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Supplementary Material

Understanding the mechanism of the Povarov reaction. A DFT study.

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Table S1. MPWB1K/6-311G** total energies (in a.u.) in acetonitrile of the stationary points involved in the Povarov reaction between the simplest N-aryl imine **13a** and 2-methylene-1,3-dioxolane **16**.

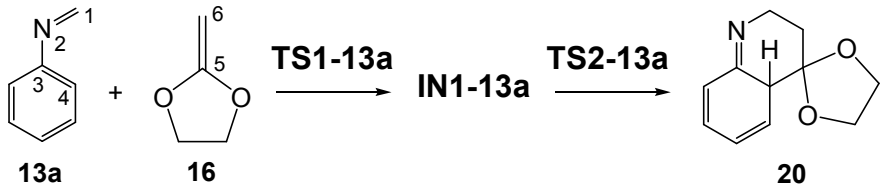
18	-650.190456
16	-306.377433
MC-18	-956.577655
TS1-18	-956.573140
IN1-18	-956.598238
TS2-18	-956.582715
19	-956.604581
20	-631.992322
TS3	-631.872594
17	-632.041117
20 + 21	-882.603678
TS4	-882.577640
IN2	-882.590566
17 + 21	-882.653181

Table S2. MPWB1K/6-311G** total energies (in a.u.) in acetonitrile of the stationary points involved in the BF_3 catalysed A-DA reaction between N-aryl-C-aryl imine **1** and MVE **23**.

22	-881.184526
23	-193.055696
TS1n-1	-1074.224892
TS1x-1	-1074.214826
INn-1	-1074.234834
INx-1	-1074.234976
TS2n-1	-1074.232694
TS2x-1	-1074.233755
24	-1074.271471
25	-1074.264715

*Study of the hetero Diels-Alder reaction between the simplest N-aryl imine **13a** and 2-methylene-1,3-dioxolane **16**.*

In order to establish the role of the Lewis Acid (LA) catalyst in Povarov reactions, the A-DA reaction between the simplest N-aryl imine **13a** and the electron-rich (ER) 2-methylene-1,3-dioxolane **16** was studied. Interestingly, the uncatalysed reaction presents also a two-step mechanism. Consequently, two TSs, an intermediate and the corresponding cycloadduct were characterised (see Scheme S1). The total and relative energies of the stationary points involved in the A-DA reaction between the simplest N-aryl imine **13a** and the ER ethylene **16** are gathered in Table S3.



13a **16** **20**

Scheme S1

The activation energy associated with the nucleophilic attack of the ER ethylene **16** on the C1 carbon of N-aryl imine **13a**, via **TS1-13a**, is 12.0 kcal/mol; formation of the corresponding intermediate **IN1-13a** is endothermic by 9.4 kcal/mol. Finally, this intermediate with a very low activation energy, 2.2 kcal/mol, yields the formal [4+2] cycloadduct **20**, via **TS2-13a**. Formation of **20** is exothermic by −17.7 kcal/mol. A comparison of these relative energies with those of the LA catalysed process allows drawing some appealing conclusions: i) coordination of the BF_3 catalyst to the imine nitrogen of N-aryl imine **13a** accelerates considerably the A-DA reaction through a strong decrease of the activation energy of 15.3 kcal/mol, ii) this larger acceleration is a consequence of the high electrophilic character of the LA complex **18** when compared with N-aryl imine **13a** (see reactivity index analysis section in the main manuscript); iii) while formation of intermediate **IN1-13a** is endothermic by 9.4 kcal/mol, formation of intermediate **IN1-18** is exothermic by 19.0 kcal/mol. This behaviour can be understood as a strong stabilisation of the zwitterionic intermediate **IN1-18** through the electron-withdrawing BF_3 LA. Note that the charge separation at **IN1-18** is 0.86e (see main manuscript); iv) the activation energy associated with **TS1-13a**, 12.0 kcal/mol, is 16.1 kcal/mol below that that associated with the A-DA reaction between N-aryl imine **13a**

and ethylene **14a**,[1] 28.1 kcal/mol, as a consequence of the low nucleophilic character of ethylene **14a**.

Table S3. MPWB1K/6-311G** total (E, a.u.) and relative (ΔE, kcal/mol) energies, in acetonitrile, of the stationary points involved in the A-DA reaction between the simplest N-aryl imine **13a** and 2-methylene-1,3-dioxolane **16**.

	E	ΔE
16	-325.586653	
TS1-13a	-631.945024	12.0
IN1-13a	-631.949034	9.4
TS2-13a	-631.945649	11.6
20	-631.992311	-17.7

The geometries of the TSs associated with A-DA reaction between the simplest N-aryl imine **13a** and the nucleophilic activated ethylene **16** are given in Figure S1. At **TS1-13a**, associated with the nucleophilic attack of the C6 carbon of the ER ethylene **16** on the C1 carbon of N-aryl imine **13a**, the distance between the C1 and C6 carbons is 1.884 Å, while the distance between the C4 and the C5 carbons, which do not participate in the nucleophilic addition, is 3.151 Å. At intermediate **IN1-13a**, the length of the C1−C6 single bond is 1.602 Å, while the distance between the C4 and the C5 carbon remains at 3.012 Å. Finally, at **TS2-13a**, associated with the ring-closure, the distance between the C4 and C5 carbons is 2.377 Å.

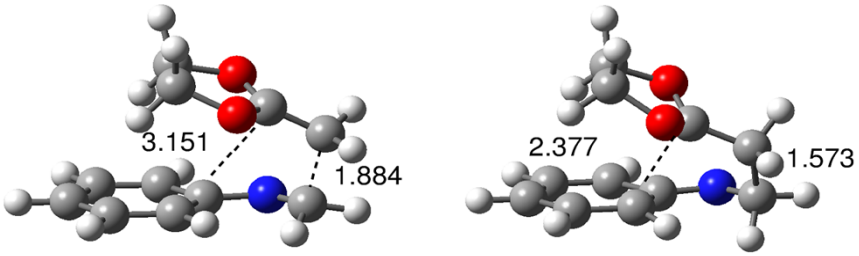
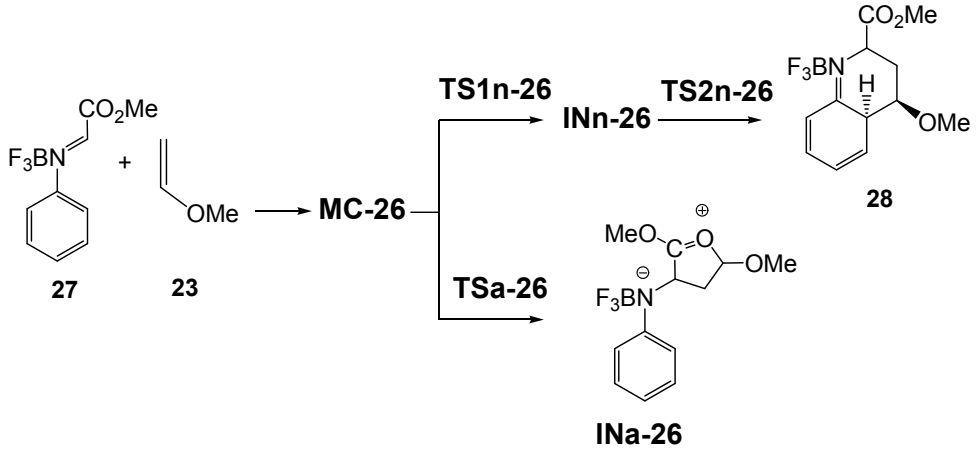


Figure S1. MPWB1K/6-311G** geometries in acetonitrile of the transition structures involved in the A-DA reaction between the simplest N-aryl imine **13a** and 2-methylene-1,3-dioxolane **16**. Lengths are given in Angstroms.

*Study of the mechanism of the BF_3 catalysed A-DA reactions of N-phenyl-C-methoxycarbonyl imine **26** with MVE **23**.*

In order to establish the role of the substituents (H, Ph, or CO_2Me) present in the C1 carbon of the imine C=N double bond in Povarov reactions, the *endo* reactive channel associated with the nucleophilic attack of MVE **23** on the BF_3 complex of N-phenyl-C-methoxycarbonyl imine **26**, BF_3:imine complex **27**, was studied (see Scheme S2). The total and relative energies are given in Table S4. A schematic representation of the energy profile for the BF_3 catalysed A-DA reactions of N-phenyl-C-methoxycarbonyl imine **26** with MVE **23** is given in Figure S2.



Scheme S2

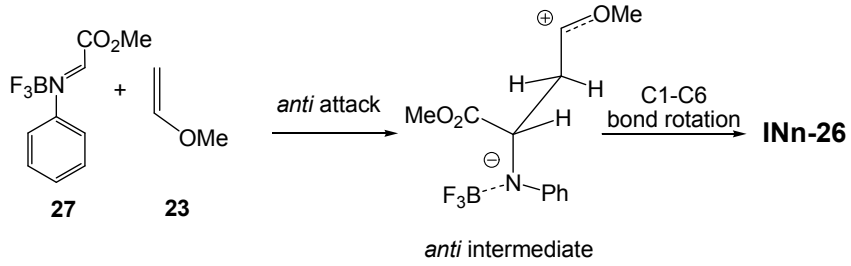
Just as the LA catalysed A-DA reaction model between imine **13a** and ER ethylene **16** (see Scheme 7), the nucleophilic attack of MVE **23** on BF_3:imine complex **27** has a low activation barrier, 5.1 kcal/mol from **MC-26**; formation of the zwitterionic intermediate **INn-26** is exothermic by −12.8. The subsequent ring-closure *via* **TS2n-26** has a unappreciable barrier, 0.8 kcal/mol. Formation of the formal [4+2] cycloadduct **28** is strongly exothermic, -29.5 kcal/mol.

The ring-closure in **INn-26** to yield the formal [4+2] CA **28** has an unappreciable barrier, 0.8 kcal/mol, while this barrier at intermediate **IN1-18** is 9.7 kcal/mol (see Table S1). Thus, the fast ring closure found in **INn-26** does not allow to justify the formation of intermediate **12** as proposed by Whiting for the formation of product **11** (see Scheme 4 in the main manuscript).[2]

Table S4. MPWB1K/6-311G** total (E, a.u.) and relative (ΔE, kcal/mol) energies, in acetonitrile, of the stationary points involved in the *endo* reactive channel of the BF_3 catalysed A-DA reaction of N-phenyl-C-methoxycarbonyl imine **26** with MVE **23**.

	E	ΔE
27	-878.012569	
MC-26	-1071.078756	-6.6
TS1n-26	-1071.070586	-1.5
INn-26	-1071.088647	-12.8
TS2n-26	-1071.086745	-11.6
28	-1071.115221	-29.5
TSa-26	-1071.078902	-6.7
INa-26	-1071.105849	-23.6

Most P-DA reactions, taking place along high asynchronous TSs, are associated with two centre reactions characterised by the most favourable nucleophile-electrophile interaction. Although usually the most favourable reaction channel is that involving the formation of the new C−C bond in a *gauche* conformation, the *anti* approach mode yielding an *anti* intermediate is also feasible, requiring a further bond rotation to yield the formal [4+2] cycloadduct (see Scheme S3).



