
C	4.57782600	-1.06279600	0.05038600
H	3.82959000	-3.02682600	-0.33147900
H	5.01367900	0.98930900	0.46488200
H	5.61032200	-1.37113400	0.07060200
C	-1.72334300	-0.64610000	-0.25782800
C	-2.66191500	-1.17947800	-1.13617200
C	-2.09475900	-0.39304100	1.06399300
C	-3.95175500	-1.42366800	-0.71892700
H	-2.37566500	-1.39072800	-2.15523300
C	-3.38438500	-0.64235800	1.47207100
H	-1.36927200	-0.00276300	1.75891200
C	-4.31862300	-1.15262400	0.58571600
H	-4.67141700	-1.83032100	-1.41103400
H	-3.66383000	-0.44674500	2.49476400
H	-5.32577100	-1.34857600	0.91650200

H	-0.06928700	1.57527900	-1.84129300
C	-1.17974500	3.25366600	-0.92460500
H	-0.63096100	4.06541400	-1.40282200
H	-2.10838700	3.13779900	-1.48297700
H	-1.42469600	3.55981200	0.08632300

trans-**16b**
E(RmPW+HF-B95) = -748.498093 au

C	-0.68995900	0.90207400	-0.62483500
N	0.64492500	0.84535800	-0.04498600
C	0.59647400	2.09788800	0.49460200
O	1.40266300	2.74624900	1.09233400
C	-0.82470700	2.30933100	0.00940400
H	-0.65619900	0.94317400	-1.71265700
C	1.62549100	-0.13318800	-0.13087400
C	1.37545000	-1.27827700	-0.87128100
C	2.84338200	0.02389100	0.51830700
C	2.33952000	-2.26117000	-0.96158400
H	0.42597000	-1.40013400	-1.36720600
C	3.79558000	-0.96850900	0.41654900
H	3.03024500	0.91743000	1.08776500
C	3.55288800	-2.11372400	-0.31908700
H	2.13599500	-3.14945800	-1.53802800
H	4.74004800	-0.84215700	0.92164900
H	4.30369600	-2.88385000	-0.38951600
C	-1.64478200	-0.15353900	-0.16925600
C	-2.66155400	-0.58218600	-1.00552500
C	-1.53992600	-0.70049400	1.09943700
C	-3.56800400	-1.53317700	-0.57781700
H	-2.74189800	-0.17178700	-2.00137300
C	-2.44138800	-1.65360700	1.52618700
H	-0.73865200	-0.38796000	1.75119400
C	-3.45919600	-2.07166300	0.68921700
H	-4.35490000	-1.85941300	-1.23913200
H	-2.34578500	-2.07697800	2.51327300
H	-4.16107000	-2.81980600	1.02127500
H	-1.52849600	2.30648900	0.83755000
C	-1.05196400	3.48035100	-0.90790000
H	-2.05971400	3.46894200	-1.31193400
H	-0.91649500	4.41346400	-0.37068400
H	-0.35235100	3.47054000	-1.73919800

cis-**17b**
E(RmPW+HF-B95) = -748.498349 au

C	-0.62796000	0.73633700	-0.91922000
N	0.66485900	0.86631000	-0.26823400
C	0.50989800	2.18471900	0.05334200
O	1.22206700	2.96141100	0.61619700

