Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

Base-Catalyzed Rearrangements of Environmentally Relevant N-Chloro-Piperidines. A Quantum-Chemical Study

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Table S1. Relative energies ΔH (in kJ/mol; at 298.15 K) for stationary points in rearrangement processes of **5-Cl**, calculated at different levels of theory.[a]

structure	B3LYP/ 6-31+G(d)	QCISD(T,FC)/ 6-31G(d)a	MP4(FC)/ 6-31G(d)	MP2(FC)/ 6-31G(d)	MP4(FC)/ 6-31+G(d)	MP2(FC)/ 6-31+G(d)	MP4(FC)/ 6-31G(2df,p)	MP2(FC)/ 6-31G(2df,p)	MP2(FULL)/ G3large	B2PLYP/ aug-def2tzvpp	HLC	ZPE[b]	Thermal Corr. (H)	ΔG_{solv}[c]	G3B3(+) (0 K)	G3B3(+) (Enthalpy)[d]	ΔH (+ΔG_{solv})
5-Cl$_{eq}$	-711,322032	-710,106829	-710,105019	-710,001717	-710,122428	-710,017517	-710,395089	-710,270694	-710,97124	-711,308742	-0,14196	0,143897	0,156963	4,6	-711,097117	-711,089487	0 (0)
5-Cl$_{ax}$	-711,318474	-710,104103	-710,102194	-709,998348	-710,118721	-710,013328	-710,392700	-710,267822	-710,968036	-711,305103	-0,14196	0,143820	0,156816	4,1	-711,094510	-711,086947	6.7 (7.2)
OH$^-$(w)$_0$	-75,785045	-75,521734	-75,521291	-75,513115	-75,596636	-75,588358	-75,587463	-75,574521	-75,728935	-75,793449	-0,02704	0,008028	0,011636	-410,1	-75,761434	-75,758129	-
OH$^-$(w)$_1$	-152,230106	-151,79452	-151,793917	-151,777378	-151,859943	-151,842451	-151,935035	-151,909037	-152,136408	-152,259023	-0,05408	0,029948	0,036269	-352,4	-152,188094	-152,182904	-
OH$^-$(w)$_2$	-228,662489	-228,048994	-228,048139	-228,021908	-228,119087	-228,091289	-228,262981	-228,222838	-228,534179	-228,716014	-0,08112	0,054965	0,064938	-316,4	-228,602899	-228,595002	-
OH$^-$(w)$_3$	-305,089581	-304,296471	-304,295404	-304,259187	-304,373191	-304,335036	-304,584061	-304,529507	-304,927199	-305,167828	-0,10816	0,079741	0,093420	-289,7	-305,013177	-305,002510	-
5'$_0$	-785,142524	-785,689587	-785,687891	-785,573983	-785,754071	-785,637399	-786,048786	-785,909612	-786,734214	-787,133237	-0,16900	0,152029	0,168687	-253,6	-786,894819	-786,883904	-95.3 (56.6)
5'$_1$	-863,574217	-861,943089	-861,941183	-861,818969	-862,011767	-861,886275	-862,375678	-862,223540	-863,133556	-863.590418	-0,19604	0,175921	0,196130	-231,4	-863,310997	-863,297433	-65.7 (50.7)
5'$_{1'}$	-863,571962	-861,941522	-861,939687	-861,817664	-862,012904	-861,887575	-862,37428	-862,222386	-863,133738	-863,589174	-0,19604	0,17679	0,196856	-236,5	-863,310023	-863,296635	-63.7 (47.6)
5'$_2$	-940,000076	-938,189436	-938,187289	-938,05574	-938,265678	-938,130375	-938,695147	-938,529161	-939,527587	-940,042385	-0,22308	0,200112	0,224230	-211,0	-939,722442	-939,705883	-56.2 (44.6)
5'$_{2'}$	-940,000061	-938,189623	-938,187499	-938,056239	-938,268951	-938,133621	-938,695392	-938,529654	-939,528981	-940,042385	-0,22308	0,201308	0,224825	-216,5	-939,722685	-939,706772	-58.5 (36.8)
5'$_{2''}$	-939,986244	-938,170334	-938,168196	-938,036008	-938,252674	-938,11663	-938,676461	-938,510004	-939,512903	-940,027733	-0,22308	0,199382	0,223653	-229,2	-939,709052	-939,692313	-20.5 (62.1)
5'$_3$	-1016,421247	-1014,430214	-1014,427838	-1014,28678	-1014,514141	-1014,368826	-1015,009761	-1014,829792	-1015,915053	-1016,487815	-0,25012	0,225913	0,252847	-201,2	-1016,125862	-1016,107462	-40.6 (43.3)