Scheme S3

Thus, the *anti* reaction channel shown in Scheme S3 was studied in order to explain Whiting's results. Interestingly, the TS associated with the *anti* approach mode of MVE **23** to BF_3:imine complex **27**, **TSa-26**, was located 6.7 below the reagents (see Table S4). Such as in the BF_3 catalysed A-DA reaction of the simplest N-aryl imine **13a**, the IRC from **TSa-26** to reagents allowed finding the molecular complex **MC-26**, which is 6.6 kcal/mol more stable than BF_3:imine complex **27** plus MVE **23**. In addition, the IRC from **TSa-26** to the products finish in a species that by full optimisation yields the cyclic intermediate **INa-26** (see Scheme S2); formation of this

intermediate is thermodynamically very favourable, −23.6 kcal/mol. Consequently, for the BF_3 catalysed A-DA reaction of the N-phenyl-C-methoxycarbonyl imine **26** with the ER MVE **23**, formation of the *anti* intermediate **INa-26** is kinetically and thermodynamically very favourable. This approach mode of the reagents seems to be responsible of obtaining Whiting's intermediate to yield the adduct **11** (see Scheme 4 in the main manuscript).

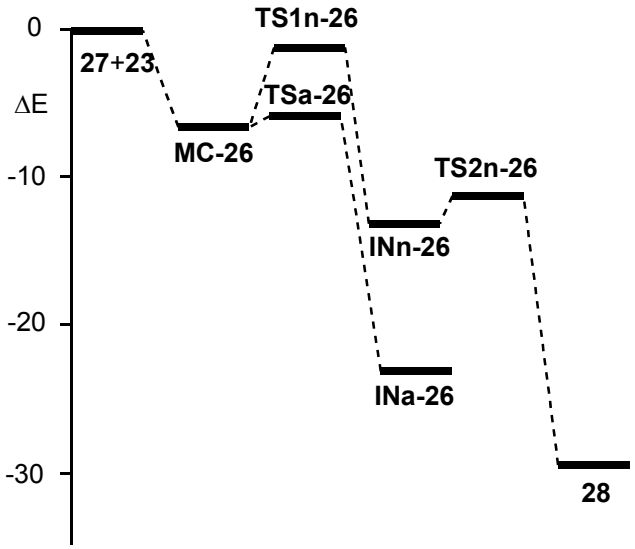


Figure S2. Energy profile (ΔE in kcal/mol) of the BF_3 catalysed A-DA reactions of N-phenyl-C-methoxycarbonyl imine **26** with MVE **23**.

The geometries of the TSs associated with the BF_3 catalysed A-DA reaction between N-aryl-C-methoxycarbonyl imine **26** and MVE **23** are given in Figure S3. At the *gauche* **TS1n-26**, associated with the nucleophilic attack of the C6 carbon of the MVE **23** on the C1 carbon of BF_3:imine complex **27**, the distance between the C1 and C6 carbons is 2.206 Å, while the distance between the C4 and the C5 carbons, which do not participate in the nucleophilic addition, is 3.115 Å. At intermediate **IN1n-26**, the length of the C1−C6 single bond is 1.559 Å while the distance between the C4 and the C5 carbon remains at 2.831 Å. At **TS2n-26**, associated with the ring-closure process, the distance between the C4 and C5 carbons is 2.301Å. Finally, at the *anti* **TSa-26** the distance between the C1 and C6 carbons is 2.120 Å, while the length of the C1−C6 single bond of the intermediate **INa-26** is 1.531 Å.

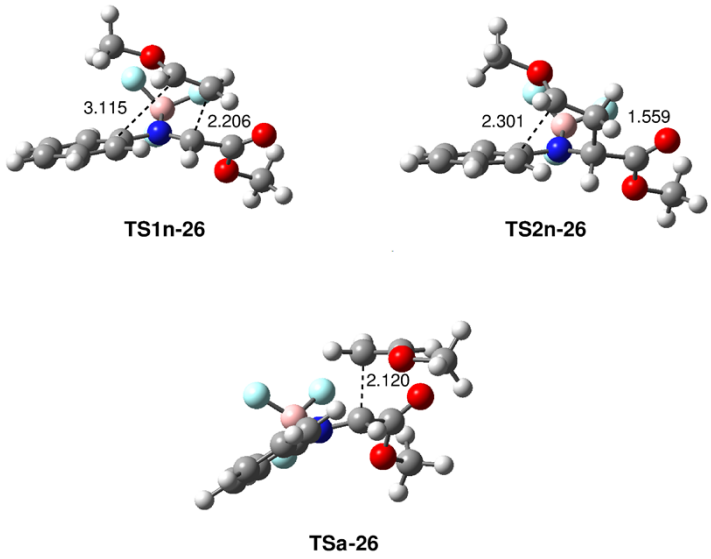


Figure S3. MPWB1K/6-311G** geometries of the TSs involved in the BF_3 catalysed A-DA reaction between N-aryl-C-methoxycarbonyl imine **26** and MVE **23**. Lengths are given in Angstroms.

The global charge transfer (GCT) that fluxes from the ER ethylene framework to BF_3:imine complex one along the BF_3 catalysed A-DA reaction of N-aryl-C-methoxycarbonyl imine **26** is 0.33e at **TS1n-26**, 0.76e at **INn-26**, 0.64e at **TS2n-26** and 0.35e at **TSa-26**. These values show the high polar character of these BF_3 catalysed A-DA reactions. NPA analysis performed at **IN1n-26** indicates the high zwitterionic character of these intermediates. At **TS2n-26** there is a reduction of the GCT as consequence of a retro-donation along the ring-closure process.

Table S5. MPWB1K/6-311G** Total and relative enthalpies (H, in au, and ΔH, kcal/mol), entropies (S, in cal/mol·K and ΔS, in cal/mol·K), Gibbs free energies (G, in au, and ΔG, in kcal/mol), computed at 25.0 °C and 1.0 atm, and scaled by a factor 0.96, in acetonitrile, of the stationary points involved in Schemes 7, 9 and S2.

	H	ΔH	S	ΔS	G	ΔG
16	-306.275954		72.4		-306.310341	
18	-650.043889		100.9		-650.091844	
MC-18	-956.326178	-4.0	135.5	-37.8	-956.390543	7.3
TS1-18	-956.321980	-1.3	126.0	-47.3	-956.381846	12.8
IN1-18	-956.344267	-15.3	124.7	-48.6	-956.403526	-0.8
TS2-18	-956.330701	-6.8	127.6	-45.7	-956.391307	6.8
19	-956.351039	-19.6	126.6	-46.7	-956.411190	-5.7
20	-631.758176		103.8		-631.807472	
TS3	-631.644450	71.4	101.8	-2.0	-631.692806	72.0
17	-631.805624	-29.8	103.5	-0.3	-631.854782	-29.7
20 + **21**	-882.227570		143.0		-882.295498	
TS4	-882.206326	13.3	136.8	-6.2	-882.271300	15.2
IN2	-882.213459	8.9	140.8	-2.2	-882.280352	9.5
17 + **21**	-882.276442	-30.7	147.2	4.2	-882.346380	-31.9
22	-880.953317		125.3		-881.012830	
23	-192.967243		74.1		-193.002453	
TS1n-1	-1073.902406	11.4	142.8	-56.6	-1073.970237	28.3
TS1x-1	-1073.892890	17.4	151.1	-48.3	-1073.964684	31.8
INn-1	-1073.910999	6.0	143.6	-55.7	-1073.979248	22.6
INx-1	-1073.911853	5.5	148.3	-51.0	-1073.982338	20.7
TS2n-1	-1073.909682	6.8	139.8	-59.6	-1073.976085	24.6
TS2x-1	-1073.910322	6.4	141.1	-58.3	-1073.977343	23.8
24	-1073.945811	-15.8	142.4	-57.0	-1074.013471	1.1
25	-1073.939500	-11.9	144.1	-55.3	-1074.007964	4.6
27	-877.822428		125.3		-877.881948	
23	-192.967243		74.1		-193.002453	
MC-26	-1070.793656	-2.5	163.6	-35.8	-1070.871376	8.2
TS1n-26	-1070.785970	2.3	142.6	-56.7	-1070.853739	19.2
INn-26	-1070.801892	-7.7	143.1	-56.3	-1070.869871	9.1
TS2n-26	-1070.801326	-7.3	142.5	-56.9	-1070.869041	9.6
TSa-26	-1070.785780	2.4	151.6	-47.8	-1070.857791	16.7
INa-26	-1070.818249	-17.9	144.3	-55.1	-1070.886792	-1.5
28	-1070.827572	-23.8	141.9	-57.5	-1070.894973	-6.6

*ELF topological analysis of bonding changes along the A-DA reaction between BF_3:imine complex **18** and ER ethylene **16**. A topological characterization of the C−C bond formation in the Povarov reaction.*

Several theoretical studies have shown that the electron localisation function (ELF) topological analysis along a reaction path can be used as a valuable tool to understand the bonding changes along the reaction path.[3] After an analysis of the electron density, the ELF provides basins, which are the domains in which the probability of finding an electron pair is maximal.[4] The basins are classified as core basins and valence basins. The latter are characterized by the synaptic order, i.e., the number of atomic valence shells in which they participate. Thus, there are monosynaptic, disynaptic, trisynaptic basins and so on.[5] Monosynaptic basins, labeled V(A), correspond to the lone pairs or non-bonding regions, while disynaptic basins connect the core of two nuclei A and B and, thus, correspond to a bonding region between A and B and are labeled V(A,B). This description recovers the Lewis bonding model, providing a very suggestive graphical representation of the molecular system.

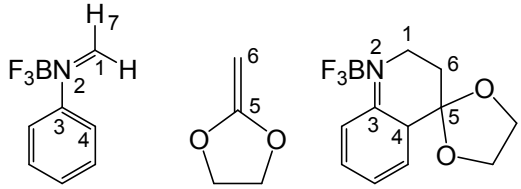
Recently, Domingo *et al.* have shown that the C−C single bond formation in organic reactions begins in the short C−C distance range of 1.9 - 2.0 Å by merging two monosynaptic basins, V(Cx) and V(Cy), into a new disynaptic basin V(Cx,Cy) associated with the formation of the new Cx−Cy single bond.[6] The Cx and Cy carbons characterized by the presence of the monosynaptic basins V(Cx) and V(Cy) have been called *pseudoradical* centres.[7]

In order to understand the C-C bond formation in Povarov reaction, an ELF topological analysis of the MPWB1K/6-31G(d) wavefunctions of some relevant points of the IRCs of the two-step reaction between BF3:imine complex **18** and ER ethylene **16** was carried out. For this ELF topological study, eight structures were selected: the stationary points **18** + **16**, **TS1-18**, **IN1-18, TS2-18**, and the formal [4+2] cycloadduct **19**, plus three relevant points of the IRCs, namely **P-I**, **P-II** and **P-III**. ELF valence basin populations *N* calculated at the eight structures are given in Table S6.

Starting from the reagents, the most remarkable feature is the topological representation of the C1=N2 and C5=C6 double bonds. In this way, the C1=N2 double bond of BF_3:imine complex **18** is topologically represented by two disynaptic basins,

V(C1,N2) and V'(C1,N2), integrating a total of 3.18e. On the other hand, the C5=C6 double bond of the ER ethylene **16** is also depicted by two disynaptic basins, V(C5,C6) and V'(C5,C6), integrating a total of 3.93e. Note that the integration of the C1=N2 double bond basins is lower than that of the C5=C6 one as a consequence of presence of the electron-withdrawing BF_3 catalyst at the N2 nitrogen.

Table S6. ELF valence basin populations *N* calculated at some selected points of the IRCs of the two-step A-DA reaction between the BF_3:imine complex **18** and the ER ethylene **16**. d(A-B) is the distance between A and B atoms (in Angstroms).