C	-0.86601700	2.23697000	-0.57934200
H	-0.52732900	0.56595300	-1.98977900
C	1.72669600	-0.02310100	-0.17754000
C	1.60814500	-1.28701200	-0.73575900
C	2.90108400	0.34761600	0.46480400
C	2.66350000	-2.17231900	-0.65579600
H	0.69107100	-1.57460000	-1.22467800
C	3.94496200	-0.54992200	0.53542100
H	2.98154100	1.33084400	0.89404600
C	3.83570700	-1.81104000	-0.02135700
H	2.56383900	-3.15337600	-1.09219700
H	4.85600900	-0.25713000	1.03268500
H	4.65739500	-2.50591900	0.03995400
C	-1.57297300	-0.25971000	-0.32887100
C	-2.69279600	-0.63345700	-1.05399600
C	-1.38217900	-0.78910800	0.93600500
C	-3.61396100	-1.51247100	-0.52124000
H	-2.84351200	-0.23357000	-2.04608200
C	-2.29928600	-1.67611400	1.46686300
H	-0.50637200	-0.51415700	1.50309100
C	-3.41812700	-2.03723200	0.74220200
H	-4.48247400	-1.79371600	-1.09527600
H	-2.13600200	-2.08753600	2.45018800
H	-4.13256100	-2.72952600	1.15810900
H	-0.85365400	2.85188600	-1.47534300
C	-2.01284900	2.61288500	0.31924200
H	-1.93876000	3.65990500	0.59459500
H	-2.96474000	2.45969000	-0.18040700
H	-2.01806300	2.02354200	1.23060400

15c

E(RmPW+HF-B95) = -309.752590 au

C	0.53216700	-0.83496000	0.00003900
C	1.73379500	-0.33742900	0.00002000
O	2.79863600	0.10689200	-0.00000200
H	0.46243600	-1.91168100	0.00004900
C	-0.72510700	0.00350300	0.00000100
C	-0.37768800	1.48103000	-0.00010900
C	-1.53833700	-0.32782300	-1.24211900
C	-1.53830900	-0.32764800	1.24218700
H	0.19924900	1.75299400	0.88088300
H	0.19917400	1.75288200	-0.88118400
H	-1.28321800	2.08115700	-0.00010600
H	-1.79300800	-1.38427300	-1.27304000
H	-2.46682500	0.23922700	-1.25330300
H	-0.98314600	-0.09054500	-2.14492700
H	-2.46681200	0.23937900	1.25329800
H	-1.79295100	-1.38410000	1.27328100
H	-0.98310900	-0.09021300	2.14494800

TS1-5cn
E(RmPW+HF-B95) = -866.307544 au

C	-0.34074000	1.78554900	0.98566200
C	0.19691500	0.69016900	1.51544000
O	0.50718000	0.15108200	2.53022700
N	0.68713100	-0.52292100	0.16956600
C	-0.10651700	-1.32816600	-0.40649100
H	0.29816400	-2.01138400	-1.14897400
C	-0.72623500	2.35846100	-0.35422700
C	-1.54424800	-1.38989500	-0.19877400
C	-2.13179300	-1.16134200	1.04004400
C	-2.34000700	-1.71694500	-1.28952900
C	-3.50213800	-1.22984700	1.16712900
H	-1.51288600	-0.95817000	1.89757500
C	-3.71202200	-1.75512400	-1.16295600
H	-1.88017800	-1.92160700	-2.24459600
C	-4.29300500	-1.50924500	0.06696500
H	-3.95626300	-1.06137000	2.12984500
H	-4.32636200	-1.98635000	-2.01768300
H	-5.36530900	-1.54986100	0.17245000
C	-0.20657900	3.79424900	-0.37975800
H	-0.54056100	4.31192800	-1.27722100
H	-0.56302400	4.35497300	0.48095500
H	0.88046500	3.81353700	-0.36017700
C	-2.24998500	2.40059000	-0.44241900
H	-2.57300200	2.90058400	-1.35478900
H	-2.66507200	1.39592500	-0.43833200
H	-2.67306300	2.93915900	0.40207000
C	-0.20556300	1.66854500	-1.60294700
H	-0.43198100	2.29567000	-2.46259500
H	0.86967400	1.51888500	-1.58528000
H	-0.68706400	0.71332900	-1.77682800
C	2.07778600	-0.64431500	-0.01063500
C	2.85803800	0.50075100	0.01530600
C	2.67811200	-1.88426000	-0.16723700
C	4.22089600	0.40536200	-0.17035100
H	2.38611500	1.45490800	0.18596500
C	4.04248900	-1.97114300	-0.34827500
H	2.08525600	-2.78265200	-0.10435300
C	4.81684100	-0.82723200	-0.35995400
H	4.82177600	1.30020900	-0.15713900
H	4.50367800	-2.93903300	-0.46070000
H	5.88398900	-0.89760100	-0.49470600
H	-0.61519100	2.44372400	1.80377800

