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Investigation of the solvent effect, regioselectivity, and the mechanism of the cycloaddition reaction between 2-chlorobenzimidazole and benzonitrile oxide

Mohamed Abdoul-Hakim[1,2], Khadija El Idrissi[1,2], Abdellah Zeroual[1]*, Hocine Garmes[2]

[1] *Molecular Modelling, Spectroscopy and Environment Research Team, Faculty of Science, Chouaïb Doukkali University, P. O. Box 20, 24000 El Jadida, Morocco; e-mail: zeroualabdellah2@gmail.com*

[2] *Analytical Chemistry and Environmental Sciences Team, Department of chemistry, Faculty of Science, Chouaib Doukkali University, P. O. Box 20, 24000 El Jadida, Morocco*

SUPPLEMENTARY INFORMATION

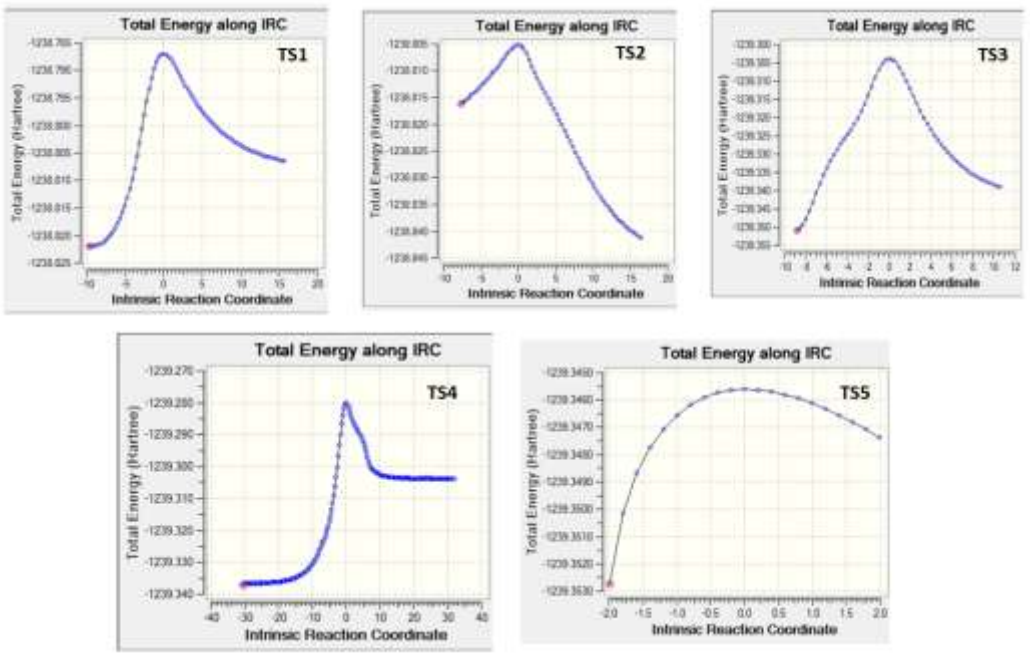
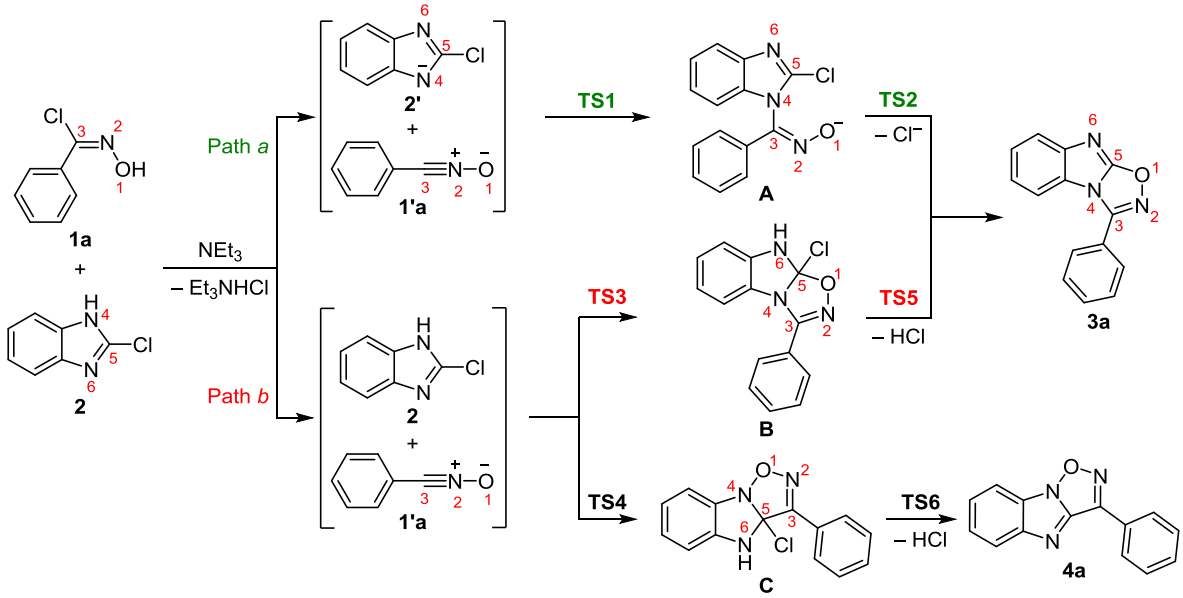


Figure S1. B3LYP/6-311G+(d,p) IRC profile associated with **TS1**–**TS5**



Scheme S1. Obtaining 3-phenyl[1,2,4]oxadiazolo[4,5-*a*]benzimidazole (**3a**) by two separate pathways

Table S1. B3LYP/6-311+G(d,p) total (a.u.) and relative enthalpies (kcal·mol^{-1}), total (a.u.) and relative (cal·mol^{-1}·K^{-1}) entropies, and total (a.u.) and relative (kcal·mol^{-1}) Gibbs energies, of the stationary points involved in the reaction of **1'a** with **2'** in gas phase and MeOH.

System	*H*	Δ*H**	*G*	Δ*G**	*S*	Δ*S**
Gas phase						
1'a	-399.638765		-399.679452		85.632	
2'	-838.945689		-838.985844		84.515	
1'a + **2'**	-1238.58445		-1238.665296		170.147	
TS1	-1238.57339	6.95	-1238.636535	18.05	132.908	-37.24
A	-1238.60597	-13.50	-1238.666528	-0.77	127.462	-42.69
TS2	-1238.59056	9.67	-1238.646989	12.26	118.759	-8.70
3a	-778.31611		-778.369258		111.859	
Cl^-	-460.301367		-460.31875		36.586	
3a + Cl^-	-1238.61748	-7.22	-1238.688008	-13.48	148.445	20.98
MeOH						
1'a	-399.646671		-399.687145		85.187	
2'	-839.024857		-839.064982		84.452	
1'a + **2'**	-1238.67153		-1238.752127		169.639	
TS1	-1238.64905	14.11	-1238.711849	25.28	132.18	-37.46
A	-1238.6854	-8.71	-1238.745847	3.94	127.216	-42.42
TS2	-1238.6681	10.86	-1238.724659	13.30	119.039	-8.18
3a	-778.328007		-778.381142		111.833	
Cl^-	-460.410401		-460.427784		36.586	
3a + Cl^-	-1238.73841	-33.26	-1238.808926	-39.58	148.419	21.20

*Relative to **1'a** + **2'** for **TS1** and **A**; relative to **A** for **TS2** and **3a**

Table S2: B3LYP/6-311+G(d,p) total (a.u.) and relative enthalpies (kcal·mol^{-1}) enthalpies, total (a.u.) and relative (cal·mol^{-1}·K^{-1}) entropies, and total (a.u.) and relative (kcal·mol^{-1}) Gibbs energies, of the stationary points involved in the reaction of **1'a** with **2'** inTHF.

System	*H*	Δ*H**	*G*	Δ*G**	*S*	Δ*S**
1'a	-399.645629		-399.686125		85.233	
2'	-839.015983		-839.056109		84.453	
1'a + **2'**	-1238.66161		-1238.742234		169.686	
TS1	-1238.64007	1355	-1238.702836	24.72	132.094	-37.592
A	-1238.6759	-8.96	-1238.736526	3.58	127.602	-42.084
TS2	-1238.6589	10.66	-1238.71543	13.23	118.973	-8.629
3a	-778.326487		-778.37962		111.828	
Cl^-	-460.398603		-460.415986		36.586	
3a + Cl^-	-1238.72509	-30.86	-1238.795606	-37.07	148.414	20.812

*Relative to **1'a** + **2'** for **TS1** and **A**; relative to **A** for **TS2** and **3a**

Table S3. B3LYP/6-311+G(d,p) total (a.u.) and relative enthalpies (kcal·mol^{-1}) enthalpies, total (a.u.) and relative (cal·mol^{-1}·K $^{-1}$) entropies, and total (a.u.) and relative (kcal·mol^{-1}) Gibbs energies, of the stationary points involved in the reaction of **1'a** with **2** in gas phase and MeOH.