18 **16** **19**

	18+16	**TS1-18**	**P-I**	**IN1-18**	**TS2-18**	**P-II**	**P-III**	**19**
d1=d(C1,C6)		2.073	1.884	1.595	1.556	1.538	1.534	1.510
d2=d(C4,C5)		3.196	3.175	3.073	2.291	2.019	1.942	1.549
V(C3,C10)	2.80	2.89	2.87	2.88	2.55	2.35	2.31	2.12
V(C4,C7)	2.81	2.84	2.81	2.80	2.49	2.28	2.22	2.06
V(C7,C8)	2.77	2.87	2.91	2.98	3.13	1.65	1.67	1.69
V'(C7,C8)						1.62	1.63	1.70
V(C8,C9)	2.78	2.73	2.71	2.69	2.49	2.33	2.31	2.23
V(C9,C10)	2.82	2.90	2.95	3.01	3.13	1.66	1.61	1.61
V'(C9,C10)						1.55	1.60	1.62
V(C3,C4)	2.88	2.77	2.69	2.60	2.47	2.41	2.39	2.34
V(N2,B)	2.41	3.17	2.65	2.49	2.51	3.18	3.11	2.68
V(N2)			0.86	1.38	1.03			
V(N2,C3)	1.98	1.99	2.00	2.02	2.35	2.60	2.67	1.56
V'(N2,C3)								1.54
V(C1,N2)	1.64	2.54	2.16	1.79	1.78	1.81	1.81	1.81
V'(C1,N2)	1.54							
V(C5,O11)	1.53	1.71	1.80	1.89	1.79	1.58	1.53	1.39
V'(C5,O12)	1.58	1.78	1.87	2.00	1.80	1.61	1.54	1.42
V(C5,C6)	2.04	2.91	2.64	2.33	2.40	2.13	2.10	2.04
V'(C5,C6)	1.89							
V(C6)		0.64						
V(C1)		0.04						
V(C1,C6)			1.14	1.61	1.78	1.81	1.83	1.87
V(C4)					0.44	0.76		
V(C5)						0.50		
V(C4,C5)							1.41	1.91

On going from reagents to **TS1-18**, d1=2.073 and d2=3.196 Å, the aforementioned pairs of disynaptic basins have merged into one disynaptic basin with lower integration, 2.54e for V(C1,N2) and 2.91e for V(C5,C6). Interestingly, two new monosynaptic basins V(C1) and V(C6), integrating 0.64e and 0.04e, respectively, appear at the most electrophilic centre of BF_3:imine complex **18**, the C1 carbon atom, and at the most nucleophilic centre of the ER ethylene **16**, the C6 carbon atom (see below). They will be responsible for the subsequent C1−C6 single bond formation.

At point **P-I**, d1=1.884 and d2=3.175 Å, the formation of the C1−C6 bond takes place through the merging of V(C1) and V(C6) monosynaptic basins which give place to the new disynaptic basin V(C1,C6) with 1.14e. Note that the formation of this C−C bond takes place at a distance of 1.884 Å. Additionally, a new monosynaptic basin, V(N2), integrating 0.86e, is observed at **P-I**, which disappears after reaching **TS2-18**.

At intermediate **IN1-18**, d1=1.595 and d2=3.073 Å, while the electron population of the disynaptic basin V(C1,C6) has reached 1.61e, indicating that the bond is practically formed, any monosynaptic basin at the C4 and C5 carbons is observed. In addition, the monosynaptic V(N2) basin has almost doubled its integration at the expense of the disynaptic basin V(C1,N2).

On going from **IN1-18** to **TS2-18**, d1=1.556 and d2=2.291 Å, the V(N2) basin starts to behave as an electronic pump, providing the necessary electronic density to promote the appearance of V(C4) monosynaptic basin. Note that this is just the phenyl ring position where the ring closure will take place. In fact, V(N2) diminishes its integration from 1.38e to 1.03e, a difference which almost covers the 0.44e of monosynaptic basin V(C4). The phenyl ring attached at N2 nitrogen, which has been almost inert towards electronic changes along the reaction path, starts to practice some interesting changes. Until **IN1-18**, the electronic picture of the phenyl ring was those of an aromatic structure with almost a symmetrical charge distribution and integration of the disynaptic V(Cphenyl,Cphenyl) basins, but from **IN1-18**, some disynaptic basins start to accumulate charge (V(C7,C8) and V(C9,C10)) while others start to lose electronic density (V(C3,C10), V(C4,C7) and V(C3,C4)). Note that at the location of those basins which accumulate charge end up being a formal double bond at the final formal [4+2] cycloadduct **19** while those that lose charge, will have a single C−C bond.

After to pass **TS2-18**, at **P-II**, d1=1.538 and d2=2.019 Å, a second monosynaptic basin appears at C5 carbon, V(C5), with a population of 0.50e. This electronic density comes partially from the disynaptic basin V(C5,C6) and from the V(C5,Ox) ones. Note that the location of this second monosynaptic basin corresponds to one of the carbon atoms participating in the formation of the second C4−C5 single bond. Furthermore, the monosynaptic basin V(C4) has increased its integration to reach 0.76e. Interestingly, at **P-II**, the C=C double bonds present in the formal [4+2] cycloadduct **19** have already topologically formed, such as shown by the presence of two pairs of disynaptic basins, V(C7,C8), V'(C7,C8), V(C9,C10) and V'(C9,C10). At **P-II**, the monosynaptic basin V(N2) has disappeared.

At **P-III**, d1=1.534 and d2=1.942 Å, the two monosynaptic basins V(C4) and V(C5) have merged in a new disynaptic basin V(C4,C5), with a population of 1.41e, thus verifying the formation of the second C4−C5 single bond. From **P-III** to formal [4+2] cycloadduct **19**, the integration of the disynaptic basin V(C4,C5) increases to reach 1.91e.

Finally, at the formal [4+2] cycloadduct **19**, the disynaptic basin V(N2,C3) has splitted into two disynaptic basins, V(N2,C3) and V'(N2,C3), integrating 1.56 and 1.54e. Such as other DA reactions, the double bond present in the formal [4+2] cycloadduct **19** is formed at the end of the reaction.

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MPWB1K/6-311G** computed total energies, unique imaginary frequency, and cartesian coordinates in acetonitrile of the stationary points involved in the studied Povarov reactions.

16

E(RmPW+HF-B95)= -306.377433 a.u.

C	0.78816500	-0.00015600	-0.00004900
C	-1.33782000	0.76019500	-0.00012300
C	-1.33800600	-0.76005800	0.00020500
O	0.03584700	-1.10426900	-0.00022000
H	-1.80239200	1.17873700	-0.88472000
H	-1.80284800	-1.17887800	-0.88407400
O	0.03589200	1.10413300	0.00006400
H	-1.80220800	-1.17844600	0.88503300
H	-1.80260700	1.17904000	0.88421500
C	2.11236700	0.00006500	0.00006400
H	2.64416200	-0.93168800	0.00007500
H	2.64375000	0.93204400	0.00013900

18

E(RmPW+HF-B95)= -650.190456 a.u.

C	-0.98777100	-0.97792900	-0.43647700
H	-0.23691000	-1.67302600	-0.76730100
C	-2.31170500	-1.35002900	-0.33466100
H	-2.59814600	-2.35927400	-0.57807700
C	-3.26467300	-0.43839100	0.07953100
H	-4.29598100	-0.73737500	0.16428800
C	-2.89173900	0.85354200	0.39693200
H	-3.62638400	1.56267200	0.73915900
C	-1.57129000	1.23928200	0.29385300
C	-0.62991300	0.32387000	-0.13756700
C	1.05438700	1.84906200	-0.70157100
H	0.30172100	2.54433800	-1.03870500
N	0.73567900	0.70746200	-0.26120400
H	-1.27265200	2.23512700	0.57678400
B	1.89069400	-0.33792200	0.17961700
F	1.46871000	-0.91327600	1.34709800
F	2.00960800	-1.25558800	-0.83766000
F	3.03766100	0.39735000	0.33620000
H	2.09754500	2.11208300	-0.73678300

MC-18

E(RmPW+HF-B95)= -956.577655 a.u.

O	-2.63551900	-1.50053100	0.24805300
C	-2.61508700	-0.16918300	0.38903400
O	-2.27701200	0.43410800	-0.75191900
C	-1.81911600	-0.55974800	-1.66067200
C	-2.48345000	-1.80412300	-1.13149900
C	-2.88176800	0.45848200	1.52785700
C	0.04462600	1.11006900	1.82808000
N	0.70349900	0.91268500	0.76328500
B	0.81957900	2.09500000	-0.33121300

F	-0.18235500	2.98761800	-0.04960700
C	1.32807400	-0.33899800	0.50724000
C	2.54885200	-0.35515300	-0.14352500
C	3.16047400	-1.56514800	-0.39682100
C	2.55326100	-2.74909400	-0.02071200
C	1.32640300	-2.72232100	0.61407500
C	0.70642100	-1.51681200	0.87879200
F	2.06377000	2.66388800	-0.17821100
F	0.67839200	1.51429400	-1.56549200
H	3.01630400	0.57072100	-0.42861300
H	4.11595700	-1.58148800	-0.89405100
H	3.03224700	-3.69142000	-0.22862500
H	0.84063300	-3.64111900	0.89724900
H	-0.01341900	0.36189300	2.60176400
H	-2.85419300	1.53088500	1.56229100
H	-0.26532700	-1.49733200	1.34511500
H	-0.43188200	2.06473400	1.95991100
H	-3.20288100	-0.10517500	2.38286000
H	-3.46318400	-1.97433600	-1.56758600
H	-2.13462800	-0.28543100	-2.65775000
H	-1.87535900	-2.69388400	-1.22474100
H	-0.73681600	-0.61048700	-1.61512200

TS1-18

E(RmPW+HF-B95)= -956.573140 a.u.

unique imaginary frequency: -286.61 cm^{-1}

C	0.52302100	2.10958200	0.28083800
H	1.48034000	2.13139300	0.76741800
C	-0.40341000	3.10939600	0.48571000
H	-0.15978300	3.92497900	1.14637400
C	-1.63068100	3.07556000	-0.15059200
H	-2.35075600	3.85987900	0.01148900
C	-1.92193700	2.02334900	-0.99540900
H	-2.87361800	1.97907400	-1.49911400
C	-1.00539000	1.01016500	-1.19894200
C	0.22858900	1.04559100	-0.56287900
C	1.01157800	-0.89907100	-1.63664100
H	0.31875900	-0.75074800	-2.44458800
C	-0.14695000	-2.63480200	-0.82144300
H	0.75409500	-2.95693800	-0.33460100
N	1.18095500	0.01971200	-0.73047600
H	-1.28291600	0.18961800	-1.83698900
B	2.38486700	-0.12990300	0.27960300
F	3.27628100	0.90925700	0.06486800
F	1.89970300	-0.09087300	1.57031500
F	2.98782500	-1.34817900	0.01854600
H	1.81933600	-1.58876700	-1.78498200
H	-0.48756400	-3.15062500	-1.69980300
C	-1.06369600	-2.00155300	-0.05141400
O	-0.76272700	-1.48018600	1.11224500
C	-2.98433600	-1.09516800	0.65072200
C	-1.85248300	-0.68061900	1.57015200
H	-3.68020500	-1.78291200	1.11485300
H	-2.03156000	-0.91631600	2.60919600
O	-2.31296100	-1.78730300	-0.40266400
H	-3.51548600	-0.25613200	0.22297700
H	-1.57627500	0.36251500	1.46226100

IN1-18

E(RmPW+HF-B95)= -956.598238 a.u.