TS1-5cx
E(RmPW+HF-B95) = -866.296682 au

C	0.46552000	1.50285500	0.41189100
C	-0.06448600	0.95776300	-0.68104900
O	-0.23521400	1.04378100	-1.85364300
N	-0.84698200	-0.61842000	-0.06416900
C	-0.20469900	-1.66581800	0.25936300
H	-0.76216900	-2.48604100	0.70524600
C	1.27068000	2.77816700	0.29754500
C	1.22406600	-1.88101200	0.11504100
C	1.99483000	-1.24829700	-0.85578700
C	1.81901300	-2.80073800	0.97000000
C	3.34278900	-1.51709900	-0.93843500
H	1.53499700	-0.57469300	-1.55884300
C	3.17301800	-3.04992300	0.89688100
H	1.21678600	-3.31073600	1.70642100
C	3.93555200	-2.40511700	-0.05744100
H	3.93574200	-1.03260600	-1.69685900
H	3.62995300	-3.75122500	1.57569700
H	4.99307900	-2.60427000	-0.12552200
C	1.73157300	3.17818600	1.68762600
H	2.32195900	4.09097200	1.65064400
H	0.88251000	3.35414900	2.34443000
H	2.34584800	2.39960800	2.13468700
C	0.43044200	3.89920400	-0.29678200
H	1.01724400	4.80979300	-0.40827600
H	0.05349600	3.61826300	-1.27648700
H	-0.42264300	4.12126700	0.33963300
C	2.48706200	2.54645300	-0.58978800
H	3.08701200	3.45089000	-0.68142800
H	3.11604500	1.75785200	-0.18383000
H	2.17676800	2.24676700	-1.58823600
C	-2.25257300	-0.60173000	0.01295500
C	-2.88519800	0.54291700	0.46983700
C	-3.00246600	-1.69575600	-0.38951900
C	-4.26034300	0.57212300	0.55967500
H	-2.28712200	1.39218800	0.75635500
C	-4.37896400	-1.65476000	-0.30131300
H	-2.51012800	-2.55947000	-0.80764300
C	-5.01115100	-0.52463700	0.17886100
H	-4.74925300	1.46112000	0.92396800
H	-4.95826100	-2.50427700	-0.62522500
H	-6.08680500	-0.49232500	0.24121100
H	0.38753700	0.99478500	1.35500500

ZW-5cn

E(RmPW+HF-B95) = -866.310499 au

C	-0.26627800	1.64030500	0.98832900
C	0.22828300	0.44984300	1.37872500
O	0.42706700	-0.08359700	2.47040300
N	0.65320600	-0.49874900	0.23055300

C	-0.18914300	-1.21299600	-0.41148000
H	0.20847500	-1.81799100	-1.21682500
C	-0.57884500	2.33460800	-0.31230900
C	-1.61957500	-1.26644500	-0.20553100
C	-2.22109200	-1.08134400	1.03749700
C	-2.40176900	-1.55361800	-1.31895400
C	-3.59150000	-1.15399500	1.14017700
H	-1.61129600	-0.90547800	1.90866100
C	-3.77505900	-1.59131100	-1.21235000
H	-1.93017500	-1.72344300	-2.27497500
C	-4.36907700	-1.38966100	0.01888900
H	-4.05881100	-1.01935300	2.10169000
H	-4.37879800	-1.78794100	-2.08284900
H	-5.44275900	-1.42981500	0.10941000
C	0.05635900	3.72157200	-0.24312500
H	-0.22273100	4.32582100	-1.10518500
H	-0.25968800	4.24926100	0.65326000
H	1.14147700	3.64809300	-0.21692700
C	-2.09312200	2.50594200	-0.41876400
H	-2.36335600	3.08032600	-1.30459500
H	-2.58924100	1.53916900	-0.47453100
H	-2.48381000	3.02866800	0.45089200
C	-0.09287400	1.68461500	-1.59842400
H	-0.23955500	2.38165300	-2.42056200
H	0.96479400	1.43681900	-1.57115200
H	-0.65518400	0.79087500	-1.85152200
C	2.04885100	-0.65587000	0.03255600
C	2.86020400	0.46123100	0.11452500
C	2.58918100	-1.90337800	-0.22071100
C	4.21531700	0.32822100	-0.09848700
H	2.41734900	1.41571400	0.34965200
C	3.94668800	-2.02467400	-0.43499400
H	1.96219900	-2.78027800	-0.20448700
C	4.76068000	-0.91016900	-0.38143300
H	4.84918800	1.19770700	-0.03868700
H	4.37016300	-2.99782000	-0.62252300
H	5.82195500	-1.00945800	-0.54124000
H	-0.53255400	2.24022300	1.85058200