System	*H*	Δ*H**	*G*	Δ*G**	*S*	Δ*S**
Gas phase						
1'a	-399.638765		-399.679452		85.632	
2	-839.47142		-839.512128		85.667	
1'a + **2**	-1239.110185		-1239.19158		171.299	
TS3	-1239.076221	21.31	-1239.136559	34.53	126.991	-44.31
TS4	-1239.053146	35.79	-1239.112964	49.33	125.897	-45.40
B	-1239.131106	-13.13	-1239.18896	1.64	121.762	-49.54
C	-1239.074989	22.09	-1239.133933	36.17	124.058	-46.64
TS5	-1239.115684	9.68	-1239.173925	9.44	122.579	0.87
TS6	-1239.069697	3.32	-1239.112964	13.16	121.337	
3a	-778.31611		-778.369258		111.859	
4a	-778.265418		-778.319505		113.836	
HCl	-460.826987		-460.848184		44.612	
3a + HCl	-1239.143097	-7,53	-1239.217442	-17.87	156.471	34.71
4a + HCl	-1239.092405	-10,93	-1239.167689	-21.18	158.448	34.39
MeOH						
1'a	-399.646671		-399.687145		85.187	
2	-839.481362		-839.521947		85.418	
1'a + **2**	-1239.128033		-1239.209092		170.605	
TS3	-1239.095179	20.67	-1239.157464	32.34	131.048	-39.56
TS4	-1239.068049	37.64	-1239.129025	50.24	128.334	-42.27
B	-1239.161687	-21.12	-1239.223066	-8.77	129.184	-41.42
C	-1239.109582	11.58	-1239.168813	25.28	124.662	-45.94
TS5	-1239.161339	0.22	-1239.22008	1.88	123.626	-5.55
TS6	-1239.109243	0.21	-1239.16862	0.12	124.968	0.32
3a	-778.328007		-778.381142		111.833	
4a	-778.27322		-778.327565		114.379	
HCl	-460.827306		-460.848504		44.613	
3a + HCl	-1239.155313	4.00	-1239.229646	-4.13	156.446	27.26
4a + HCl	-1239.100526	5.68	-1239.176069	-4.55	158.449	34.33

*Relative to **1'a** + **2** for **TS3**, **TS4**, **B,** and **C** ; relative to **A** for **TS5**, **TS6**, **3a** + HCl, and **4a** + HCl

Table S4. Valence pool populations calculated from the ELF of the most relevant points along the IRC curve associated with **TS1** in the nucleophilic addition step of **1'a** to **2'**

IRC	Distance, Å		ΔE, kcal·mol^{-1}	Bassins																					
	(N3,C1)	(C5,O)		V(N3,O)	V(N3,C1)	V'(N3,C1)	V(N2,C1)	V(C5,N2)	V(C5,Cl)	V(C5,N1)	V(C5,O)	V(Asyn) (C5,Cl)	V(O)	V'(O)	V'' (O)	V(N3)	V(C1)	V'(C1)	V(N2)	V'(N2)	V'' (N2)	V(C5)	V(Cl)	V' (Cl)	V'' (Cl)	V(N1)
P1	3.50	4.75	0	1.61	3.39	2.58		2.49	1.51	2.74			2.73	2.96					3.13				3.16	3.20		3.09
P2	3.47	4.72	0,07	1.61	3.38	2.58		2.49	1.51	2.74			2.73	2.97					3.13				3.16	3.20		3.09
P3	3.45	4.70	0,13	1.61	3.38	2.58		2.50	1.51	2.74			2.72	2.96					3.13				3.16	3.20		3.09
P4	3.42	4.68	0,21	1.61	3.38	2.58		2.50	1.51	2.73			2.73	2.97					3.13				3.16	3.20		3.09
P5	3.39	4.66	0,28	1.60	3.39	2.59		2.49	1.51	2.74			2.73	2.96					3.13				3.17	3.20		3.09
P6	3.37	4.64	0,35	1.60	3.39	2.58		2.49	1.51	2.73			2.75	2.95					3.14				3.17	3.20		3.09
P7	3.34	4.61	0,43	1.60	3.39	2.58		2.49	1.51	2.74			2.74	2.95					3.14				3.17	3.20		3.09
P8	3.31	4.59	0,51	1.59	3.38	2.59		2.50	1.51	2.74			2.74	2.95					3.13				3.17	3.20		3.09
P9	3.28	4.58	0,6	1.60	3.37	2.60		2.49	1.51	2.74			2.74	2.94					3.13				3.17	3.20		3.09
P10	3.26	4.56	0,69	1.61	3.37	2.60		2.49	1.51	2.74			2.75	2.94					3.13				3.17	3.19		3.09
P11	3.23	4.54	0,79	1.60	3.37	2.61		2.49	1.51	2.74			2.76	2.94					3.13				3.18	3.19		3.09
P12	3.20	4.53	0,88	1.59	3.36	2.62		2.49	1.51	2.74			2.76	2.93					3.13				3.17	3.19		3.09
P13	3.17	4.51	0,99	1.59	3.36	2.62		2.49	1.51	2.74			2.77	2.94					3.14				3.18	3.19		3.10
P14	3.14	4.50	1,1	1.59	3.35	2.63		2.49	1.51	2.74			2.78	2.93					3.13				3.17	3.19		3.09
P15	3.11	4.48	1,22	1.59	3.35	2.63		2.49	1.51	2.74			2.79	2.93					3.14				3.18	3.18		3.09
P16	3.08	4.47	1,35	1.59	3.35	2.63		2.50	1.51	2.74			2.79	2.92					3.13				3.18	3.18		3.10
P17	3.06	4.46	1,48	1.59	3.35	2.64		2.49	1.51	2.74			2.78	2.92					3.12				3.18	3.19		3.09
P18	3.03	4.45	1,61	1.59	3.34	2.64		2.49	1.51	2.74			2.80	2.91					3.13				3.18	3.19		3.09
P19	3.00	4.43	1,76	1.59	3.34	2.65		2.49	1.51	2.74			2.80	2.91					3.13				3.18	3.18		3.09
P20	2.97	4.42	1,92	1.59	3.34	2.65		2.49	1.51	2.74			2.80	2.90					3.13				3.18	3.18		3.09
P21	2.94	4.41	2,09	1.59	3.34	2.65		2.48	1.51	2.74			2.81	2.89					3.13				3.19	3.18		3.09
P22	2.92	4.40	2,26	1.59	3.34	2.65		2.49	1.50	2.75			2.82	2.88					3.13				3.19	3.18		3.09

Table S4 (continued)**.** Valence pool populations calculated from the ELF of the most relevant points along the IRC curve associated with **TS1** in the nucleophilic addition step of **1'a** to **2'**

IRC	Distance, Å		ΔE, kcal·mol^{-1}	Basin																					
	(N3,C1)	(C5,O)		V(N3,O)	V(N3,C1)	V'(N3,C1)	V(N2,C1)	V(C5,N2)	V(C5,Cl)	V(C5,N1)	V(C5,O)	V(Asyn)(N2,C1)	V(O)	V'(O)	V'' (O)	V(N3)	V(C1)	V'(C1)	V(N2)	V'(N2)	V'' (N2)	V(C5)	V(Cl)	V' (Cl)	V'' (Cl)	V(N1)
P23	2.89	4.39	2,45	1.58	3.35	2.65		2.49	1.51	2.75			2.82	2.89					3.12				3.19	3.18		3.09
P24	2.86	4.38	2,64	1.58	3.35	2.65		2.49	1.51	2.75			2.83	2.89					3.12				3.19	3.17		3.09
P25	2.83	4.36	2,85	1.57	3.36	2.64		2.49	1.51	2.75			2.84	2.88					3.12				3.19	3.17		3.09
P26	2.81	4.35	3,07	1.58	3.37	2.63		2.49	1.51	2.75			2.84	2.87					3.11				3.19	3.18		3.09
P27	2.78	4.34	3,3	1.58	3.38	2.63		2.48	1.51	2.75			2.84	2.86					3.11				3.19	3.17		3.09
P28	2.75	4.33	3,54	1.58	3.39	2.62		2.48	1.51	2.75			2.85	2.86					3.10				3.20	3.17		3.09
P29	2.72	4.32	3,8	1.57	3.39	2.62		2.48	1.51	2.76			2.86	2.85					3.11				3.20	3.16		3.09
P30	2.69	4.31	4,06	1.57	3.41	2.61		2.48	1.51	2.76			2.87	2.85					3.11				3.20	3.16		3.09
P31	2.67	4.30	4,35	1.56	3.43	2.60		2.48	1.51	2.75			2.88	2.84					3.11				3.20	3.16		3.10
P32	2.64	4.29	4,64	1.56	3.44	2.59		2.48	1.51	2.76			2.89	2.84					3.10				3.20	3.17		3.10
P33	2.61	4.27	4,96	1.55	3.46	2.57		2.48	1.51	2.76			2.90	2.83					3.09				3.20	3.16		3.10
P34	2.58	4.26	5,29	1.55	3.49	2.55		2.48	1.51	2.76			2.92	2.83					3.09				3.21	3.16		3.09
P35	2.56	4.25	5,64	1.54	3.51	2.53		2.48	1.51	2.76			2.92	2.82					3.08				3.21	3.16		3.10
P36	2.59	4.23	6	1.54	3.54	2.51		2.47	1.51	2.77			2.92	2.83					3.08				3.21	3.15		3.09
P37	2.50	4.22	6,39	1.54	3.56	2.49		2.47	1.51	2.77			2.93	2.81					3.08				3.20	3.17		3.09
P38	2.47	4.20	6,79	1.54	3.60	2.47		2.48	1.51	2.77			2.94	2.80					3.07				3.20	3.16		3.08
P39	2.44	4.19	7,22	1.53	3.63	2.44		2.47	1.51	2.77			2.95	2.80					3.07				3.20	3.16		3.09
P40	2.41	4.17	7,67	1.52	3.68	2.39		2.47	1.52	2.77			2.97	2.79					3.07				3.19	3.16		3.09
P41	2.38	4.15	8,14	1.51	3.74	2.35		2.46	1.52	2.78			2.97	2.78					3.06				3.19	3.16		3.09
P42	2.35	4.13	8,62	1.50	3.79	2.31		2.46	1.52	2.78			2.98	2.78					3.05				3.19	3.17		3.08
P43	2.31	4.11	9,13	1.50	3.86	2.26		2.45	1.52	2.79			3.00	2.77					3.04				3.19	3.17		3.08
P44	2.28	4.09	9,64	1.48	3.93	2.22		2.44	1.52	2.80			3.01	2.75					3.04				3.18	3.17		3.09