5'$_{3a}$	-1016,421825	-1014,429345	-1014,426839	-1014,28599	-1014,514611	-1014,369315	-1015,00882	-1014,82896	-1015,914171	-1016,488539	-0,25012	0,225765	0,252671	-203,1	-1016,125339	-1016,106961	-39.3 (42.7)
5'$_{3b}$	-1016,418432	-1014,419727	-1014,417073	-1014,276358	-1014,507974	-1014,362886	-1014,999032	-1014,819178	-1015,909705	-1016,472815	-0,25012	0,223481	0,251338	-	-1016,123225	-1016,103810	-31.0 (-)
5'$_{3''}$	-1016,410748	-1014,415409	-1014,413042	-1014,271521	-1014,505922	-1014,360117	-1014,994684	-1014,814454	-1015,906583	-1016,478792	-0,25012	0,22366	0,251903	-214,6	-1016,119924	-1016,100130	-21.4 (49.1)
5-TS$_0$	-787,154346	-785,693165	-785,692173	-785,573679	-785,748963	-785,626463	-786,050439	-785,906859	-786,723578	-787,133853	-0,16900	0,147812	0,164075	-251,2	-786,893344	-786,882665	-92.0 (62.3)
5-TS$_{1(anti)}$	-863,574502	-861,934859	-861,932838	-861,807677	-862,001759	-861,872992	-862,366403	-862,211273	-863,120033	-863,583683	-0,19604	0,174069	0,193826	-220,2	-863,302761	-863,289579	-45.1 (82.5)
5-TS$_{1(syn)}$	-863,554296	-861,909337	-861,906981	-861,781395	-861,975694	-861,846503	-862,340551	-862,184868	-863,094534	-863,560749	-0,19604	0,172573	0,192151	-243,5	-863,279645	-863,266586	-15,3 (119,6)
5-TS$_2$	-939,996579	-938,176023	-938,174279	-938,037969	-938,248402	-938,107821	-938,681769	-938,511072	-939,504359	-940,029004	-0,22308	0,197839	0,221141	-201,7	-939,706312	-939,690483	-15.7 (94.4)
5-TS$_{2'}$	-939,99628	-938,174292	-938,172520	-938,03649	-938,249629	-938,109387	-938,680226	-938,509759	-939,505248	-940.029021	-0,22308	0,198066	0,221239	-210,4	-939,706713	-939,691022	-17.2 (84.2)
5-TS$_{2''}$	-939,987163	-938,165266	-938,162985	-938,028865	-938,246784	-938,108716	-938,670514	-938,502158	-939,504649	-940.027733	-0,22308	0,198079	0,221902	-219,4	-939,704235	-939,687894	-8.9 (83.5)
5-TS$_3$	-1016,409662	-1014,402831	-1014,400622	-1014,254558	-1014,491403	-1014,340720	-1014,982000	-1014,79717	-1015,886676	-1016,468628	-0,25012	0,221332	0,248998	-203,8	-1016,107122	-1016,087817	11.0 (92.3)
5-TS$_{3'}$	-1016,41581	-1014,410511	-1014,408736	-1014,262748	-1014,49327	-1014,342419	-1014,990681	-1014,805857	-1015,888053	-1016,472161	-0,25012	0,222247	0,248817	-205,4	-1016,107388	-1016,089213	7.3 (87.0)
5A	-250,555390	-249,906004	-249,904252	-249,818234	-249,918431	-249,831658	-250,122985	-250,024823	-250,376843	-250,589029	-0,11492	0,130030	0,141273	-7.7	-250,4624019	-250,456071	-
Cl$^-$(w)$_1$	-536.693139	-535.900561	-535.899740	-535.875537	-535.930437	-535.905476	-536.037866	-536.000366	-536.460328	-536,632979	-0,05408	0,022192	0,027885	-287,0	-536,531295	-536,526440	-354.2 (-244.1)[e]
Cl$^-$(w)$_2$	-613,111866	-612,137170	-612,135907	-612,101701	-612,176371	-612,141037	-612,347559	-612,295809	-612.846195	-613,093633	-0,08112	0,046746	0,055803	-281,5	-612,934710	-612,927419	-291.7 (-175.4)[e]
Cl$^-$(w)$_3$	-689,531022	-688,380965	-688,379326	-688,335169	-688,411276	-688,378303	-688,664365	-688,598390	-689,233906	-689,539449	-0,10816	0,072721	0,084796	-242.8	-689,3257750	-689,316447	-231.7 (-162.7)[e]
Cl$^-$(w)$_4$	-765,948769	-764,617290	-764,615275	-764,561386	-764,669584	-764,613402	-764,973880	-764,893727	-765,618258	-765,982346	-0,13520	0,097824	0,113247	-231,3	-765,7400953	-765,728367	-242.7 (-188.9)[e]