ZW-5cx
E(RmPW+HF-B95) = -866.300264 au

C	0.35148300	1.47611300	0.48632100
C	-0.16658600	0.76763400	-0.53536000
O	-0.27711500	0.89905300	-1.75043600
N	-0.77239000	-0.56848300	-0.01305000
C	-0.04987700	-1.57559400	0.30368000
H	-0.57453100	-2.41641400	0.74098100
C	1.02739300	2.80412600	0.27096000
C	1.37810300	-1.73008600	0.14666400

C	2.13064400	-1.04017900	-0.80383700
C	1.99272600	-2.68424900	0.95103900
C	3.47799700	-1.29363700	-0.91286200
H	1.65413400	-0.33490500	-1.46494800
C	3.34810100	-2.91354100	0.85188400
H	1.40501600	-3.23663600	1.66817300
C	4.09046200	-2.21619500	-0.08095900
H	4.05757500	-0.76744200	-1.65336500
H	3.82043400	-3.64043500	1.49177400
H	5.14909300	-2.40009800	-0.17080800
C	1.49252100	3.34445100	1.61107100
H	1.99113400	4.30401800	1.49107600
H	0.65203700	3.48595000	2.28760500
H	2.19297700	2.66085500	2.08681400
C	0.06557100	3.79884800	-0.36496000
H	0.55957300	4.74957800	-0.56294900
H	-0.31513400	3.40754800	-1.30310900
H	-0.78055800	3.98869800	0.29173800
C	2.23360500	2.63059300	-0.64435900
H	2.73567400	3.58191600	-0.81790700
H	2.95369500	1.94194400	-0.20717700
H	1.92082500	2.23139600	-1.60537400
C	-2.18785400	-0.65537400	0.02208100
C	-2.91596700	0.43459400	0.46182400
C	-2.82495500	-1.81031500	-0.39432500
C	-4.29058900	0.34824700	0.51441100
H	-2.39326400	1.32896700	0.75852000
C	-4.20132500	-1.88651000	-0.33470800
H	-2.25195000	-2.62626300	-0.80482300
C	-4.93571500	-0.81077800	0.12389800
H	-4.86156100	1.19404700	0.86100700
H	-4.69958700	-2.78204800	-0.66824900
H	-6.01133500	-0.86898500	0.16186800
H	0.32497600	1.05638100	1.47920600

TS2-5cn

E(RmPW+HF-B95) = -866.297831 au

C	-0.44731000	-0.44682800	-0.60741900
N	0.55532500	-0.32391200	0.25595100
C	0.14843500	0.52632500	1.35251500
O	0.26982600	0.16785000	2.51186100
C	-0.50051400	1.65641000	0.83359100
H	-0.17319200	-0.50061200	-1.65622800
C	-1.79373700	-0.85748700	-0.28914700
C	-2.74817000	-0.82851500	-1.30250900
C	-2.14064000	-1.38969400	0.95547500
C	-4.03066400	-1.27685300	-1.07158900
H	-2.48114800	-0.44276500	-2.27475300
C	-3.42060700	-1.83981900	1.17394400