Table S4 (continued)**.** Valence pool populations calculated from the ELF of the most relevant points along the IRC curve associated with **TS1** in the nucleophilic addition step of **1'a** to **2'**

IRC	Distance, Å		ΔE, kcal·mol^{-1}	Basin																					
	(N3,C1)	(C5,O)		V(N3,O)	V(N3,C1)	V'(N3,C1)	V(N2,C1)	V(C5,N2)	V(C5,Cl)	V(C5,N1)	V(C5,O)	V(Asyn)(N2,C1)	V(O)	V'(O)	V" (O)	V(N3)	V(C1)	V'(C1)	V(N2)	V'(N2)	V" (N2)	V(C5)	V(Cl)	V' (Cl)	V" (Cl)	V(N1)
P45	2.25	4.07	10,16	1.48	3.97	2.21		2.44	1.53	2.81			3.01	2.76					3.02				3.18	3.17		3.08
P46	2.21	4.05	10,67	1.47	4.01			2.42	1.53	2.81			3.02	2.75		2.20			3.02				3.18	3.17		3.07
P47	2.17	4.02	11,14	1.46	4.03			2.41	1.54	2.82			3.02	2.77		2.21			3.01				3.17	3.17		3.07
P48	2.14	4.00	11,56	1.45	3.33			2.40	1.54	2.83			3.02	2.77		2.23	0.36	0.36	3.00				3.17	3.17		3.07
P49	2.10	3.98	11,9	1.44	3.29			2.38	1.55	2.84			3.01	2.79		2.27	0.39	0.39	2.99				3.17	3.17		3.06
P50	2.06	3.95	12,12	1.44	3.22			2.37	1.55	2.85			3.01	2.79		2.29	0.42	0.42	2.98				3.17	3.16		3.05
P51	2.02	3.93	12,2	1.43	3.12			2.35	1.56	2.86			2.99	2.79		2.33	0.47	0.47	2.98				3.17	3.16		3.04
P52	1.98	3.91	12,11	1.43	3.03			2.33	1.57	2.87			2.99	2.81		2.36	0.52	0.52	2.97				3.17	3.15		3.04
P53	1.94	3.88	11,82	1.43	2.91			2.31	1.58	2.88			2.99	2.84		2.40	0.56	0.59	2.96				3.17	3.14		3.03
P54	1.89	3.86	11,29	1.43	2.79			2.30	1.58	2.90		0.05	2.99	2.83		2.46	0.58	0.57	2.98				3.18	3.13		3.02
P55	1.85	3.84	10,53	1.43	2.70		3.08	2.28	1.59	2.91			2.95	2.86		2.51	0.58	0.58					3.19	3.12		3.01
P56	1.81	3.82	9,50	1.44	2.63		1.89	2.26	1.60	2.92			3.00	2.83		2.55	0.59	0.59		1.25			3.19	3.11		3.01
P57	1.76	3.80	8,25	1.43	2.57		1.89	2.24	1.61	2.93			2.96	2.88		2.58	0.60	0.60		1.28			3.20	3.09		3.00
P58	1.72	3.77	6,80	1.43	2.51		1.51	2.22	1.61	2.94			2.98	2.84		2.61	0.61	0.61		1.28	0.40		3.21	3.08		2.99
P59	1.68	3.75	5,23	1.44	2.46		1.53	2.21	1.62	2.94			2.95	2.88		2.64	0.61	0.61		1.28	0.43		3.21	3.07		2.99
P60	1.64	3.73	3,61	1.45	2.43		1.55	2.19	1.62	2.96			2.96	2.86		2.66	0.61	0.61		1.26	0.46		3.22	3.07		2.97
P61	1.60	3.70	2,02	1.45	2.41		1.59	2.18	1.62	2.96			2.94	2.87		2.67	0.60	0.61		1.24	0.48		3.23	3.05		2.97
P62	1.57	3.68	0,53	1.45	2.39		1.62	2.17	1.63	2.96			2.95	2.86		2.69	0.59	0.60		1.22	0.50		3.23	3.05		2.97
P63	1.55	3.65	-0,85	1.45	2.38		1.66	2.17	1.63	2.97			2.94	2.87		2.70	0.59	0.60		1.20	0.50		3.23	3.04		2.97
P64	1.53	3.62	-2,1	1.46	2.37		1.69	2.16	1.64	2.97			2.94	2.85		2.70	0.58	0.59		1.17	0.51		3.23	3.04		2.96
P65	1.51	3.59	-3,22	1.45	2.38		1.71	2.16	1.63	2.97			2.94	2.86		2.71	0.57	0.58		1.14	0.52		3.24	3.04		2.96
P66	1.50	3.56	-4,21	1.45	2.38		1.73	2.16	1.63	2.98			2.94	2.86		2.71	0.56	0.57		1.13	0.52		3.24	3.04		2.95

Table S4 (continued)**.** Valence pool populations calculated from the ELF of the most relevant points along the IRC curve associated with **TS1** in the nucleophilic addition step of **1'a** to **2'**

IRC	Distance, Å		ΔE, kcal·mol^{-1}	Basin																						
	(N3,C1)	(C5,O)		V(N3,O)	V(N3,C1)	V'(N3,C1)	V(N2,C1)	V(C5,N2)	V(C5,Cl)	V(C5,N1)	V(C5,O)	V(Asyn)(N2,C1)	V(O)	V'(O)	V'' (O)	V(N3)	V(C1)	V'(C1)	V(N2)	V'(N2)	V'' (N2)	V(C5)	V(Cl)	V' (Cl)	V'' (Cl)	V(N1)
P67	1.49	3.54	-5,08	1.43	2.40		1.84	2.23	1.63	2.97			2.96	2.86		2.73	0.51	0.51		1.07	0.39		3.28	3.00		2.96
P68	1.48	3.51	-5,85	1.45	2.38		1.77	2.17	1.64	2.97			2.95	2.86		2.72	0.55	0.55		1.09	0.51		3.24	3.04		2.96
P69	1.47	3.48	-6,52	1.45	2.39		1.78	2.18	1.63	2.97			2.95	2.86		2.71	0.54	0.54		1.08	0.50		3.25	3.03		2.96
P70	1.47	3.46	-7,09	1.44	2.39		1.79	2.19	1.63	2.97			2.94	2.85		2.72	0.54	0.53		1.08	0.49		3.25	3.03		2.96
P71	1.46	3.43	-7,6	1.44	2.40		1.80	2.20	1.63	2.97			2.96	2.87		2.72	0.53	0.53		1.07	0.47		3.26	3.02		2.96
P72	1.46	3.41	-8,04	1.44	2.39		1.81	2.20	1.63	2.98			2.94	2.86		2.72	0.53	0.53		1.07	0.46		3.26	3.02		2.96
P73	1.45	3.38	-8,42	1.44	2.39		1.82	2.21	1.63	2.97			2.95	2.86		2.73	0.52	0.52		1.07	0.44		3.26	3.01		2.96
P74	1.45	3.36	-8,75	1.43	2.40		1.82	2.23	1.63	2.97			2.95	2.86		2.74	0.52	0.52		1.07	0.42		3.27	3.01		2.95
P75	1.45	3.34	-9,02	1.43	2.40		1.83	2.23	1.63	2.97			2.96	2.87		2.74	0.51	0.51		1.07	0.40		3.28	3.00		2.96
P76	1.45	3.32	-9,24	1.43	2.40		1.84	2.23	1.63	2.97			2.96	2.86		2.73	0.51	0.51		1.07	0.39		3.28	3.00		2.96
P77	1.44	3.30	-9,4	1.43	2.40		1.84	2.22	1.63	2.97			2.96	2.86		2.74	0.51	0.51		1.07	0.38		3.28	3.01		2.96
P78	1.44	3.28	-9,53	1.42	2.40		1.85	2.21	1.63	2.98			3.28	2.86		2.74	0.51	0.51		1.08	0.37		3.28	3.00		2.96
P79	1.44	3.27	-9,62	1.41	2.40		1.85	2.57	1.63	2.96			2.96	2.86		2.75	0.50	0.50		1.08			3.28	3.00		2.97
P80	1.44	3.26	-9,66	1.42	2.40		1.85	2.57	1.63	2.96			2.96	2.86		2.75	0.50	0.50		1.07			3.29	3.00		2.97
P81	1.44	3.26	-9,69	1.42	2.40		1.86	2.57	1.63	2.96			2.96	2.86		2.74	0.50	0.50		1.07			3.28	3.00		2.97
P82	1.44	3.26	-9,7	1.43	2.40		1.86	2.58	1.63	2.96			2.96	2.86		2.75	0.50	0.50		1.06			3.29	3.00		2.97
P83	1.44	3.26	-9,71	1.42	2.41		1.86	2.60	1.63	2.96			2.96	2.86		2.75	0.50	0.49		1.04			3.29	3.00		2.98