C	0.18320400	1.97406400	0.38753300
H	1.06463200	2.10207100	0.98805400
C	-0.87594500	2.82959800	0.58371500
H	-0.78896900	3.59255500	1.34146000
C	-2.04295700	2.72440700	-0.15646400
H	-2.86853700	3.39578300	0.00829500
C	-2.10791700	1.73909900	-1.11705300
H	-2.99195200	1.63300300	-1.72639300
C	-1.04958200	0.87054200	-1.32885600
C	0.13369200	0.96038000	-0.58340800
C	1.00491100	-1.12272800	-1.44120900
H	0.32949600	-1.03358900	-2.28195500
C	0.50956100	-2.26776500	-0.50491900
H	1.25159900	-2.41657600	0.26968200
N	1.20254800	0.11114300	-0.75528900
H	-1.15830200	0.13601000	-2.10755500
B	2.39600900	0.16142200	0.19748500
F	3.05494700	1.39121500	0.12634900
F	1.99267200	-0.05149000	1.52509000
F	3.28642000	-0.86083200	-0.15256100
H	1.95120000	-1.47408500	-1.82805500
H	0.35484500	-3.17425300	-1.07724400
C	-0.74327600	-1.87366200	0.11686400
O	-0.76725700	-1.25400500	1.22046100
C	-2.90614600	-1.45261000	0.36596400
C	-2.10850000	-0.76945400	1.46313100
H	-3.55176900	-2.24657800	0.71051800
H	-2.38480100	-1.06558700	2.46311200
O	-1.86931000	-2.06595600	-0.43944900
H	-3.43678000	-0.76320700	-0.27378400
H	-2.06462900	0.30776500	1.36368000

TS2-18

E(RmPW+HF-B95)= -956.582715 a.u.

unique imaginary frequency: -410.77 cm^{-1}

C	0.60106700	1.88000900	0.21200600
H	1.51020100	2.06094100	0.75430200
C	-0.42027400	2.77554000	0.26938900
H	-0.29409700	3.66782500	0.86181200
C	-1.63365000	2.57886400	-0.41730300
H	-2.41444400	3.31759600	-0.35926700
C	-1.78141400	1.45878800	-1.16952400
H	-2.67580200	1.30098100	-1.75126800
C	-0.76679100	0.47529900	-1.21766800
C	0.46264300	0.69123500	-0.54163800
C	1.00523100	-1.49423400	-1.15073900
H	0.78077300	-1.35398300	-2.20668400
C	-0.21343600	-2.12037100	-0.45764700
H	0.11696200	-2.61556400	0.44929600
N	1.39195000	-0.26572300	-0.53639300
H	-0.79524600	-0.20588900	-2.05190300

B	2.70974700	-0.14081400	0.26023200
F	3.40924900	0.98648200	-0.16654300
F	2.44180800	-0.01565900	1.62342400
F	3.46933500	-1.28234900	0.03683700
H	1.82498800	-2.19298200	-1.08749700
H	-0.66207900	-2.85826700	-1.11202900
C	-1.30715300	-1.20786600	-0.03131500
O	-1.28085400	-0.75604300	1.19683800
C	-3.45895500	-0.82046000	0.42070700
C	-2.58958700	-0.29993800	1.55446900
H	-4.17238100	-1.57196900	0.72801800
H	-2.82872100	-0.73017000	2.51639800
O	-2.52170800	-1.45635200	-0.45240800
H	-3.95861600	-0.03148200	-0.12548800
H	-2.57305700	0.77878700	1.61459200

19

E(RmPW+HF-B95)= -956.604581 a.u.

C	0.96920400	2.03278500	0.23891600
H	1.96101600	2.19900400	0.60826900
C	0.06340800	3.02513200	0.23459700
H	0.35791700	3.99036200	0.61426100
C	-1.28105200	2.87071000	-0.25020300
H	-1.94514000	3.71742400	-0.22774600
C	-1.68224500	1.69277900	-0.71553900
H	-2.68121700	1.53735700	-1.08769300
C	-0.78271400	0.52538800	-0.75280200
C	0.60200600	0.73976100	-0.24555400
C	0.82464700	-1.53458900	-0.73570100
H	0.60293500	-1.46934700	-1.80110200
C	-0.42042600	-1.81925700	0.06892700
H	-0.14482100	-1.89376800	1.11525500
N	1.40038300	-0.27707200	-0.28547100
H	-0.68033800	0.21039600	-1.79736400
B	2.91017800	-0.43007300	0.14926900
F	3.47252000	0.77447400	0.50220200
F	2.91767200	-1.31603100	1.21253400
F	3.56492400	-0.97914800	-0.93871100
H	1.56496300	-2.30975300	-0.60226900
H	-0.87242900	-2.75543000	-0.23942500
C	-1.43969800	-0.70630300	-0.08160100
O	-1.96706000	-0.38317500	1.17284600
C	-3.58802000	-1.39524900	-0.04438600
C	-3.37743800	-0.43739900	1.09587800
H	-3.50122100	-2.43026200	0.28186600
H	-3.76249400	-0.78838200	2.04452700
O	-2.51710000	-1.05253100	-0.89880600
H	-4.51571900	-1.25469100	-0.58230500
H	-3.78581600	0.54639900	0.87394500

20

E(RmPW+HF-B95)= -631.992322 a.u.

C	-2.71885300	0.01591500	0.44864800
H	-3.49627600	0.59523000	0.91892200

C	-2.81614200	-1.30659600	0.28972700
H	-3.69607100	-1.82606200	0.63389500
C	-1.76067200	-2.07969500	-0.33202300
H	-1.89127200	-3.14521600	-0.42680600
C	-0.65544000	-1.49354200	-0.77847700
H	0.12926900	-2.06558500	-1.24745000
C	-0.44698800	-0.03062900	-0.67434500
C	-1.54458800	0.73342100	0.00575400
C	-0.20884100	2.55351400	-0.27976000
H	-0.15962100	2.51024000	-1.37284700
C	0.96183700	1.79216500	0.31574600
H	0.91426800	1.88018900	1.39619400
N	-1.45523600	1.99171200	0.17890400
H	-0.35826100	0.38178100	-1.68626600
H	-0.16195800	3.60011400	-0.00152500
H	1.90999600	2.20052400	-0.01963400
C	0.90775900	0.31499600	-0.03630800
O	1.13823100	-0.44396400	1.12506400
C	2.94314600	-0.65037300	-0.22633600
C	2.18849500	-1.34957600	0.87122100
H	3.60812400	0.11488400	0.17288800
H	2.75935700	-1.48661200	1.78123300
O	1.89146900	-0.06597200	-0.95990400
H	3.49635600	-1.31135400	-0.88046300
H	1.79687500	-2.30823600	0.53517000

20+21

E(RmPW+HF-B95)= -882.603678 a.u.

C	2.69630000	-2.30149400	0.19279300
H	2.98036900	-3.08785400	0.87267400
C	3.21828400	-2.20400900	-1.03146000
H	3.92262700	-2.94423600	-1.37636900
C	2.90355700	-1.08713000	-1.90335600
H	3.44062100	-0.98785200	-2.83244000
C	1.97336500	-0.20613300	-1.55784400
H	1.71819800	0.62263100	-2.19859900
C	1.17150600	-0.36958100	-0.31586300
C	1.80105800	-1.27684000	0.71265800
C	0.82552100	-0.15456300	2.53378400
C	-0.03154500	0.63235400	1.56350900
N	1.61007500	-1.22275700	1.96427200
H	0.22812100	-0.85113300	-0.60371500
C	0.76561000	0.93826100	0.32445500
O	1.90243300	1.69803400	0.67561900
C	0.44272700	3.03964600	-0.42918300
C	1.90003700	2.88375300	-0.08725700
H	-0.11127300	3.50201100	0.38681800
H	2.29842100	3.69211800	0.51373700
O	0.04894100	1.69841800	-0.60514200
H	0.25623700	3.57969100	-1.34826500
H	2.50615700	2.76102800	-0.98362000
H	0.20932000	-0.57545900	3.32431900
H	1.52743100	0.51774600	3.02735700
H	-0.36883100	1.55839500	2.02186600
H	-0.90438900	0.05804800	1.26231400
C	-4.00723900	-1.00496000	0.79284500

C	-2.98366600	-1.73718200	0.36209600
C	-2.73379100	-0.40363100	-1.61372200
C	-3.30467100	0.74408500	-0.80862900
N	-2.19109200	-1.40141300	-0.71914700
C	-4.40967000	0.26483600	0.11554300
H	-1.93750300	-0.04858800	-2.26118500
H	-3.51949600	-0.82866100	-2.24541900
H	-3.67031400	1.51230500	-1.48442100
H	-2.49785900	1.18283200	-0.22709300
H	-5.33549800	0.12181400	-0.44418300
H	-4.62837900	1.03276600	0.85585700
H	-4.54305000	-1.33157400	1.66908500
H	-2.68881200	-2.63967800	0.87456400
H	-1.79027700	-2.19323700	-1.18519200

TS3

E(RmPW+HF-B95)= -631.872594 a.u.
unique imaginary frequency: -1795.64 cm^{-1}

O	1.94032000	-0.05996400	-0.91280900
C	0.87804000	0.40593400	-0.13303000
O	0.99580900	-0.20694600	1.11800100
C	1.88853600	-1.28885000	0.99278600
C	2.81560100	-0.79560400	-0.08448900
C	0.92132300	1.91491600	0.04388000
C	-0.44940000	2.53498800	0.35796700
N	-1.32884900	1.89988300	-0.59670500
C	-1.50995400	0.60817500	-0.17334500
C	-0.45639700	-0.09321400	-0.82327100
C	-2.41250200	-0.02680400	0.65712400
C	-2.46650700	-1.39945500	0.51734400
C	-1.61343100	-2.11576500	-0.34334000
C	-0.59140300	-1.49652100	-1.00516200
H	-3.13977100	0.50953500	1.24421200
H	-3.23583900	-1.94617700	1.03966600
H	-1.77096300	-3.17571300	-0.45681000
H	0.09681300	-2.05111600	-1.62255800
H	-0.51825200	0.99833400	-1.52632700
H	3.59018000	-0.14681400	0.31994400
H	2.36940300	-1.45470700	1.94817900
H	3.26799400	-1.58428700	-0.67218600
H	1.35756500	-2.18789400	0.68461000
H	-0.41284600	3.61243300	0.23065200
H	-0.73521500	2.31126700	1.38980200
H	1.65564800	2.12863000	0.81352500
H	1.26474400	2.33581100	-0.89609000

TS4

E(RmPW+HF-B95)= -882.577640 a.u.
unique imaginary frequency: -1478.58 cm^{-1}

C	3.54196000	-1.66251700	0.33829400
C	3.38087000	-0.38206200	1.08299500
C	2.62511800	0.61218400	0.65301500
N	1.89053800	0.55565500	-0.56247100
C	2.29394800	-0.51012100	-1.48385000

C	2.47032600	-1.80102400	-0.72382200
C	-0.79253500	0.63637600	-0.21517700
C	-0.97868400	1.03986600	-1.57349100
C	-0.67728000	2.29324500	-1.97965700
C	-0.28799900	3.24757600	-0.99211400
C	-0.27572800	2.95425900	0.32518300
C	-0.66346300	1.65273200	0.82565400
N	-0.77436200	1.47279400	2.09671600
C	-1.22866700	0.17299400	2.53249700
C	-0.81604000	-0.96653200	1.62477500
C	-1.31288800	-0.68926000	0.22585700
O	-0.91405100	-1.67673500	-0.69131500
C	-1.95808300	-2.61699100	-0.76264700
C	-3.16805000	-1.72871000	-0.65649200
O	-2.73707900	-0.73335400	0.23951600
H	-0.03356700	3.70596000	1.05984600
H	-0.01845800	4.24365500	-1.30979700
H	-0.73584000	2.57875600	-3.01604300
H	-1.26953100	0.28107100	-2.28484700
H	0.60599400	0.48788300	-0.34641700
H	-1.90598200	-3.32029800	0.06792700
H	-4.03984100	-2.22672400	-0.24783200
H	-1.88007700	-3.15422100	-1.69910900
H	-3.42022400	-1.29189600	-1.62240500
H	-0.85161700	-0.00767600	3.53662800
H	-2.31963600	0.17392700	2.61309200
H	-1.21447300	-1.91434300	1.97776500
H	0.27084300	-1.03700500	1.59119800
H	1.51365800	-0.59900300	-2.23333000
H	3.21967100	-0.22118500	-1.97625800
H	2.71670700	-2.59271300	-1.42406200
H	1.51918000	-2.06044400	-0.26675200
H	4.53609900	-1.70255400	-0.10752400
H	3.49218600	-2.49702600	1.03352600
H	3.89190600	-0.25614300	2.02361900
H	2.48330700	1.52517700	1.20594600
H	1.91867200	1.45428000	-1.02661000

IN2

E(RmPW+HF-B95)= -882.590566 a.u.