H	-1.40457700	-1.44389200	1.74071000
C	-4.37302900	-1.77948100	0.16847100
H	-4.76214700	-1.23930800	-1.86259400
H	-3.67938700	-2.25209500	2.13585000
H	-5.37358800	-2.13724600	0.35011100
C	-0.14888200	2.58814600	-0.30085300
C	0.18728800	3.93254600	0.35284600
H	0.42098200	4.67838200	-0.40432500
H	-0.65020500	4.30169900	0.93894800
H	1.04393100	3.84136000	1.01521900
C	1.04802400	2.20095000	-1.15080800
H	1.92905800	2.01899100	-0.54235200
H	0.88007200	1.32474100	-1.76837600
H	1.27917400	3.01923500	-1.82830300
C	-1.36306300	2.79467600	-1.19798500
H	-1.18715100	3.60003300	-1.90876600
H	-1.58636700	1.88820800	-1.75497600
H	-2.24591500	3.04731400	-0.61582600
C	1.84557100	-0.80986200	0.03945200
C	2.91164200	-0.27202600	0.74708100
C	2.06291800	-1.81551100	-0.88862200
C	4.18665800	-0.72673200	0.50086200
H	2.72774200	0.48567200	1.49056900
C	3.35019400	-2.24502300	-1.14393600
H	1.22746600	-2.28587100	-1.38168500
C	4.41491700	-1.70361600	-0.45374000
H	5.01224900	-0.31067600	1.05517200
H	3.51455700	-3.02458600	-1.87014400
H	5.41729100	-2.05091000	-0.64390800
H	-1.08891500	2.16126600	1.59333800

TS2-5cx

E(RmPW+HF-B95) = -866.280138 au

C	0.16939700	-0.95561600	-0.78360600
N	0.96523600	-0.19302600	-0.04659600
C	0.17614700	0.89230200	0.52192100
O	0.21021700	1.16245600	1.70983000
C	-0.59747800	1.39103100	-0.52745100
H	0.57999500	-1.34366900	-1.71027600
C	2.36050300	-0.25964800	-0.05046500
C	2.99115100	-1.44810400	-0.38122000
C	3.10977900	0.85936400	0.28132700
C	4.36984300	-1.50337800	-0.42396100
H	2.40506800	-2.33367000	-0.56916600
C	4.48412100	0.78421100	0.25776900
H	2.61091700	1.77217000	0.56067300
C	5.12068000	-0.39048300	-0.10440300
H	4.85588700	-2.42949600	-0.68490500
H	5.06485800	1.65377300	0.51979500

H	6.19717400	-0.43918800	-0.12252700
C	-1.06735800	-1.53194700	-0.30887800
C	-1.95818000	-2.08475100	-1.22363200
C	-1.35174100	-1.61153900	1.05519200
C	-3.13433700	-2.65679600	-0.79122600
H	-1.73420300	-2.04051400	-2.27852000
C	-2.52553900	-2.19153100	1.47760100
H	-0.65289700	-1.20819600	1.76963200
C	-3.42540400	-2.70623600	0.55992000
H	-3.82517500	-3.06886700	-1.50909700
H	-2.73995200	-2.24831000	2.53258300
H	-4.34346300	-3.15866300	0.89846300
C	-1.74112400	2.33004000	-0.32190900
C	-2.38120000	2.63716300	-1.66416300
H	-1.67407000	3.11999700	-2.33536100
H	-2.73625700	1.72857900	-2.14565300
H	-3.23162500	3.30314800	-1.54006400
C	-1.25250800	3.62798600	0.31574700
H	-0.78447700	3.42808200	1.27316000
H	-0.52812800	4.12709000	-0.32351000
H	-2.08911800	4.30723700	0.47165100
C	-2.76646600	1.67074300	0.59384500
H	-3.59104100	2.35173600	0.79610400
H	-3.17472400	0.77105100	0.13768700
H	-2.31073800	1.39267100	1.53956000
H	-0.21814300	1.24972000	-1.52714500