Table S5. Valence pool populations calculated from the ELF of the most relevant points along the IRC curve associated with **TS2** in the nucleophilic addition step of **1'a** to **2'**

IRC	Distance, Å		ΔE, kcal·mol^{-1}	Basin																				
	(C5,Cl)	(C5,O)		V(N3,O)	V(N3,C1)	V(N2,C1)	V(C5,N2)	V(C5,Cl)	V(C5,N1)	V(C5,O)	V(Asyn)(C5,O)	V(Asyn)(C5,Cl)	V(O)	V'(O)	V'' (O)	V(N3)	V(C1)	V'(C1)	V(N2)	V'(N2)	V(C5)	V(Cl)	V' (Cl)	V'' (Cl)	V(N1)
S1	1,73	2,63	0	1.39	2.46	1.80	2.28	1.66	2.93				3.02	2.81		2.75	0.34	0.55	1.47			3.43	2.85		2.98
S2	1,73	2,62	0,25	1.40	2.46	1.79	2.28	1.65	2.94				3.02	2.79		2.75	0.34	0.55	1.49			3.44	2.83		2.97
S3	1,73	2,60	0,5	1.39	2.47	1.79	2.27	1.65	2.94				3.03	2.79		2.75	0.34	0.54	1.51			3.45	2.83		2.98
S4	1,73	2,58	0,77	1.39	2.47	1.79	2.26	1.65	2.94				3.03	2.77		2.76	0.34	0.54	1.53			3.48	2.80		2.98
S5	1,73	2,56	1,05	1.39	2.48	1.78	2.25	1.66	2.93				3.04	2.76		2.76	0.33	0.53	1.55			3.51	2.78		2.97
S6	1,74	2,53	1,35	1.39	2.49	1.78	2.24	1.65	2.94				3.04	2.77		2.76	0.33	0.53	1.57			3.54	2.75		2.98
S7	1,74	2,51	1,65	1.39	2.50	1.78	2.22	1.65	2.94				3.04	2.76		2.75	0.33	0.52	1.58			3.56	2.73		2.99
S8	1,74	2,48	1,97	1.38	2.51	1.77	2.22	1.65	2.93				3.06	2.74		2.75	0.33	0.51	1.60			3.58	2.71		2.99
S9	1,74	2,46	2,3	1.38	2.51	1.77	2.21	1.65	2.93				3.08	2.73		2.75	0.32	0.50	1.62			3.61	2.69		2.99
S10	1,74	2,43	2,64	1.37	2.52	1.77	2.20	1.65	2.92				3.09	2.71		2.76	0.32	0.49	1.64			3.65	2.65		2.99
S11	1,75	2,39	2,99	1.37	2.54	1.77	2.18	1.65	2.92				3.12	2.68		2.76	0.32	0.47	1.66			3.68	2.63		2.99
S12	1,75	2,36	3,36	1.36	2.55	1.77	2.17	1.65	2.92				3.13	2.66		2.76	0.32	0.45	1.68			3.72	2.60		3.00
S13	1,75	2,32	3,74	1.36	2.56	1.77	2.15	1.64	2.91				3.18	2.62		2.76	0.33	0.44	1.71			3.74	2.58		3.01
S14	1,76	2,27	4,14	1.35	2.88	1.77	2.14	1.64	2.91				3.24	2.56		2.77		0.43	1.73			3.78	2.55		3.02
S15	1,76	2,23	4,55	1.34	3.31	1.77	2.13	1.63	2.90				3.31	2.47		2.77			1.76			2.53	2.27	1.54	3.02
S16	1,77	2,18	4,98	1.44	3.42	1.83	2.13	1.74	2.75				3.36	2.59		2.58			1.80			2.41	1.99	1.85	3.01
S17	1,77	2,12	5,42	1.31	3.29	1.77	2.10	1.61	2.89				3.61	2.16		2.78			1.81			2.48	2.07	1.82	3.07
S18	1.78	2,07	5,85	1.30	3.28	1.78	2.09	1.60	2.88				3.89	1.87		2.79			1.83			2.47	1.99	1.93	3.09
S19	1.79	2.01	6,25	1.29	3.27	1.79	2.07	1.58	2.85				4.27	1.48		2.80			1.85			2.45	1.93	2.02	3.14
S20	1.80	1.95	6,6	1.37	3.36	1.86	2.09	1.68	2.65				4.63	1.30		2.63			1.89			2.37	1.77	2.19	3.18
S21	1.89	1.82	6,88	1.24	3.24	1.81	2.04	1.53	2.54	0.32			4.81	0.93		2.83			1.89			2.44	1.81	2.20	3.18
S22	1.83	1.83	6,97	1.22	3.22	1.83	2.03	1.50	2.49	0.37			4.92	0.81		2.85			1.90			2.43	1.77	2.29	3.21
S23	1,85	1,77	6,86	1.17	3.21	1.84	2.02	1.46	2.43	0.40			2.71	0.76	2.28	2.87			1.91			2.42	1.73	2.37	3.25

Table S5 (continued). Valence pool populations calculated from the ELF of the most relevant points along the IRC curve associated with **TS2** in the nucleophilic addition step of **1'a** to **2'**