C	3.49031200	-1.81033300	0.66675700
C	3.05507600	-0.66039600	1.50364100
C	2.35161200	0.35737100	1.05649300
N	1.96718100	0.45110300	-0.34062900
C	2.73732300	-0.43006700	-1.24652000
C	2.77042500	-1.81863500	-0.66594300
C	-1.04051900	0.77858900	-0.30886400
C	-0.80261900	0.98510600	-1.66106100
C	-0.16962900	2.11413100	-2.13509900
C	0.23205100	3.07259400	-1.19222300
C	-0.00349100	2.90790400	0.14328400
C	-0.71182800	1.77648100	0.67278300
N	-0.96826600	1.70773600	1.95509200
C	-1.76611200	0.57021000	2.33038800
C	-1.35685800	-0.70492800	1.62651100
C	-1.56387600	-0.54443200	0.13897800

O	-0.88250100	-1.59768300	-0.54562600
C	-1.82867500	-2.45561600	-1.13920400
C	-3.11223700	-2.07247500	-0.44627900
O	-2.91816200	-0.70014200	-0.21940900
H	0.30801200	3.66078700	0.85136400
H	0.74826500	3.96117000	-1.52559100
H	0.01082800	2.25625000	-3.18670200
H	-1.08723000	0.19988900	-2.34744800
H	0.95327200	0.26130900	-0.42879300
H	-1.54161600	-3.48846400	-0.97396900
H	-3.23533000	-2.61445900	0.49120600
H	-1.88663600	-2.26470100	-2.21008700
H	-3.99745900	-2.20483400	-1.05522400
H	-1.70439500	0.42886600	3.40772600
H	-2.82904000	0.74522200	2.10730800
H	-1.91129300	-1.57065700	1.98192100
H	-0.29700300	-0.88978900	1.79974800
H	2.25109000	-0.38853800	-2.21295500
H	3.73323800	-0.00879500	-1.32944300
H	3.25783400	-2.48481200	-1.36878400
H	1.74796800	-2.16676600	-0.53752300
H	4.56953400	-1.75672500	0.52592500
H	3.30336600	-2.73392000	1.20759000
H	3.31856700	-0.65468800	2.54902200
H	1.98317600	1.17065300	1.65540700
H	2.03201400	1.42071000	-0.64351500

17

E(RmPW+HF-B95)= -632.041117 a.u.

C	-2.85060300	0.31005100	0.09831000
H	-3.61683100	1.06758700	0.15453400
C	-3.18939400	-1.02173000	0.12785600
H	-4.22787200	-1.29941300	0.21292700
C	-2.21264300	-2.00290100	0.04799500
H	-2.47936600	-3.04614600	0.06563600
C	-0.89459100	-1.61707800	-0.05716100
H	-0.11315900	-2.35677900	-0.13121100
C	-0.53235400	-0.28235200	-0.08196600
C	-1.51619100	0.70549100	-0.01032300
C	0.17450500	2.42675400	0.13819400
C	1.07338200	1.51922100	-0.66114900
N	-1.19313000	2.03666900	-0.08812800
C	0.91624000	0.09506800	-0.17581900
O	1.50799700	-0.06828300	1.09130900
C	2.72357900	-1.31656400	-0.35198900
C	2.84939900	-0.41824800	0.85212600
H	3.59287200	-1.29401800	-0.99930000
H	3.45206700	0.46291400	0.63471500
O	1.61306600	-0.77864700	-1.03697100
H	2.51664700	-2.34452900	-0.05990800
H	3.24092800	-0.91264400	1.73146800
H	0.29735700	3.45784500	-0.17398000
H	0.44702400	2.35933000	1.19491100
H	2.11250700	1.81916600	-0.56710100
H	0.80090000	1.55932200	-1.71278900
H	-1.88762300	2.65985100	0.27584200

17+21

E(RmPW+HF-B95)= -882.653181 a.u.

C	-0.20843900	2.46372300	-0.29272700
H	0.79325900	2.78157500	-0.53715500
C	-1.13302100	3.37090800	0.16615600
H	-0.84450500	4.40354600	0.28259200
C	-2.42485400	2.97230500	0.47620800
H	-3.15060500	3.68584400	0.82834100
C	-2.76118200	1.64507800	0.32310100
H	-3.75997300	1.30563500	0.54862400
C	-1.84327300	0.71402500	-0.12769900
C	-0.54587500	1.11651800	-0.45448900
C	0.12507500	-1.17666100	-0.79142100
C	-1.30373500	-1.47492800	-1.16714000
N	0.37012300	0.23235500	-0.95472000
H	3.59864700	1.81515800	-0.57830700
C	-2.23675000	-0.72861900	-0.24025000
O	-2.21816500	-1.29803200	1.04905300
C	-4.30063200	-1.62512100	0.23624100
C	-3.22363100	-2.28123600	1.06018200
H	-4.93215700	-2.32991400	-0.29230900
H	-2.87486600	-3.20588700	0.60133700
O	-3.56514600	-0.86452000	-0.69737900
H	-4.92044400	-0.96945300	0.84569800
H	-3.50921800	-2.47441800	2.08601600
H	0.81111800	-1.72478400	-1.42808900
H	0.29633800	-1.49968800	0.24012400
H	-1.51118800	-2.53889500	-1.10370000
H	-1.49551300	-1.15013400	-2.18680400
C	4.54664700	-1.18994100	-0.73835300
C	4.01896000	-0.05644200	-1.18792400
C	3.26452200	0.53765800	1.02427800
C	4.48407900	-0.21162400	1.52002900
N	3.34978600	0.86142300	-0.38756900
C	4.64967200	-1.49017800	0.72135800
H	3.10536200	1.45706900	1.57677300
H	2.38246600	-0.08615200	1.17923400
H	4.38426000	-0.42130800	2.58103200
H	5.36396000	0.41604500	1.38863000
H	3.90135700	-2.22249400	1.02796000
H	5.61605000	-1.94343800	0.93299800
H	4.95742200	-1.88640800	-1.45098600
H	4.03602900	0.19445900	-2.23756200
H	1.33393200	0.52481700	-0.88711700

22

E(RmPW+HF-B95)= -881.184526 a.u.

C	2.65368100	0.38812500	-0.85791300
H	2.26410100	1.24819300	-1.37615300
C	3.96986100	0.00391600	-0.99297900
H	4.62961700	0.57913800	-1.62074000
C	4.44221900	-1.11078300	-0.32279600
H	5.47330200	-1.40500000	-0.42568200

C	3.59268400	-1.83997100	0.48476200
H	3.95714800	-2.70153900	1.01857400
C	2.27112100	-1.46045000	0.62774800
C	1.81046200	-0.35701700	-0.05385100
C	-0.46183300	-0.82412100	-0.11007900
H	-0.11554200	-1.84054700	-0.24919200
N	0.44803900	0.06132600	0.05189000
H	1.61297100	-2.00806900	1.28247200
B	0.23176500	1.61597400	0.44886200
F	1.38532200	2.01315700	1.07337100
F	0.02722400	2.31900200	-0.72113800
F	-0.83905300	1.69049900	1.30003400
C	-1.89615600	-0.66291600	-0.14488500
C	-2.64991400	-1.78595000	0.18427700
C	-2.53930200	0.49333600	-0.57623000
C	-4.02567900	-1.72824100	0.16202300
H	-2.15044100	-2.69564100	0.47710000
C	-3.91450200	0.52668400	-0.63416300
H	-1.96583500	1.34507400	-0.89223800
C	-4.65501900	-0.56570800	-0.24507200
H	-4.60537600	-2.59046600	0.44427800
H	-4.41102800	1.41740300	-0.98038900
H	-5.73118100	-0.52304400	-0.28102300

23

E(RmPW+HF-B95)= -193.055696 a.u.

C	1.85758900	-0.06769000	0.00504300
H	2.65502700	0.65281100	0.00447400
H	2.10121200	-1.11699100	0.01276300
C	0.60315700	0.34460500	-0.00474100
O	-0.43810800	-0.50170100	-0.00878000
C	-1.70582900	0.10999800	0.00591600
H	-1.84447900	0.70182800	0.90775700
H	-1.84451500	0.74394200	-0.86686800
H	0.34660100	1.39598000	-0.01221200
H	-2.43848200	-0.68544400	-0.01298200

TS1n-1

E(RmPW+HF-B95)= -1074.224892 a.u.

unique imaginary frequency: -395.24 cm^{-1}

C	-2.31045500	1.19755100	-1.03776100
H	-1.99499700	2.18397400	-0.74995100
C	-3.56200100	1.01433200	-1.57927000
H	-4.19775300	1.87172700	-1.72932200
C	-4.00467400	-0.24760600	-1.93706100
H	-4.98481500	-0.38509200	-2.36187300
C	-3.16489800	-1.32227500	-1.74857300
H	-3.48111000	-2.31445900	-2.02620000
C	-1.90449700	-1.15077700	-1.20249800
C	-1.46116300	0.11338600	-0.82340700
C	0.71773700	-0.62404900	-0.33523600
H	0.45214000	-1.40757500	-1.02502000
C	0.69732500	-1.74745700	1.32205900
H	1.18893500	-0.98959900	1.91001300

N	-0.20619200	0.34661200	-0.23798600
H	-1.28880200	-2.02552500	-1.08846400
B	-0.09380100	1.53486300	0.78522200
F	-1.30378100	1.72268300	1.43148800
F	0.88647400	1.20770100	1.71037500
F	0.23719000	2.71352600	0.11531900
H	1.25430400	-2.62795200	1.05789900
C	-0.64851200	-1.90662100	1.52088800
O	-1.31959000	-0.93647400	2.02844100
C	-2.74152900	-0.96959200	2.01991900
H	-3.07628500	-0.86963500	3.04343400
H	-3.07082200	-0.12390800	1.42903200
C	2.17784100	-0.36678100	-0.42310700
C	2.99652200	-1.46410200	-0.66703100
C	2.74314100	0.89849300	-0.41283600
C	4.35219000	-1.31093100	-0.85206000
H	2.56419300	-2.45097400	-0.72189000
C	4.10321100	1.05077500	-0.60497300
H	2.12555200	1.76572500	-0.27660900
C	4.91333800	-0.04740400	-0.81376700
H	4.96871900	-2.17505600	-1.03590700
H	4.52921600	2.04061000	-0.59729100
H	5.97328400	0.08003500	-0.95992200
H	-1.19648900	-2.77984900	1.19066700
H	-3.09660000	-1.89809100	1.58731600

TS1x-1

E(RmPW+HF-B95)= -1074.214826 a.u.