trans-**16c**
E(RmPW+HF-B95) = -866.386444 au

C	0.57103100	0.17259000	-0.39896100
N	-0.43006200	-0.73599000	0.14187800
C	0.45696700	-1.48209300	0.86043400
O	0.31878100	-2.45926200	1.53709800
C	1.62280200	-0.61831500	0.42082500
H	0.68855500	0.04843100	-1.47400100
C	-1.79680300	-0.82179400	-0.08590800
C	-2.40519400	0.08538600	-0.93986400
C	-2.55297400	-1.80642200	0.53717500
C	-3.76362900	0.00516700	-1.16947500
H	-1.81738900	0.85456900	-1.41414300
C	-3.90881700	-1.87168700	0.29567400
H	-2.07129100	-2.50659700	1.19671200
C	-4.52272400	-0.97072300	-0.55467600
H	-4.22937500	0.71543100	-1.83388000
H	-4.49162000	-2.63884000	0.78028500
H	-5.58362800	-1.02950200	-0.73580600
C	0.40059000	1.61843100	-0.05858000
C	0.89758200	2.59284700	-0.90719400
C	-0.22306200	2.00267600	1.11740300

C	0.78694100	3.93074500	-0.58137300
H	1.37418600	2.30251400	-1.83205600
C	-0.33816600	3.33909300	1.44205600
H	-0.63170600	1.25118700	1.77546800
C	0.16845800	4.30670400	0.59499400
H	1.17870800	4.68007700	-1.25066900
H	-0.83061800	3.62675200	2.35721700
H	0.07560700	5.35067400	0.84818300
C	2.76229100	-1.32654200	-0.29932700
C	3.56821100	-2.08139100	0.74533100
H	4.00603500	-1.39839100	1.46984000
H	2.94011900	-2.78572000	1.28310200
H	4.37852600	-2.63429600	0.27636400
C	3.64037500	-0.29278400	-0.98138500
H	3.10303600	0.23668600	-1.76547000
H	4.00687600	0.44520400	-0.27165800
H	4.50216100	-0.76967200	-1.44204500
C	2.22829400	-2.31292700	-1.32477000
H	3.05172700	-2.79626800	-1.84370400
H	1.63477900	-3.09106700	-0.85136000
H	1.61071200	-1.82919200	-2.07844800
H	2.01174300	-0.01972900	1.24188000

cis-**17c**
E(RmPW+HF-B95) = -866.392612 au

C	0.34767600	-0.04512200	-0.93320900
N	-0.74718600	-0.74848100	-0.28336700
C	-0.05609900	-1.90859300	-0.08925500
O	-0.37512900	-2.95225300	0.40103200
C	1.19336500	-1.34943600	-0.73927900
H	0.14008600	0.11239300	-1.99122800
C	-2.09511200	-0.42709500	-0.18275000
C	-2.55609000	0.77672400	-0.69379300
C	-2.98020300	-1.31121100	0.42130900
C	-3.89712400	1.09087000	-0.60252300
H	-1.86701200	1.46483700	-1.15616300
C	-4.31639100	-0.98162800	0.50151900
H	-2.61161500	-2.24347700	0.81181200
C	-4.78384100	0.21672200	-0.00583900
H	-4.24713300	2.02933900	-1.00208700
H	-5.00020700	-1.67291100	0.96793600
H	-5.83012500	0.46622200	0.06367200
C	0.73172400	1.26940500	-0.32655600
C	1.47256900	2.16481100	-1.08178700
C	0.33315800	1.63946600	0.94733600
C	1.84493500	3.38795700	-0.56311500
H	1.76475700	1.89805100	-2.08699100
C	0.69752900	2.86675800	1.46601700
H	-0.26297800	0.96116700	1.53730500

C	1.45963900	3.74135500	0.71633200
H	2.42897100	4.06953700	-1.16069700
H	0.38018200	3.14067700	2.45951000
H	1.74293900	4.69885400	1.12319400
C	2.50840600	-1.47387400	0.02465200
C	3.59298600	-0.65822600	-0.65553100
H	3.69161500	-0.93116400	-1.70436900
H	3.39352900	0.40692600	-0.59778100
H	4.55250900	-0.84084100	-0.17709300
C	2.88979800	-2.94781900	-0.02558100
H	2.11725700	-3.56784900	0.41866100
H	3.04068200	-3.27980800	-1.05070100
H	3.81694800	-3.11401800	0.51752700
C	2.37767600	-1.05795500	1.47967800
H	3.30985700	-1.25639600	2.00316400
H	2.16207200	-0.00098000	1.58426900
H	1.59523600	-1.62194500	1.98261800
H	1.32615900	-1.81989400	-1.71299300