IRC	Distance, Å		ΔE, kcal·mol^{-1}	V(N3,O)	V(N3,C1)	V(N2,C1)	V(C5,N2)	V(C5,Cl)	V(C5,N1)	V(C5,O)	V(Asyn)(C5,O)	V(Asyn)(C5,Cl)	V(O)	V'(O)	V'' (O)	V(N3)	V(C1)	V'(C1)	V(N2)	V'(N2)	V(C5)	V(Cl)	V' (Cl)	V'' (Cl)	V(N1)
	(C5,Cl)	(C5,O)																							
S24	1,86	1,71	6,52	1.14	3.20	1.86	2.02	1.44	2.39	0.82	0.28		2.68		2.36	2.90			1.92			2.41	1.70	2.45	3.29
S25	1.88	1.65	5,94	1.12	3.18	1.88	2.01	1.39	2.34	1.23			2.62		2.35	2.92			1.92			2.39	1.68	2.52	3.33
S26	1.90	1.59	5,19	1.08	3.16	1.90	2.00	1.34	2.29	1.28			2.62		2.33	2.95			1.92			2.37	1.68	2.59	3.35
S27	1.93	1.54	4,39	1.06	3.13	1.91	2.00	1.29	2.27	1.34			2.60		2.32	2.98			1.91			2.36	1.69	2.64	3.38
S28	1.96	1.50	3,65	1.04	3.12	1.93	2.01	0.83	2.27	1.40		0.35	2.59		2.28	3.00			1.89			2.35	1.74	2.71	3.37
S29	1,99	1,47	3,01	1.03	3.11	1.94	2.01	0.71	2.28	1.44		0.39	2.59		2.25	3.02			1.87			2.34	1.78	2.75	3.36
S30	2,02	1,45	2,42	1.02	3.10	1.95	2.02	0.54	2.28	1.46			2.59		2.23	3.04			1.84		0.57	2.31	1.81	2.78	3.35
S31	2,06	1,44	1,84	1.02	3.10	1.95	2.03	0.49	2.31	1.48			2.60		2.21	3.04			1.82		0.55	2.30	1.84	2.82	3.33
S32	2,09	1,43	1,26	1.02	3.09	1.96	2.05	0.45	2.33	1.51			2.60		2.18	3.05			1.78		0.53	2.30	1.87	2.86	3.31
S33	2,13	1,42	0,67	1.03	3.08	1.98	2.07	0.40	2.36	1.52			2.62		2.15	3.06			1.75		0.51	2.31	1.90	2.89	3.29
S34	2,16	1,42	0,06	1.03	3.07	1.98	2.08	0.35	2.38	1.55			2.61		2.14	3.06			1.71		0.48	2.33	1.90	2.94	3.27
S35	2,19	1,41	-0,6	1.02	3.07	1.99	2.10	0.30	2.41	1.56			2.62		2.11	3.07			1.67		0.45	2.34	1.91	2.99	3.25
S36	2,23	1,40	-1,2	1.02	3.07	2.00	2.12	0.25	2.46	1.58			2.63		2.09	3.07			1.64		0.41	2.37	1.92	3.02	3.24
S37	2,27	1,40	-1,8	1.02	3.06	2.01	2.14	0.19	2.82	1.60			2.64		2.06	3.08			1.60			2.42	1.91	3.07	3.26
S38	2,30	1,39	-2,5	1.02	3.06	2.02	2.16		2.86	1.61			2.65		2.04	3.09			1.57			2.59	1.90	3.13	3.20
S39	2,34	1,39	-3,1	1.02	3.06	2.03	2.19		2.87	1.62			2.68		2.01	3.09			1.53			2.62	1.85	3.16	3.19
S40	2,37	1,38	-3,8	1.02	3.05	2.03	2.20		2.86	1.64			2.70		1.97	3.09			1.50			2.69	1.75	3.21	3.17
S41	2,41	1,38	-4,4	1.02	3.05	2.03	2.22		2.87	1.66			2.71		1.95	3.09			1.46			2.78	1.69	3.20	3.15
S42	2,44	1,37	-5	1.02	3.04	2.05	2.24		2.86	1.69			2.72		1.91	3.11			1.43			3.31		4.38	3.14
S43	2,48	1,37	-5,7	1.03	3.04	2.05	2.26		2.86	1.71			4.60			3.11			1.40			3.36		4.34	3.13
S44	2,51	1,37	-6,3	1.04	3.04	2.06	2.13		2.87	1.72			4.59			3.11			1.36	0.15		3.42		4.31	3.12
S45	2,55	1,36	-6,9	1.04	3.04	2.06	2.15		2.87	1.73			4.58			3.11			1.33	0.17		4.09	0.15	3.50	3.11
S46	2,59	1,36	-7,5	1.04	3.04	2.06	2.16		2.87	1.73			4.58			3.11			1.30	0.17		4.23		3.51	3.10
S47	2,62	1,36	-8,1	1.04	3.03	2.07	2.18		2.87	1.74			4.57			3.12			1.26	0.17		4.18		3.59	3.09

Table S5 (continued). Valence pool populations calculated from the ELF of the most relevant points along the IRC curve associated with **TS2** in the nucleophilic addition step of **1'a** to **2'**

IRC	Distance, Å		ΔE, kcal·mol^{-1}	V(N3,O)	V(N3,C1)	V(N2,C1)	V(C5,N2)	V(C5,Cl)	V(C5,N1)	V(C5,O)	V(Asyn)(C5,O)	V(Asyn)(C5,Cl)	V(O)	V'(O)	V'' (O)	V(N3)	V(C1)	V'(C1)	V(N2)	V'(N2)	V(C5)	V(Cl)	V' (Cl)	V'' (Cl)	V(N1)
	(C5,Cl)	(C5,O)																							
S48	2,67	1,36	-8,7	1.03	3.03	2.08	2.18		2.87	1.75			4.56			3.12			1.23	0.18		4.16		3.62	3.09
S49	2,69	1,35	-9,3	1.04	3.04	2.08	2.19		2.87	1.74			4.56			3.12			1.20	0.19		4.14		3.65	3.08
S50	2,72	1,35	-9,8	1.03	3.03	2.08	2.19		2.88	1.76			4.55			3.13			1.17	0.20		4.13		3.67	3.07
S51	2,76	1,35	-10	1.03	3.03	2.09	2.20		2.88	1.76			4.55			3.13			1.15	0.21		4.16		3.66	3.07
S52	2,79	1,35	-11	1.03	3.04	2.09	2.19		2.88	1.76			4.54			3.13			1.13	0.23		4.14		3.67	3.06
S53	2,82	1,34	-11	1.03	3.03	2.10	2.20		2.89	1.77			4.53			3.14			1.09	0.24		4.13		3.70	3.06
S54	2,85	1,34	-12	1.03	3.03	2.10	2.20		2.89	1.76			4.53			3.13			1.07	0.26		4.13		3.70	3.07
S55	2,88	1,34	-12	1.04	3.03	2.11	2.20		2.89	1.78			4.52			3.13			1.05	0.27		4.15		3.69	3.06
S56	2,91	1,34	-13	1.04	3.03	2.11	2.20		2.89	1.77			4.52			3.13			1.02	0.29		4.16		3.69	3.05
S57	2,94	1,34	-13	1.03	3.02	2.11	2.20		2.90	1.77			4.52			3.13			1.00	0.30		4.17		3.68	3.05
S58	2,97	1,34	-13	1.03	3.02	2.11	2.20		2.90	1.77			4.51			3.13			0.98	0.32		4.18		3.68	3.05
S59	2,99	1,34	-14	1.03	3.02	2.12	2.20		2.90	1.77			4.51			3.13			0.97	0.33		3.93	0.26	3.67	3.06
S60	3,02	1,34	-14	1.03	3.02	2.12	2.20		2.91	1.77			4.51			3.14			0.95	0.34		3.88	0.31	3.67	3.05
S61	3,05	1,34	-14	1.03	3.03	2.11	2.20		2.92	1.77			4.51			3.14			0.93	0.36		3.87	0.34	3.65	3.05
S62	3,07	1,34	-15	1.03	3.02	2.11	2.20		2.91	1.77			4.51			3.14			0.91	0.38		3.84	0.38	3.64	3.04
S63	3,09	1,34	-15	1.04	3.02	2.11	2.20		2.91	1.77			4.50			3.14			0.90	0.39		3.83	0.41	3.64	3.04
S64	3,11	1,34	-15	1.04	3.02	2.11	2.20		2.92	1.77			4.51			3.14			0.89	0.40		3.81	0.43	3.64	3.04
S65	3,13	1,34	-15	1.04	3.02	2.11	2.20		2.92	1.77			4.51			3.14			0.87	0.41		3.80	0.46	3.60	3.05
S66	3,15	1,34	-15	1.03	3.02	2.11	2.21		2.92	1.77			4.51			3.14			0.86	0.42		3.77	0.49	3.61	3.04
S67	3,17	1,34	-16	1.03	3.02	2.12	2.21		2.93	1.77			4.50			3.14			0.84	0.43		3.75	0.53	3.59	3.04

Table S6. Summary of table S4

Structure IRC	P1 (**1'a** + **2'**)	P45	P46	P48	P50	P51	P52	P54	P55 **(TS1)**	P56	P58	P83 **(A)**
d(N2-C1)	3.50	2.25	2.21	2.14	2.06	2.02	1.98	1.89	1.85	1.81	1.72	1.38
ΔE	00	10.16	10.66	11.56	12.12	12.20	12.11	11.29	10.53	9.51	6.80	-19.71
V(N3,C1)	3.39	3.97	4.01	3.33	3.22	3.12	3.03	2.79	2.70	2.63	2.51	2.41
V'(N3,C1)	2.59	2.21										
V(C1)				0.36	0.42	0.47	0.52	0.57	0.58	0.59	0.61	0.49
V'(C1)				0.36	0.42	0.47	0.52	0.58	0.58	0.59	0.61	0.50
V(N3)			2.20	2.23	2.29	2.33	2.36	2.46	2.51	2.55	2.61	2.75
V(N2,C1)									3.08	1.89	1.51	1.86
V(N2) / V'(N2)	3.13 / -	3.02 / -	3.02 / -	3.00 / -	2.98 / -	2.98 / -	2.97 / -	2.98 / -		1.25 / -	1.28 / 0.40	1.04 / -
V(Asyn)(N2,C1)								0.05				

Table S7. Summary of table S5.