unique imaginary frequency: -438.20 cm^{-1}

C	-2.08137900	-2.05422800	0.55101600
H	-1.53489400	-2.92731700	0.24524200
C	-3.32490200	-2.20585900	1.12014800
H	-3.73450000	-3.19754800	1.22349100
C	-4.04580000	-1.10979700	1.56278800
H	-5.02107500	-1.23587100	2.00208600
C	-3.48203400	0.14127300	1.45357600
H	-4.01098700	1.01039900	1.80933600
C	-2.22313800	0.30220500	0.90056100
C	-1.50538800	-0.79114500	0.42676900
C	0.53034000	0.37606800	0.31148300
H	0.09260700	0.88603700	1.15525200
C	0.51542300	1.89289300	-0.93423000
H	0.97006100	1.31789400	-1.72070100
N	-0.20825300	-0.67317500	-0.10032600
H	-1.80399100	1.29173200	0.88652600
B	0.23737400	-1.57983900	-1.29717200
F	-0.85682800	-2.23844800	-1.82237800
F	0.76034200	-0.74936600	-2.29946100
F	1.19928700	-2.48616500	-0.88831500
H	1.13147600	2.60612000	-0.41103700
C	-0.79063800	2.24739200	-1.14567000
O	-1.32593100	3.25661200	-0.54236800
C	-2.71028400	3.51092900	-0.78393000
H	-2.83631000	3.88911800	-1.79099200
H	-3.28342100	2.60086900	-0.64287900
C	2.00524600	0.29142300	0.50934800

C	2.44238700	0.63908600	1.78095400
C	2.94222900	-0.09202800	-0.43894100
C	3.78080600	0.57484600	2.11421900
H	1.72570500	0.95555600	2.52229400
C	4.27970100	-0.14722700	-0.10571200
H	2.63172000	-0.34574200	-1.43462000
C	4.70488300	0.17926000	1.16916400
H	4.09690500	0.83971300	3.10952400
H	4.99733900	-0.44678200	-0.85165700
H	5.75184800	0.13241500	1.41969000
H	-1.43601400	1.65944200	-1.78815100
H	-3.00802900	4.25773800	-0.06418000

IN1n-1

E(RmPW+HF-B95)= -1074.234834 a.u.

C	2.23087000	-1.58652600	-0.10714400
H	1.84427900	-2.24738100	0.64815500
C	3.50585300	-1.75095600	-0.58310600
H	4.11258500	-2.54907300	-0.18573900
C	4.02160500	-0.91514200	-1.56814800
H	5.02604600	-1.05043200	-1.93214800
C	3.21214900	0.06662100	-2.08321400
H	3.57237300	0.71044100	-2.86940000
C	1.91413700	0.24231100	-1.61947900
C	1.39866800	-0.56566200	-0.59800500
C	-0.69015900	0.56962500	-0.67062900
H	-0.46601300	0.59406400	-1.73212500
C	-0.43721300	2.05774500	-0.14838100
H	-0.94097100	2.10958200	0.81162400
N	0.15435100	-0.38224300	-0.04945500
H	1.30884400	0.97965100	-2.11734000
B	-0.09966600	-0.79088900	1.41931600
F	1.05578100	-0.63008000	2.19007500
F	-1.10018300	0.03761800	1.92692100
F	-0.49025100	-2.12987800	1.50987500
H	-0.83544900	2.76782600	-0.86037000
C	0.97077700	2.28143100	0.05627500
O	1.45922700	1.84316600	1.12073400
C	2.87884900	1.76571100	1.30342900
H	3.06910100	2.03729200	2.33050500
H	3.13902400	0.72866000	1.11926900
C	-2.16060800	0.23016400	-0.58493300
C	-3.14973200	1.19921300	-0.59822300
C	-2.53759200	-1.10435400	-0.60982200
C	-4.48593600	0.84424700	-0.63097300
H	-2.89899100	2.24646100	-0.58212500
C	-3.87106800	-1.45823700	-0.63975600
H	-1.77610700	-1.86410700	-0.58583800
C	-4.85336200	-0.48555000	-0.65172500
H	-5.23918200	1.61514400	-0.63979800
H	-4.14386700	-2.50115700	-0.65187300
H	-5.89463200	-0.76227400	-0.67510700
H	1.61663200	2.79468900	-0.64467500
H	3.37884500	2.43263800	0.61187100

IN1x-1

E(RmPW+HF-B95)= -1074.234976 a.u.

C	2.06100700	-1.91662100	-0.26136600
H	1.60175900	-2.67570700	0.34673300
C	3.34869400	-2.07155000	-0.70417900
H	3.89085100	-2.96325600	-0.43233800
C	3.96137600	-1.10515800	-1.49501800
H	4.97397600	-1.23642600	-1.83724500
C	3.24045200	0.01078700	-1.83975000
H	3.67968800	0.77034900	-2.46645300
C	1.93169100	0.18159600	-1.40311600
C	1.30910000	-0.77902000	-0.59486200
C	-0.67266500	0.53499000	-0.49200700
H	-0.40392500	0.75447300	-1.52109000
C	-0.24760200	1.78273700	0.34370300
H	-0.77372600	1.68541700	1.29715500
N	0.03991700	-0.63254100	-0.08267500
H	1.40512300	1.05073500	-1.75954100
B	-0.22910600	-1.19359600	1.32671400
F	0.91035200	-1.00496100	2.13421200
F	-1.28071700	-0.48459800	1.90285100
F	-0.52980300	-2.55359200	1.29338700
H	-0.49989000	2.72491800	-0.12570500
C	1.15888100	1.76860400	0.69799600
O	1.85230400	2.79722600	0.53750000
C	3.24922000	2.78590800	0.88582600
H	3.46499500	1.92945700	1.51096700
H	3.79710400	2.74229200	-0.04573400
C	-2.17156300	0.36070600	-0.51879400
C	-2.72567500	-0.90538800	-0.62360900
C	-3.01337600	1.46015100	-0.54417200
C	-4.09104700	-1.06483500	-0.75072300
H	-2.07670700	-1.76432100	-0.58492400
C	-4.38071700	1.30061100	-0.66936200
H	-2.61304100	2.45815400	-0.47069200
C	-4.92598000	0.03683100	-0.77496500
H	-4.50583100	-2.05721000	-0.82524400
H	-5.01847500	2.16937900	-0.68534700
H	-5.99176600	-0.08983900	-0.87195500
H	1.59035200	0.91172400	1.20585900
H	3.43793200	3.71408700	1.40306600

TS2n-1

E(RmPW+HF-B95)= -1074.232694 a.u.

unique imaginary frequency: -198.81 cm^{-1}

C	-2.25745500	1.53092100	-0.48781600
H	-1.87946400	2.41443700	-0.00854600
C	-3.55830200	1.46227100	-0.88568900
H	-4.19995000	2.31263700	-0.71942800
C	-4.07857400	0.31837900	-1.50895900
H	-5.11150900	0.28571600	-1.81038900
C	-3.24327300	-0.72727700	-1.75767500
H	-3.59837900	-1.59729700	-2.28578800
C	-1.89063800	-0.68722200	-1.36897600
C	-1.37247200	0.45019600	-0.70590900

C	0.67530100	-0.65747700	-0.59642700
H	0.49051000	-0.86408300	-1.64833400
C	0.19758000	-1.93268500	0.17306600
H	0.66708300	-1.89745900	1.15148500
N	-0.11014700	0.47607300	-0.23281800
H	-1.24262500	-1.40504400	-1.84148900
B	0.26130900	1.27825700	1.05443600
F	-0.86902900	1.50832300	1.83288400
F	1.15612200	0.50270800	1.78575600
F	0.83461200	2.50140700	0.72145900
H	0.50772600	-2.82051200	-0.36578400
C	-1.24608100	-1.97598200	0.41059100
O	-1.62976100	-1.36266500	1.46443400
C	-3.02554200	-1.29073800	1.73520500
H	-3.12514400	-1.15236900	2.80079300
H	-3.41576300	-0.43334900	1.20033100
C	2.16206300	-0.43303000	-0.51039300
C	3.04003200	-1.39237500	-0.03961800
C	2.67622600	0.74867600	-1.02311700
C	4.40541100	-1.17187500	-0.06946600
H	2.67474100	-2.32249500	0.36248700
C	4.03714300	0.97063400	-1.05057800
H	1.99567000	1.50151400	-1.38402100
C	4.90973000	0.00971200	-0.57240700
H	5.07397400	-1.92958500	0.30567100
H	4.41878600	1.89771300	-1.44682600
H	5.97329400	0.18234800	-0.59248400
H	-1.89206800	-2.73698800	-0.00193100
H	-3.51652900	-2.20236400	1.41445200

TS2x-1

E(RmPW+HF-B95)= -1074.233755 a.u.
unique imaginary frequency: -185.60 cm^{-1}

C	2.03071000	-1.89243500	-0.39905800
H	1.53320800	-2.74760200	0.02330600
C	3.35404000	-1.92882700	-0.71807000
H	3.91536400	-2.82885700	-0.52520800
C	3.99961700	-0.82513600	-1.29422300
H	5.04668700	-0.87668800	-1.53893200
C	3.27011100	0.28894600	-1.57851100
H	3.72606600	1.12769400	-2.07932300
C	1.90117200	0.36181600	-1.26088500
C	1.25647800	-0.74402100	-0.65859900
C	-0.68333300	0.55389800	-0.54199200
H	-0.45928500	0.78374400	-1.58191400
C	-0.07936300	1.69905800	0.29872700
H	-0.57989600	1.67724000	1.26800900
N	-0.02108300	-0.67572900	-0.22052200
H	1.34282700	1.15783800	-1.72221200
B	-0.35215000	-1.38693100	1.12513000
F	0.78340900	-1.35726700	1.94935200
F	-1.36249900	-0.68614700	1.76593500
F	-0.72259300	-2.70822800	0.90790300
H	-0.22418700	2.67240900	-0.15681800
C	1.35231800	1.52328100	0.60038700
O	2.07447800	2.57760300	0.61057500

C	3.41645400	2.48260200	1.08881300
H	3.50276800	1.66922800	1.79902700
H	4.06725400	2.31947200	0.23915700
C	-2.18554900	0.47011400	-0.49107700
C	-2.80852800	-0.73430800	-0.77964600
C	-2.96676400	1.58728800	-0.25543400
C	-4.18410400	-0.81842300	-0.82938300
H	-2.20434800	-1.61235500	-0.93831000
C	-4.34699800	1.50297100	-0.30486400
H	-2.50984000	2.53688300	-0.02841600
C	-4.96121400	0.30134400	-0.59278700
H	-4.65299100	-1.76440300	-1.04730300
H	-4.94040700	2.38264400	-0.11530600
H	-6.03625100	0.23515200	-0.62884400
H	1.67060100	0.67870500	1.19859600
H	3.63980100	3.42858500	1.55878800

24

E(RmPW+HF-B95)= -1074.271471 a.u.