18

E(RmPW+HF-B95) = -284.0803863 au

C	0.02596700	0.30543600	-0.00001900
C	-1.10263100	-0.37175600	-0.00004200
O	-2.09589600	-0.93415800	-0.00005700
C	1.22814100	-0.43201900	0.00001600
N	2.22551300	-0.99597600	0.00004700
C	0.03054600	1.80998400	0.00004000
H	0.53833500	2.18711400	0.88128800
H	-0.98026100	2.20092100	0.00003900
H	0.53836500	2.18718400	-0.88116100

19

E(RmPW+HF-B95) = -364.8784705 au

N	2.26496300	-0.42128700	0.00002300
C	1.40168300	0.48990300	-0.00005100
H	1.68713400	1.54741900	-0.00011600
C	-0.03589300	0.21909700	-0.00002400
C	-0.51492000	-1.08376200	-0.00002700
C	-0.93378100	1.27335300	-0.00000200
C	-1.87046800	-1.32142000	-0.00000400
H	0.19949300	-1.89075200	-0.00004500
C	-2.29413700	1.03485300	0.00002300
H	-0.56368400	2.28812100	-0.00000500
C	-2.76338000	-0.26287800	0.00002200
H	-2.23824700	-2.33525800	-0.00000900
H	-2.98671600	1.86135600	0.00004100
H	-3.82511400	-0.45255600	0.00003900
C	3.64444400	-0.04386400	0.00003400

H	3.80254500	1.03765000	0.00002200
H	4.13428100	-0.46933500	-0.87195400
H	4.13427900	-0.46931800	0.87203200

TS1-6n
E(RmPW+HF-B95) = -648.9630930 au

C	-2.04150400	-0.90040100	-0.44710300
C	-1.81910700	-0.57673100	0.82887300
O	-1.86864700	-0.72858400	1.97343600
N	-0.83199500	1.34862200	0.58496600
C	0.36301900	1.63377300	0.31246500
H	0.63640500	2.67127800	0.11405500
C	-1.67793900	-0.09016500	-1.53306000
N	-1.42592900	0.52992600	-2.46525800
C	-2.74811100	-2.20457100	-0.71150500
C	1.43989600	0.65642100	0.20622800
C	1.40854800	-0.54569500	0.89976200
C	2.52774900	0.95039700	-0.60225100
C	2.44281500	-1.44553200	0.76520800
H	0.59004100	-0.75524400	1.56774800
C	3.55433900	0.04146400	-0.74725000
H	2.55788200	1.88855600	-1.13512400
C	3.51183600	-1.15784300	-0.06369600
H	2.41917200	-2.37377900	1.31294500
H	4.38861700	0.26991700	-1.39048200
H	4.31762500	-1.86662700	-0.16947300
C	-1.81371400	2.39086200	0.65643800
H	-1.37865000	3.38385500	0.55569000
H	-2.54172900	2.24251400	-0.13690700
H	-2.33580300	2.32415200	1.60628100
H	-2.12899100	-2.86343400	-1.31310800
H	-2.97431000	-2.71392200	0.21811500
H	-3.68258000	-2.04031300	-1.23984500

ZW-6n
E(RmPW+HF-B95) = -648.9741149 au

C	0.05004500	-1.55155100	0.17342200
N	1.24229000	-1.17241700	0.39694700
C	1.64463100	0.28067200	0.64382200
O	1.97359600	0.51021600	1.78938600
C	1.58962500	1.03202400	-0.50122000
C	1.14113800	0.45903600	-1.69963600
N	0.75821000	-0.03136200	-2.66897800
H	-0.08241500	-2.59797900	-0.07359000
C	-1.13578500	-0.72557400	0.21478600
C	-2.18394700	-1.05834800	-0.63291600
C	-1.26474900	0.33695500	1.10396100