IRC	S1 **(A)**	S14	S16	S21	S22 (**TS2)**	S23	S24	S28	S29	S30	S36	S37	S38	S67 (**3a** + Cl^-)
d(N2-C1)	1.44	1.45	1.44	1.43	1.42	1.42	1.42	1.40	1.40	1.39	1.38	1.38	1.38	1.38
d(C5-Cl)	1.73	1.76	1.77	1.82	1.83	1.85	1.86	1.96	1.99	2.02	2.23	2.26	2.30	3.17
d(C5-O)	4.10	2.27	2.18	1.89	1.83	1.77	1.71	1.50	1.47	1.45	1.41	1.40	1.39	1.34
ΔE	0.00	7.73	8.57	10.47	10.56	10.45	10.10	7.24	6.60	6.01	2.41	1.73	1.13	-12.10
V(N3,C1)	2.41	2.88	3.30	3.24	3.22	3.21	3.20	3.12	3.11	3.10	3.07	3.06	3.06	2.12
V(N3)	2.75	2.77	2.77	2.83	2.85	2.87	2.90	3.00	3.02	3.04	3.07	3.08	3.09	3.14
V(N2,C1)	1.86	1.77	1.77	1.81	1.83	1.84	1.86	1.93	1.94	1.95	2.00	2.01	2.02	2.12
V(N2) / V'(N2)	1.04 / -	1.73 / -	1.80 / -	1.89 / -	1.90 / -	1.91 / -	1.92 / -	1.89 / -	1.87 / -	1.84 / -	1.64 / -	1.60 / -	1.57 / -	0.84 / 0.43
V(C1)	0.49	0.43												
V'(C1)	0.50													
V(C5,Cl)	1.63	1.64	1.62	1.53	1.50	1.46	1.44	0.83	0.71	0.54	0.25	0.19		
V(C5,O)				0.32	0.37	0.40	0.82	1.40	1.44	1.46	1.59	1.60	1.61	1.77
V(C5)										0.32	0.41			
V(O)	2.96	3.24	3.42	4.81	4.92	2.71	2.68	2.59	2.59	2.23	2.63	2.64	2.65	4.50
V'(O)	2.86	2.56	2.35	0.93	0.81	2.28	2.36	2.28	2.25	2.23	2.09	2.06	2.04	
V''(O)						0.76								
V(Cl)	3.29	2.55	2.52	2.44	2.43	2.42	2.41	2.35	2.34	2.31	2.73	2.42	2.59	3.75
V'(Cl)	3.00	3.78	2.14	1.81	1.77	1.73	1.70	1.74	1.78	1.81	1.92	1.91	1.90	0.49
V''(Cl)			1.70	2.20	2.29	2.37	2.45	271	2.75	2.78	3.02	3.07	3.13	3.59
V(Asyn)(C5,O)							0.28							
V(Asyn)(C5,Cl)								0.35	0.39					

B3LYP/B3LYP/6-311G+(d,p) Cartesian coordinates and electronic energies for TSs structures, together with the single imaginary frequencies.

TS-1 (Gas)

E(RB3LYP) = -1238.78699205 A.U.

1 imaginary frequency -270.6595 cm^{-1}

C	1.62987100	-0.57431000	0.00321800
C	2.80994900	0.06746300	-0.47494100
C	4.02118500	-0.63121100	-0.52817100
C	4.03560600	-1.95578400	-0.10038500
C	2.86656400	-2.58309500	0.37525400
C	1.65241600	-1.90447400	0.43352000
C	1.22274700	1.44150000	-0.55837700
H	4.92007400	-0.14433700	-0.89196700
H	4.96394500	-2.51805000	-0.12866500
H	2.91656900	-3.61532600	0.70757400
H	0.75589300	-2.38604900	0.80841200
N	2.51077400	1.36974500	-0.83181400
N	0.60181700	0.34406600	-0.08185300
N	-0.94340300	0.64156000	2.20947100
C	-2.15899000	-0.22840400	0.25776300
C	-2.01513900	-0.57772200	-1.09512100
C	-3.42941700	-0.38972900	0.85316100
C	-3.09696800	-1.07066100	-1.81999200
H	-1.04641800	-0.45566800	-1.55815100
C	-4.50241200	-0.88095700	0.12100800
H	-3.55137200	-0.12123100	1.89540200
C	-4.34715200	-1.22719600	-1.22352500
H	-2.95761800	-1.33349800	-2.86375800
H	-5.46810200	-0.99436800	0.60379000
H	-5.18641100	-1.61099900	-1.79378200
C	-1.06553100	0.28197800	1.05484600
O	-0.18632000	1.08502800	3.09434500
Cl	0.30725400	2.90631300	-0.84669400

TS-1 (CH_3OH)

E(RB3LYP) = -1238.86297440 A.U.

1 imaginary frequency -310.2206 cm^{-1}

C	1.61410200	-0.61196200	-0.08034400
C	2.82373000	0.04589200	-0.44372100
C	4.03736500	-0.65300800	-0.45284800
C	4.01930500	-1.99773800	-0.09315700
C	2.81917700	-2.64401500	0.26850200
C	1.60387000	-1.96458800	0.27922300
C	1.23979100	1.43214000	-0.55254500
H	4.96220700	-0.15902200	-0.73145000

H	4.94526800	-2.56252200	-0.09010200
H	2.84544000	-3.69272500	0.54401500
H	0.68388300	-2.46632100	0.55833100
N	2.54666700	1.37097100	-0.74701700
N	0.59141000	0.31642000	-0.17959900
N	-0.82771900	0.64384700	2.15286600
C	-2.19768000	-0.21473400	0.27100800
C	-2.12116300	-0.50092400	-1.09948200
C	-3.42466500	-0.40909400	0.93814300
C	-3.24125800	-0.96841800	-1.78413900
H	-1.18135300	-0.35414800	-1.61212900
C	-4.53573800	-0.87524500	0.24590300
H	-3.49300800	-0.19084900	1.99675100
C	-4.45170500	-1.15801000	-1.11965600
H	-3.16415800	-1.18447000	-2.84383600
H	-5.47108000	-1.01897000	0.77510100
H	-5.32011800	-1.52189800	-1.65656800
C	-1.06449800	0.27803500	1.02841300
O	0.03811100	1.07746500	2.96372900
Cl	0.35245400	2.92132600	-0.80385400

TS-1 (THF)

E(RB3LYP) = -1238.85397603 A.U.

1 imaginary frequency - -304.1028 cm^{-1}

C	1.62242700	-0.60140000	-0.07344200
C	2.82220000	0.06531400	-0.45388800
C	4.04015100	-0.62515700	-0.48032300
C	4.03700700	-1.97011800	-0.12102300
C	2.84684700	-2.62486800	0.25754400
C	1.62714800	-1.95390000	0.28593200
C	1.22842300	1.44028400	-0.54049200
H	4.95700200	-0.12346600	-0.77127300
H	4.96714800	-2.52815500	-0.13071000
H	2.88446300	-3.67325400	0.53342100
H	0.71488900	-2.46138800	0.57970000
N	2.53219900	1.38782600	-0.75321400
N	0.59263700	0.31959500	-0.15846000
N	-0.84172000	0.59677500	2.17641800
C	-2.19221600	-0.22639700	0.26904500
C	-2.10594400	-0.50117300	-1.10343300
C	-3.42657200	-0.42188900	0.92252500
C	-3.22174400	-0.95822300	-1.80188100
H	-1.16110400	-0.35310300	-1.60638800
C	-4.53341000	-0.87747000	0.21674100
H	-3.50267000	-0.21204900	1.98231000
C	-4.43909000	-1.14896200	-1.15044700
H	-3.13562200	-1.16512000	-2.86284100
H	-5.47398700	-1.02158600	0.73679400
H	-5.30425200	-1.50457300	-1.69827600
C	-1.06342200	0.25375300	1.04056100

O	0.00859200	1.01666800	3.00656100
Cl	0.32663200	2.92242400	-0.78076300

TS-2 (Gas)

E(RB3LYP) = -1238.80508340 A.U.

1 imaginary frequency -251.3436 cm^{-1}

C	-1.15705000	0.87553700	-0.09979400
C	-2.52902500	0.53789300	0.04273100
C	-3.46609900	1.56457800	0.19577800
C	-3.01770400	2.88900300	0.21376500
C	-1.66071000	3.20101900	0.08661000
C	-0.70593500	2.18295300	-0.07542600
C	-1.50545700	-1.33657600	-0.08571600
H	-4.51700200	1.32336100	0.31190300
H	-3.73834300	3.69209400	0.33746100
H	-1.33692800	4.23601400	0.11562000
H	0.34698200	2.42127900	-0.16617600
N	-2.72204700	-0.82453000	-0.01707000
N	-0.47243600	-0.35860300	-0.28231600
N	0.49366300	-1.56924800	1.40612000
C	2.00511600	-0.13303100	0.16757700
C	2.24744300	0.51334300	-1.05601900
C	3.06597600	-0.24124100	1.08713100
C	3.50658700	1.03225000	-1.35006900
H	1.44129600	0.59208000	-1.77539400
C	4.31887100	0.27591100	0.78642200
H	2.88320500	-0.73827100	2.03186100
C	4.55059700	0.91937100	-0.43363500
H	3.67152200	1.52459000	-2.30323300
H	5.12286100	0.18323700	1.50995300
H	5.52994600	1.32609000	-0.66260000
C	0.69282900	-0.69479400	0.46739200
O	-0.75312200	-2.01268300	1.44212100
Cl	-1.32620300	-2.86527300	-1.08023400

TS-2 (CH_3OH)

E(RB3LYP) = -1238.88300401 A.U.