C	-1.96742000	1.71348400	-0.59086500
H	-1.49678600	2.64252200	-0.33431800
C	-3.22822100	1.69714700	-1.05090700
H	-3.74190600	2.63675000	-1.17653400
C	-3.93652600	0.48809500	-1.37064800
H	-4.96705500	0.54487100	-1.67515600
C	-3.29793900	-0.67430700	-1.30079800
H	-3.77792900	-1.60148000	-1.57241100
C	-1.85715300	-0.75919600	-0.95765900
C	-1.25446300	0.48330200	-0.39242600
C	0.66414300	-0.75258900	0.44902200
H	0.69274400	-0.89187700	1.52525100
C	0.07099000	-2.00218200	-0.18657200
H	0.45744300	-2.86455200	0.34599600
N	-0.12608300	0.46193500	0.23768400
H	-1.37035000	-0.89799100	-1.93170100
B	0.41144400	1.76474800	0.98399800
F	-0.61324200	2.26569400	1.76736600
F	1.46869600	1.38738700	1.77916600
F	0.79615500	2.69065900	0.03179600
H	0.38595600	-2.08581500	-1.22231000
C	-1.42818000	-1.97012700	-0.12886800
O	-1.78232200	-1.86772200	1.21494500
C	-3.14729000	-2.03016900	1.48962800
H	-3.24507700	-2.14898900	2.56147300
H	-3.72805600	-1.16407600	1.17787600
C	2.07512100	-0.56867800	-0.04294200
C	3.10754900	-1.22071100	0.60872700
C	2.35236900	0.16843300	-1.18081000
C	4.39954400	-1.14284600	0.12792100
H	2.89837500	-1.78842300	1.50236100
C	3.64604500	0.25206300	-1.65927200
H	1.55748200	0.69708300	-1.68248300
C	4.67273100	-0.40542100	-1.00901200
H	5.19532200	-1.65300100	0.64588600
H	3.85211500	0.83537300	-2.54200000
H	5.68133400	-0.33920800	-1.38271500

H	-1.85993300	-2.87010900	-0.56992700
H	-3.54201900	-2.91802900	0.99530600

25

E(RmPW+HF-B95)= -1074.264715 a.u.

C	-2.26013800	-2.05143400	0.24330700
H	-1.78650300	-3.00113700	0.10894400
C	-3.59244600	-1.97064600	0.40716400
H	-4.16339800	-2.88536200	0.39681600
C	-4.29693700	-0.73583000	0.59937500
H	-5.36850600	-0.75098000	0.69845300
C	-3.61084900	0.40002400	0.66503300
H	-4.08824100	1.35286900	0.82242900
C	-2.14192100	0.43328600	0.53652300
C	-1.46121500	-0.86519500	0.27103400
C	0.43626000	0.49006100	0.26334800
H	0.12392500	0.84257200	1.24666200
C	-0.21543100	1.39007700	-0.76892000
H	-0.05531200	0.95845300	-1.75203900
N	-0.17146700	-0.84249000	0.10210900
H	-1.75346600	0.80401900	1.49364100
B	0.72434000	-1.97910100	-0.56622000
F	-0.03497300	-3.08240000	-0.89578800
F	1.22268700	-1.40500400	-1.72488800
F	1.72556400	-2.33818800	0.30530800
H	0.24360300	2.37306900	-0.74872300
C	-1.69762000	1.52393300	-0.45961400
O	-2.00314300	2.72607200	0.18628400
C	-2.11241200	3.81768500	-0.68664400
H	-1.17710300	4.01247500	-1.21003500
H	-2.89810800	3.64964000	-1.42287200
C	1.93919100	0.54212900	0.30026300
C	2.57620700	0.32786600	1.51168600
C	2.70030100	0.88453400	-0.80359300
C	3.94726600	0.43734700	1.61983100
H	1.98775600	0.07130900	2.37897000
C	4.07288800	1.00145600	-0.69889600
H	2.22305300	1.05182600	-1.75432600
C	4.70016900	0.77626300	0.51133000
H	4.42690000	0.26618700	2.56961100
H	4.65352200	1.27007500	-1.56627800
H	5.77089300	0.86981500	0.59165400
H	-2.29162200	1.43723500	-1.36888900
H	-2.36305900	4.68329200	-0.08700400

27

E(RmPW+HF-B95)= -878.012569 a.u.

C	-2.33441800	0.64272600	0.55781900
H	-1.94239500	1.56721800	0.94502500
C	-3.68611900	0.37363800	0.57443000
H	-4.36697600	1.10293900	0.97964400
C	-4.16688600	-0.82131800	0.07099800
H	-5.22507600	-1.02189900	0.07924300
C	-3.29284000	-1.75252400	-0.45485900

H	-3.66449200	-2.67545200	-0.86669500
C	-1.93600000	-1.49903100	-0.46967100
C	-1.46939200	-0.30821400	0.05020900
C	0.74447200	-0.93120700	0.41107100
H	0.38103800	-1.90808300	0.70125800
N	-0.07151900	-0.02764300	0.07307700
H	-1.25232200	-2.20663900	-0.90903000
C	2.21673500	-0.69914600	0.54023000
O	2.67515200	-0.15637100	1.49521700
O	2.87080000	-1.25265000	-0.44004500
C	4.29181600	-1.12054100	-0.38616400
H	4.66432200	-1.62823200	-1.26212300
H	4.55988400	-0.07157400	-0.40686300
H	4.67133500	-1.58161000	0.51711000
F	0.32262100	2.24631400	0.77331100
F	1.69444200	1.34586400	-0.80906300
F	-0.45342500	1.87627600	-1.33379000
B	0.40614900	1.47332600	-0.35379700

MC-26

E(RmPW+HF-B95)= -1071.078756 a.u.

C	2.86397200	0.00438800	0.26546400
H	2.94486700	-0.07904800	1.33561300
C	3.98603100	0.10505200	-0.52808900
H	4.96090000	0.10649100	-0.07052100
C	3.86213500	0.20723800	-1.90188300
H	4.74224600	0.29428100	-2.51672500
C	2.61025800	0.20766400	-2.48464800
H	2.50875200	0.30370000	-3.55248400
C	1.47671700	0.09750300	-1.70280700
C	1.61758300	-0.01464700	-0.33343500
C	-0.46796200	-0.92254000	0.15058100
H	-0.40532500	-1.46682300	-0.78123500
C	-1.85475300	1.58523300	-1.37279400
H	-1.10790800	2.31495100	-1.63919000
N	0.47569600	-0.16076500	0.50771200
H	0.49892000	0.12796300	-2.15555800
B	0.41461100	0.74757000	1.86429000
F	1.08368100	1.90148200	1.56825100
F	-0.91708500	0.98302200	2.10693300
F	1.01959700	0.02858600	2.85806700
H	-2.31521400	1.63574200	-0.40294900
C	-2.21138300	0.62417300	-2.20748000
O	-1.64374300	0.47024700	-3.41463800
C	-2.23320900	-0.51657700	-4.23035300
H	-3.25295200	-0.24522600	-4.49155200
H	-1.63776200	-0.57635600	-5.13113000
H	-2.95839100	-0.11091300	-1.94201200
H	-2.23182500	-1.48401700	-3.73374500
C	-1.69434600	-1.16044200	0.97455700
O	-2.79060600	-0.94203900	0.56341600
O	-1.38346400	-1.70621900	2.11685600
C	-2.47572000	-1.96909300	2.99521700
H	-3.18953400	-2.62682500	2.51488600
H	-2.04351100	-2.44071900	3.86380300
H	-2.95460600	-1.03529700	3.26348400

TS1n-26

E(RmPW+HF-B95)= -1071.070586 a.u.
unique imaginary frequency: cm^{-1}

C	1.89581200	-1.58729600	0.17257000
H	1.39992300	-2.17818500	0.92080600
C	3.20556400	-1.86206600	-0.15145600
H	3.71875500	-2.65489500	0.36720500
C	3.86002100	-1.13688200	-1.13044600
H	4.88600800	-1.35368300	-1.37604600
C	3.17855000	-0.14131000	-1.79746900
H	3.66693500	0.42831000	-2.57051900
C	1.85985100	0.13755000	-1.48906400
C	1.20854500	-0.57952800	-0.49395100
C	-0.88873500	0.37209100	-0.93726700
H	-0.54266200	0.56354900	-1.93982300
C	-0.79918100	2.50920300	-0.39974900
H	-1.53586400	2.29736900	0.35521200
N	-0.13246400	-0.33245700	-0.14151300
H	1.35953000	0.91023700	-2.04606600
B	-0.65736100	-0.75628400	1.30216800
F	0.32893500	-0.50149100	2.23061800
F	-1.77643600	0.02605300	1.54835100
F	-0.96765100	-2.09998300	1.29893900
H	-1.11289500	3.00407800	-1.30023500
C	0.50354700	2.53930500	-0.04149700
O	0.86275000	1.99912400	1.08473100
C	2.24007700	1.90579200	1.40876500
H	2.45424400	2.60487500	2.20785800
H	2.41241000	0.89098500	1.74191900
H	1.28736200	2.92649600	-0.67896000
H	2.85458500	2.12465700	0.54193600
C	-2.39225700	0.25734100	-0.87188300
O	-3.16934500	1.15517600	-0.96679400
O	-2.71310000	-1.01364800	-0.83665200
C	-4.10732700	-1.29433200	-0.81433100
H	-4.58200100	-0.90315200	-1.70608400
H	-4.18828900	-2.37009600	-0.77863800
H	-4.55685600	-0.84755900	0.06441700

TSa-26

E(RmPW+HF-B95)= -1071.078902 a.u.
unique imaginary frequency: -313.08 cm^{-1}

C	2.74490900	-0.86786500	-0.36854000
H	2.57815800	-1.92893300	-0.30901300
C	3.99980600	-0.35271500	-0.60489800
H	4.83324700	-1.02477800	-0.72577000
C	4.19253800	1.01493300	-0.69197500
H	5.17605200	1.41378600	-0.87596100
C	3.11689000	1.86388700	-0.53258900
H	3.25630900	2.93101600	-0.58300900
C	1.85314400	1.35906300	-0.29194000
C	1.66062400	-0.01277800	-0.22344400
C	-0.67901400	0.11836800	-0.32790100

H	-0.53494300	0.96738100	-0.98099100
C	-1.17358500	1.21335900	1.41828100
H	-0.16246300	1.34089900	1.76785800
N	0.38522400	-0.57631600	-0.01522500
H	1.03432800	2.04372200	-0.14079400
B	0.25336900	-1.88484100	0.86733900
F	1.14101900	-1.77603600	1.91683700
F	-1.05244600	-1.91542700	1.34367300
F	0.52866500	-2.99864100	0.10287500
H	-1.77447800	0.43686100	1.85351500
C	-1.79524800	2.25247100	0.81411600
O	-1.12152700	3.29213000	0.40326400
C	-1.84432000	4.28712500	-0.31524800
H	-2.63266700	4.69350800	0.30784200
H	-1.13151300	5.06043100	-0.55843300
H	-2.84772200	2.21770100	0.57105600
H	-2.25838700	3.86508200	-1.22385800
C	-1.99971300	-0.57347000	-0.55846200
O	-3.06430700	-0.14893000	-0.22856200
O	-1.80564600	-1.64650600	-1.28217400
C	-2.97265100	-2.39612100	-1.60043600
H	-3.66348200	-1.78812100	-2.17176900
H	-2.62943900	-3.23618800	-2.18477300
H	-3.45000700	-2.73411300	-0.68848300

INn-26

E(RmPW+HF-B95)= -1071.088647 a.u.