[a] All single point energy calculations (values in Hartree) performed for B3LYP/6-31+G(d) optimized geometries. [b] ZPE (obtained from B3LYP/6-31+G(d) frequency calculation) is scaled by 0.9636 (according to Jeffrey P. Merrick, Damian Moran, and Leo Radom, An evaluation of harmonic vibrational frequency scale factors. *J. Phys. Chem. A* **2007**, *111*, 11683-11700.). [c] Solvation energies calculated with CPCM/B3LYP/6-31+G(d) method in the model solvent ε = 78.4 (water). [d] G3B3(+) (Enthalpy) = G3B3(+) (0K) + [(Thermal correction to enthalpy) – (Zero-point correction)]; at 298.15 K. [e] Energies calculated for both products **5A** and **Cl$^-$(w)$_n$**, where *n* is 1,2,3, or 4.

Table S2. Relative energies ΔH (in kJ/mol) for stationary points in conformational/configurational processes of **5-Cl** and **5-H**, calculated at different levels of theory.[a]

structure	B3LYP/ 6-31+G(d)	QCISD(T,FC)/ 6-31G(d)[a]	MP4(FC)/ 6-31G(d)	MP2(FC)/ 6-31G(d)	MP4(FC)/ 6-31+G(d)	MP2(FC)/ 6-31+G(d)	MP4(FC)/ 6-31G(2df,p)	MP2(FC)/ 6-31G(2df,p)	MP2(FULL)/ G3large	B2PLYP/ aug-def2tzvpp	HLC	ZPE[b]	Thermal Corr. (G)	ΔG_{solv} [c]	G3B3(+) (0 K)	G3B3(+)[d]	ΔG (+ΔG_{solv})
5-Cl$_{eq}$	-711,322032	-710,106829	-710,105019	-710,001717	-710,122428	-710,017517	-710,395089	-710,270694	-710,97124	-711,308742	-0,14196	0,143897	0,156963	-2,1	-711,097117	-711,089487	0 (0)
5-Cl$_{ax}$	-711,318474	-710,104103	-710,102194	-709,998348	-710,118721	-710,013328	-710,392700	-710,267822	-710,968036	-711,305103	-0,14196	0,143820	0,156816	-3,1	-711,094510	-711,086947	6,7 (5,7)
5-Cl$_{ni}$	-711,302525	-710,082538	-710,080617	-709,977905	-710,097685	-709,993353	-710,372033	-710,248072	-710,949186	-711,288319	-0,14196	0,142794	0,155511	-6,1	-711,075854	-711,068531	55.0 (51,0)
5-Cl$_{ri}$	-711,298735	-710,079585	-710,077524	-709,974137	-710,094481	-709,989518	-710,368870	-710,244243	-710,945087	-711,284669	-0,14196	0,142929	0,155913	-3,2	-711,072382	-711,064797	64.8 (63,7)
5-H$_{eq}$	-251,748048	-251,094587	-251,092032	-251,002428	-251,107523	-251,016706	-251,332508	-251,229399	-251,586210	-251,796534	-0.12168	0,153598	0,165904	-1,7	-251,661169	-251,654665	0 (0)
5_H$_{ax}$	-251,746848	-251,094014	-251,091504	-251,001623	-251,106145	-251,015094	-251,331898	-251,228499	-251,584714	-251,795211	-0.12168	0,153434	0,165800	-3,3	-251,660039	-251,653469	3,1 (1,5)
5-H$_{ni}$	-251,741608	-251,083507	-251,080966	-250,991659	-251,097721	-251,007274	-251,321998	-251,219136	-251,577527	-251,788237	-0.12168	0,152211	0,164405	+5,1	-251,653539	-251,647095	19,9 (26,7)
5-H$_{ri}$	-251,730024	-251,048823	-251,045974	-250,981857	-251,087132	-250,995404	-251,313443	-251,209251	-251,565087	-251,777485	-0.12168	0,153370	0,165509	-4,1	-251,647763	-251,635621	50,0 (47,6)

[a] All single point energy calculations (values in Hartree) performed for B3LYP/6-31+G(d) optimized geometries. [b] ZPE (obtained from B3LYP/6-31+G(d) frequency calculation) is scaled by 0.9636 (according to Merrick, J. P.; Moran, D.; Radom, L. *J. Phys. Chem. A* **2007**, *111*, 11683-11700.). [c] CPCM/B3LYP/6-31+G(d), ε = 8.93 (dichloromethane). [d] G3B3(+) (Gibbs Free Energy) = G3B3(+) (0K) + [(Thermal correction to Gibbs free energy) – (Zero-point correction)]; at 298.15 K for **5-Cl$_{ri}$** and **5-H$_{ri}$**, at 175.15 K for **5-Cl$_{ni}$** and **5-H$_{ni}$**.