1 imaginary frequency -273.3131 cm^{-1}

C	-1.13571300	0.88208000	-0.10448900
C	-2.51330200	0.58427500	0.02198800
C	-3.43019500	1.62782400	0.16671500
C	-2.94832400	2.94079600	0.19001100

C	-1.58153900	3.21640900	0.07436600
C	-0.64941100	2.17874600	-0.07855000
C	-1.52897600	-1.31825800	-0.09410400
H	-4.48938300	1.41864700	0.26819100
H	-3.64851200	3.76121300	0.30501100
H	-1.23380000	4.24268200	0.10176800
H	0.40819300	2.39273300	-0.16806700
N	-2.73650700	-0.78543900	-0.04975600
N	-0.47811500	-0.37196200	-0.27704100
N	0.47084800	-1.57287200	1.42904900
C	1.99989500	-0.15787900	0.17029300
C	2.25897200	0.39055700	-1.09523200
C	3.03236000	-0.17597500	1.12434400
C	3.51943400	0.90081500	-1.40129600
H	1.47279300	0.40619600	-1.84041700
C	4.28826500	0.33195200	0.81264800
H	2.83803500	-0.58558100	2.10790100
C	4.53929500	0.87350600	-0.45130200
H	3.70356200	1.31743600	-2.38522900
H	5.07383100	0.31337900	1.55985700
H	5.51872100	1.27256600	-0.68906600
C	0.68243200	-0.71917800	0.47966200
O	-0.80347500	-1.98943600	1.48312800
Cl	-1.36519900	-2.87328900	-1.04300300

TS-2 (THF)

E(RB3LYP) = -1238.87376814 A.U.

1 imaginary frequency -269.0933 cm^{-1}

C	-1.13872100	0.88082400	-0.10387500
C	-2.51574100	0.57761000	0.02356300
C	-3.43545300	1.61878600	0.16956100
C	-2.95810500	2.93336000	0.19349200
C	-1.59245000	3.21397700	0.07755800
C	-0.65716700	2.17898200	-0.07667100
C	-1.52584900	-1.32087500	-0.09416800
H	-4.49359100	1.40509500	0.27234900
H	-3.66117100	3.75132200	0.30992600
H	-1.24790700	4.24141000	0.10641500
H	0.39994300	2.39617900	-0.16521700
N	-2.73477900	-0.79092700	-0.04762700
N	-0.47731000	-0.37019200	-0.27826500
N	0.47331400	-1.57101900	1.42698200
C	2.00064100	-0.15452000	0.16983100
C	2.25697600	0.40749200	-1.09042000
C	3.03721600	-0.18497200	1.11942100
C	3.51713400	0.91920900	-1.39521800
H	1.46789700	0.43163000	-1.83229700
C	4.29264200	0.32438300	0.80892900
H	2.84492900	-0.60674900	2.09819800
C	4.54057800	0.88016000	-0.44956200

H	3.69826200	1.34610800	-2.37545000
H	5.08090100	0.29547300	1.55317100
H	5.51991600	1.28030300	-0.68636900
C	0.68371300	-0.71570700	0.47824300
O	-0.79656400	-1.99169800	1.47880100
Cl	-1.35868900	-2.87261600	-1.04722700

TS-3 (Gas)

E(RB3LYP) = -1239.30380939 A.U.

1 imaginary frequency -269.0933 cm^{-1}

C	1.31513300	0.81096000	0.23022500
C	2.67333600	0.45226100	0.14966000
C	3.67608300	1.38789300	-0.08583300
C	3.27372600	2.71116900	-0.23778000
C	1.92081200	3.08059700	-0.15617900
C	0.92348500	2.13978300	0.07870500
C	1.41299000	-1.33528800	0.48215900
H	4.71949400	1.10391700	-0.15165200
H	4.02130400	3.47290500	-0.42479400
H	1.64912400	4.12186800	-0.28220400
H	-0.11992700	2.42297900	0.13415000
N	2.70516600	-0.92034900	0.36395300
N	0.54524200	-0.33785400	0.48368200
N	-0.47531400	-1.22554000	-1.66966500
C	-2.16595300	-0.06817400	-0.23841800
C	-2.33592300	0.37492600	1.08195900
C	-3.24791000	0.02994900	-1.13581000
C	-3.55657200	0.90392700	1.49276500
H	-1.51103300	0.29251400	1.77689600
C	-4.46093500	0.55597300	-0.71212100
H	-3.12034400	-0.31129000	-2.15549200
C	-4.62379500	0.99803100	0.60240400
H	-3.67287200	1.23928500	2.51732700
H	-5.28467400	0.62386800	-1.41397900
H	-5.57269600	1.40933300	0.92665000
C	-0.91769400	-0.62717300	-0.69421900
O	0.62844500	-1.71680500	-2.00235500
H	3.48590400	-1.54056000	0.21630100
Cl	1.03716500	-2.95312900	0.91086800

TS-3 (CH_3OH)

E(RB3LYP) = -1239.32271925 A.U.

1 imaginary frequency -369.6278 cm^{-1}

C	1.49562100	0.69104100	0.06964300
C	2.76705200	0.16343800	0.36956400
C	3.92431800	0.93767900	0.32204500

C	3.76512300	2.26979100	-0.04385000
C	2.49951200	2.80638500	-0.34867800
C	1.34773700	2.03015200	-0.29623300
C	1.21820600	-1.39760100	0.55840500
H	4.89680500	0.52378500	0.55642400
H	4.63711500	2.91065200	-0.09575500
H	2.42349000	3.84976900	-0.63035500
H	0.37502700	2.44367300	-0.53034000
N	2.54666600	-1.17279600	0.68032400
N	0.54332700	-0.31973700	0.22213900
N	-0.74282900	-0.93817900	-1.98573700
C	-2.17769700	0.12682700	-0.25604900
C	-2.17371200	0.49543000	1.09718100
C	-3.35850300	0.30078900	-1.00621300
C	-3.32119200	1.02360000	1.68508800
H	-1.27387500	0.36646000	1.68239000
C	-4.49730300	0.82639300	-0.40878900
H	-3.36918700	0.02028100	-2.05198800
C	-4.48648000	1.19169300	0.93966900
H	-3.30083000	1.30260100	2.73241100
H	-5.39725700	0.95360800	-0.99970200
H	-5.37673900	1.60279900	1.40113700
C	-1.01288400	-0.43620100	-0.90717500
O	0.24073400	-1.43913300	-2.60965600
H	3.23607600	-1.86293700	0.94497900
Cl	0.52085600	-2.92700700	0.87078400

TS-3 (THF)

E(RB3LYP) = -1239.31988008 A.U.

1 imaginary frequency -377.0169 cm^{-1}

C	1.45822500	0.72091700	0.10035100
C	2.75661800	0.22155200	0.32090200
C	3.89005400	1.02552500	0.22502800
C	3.67864800	2.35947000	-0.10669700
C	2.38557400	2.86838600	-0.33166200
C	1.25795500	2.06176100	-0.23140000
C	1.25892400	-1.38249700	0.56223400
H	4.88401500	0.63256800	0.39761600
H	4.53055700	3.02302300	-0.19469200
H	2.26830200	3.91413400	-0.58941400
H	0.26392800	2.45393100	-0.40480800
N	2.58632800	-1.12439200	0.62018500
N	0.53842300	-0.31598700	0.28646400
N	-0.68994200	-1.02712900	-1.90540900
C	-2.17761000	0.08830300	-0.25150300
C	-2.20808600	0.50430100	1.08771600
C	-3.34203200	0.22524600	-1.03421400
C	-3.37303000	1.04267400	1.63004600
H	-1.32085100	0.40190400	1.69715300
C	-4.49837200	0.76138100	-0.48185100

H	-3.32554800	-0.09254400	-2.06918000
C	-4.52195100	1.17423900	0.85260700
H	-3.37958300	1.35815100	2.66720300
H	-5.38546500	0.85946700	-1.09731600
H	-5.42607400	1.59333200	1.27863400
C	-0.99303500	-0.48583300	-0.85285300
O	0.32113100	-1.54120900	-2.46649300
H	3.30601400	-1.80346400	0.82376000
Cl	0.62004100	-2.93240100	0.89894600

TS-4 (Gas)

E(RB3LYP) = - -1239.27999397 A.U.

1 imaginary frequency -437.9453 cm^{-1}

C	2.37961800	0.19504400	0.10560300
C	1.75435800	-0.67613800	-0.82994500
C	2.31394600	-1.90228400	-1.19000600
C	3.53793700	-2.22444300	-0.61651100
C	4.18346200	-1.36082900	0.29604600
C	3.62030600	-0.15201400	0.66621600
C	0.47832000	1.11118200	-0.38722200
H	1.82843500	-2.56914900	-1.89256100
H	4.01309400	-3.16247300	-0.87949200
H	5.13683000	-1.65936800	0.71579400
H	4.09786400	0.51129500	1.37628400
N	0.61537700	-0.02280100	-1.23913800
N	1.63368500	1.32299200	0.29250200
N	-0.42314500	0.84364600	1.99373300
O	0.59454200	1.22130000	2.53875000
C	-2.05003000	-0.08997600	0.42675200
C	-2.71491500	0.20032300	-0.77442100
C	-2.54748900	-1.12246400	1.24359100
C	-3.84555300	-0.52499400	-1.14551000
H	-2.36883200	1.01043100	-1.40223500
C	-3.68307400	-1.83088200	0.87232100
H	-2.03598600	-1.35675600	2.16918700
C	-4.33481000	-1.53965800	-0.32684500
H	-4.35180700	-0.28299700	-2.07302200
H	-4.05634300	-2.61797000	1.51761000
H	-5.21785200	-2.09711300	-0.61703000
C	-0.84708200	0.62811600	0.84988600
Cl	-0.22817100	2.56778500	-1.17727500
H	-0.17421300	-0.47141000	-1.68027600

TS-4 (CH_3OH)

E(RB3LYP) = -1239.29463356 A.U.