C	-3.34020800	-0.30984800	-0.62465200
H	-2.07554900	-1.88195900	-1.32104800
C	-2.43497100	1.06047800	1.12504800
H	-0.46514600	0.57484400	1.78647600
C	-3.46534900	0.74624700	0.25686500
H	-4.14267100	-0.55222900	-1.30143600
H	-2.54341300	1.87670100	1.82000100
H	-4.37483200	1.32532100	0.27269700
C	1.98711100	2.47090100	-0.45536300
C	2.36042600	-2.08356300	0.44796700
H	3.03233900	-1.85260800	-0.37102300
H	2.87319300	-1.91603600	1.38747300
H	2.02142500	-3.10946200	0.37942000
H	2.35625800	2.70360300	0.53687500
H	2.77243700	2.69881800	-1.17161300
H	1.14830900	3.13112800	-0.66760200

TS2-6n
E(RmPW+HF-B95) = -648.9435846 au

C	-0.25795100	0.03880400	1.08343900
N	-1.13936800	-0.93778000	0.83372500
C	-1.39232900	-0.85285800	-0.57971800
O	-1.45473600	-1.78825200	-1.32476000
C	-1.40752300	0.55112500	-0.88846500
C	-2.12336600	1.40473000	-0.01624400
N	-2.71509600	2.11404700	0.66996500
H	-0.46949000	0.70013300	1.91726700
C	1.09799700	0.03210000	0.58578400
C	1.92024200	1.11562700	0.87844000
C	1.61544200	-1.04935300	-0.12605300
C	3.22695500	1.13404000	0.44495800
H	1.52327500	1.94818800	1.43885900
C	2.92216500	-1.02214300	-0.55540900
H	0.99000300	-1.90330200	-0.33031200
C	3.72951500	0.06730100	-0.27577600
H	3.85652500	1.97903800	0.67192100
H	3.31994100	-1.86107900	-1.10308300
H	4.75423700	0.07784500	-0.61072800
C	-1.25492000	0.98090600	-2.30287100
C	-2.15213000	-1.35455300	1.76985100
H	-2.74629600	-0.50261500	2.09900300
H	-2.79700000	-2.06422100	1.26771300
H	-1.70313700	-1.84250600	2.62689900
H	-0.57283500	0.31305200	-2.81769500
H	-2.20529300	0.95697100	-2.83549600
H	-0.87536800	1.99629000	-2.35971800

trans-**20**
E(RmPW+HF-B95) = -649.0221015 au

C	-0.57501700	0.53529900	-0.03315300
N	-0.91668500	0.26321500	1.34604200
C	0.11774900	0.92859200	1.90282000
O	0.44036500	1.14569300	3.02474300
C	0.70898600	1.25353700	0.51434600
C	0.72747900	2.66653600	0.21059200
N	0.73402200	3.77940000	-0.04901800
H	-1.25640200	1.24613200	-0.49775800
C	-0.39141000	-0.65188400	-0.91879400
C	-0.50641600	-0.50813500	-2.29129800
C	-0.08715000	-1.89768100	-0.39520100
C	-0.30971300	-1.58807800	-3.12812700
H	-0.75397000	0.45716000	-2.70746700
C	0.10196000	-2.98040900	-1.23045600
H	0.00086300	-2.01854800	0.67397100
C	-0.00687300	-2.82744700	-2.59878700
H	-0.40059500	-1.46280100	-4.19518100
H	0.33397100	-3.94645200	-0.81138600
H	0.13965800	-3.67309700	-3.25132400
C	2.04700100	0.60331600	0.24485300
C	-2.08286800	-0.32041100	1.92787300
H	-2.96718700	0.27888100	1.72522800
H	-1.93140700	-0.36953600	2.99945800
H	-2.24410400	-1.32368700	1.54453100
H	2.01394900	-0.44798200	0.50690900
H	2.81275600	1.08426200	0.84272000
H	2.31379600	0.68597800	-0.80343300