C	1.79109300	-1.62849500	0.09128900
H	1.31815900	-2.22957400	0.84619400
C	3.09584400	-1.86193400	-0.25781500
H	3.63461600	-2.65241300	0.24000700
C	3.72898100	-1.10488200	-1.23736900
H	4.75531400	-1.29460900	-1.50169700
C	3.00855700	-0.12192300	-1.87039500
H	3.46240900	0.46771700	-2.65069200
C	1.68313400	0.12767500	-1.53292400
C	1.04378300	-0.61342600	-0.53065100
C	-0.92699300	0.69409100	-0.73280100
H	-0.67316300	0.74899900	-1.78829400
C	-0.62652500	2.10554400	-0.09261800
H	-1.10427300	2.09814400	0.88310000
N	-0.24059600	-0.36948600	-0.11507200
H	1.15647000	0.86219300	-2.11718800
B	-0.73675000	-0.88729700	1.25057000
F	0.21776500	-0.67065500	2.24411500
F	-1.89278300	-0.16485200	1.57816700
F	-1.02571500	-2.24808600	1.20072000
H	-1.04875300	2.87197500	-0.73189600
C	0.79692700	2.29080800	0.06469300
O	1.32016300	1.88311400	1.12695900
C	2.75122200	1.81542000	1.24978900
H	2.97749100	2.05276700	2.27785400
H	3.02054000	0.79257200	1.01434000
C	-2.43360100	0.53631000	-0.73707000
H	1.42507300	2.77554000	-0.67376600
H	3.21468000	2.51321800	0.56394000

C	-4.18019400	-0.94253000	-1.06840000
H	-4.65881800	-0.30896300	-1.80426200
H	-4.28621700	-1.98225500	-1.33632300
H	-4.61410300	-0.75654600	-0.09322400
O	-2.78175100	-0.69286000	-1.03303900
O	-3.20069500	1.43930900	-0.57602200

INa-26

E(RmPW+HF-B95)= -1071.105849 a.u.

C	3.13303000	-0.32596300	-0.20889000
H	3.08407900	-1.39589200	-0.10657400
C	4.34074100	0.29234800	-0.43721400
H	5.23258400	-0.31097200	-0.50116800
C	4.42340500	1.66568800	-0.59554100
H	5.37096400	2.14421500	-0.77801700
C	3.26333200	2.40702200	-0.50951600
H	3.29780800	3.47967000	-0.61665600
C	2.04462800	1.79974700	-0.26984300
C	1.95055400	0.41577700	-0.12367900
C	-0.45865400	0.46015700	-0.04390300
H	-0.36380700	1.24458600	-0.79727700
C	-1.13894600	1.02299700	1.20699300
H	-0.83933500	2.03612600	1.43768000
N	0.75992000	-0.24110900	0.10629300
H	1.17144000	2.42369900	-0.17310400
B	0.71049400	-1.62549900	0.74905000
F	1.51968900	-1.69867400	1.87571900
F	-0.63789700	-1.83865400	1.13371400
F	1.07653500	-2.63803100	-0.13677600
H	-0.92460000	0.37165200	2.04345900
C	-2.60257400	0.97838900	0.87541500
O	-2.98663000	2.07515800	0.20621900
C	-4.37630300	2.15488900	-0.05860800
H	-4.94029200	2.05945300	0.86551300
H	-4.55235400	3.12689500	-0.49584400
H	-3.28053200	0.69248800	1.67094000
H	-4.67752400	1.37992800	-0.75618900
C	-1.54900800	-0.41286100	-0.56338100
O	-2.69133800	-0.19969200	-0.07353000
O	-1.36276600	-1.26611800	-1.46326900
C	-2.46729600	-2.09922300	-1.86963700
H	-3.24935900	-1.47767400	-2.28346700
H	-2.05708500	-2.76145800	-2.61384300
H	-2.82043900	-2.64780600	-1.00721000

TS2n-26

E(RmPW+HF-B95)= -1071.086745 a.u.

unique imaginary frequency: -176.89 cm^{-1}

C	-1.78548400	1.60178000	-0.40635700
H	-1.30122300	2.45648400	0.02990300
C	-3.10244800	1.65259900	-0.75224500
H	-3.65783100	2.55619800	-0.55878800
C	-3.75035900	0.56137400	-1.35009000
H	-4.79453900	0.62294400	-1.60430300

C	-3.02584400	-0.55519900	-1.63637300
H	-3.48262400	-1.38839600	-2.14515700
C	-1.65881700	-0.63661400	-1.31131100
C	-1.01472200	0.45017900	-0.67864800
C	0.91755800	-0.84028300	-0.63593300
H	0.75742500	-1.01681000	-1.69961000
C	0.36366200	-2.09101700	0.11142800
H	0.91615900	-2.17486100	1.04199300
N	0.26744300	0.36522000	-0.27295500
H	-1.09323700	-1.40586800	-1.80939000
B	0.79425600	1.25847200	0.88733700
F	-0.18477500	1.40203600	1.86477100
F	1.90030800	0.61623700	1.44153000
F	1.14450200	2.51546500	0.41240300
H	0.53805300	-2.97379500	-0.49095200
C	-1.05555600	-1.98556100	0.45231400
O	-1.30221300	-1.33387200	1.52062800
C	-2.66258200	-1.11966500	1.88692100
H	-2.66858700	-0.94517100	2.95164600
H	-3.00608500	-0.24153500	1.35346600
C	2.42013300	-0.79840600	-0.50873400
H	-1.80534600	-2.66837800	0.08075600
H	-3.25927200	-1.98771000	1.63179200
O	2.91078700	0.27244800	-1.09029800
O	3.07843800	-1.67406000	-0.03141000
C	4.31922600	0.42404400	-1.00490600
H	4.54893800	1.34798100	-1.51453800
H	4.61990600	0.48002100	0.03493600
H	4.81986800	-0.40917800	-1.48384700

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E(RmPW+HF-B95)= -1071.115221 a.u.

C	-1.51809100	1.89979800	-0.25419700
H	-0.93085600	2.72126400	0.11017900
C	-2.81354900	2.06167700	-0.57448300
H	-3.26139600	3.03349000	-0.44328800
C	-3.63213900	1.00476200	-1.09778300
H	-4.66410000	1.20854400	-1.32551900
C	-3.10217300	-0.19421100	-1.32484900
H	-3.68619200	-0.99212500	-1.75514200
C	-1.68581600	-0.48988900	-1.03720900
C	-0.89808400	0.63477400	-0.46512400
C	0.83074500	-0.89390600	-0.59029800
H	0.70243400	-0.92603700	-1.67414600
C	0.00847700	-2.00857200	0.02025300
H	0.27390900	-2.13467300	1.06318100
N	0.34038800	0.39983500	-0.15085300
H	-1.22490900	-0.80382800	-1.98040400
B	1.15950200	1.36357200	0.81785600
F	0.30067100	1.79966700	1.80741100
F	2.16953700	0.61150100	1.38716000
F	1.64836000	2.42372600	0.09004400
H	0.23419600	-2.93240100	-0.49993900
C	-1.47601600	-1.68640100	-0.06491000
O	-1.93245600	-1.34712700	1.20975000
C	-3.23369300	-1.78121800	1.50931500

H	-3.43865900	-1.48202600	2.52943300
H	-3.97564500	-1.32791800	0.85615100
H	-2.03298800	-2.53789500	-0.44979900
H	-3.30742800	-2.86549500	1.43426900
C	2.31396000	-1.07293300	-0.39892600
O	2.81498400	-1.98642900	0.18266700
O	2.97452600	-0.13830300	-1.04856600
C	4.37967100	-0.13323100	-0.85259600
H	4.81887200	-1.04871400	-1.23102900
H	4.75294700	0.71992300	-1.39927700
H	4.59628000	-0.03189600	0.20452200

TS1-13a

E(RmPW+HF-B95)= -631.945024 a.u.
unique imaginary frequency: -458.42 cm^{-1}

C	-2.03089200	0.94738600	0.89012800
H	-2.09644400	1.59800200	1.74794700
C	-2.97037700	-0.04051000	0.71633500
H	-3.76682900	-0.14251900	1.43744800
C	-2.90768600	-0.90399900	-0.36995600
H	-3.64580100	-1.67674700	-0.50595200
C	-1.87190300	-0.74601000	-1.26834900
H	-1.79770200	-1.40120600	-2.12338000
C	-0.91388700	0.23863100	-1.09468900
C	-0.96248700	1.12946700	-0.00665300
C	0.98629600	2.23628300	-0.54176600
H	0.92871400	1.93709200	-1.58784200
C	2.44657700	1.15318700	-0.04730300
H	2.71215000	1.65241800	0.86822500
N	-0.06904500	2.12423800	0.26345800
H	-0.12222600	0.30955500	-1.82259500
H	1.54277400	3.15835000	-0.42793600
H	3.15085300	1.24726700	-0.85685700
C	1.95608100	-0.12448200	0.15309700
O	1.34596300	-0.44929700	1.25036600
C	1.26004500	-2.20591900	-0.24128200
C	0.66974800	-1.69674000	1.06150900
H	1.96487700	-3.01644200	-0.11211400
H	0.88448700	-2.32564400	1.91291500
O	1.98423500	-1.07350800	-0.73807400
H	0.50848600	-2.46954600	-0.97235100
H	-0.39068900	-1.48156200	0.99352800

IN1-13a

E(RmPW+HF-B95)= -631.949034 a.u.

C	2.04716700	0.97982900	-0.84492100
H	2.13474400	1.67685100	-1.66455300
C	2.96242000	-0.02512200	-0.68745700
H	3.77644600	-0.10827900	-1.39271600
C	2.86602400	-0.93839300	0.36399000
H	3.59055100	-1.72593500	0.48683200
C	1.81530500	-0.78834100	1.24530300
H	1.71873200	-1.46498500	2.08277600
C	0.86884200	0.21316900	1.09068000

C	0.93571500	1.15193900	0.02601600
C	-1.08549100	2.17360500	0.54609200
H	-0.97361700	1.90950900	1.60259300
C	-2.27797700	1.26157700	-0.01222800
H	-2.54388100	1.65780400	-0.98340700
N	0.07081400	2.13462900	-0.23821500
H	0.08462300	0.28179900	1.82753100
H	-1.53533500	3.16360700	0.51863100
H	-3.11611300	1.29670000	0.67157900
C	-1.84226500	-0.09788800	-0.18486700
O	-1.22895800	-0.46069500	-1.24144700
C	-1.33938400	-2.21127500	0.26054000
C	-0.68354300	-1.77977300	-1.03957500
H	-2.09227500	-2.97756000	0.14644700
H	-0.95581300	-2.38081100	-1.89364000
O	-2.01419900	-1.01119000	0.69328800
H	-0.62895000	-2.47537200	1.03033300
H	0.38958700	-1.65661600	-0.96106500

TS2-13a

E(RmPW+HF-B95)= -631.945649 a.u.

unique imaginary frequency: -265.40 cm^{-1}

C	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.07900542
C	1.15176407	0.00000000	-0.71934559
H	2.09950177	-0.00128181	-0.20221924
C	1.13580108	-0.00275798	-2.13047405
H	2.05829164	-0.00879090	-2.68651468
C	-0.07282452	-0.01350362	-2.76726260
H	-0.11169793	-0.05650774	-3.84616886
C	-1.28129830	0.00346294	-2.05134843
C	-1.28566377	-0.00414168	-0.62535982
C	-3.55066560	0.14714577	-0.64935719
H	-3.65974689	-0.65821141	-1.38456920
C	-3.69125665	1.49018052	-1.45603753
H	-4.08815720	2.23410793	-0.77221069
N	-2.37065387	0.06362286	0.11694408
H	-2.17967807	-0.23533485	-2.59692185
H	-4.42534249	0.10367701	-0.00777157
H	-4.38208670	1.36519960	-2.28096115
C	-2.45831036	2.06737129	-1.98243021
O	-1.68903114	2.74282890	-1.18672261
C	-1.11462253	3.14741185	-3.37946905
C	-0.58408226	3.22509508	-1.95863611
H	-1.39512690	4.10466074	-3.79708105
H	-0.35907648	4.22722988	-1.62626617
O	-2.31622884	2.37504737	-3.23658609
H	-0.45211950	2.61802161	-4.05006594
H	0.24775246	2.55560910	-1.78056793