1 imaginary frequency -453.9503 cm^{-1}

C	-2.42346900	-0.37957100	-0.00605300
C	-1.88927400	0.80276600	-0.60040000
C	-2.61414700	1.99659700	-0.66098100
C	-3.90178800	1.96970900	-0.14634000
C	-4.45708200	0.79913700	0.42790000
C	-3.73509500	-0.37646700	0.50754000
C	-0.37841700	-0.84853100	-0.56836200
H	-2.19658200	2.89463700	-1.09857200
H	-4.50421900	2.86963700	-0.18597400
H	-5.46810000	0.83581400	0.81555400
H	-4.14899200	-1.27061300	0.95730900
N	-0.64643000	0.45735300	-1.05078300
N	-1.52465800	-1.39982000	-0.06858900
N	0.45171500	-1.19848500	1.83757600
O	-0.55074500	-1.79710500	2.22480200
C	2.07521200	0.10175200	0.50888100
C	3.24137200	-0.56731200	0.11216600
C	2.08069200	1.49965800	0.61886400
C	4.40054400	0.15526600	-0.15779600
H	3.23741800	-1.64657200	0.02565500
C	3.24246900	2.21660900	0.34147800
H	1.18424200	2.01933900	0.93604500
C	4.40194100	1.54620700	-0.04797400
H	5.30167100	-0.36810700	-0.45526000
H	3.24197700	3.29623000	0.43471500
H	5.30501000	2.10576700	-0.26287700
C	0.84706400	-0.65221600	0.80071700
Cl	0.53463500	-1.88516100	-1.72813500
H	0.06021000	1.09348000	-1.39197600

TS-4 (THF)

E(RB3LYP) = -1239.29240780 A.U.

1 imaginary frequency -445.2895 cm^{-1}

C	2.37651800	0.19691200	0.09608700
C	1.73620400	-0.70509800	-0.80445200
C	2.28986400	-1.94527800	-1.13305700
C	3.52042700	-2.24708300	-0.56772800
C	4.18234400	-1.35384700	0.31001200
C	3.62755700	-0.13458000	0.65106900
C	0.46566800	1.09293600	-0.40786500
H	1.79014900	-2.63242800	-1.80427900
H	3.99240400	-3.19302100	-0.80613600
H	5.14160000	-1.64154900	0.72341400
H	4.12176700	0.54753000	1.33178000
N	0.59503500	-0.06919700	-1.21279000
N	1.63507300	1.32789000	0.25380200
N	-0.47280600	0.97423800	1.97996200
O	0.53549600	1.39416100	2.53463400
C	-2.03779800	-0.07994200	0.42778500
C	-2.77263100	0.23675900	-0.72417600

C	-2.44185700	-1.17193400	1.21710700
C	-3.88754000	-0.52238800	-1.07463300
H	-2.49076300	1.08332800	-1.33511500
C	-3.56190600	-1.91674200	0.86642300
H	-1.87344800	-1.42693400	2.10316000
C	-4.28648600	-1.59772400	-0.28324200
H	-4.44942700	-0.26342500	-1.96440400
H	-3.86506100	-2.75157800	1.48761000
H	-5.15627100	-2.18292300	-0.55819400
C	-0.85127600	0.67952800	0.83752100
Cl	-0.22196300	2.52931700	-1.25730900
H	-0.17716700	-0.51031900	-1.69259000

TS-5 (Gas)

E(RB3LYP) = -1239.34559587 A.U.

1 imaginary frequency -189.2127 cm^{-1}

C	1.01284800	0.96127800	-0.16662200
C	2.35367800	0.64375500	-0.45024700
C	3.36356800	1.56320100	-0.21707700
C	2.99193900	2.80616100	0.29311400
C	1.65494900	3.11674400	0.56577500
C	0.63450900	2.19228500	0.34306400
C	1.18915000	-1.16214000	-0.83689400
H	4.39930700	1.31725200	-0.41250600
H	3.75870100	3.54527700	0.49079800
H	1.40503400	4.08999600	0.96968300
H	-0.39496000	2.42081500	0.58080200
N	2.44110900	-0.68265700	-0.95053600
N	0.29543600	-0.21958500	-0.48198500
N	-0.81273300	-2.06649000	-0.96783200
C	-2.24013600	-0.25878700	-0.17721100
C	-3.14028100	-1.02020900	0.57771000
C	-2.59297700	1.02620000	-0.60804300
C	-4.38426600	-0.49017500	0.90421600
H	-2.85435400	-2.01007700	0.91025500
C	-3.84043800	1.54611700	-0.27869400
H	-1.91025600	1.60544100	-1.21897200
C	-4.73468700	0.79051100	0.47948600
H	-5.07763000	-1.07648100	1.49524500
H	-4.11706400	2.53677300	-0.61964300
H	-5.70439800	1.20007300	0.73752400
C	-0.94539700	-0.84414400	-0.53953200
O	0.58870300	-2.26214000	-1.20226700
H	3.13137000	-1.31563100	-0.50475600
Cl	2.42665800	-2.27411700	1.45046500

TS-5 (CH_3OH)

E(RB3LYP) = -1239.39184869 A.U.

1 imaginary frequency -203.6471 cm^{-1}

C	-0.58288400	0.94121700	-0.04763500
C	-1.97115300	0.65340800	-0.03489600
C	-2.89481000	1.69295500	-0.12673200
C	-2.40249400	2.99100400	-0.23731400
C	-1.02531000	3.25766300	-0.25977400
C	-0.08635900	2.23249900	-0.16465200
C	-0.99654100	-1.23323700	0.10760100
H	-3.95780200	1.49118600	-0.11674500
H	-3.10156400	3.81545900	-0.31170900
H	-0.68081200	4.28016000	-0.35399700
H	0.97444500	2.43919300	-0.19003400
N	-2.19766600	-0.73738100	0.06112900
N	0.02292500	-0.32522200	0.06853800
N	0.93580100	-2.33707600	0.14228500
C	2.56378200	-0.53035800	0.04328700
C	2.91393200	0.58429500	0.81621900
C	3.52963900	-1.17317300	-0.74221500
C	4.22417100	1.05262200	0.79775600
H	2.17843500	1.06649600	1.44842400
C	4.83642100	-0.69559300	-0.75638300
H	3.25120000	-2.02948100	-1.34343500
C	5.18467600	0.41627800	0.01097600
H	4.49498200	1.91056600	1.40123400
H	5.58067800	-1.18826100	-1.37042500
H	6.20301000	0.78663600	-0.00367200
C	1.19725800	-1.06116100	0.07981000
O	-0.50054200	-2.46301000	0.15247600
H	-3.61924800	-1.29361500	0.06682300
Cl	-5.03461100	-1.32629600	0.04316300

TS-5 (THF)

E(RB3LYP) = -1239.38517939 A.U.

1 imaginary frequency -360.3204 cm^{-1}

C	0.95516700	1.02643900	-0.16301700
C	2.30478100	0.77261600	-0.47591100
C	3.29385000	1.70987200	-0.21822400
C	2.88766200	2.90792600	0.36518800
C	1.54410000	3.15665700	0.67755000
C	0.54793100	2.21752300	0.41848600
C	1.17565500	-1.02766900	-1.01703200
H	4.33173300	1.51431300	-0.45343900
H	3.63143900	3.66337000	0.58578900
H	1.27018300	4.09868000	1.13550700
H	-0.48510500	2.40706000	0.67233600
N	2.39527000	-0.51677100	-1.04547100
N	0.26788600	-0.14913900	-0.55369700

N	-0.78863300	-2.02225600	-1.07478900
C	-2.25422000	-0.29721400	-0.17793600
C	-2.65261300	0.99335500	-0.55118400
C	-3.11423600	-1.11807700	0.56324000
C	-3.90845700	1.45875000	-0.17585100
H	-2.00366800	1.61815100	-1.15305600
C	-4.36660500	-0.64074700	0.93552800
H	-2.79418100	-2.11073600	0.85341000
C	-4.76341200	0.64514100	0.56864100
H	-4.22097100	2.45355100	-0.46923800
H	-5.02939800	-1.27096000	1.51589700
H	-5.73922200	1.01399600	0.86201700
C	-0.95244100	-0.82251500	-0.59457900
O	0.62619400	-2.16022100	-1.35181200
H	3.23839600	-1.07156400	-1.12888900
Cl	2.67568300	-2.47701600	1.54014500