Table S3. Relative energies ΔH (in kJ/mol; at 298.15 K) for stationary points in rearrangement processes of **6**, calculated at different levels of theory.[a]

structure	B3LYP/ 6-31+G(d)	QCISD(T,FC)/ 6-31G(d)a	MP4(FC)/ 6-31G(d)	MP2(FC)/ 6-31G(d)	MP4(FC)/ 6-31+G(d)	MP2(FC)/ 6-31+G(d)	MP4(FC)/ 6-31G(2df,p)	MP2(FC)/ 6-31G(2df,p)	MP2(FULL)/ G3large	B2PLYP/ aug-def2tzvpp	HLC	ZPE[b]	Thermal Corr. (H)	ΔG_{solv} [c]	G3B3 (0 K)	G3B3 (Enthalpy)[d]	ΔH/G3B3 (+ΔG_{solv})
6_{eq}	-825.813216	-824,318269	-824,316616	-824,192239	-824,346778	-824,220009	-824,700469	-824,549828	-825,393976	-825,816617	-0,18252	0,175404	0,192309	-10,5	-825,555778	-825,545499	0 (0)
$OH^-(H_2O)$	-152,230106	-151,79452	-151,793917	-151,777378	-151,859943	-151,842451	-151,935035	-151,909037	-152,136408	-152,259023	-0,05408	0,029948	0,036269	-352,4	-152,188094	-152,182904	-
6-TS_{A1}	-978,079390	-976,168308	-976,168737	-976,018910	-976,238547	-976,084052	-976,695578	-976,510592	-977,549287	-978,102065	-0,2366	0,205419	0,228634	-218,0	-977,769693	-977,754238	-67.8 (77,1)
6-TS_{A2}	-978,077062	-976,162566	-976,161474	-976,014226	-976,237851	-976,085644	-976,689551	-976,506890	-977,551833	-978,100803	-0,2366	0,206809	0,229100	-216,8	-977,770336	-977,755857	-72,1 (74,0)
6-TS_{A3}	-978,069822	-976,152270	-976,150626	-976,003659	-976,231349	-976,079759	-976,678265	-976,496106	-977,546422	-978,095159	-0,2366	0,205470	0,228972	-224,9	-977,765978	-977,750238	-57,3 (80,7)
6-TS_{B1}	-978,076350	-976,167608	-976,167065	-976,018847	-976,236341	-976,083576	-976,695308	-976,511748	-977,550366	-978,099731	-0,2366	0,205706	0,228773	-211,1	-977,769910	-977,754613	-68,8 (83,0)
6-TS_{B2}	-978,081455	-976,165627	-976,164404	-976,017384	-976,240734	-976,088721	-976,692170	-976,509677	-977,554512	-978,104123	-0,2366	0,206250	0,228446	-211,7	-977,773571	-977,759166	-80,7 (70,5)
6-TS_{B3}	-978,07158	-976,154833	-976,153289	-976,006458	-976,233409	-976,081919	-976,680930	-976,498853	-977,548599	-978,097019	-0,2366	0,205752	0,229052	-217,9	-977,767727	-977,752199	-62,5 (82,5)
6A[e]	-365,045707	-364,116643	-364,115157	-364,008147	-364,141664	-364,033159	-364,428028	-364,303666	-364,799088	-365,096303	-0,15548	0,161854	0,176790	-25,2	-364,906537	-364,897715	-254,0 (-197,8)
6B[e]	-365,047801	-364,118109	-364,116487	-364,009431	-364,143360	-364,034806	-364,428923	-364,304560	-364,800320	-365,097861	-0,15548	0,161614	0,176614	-26,8	-364,908149	-364,899254	-258,0 (-203,4)
"7"[f]	-364,995901	-364,073904	-364,073226	-363,965059	-364,094990	-363,984693	-364,384559	-364,258485	-364,746803	-365,043001	-0,15548	0,165255	0,176665	-16,9	-364,854054	-364,847161	-121,2 (-58,3)
"8"[g]	-365,050345	-364,128591	-364,127772	-364,022348	-364,151682	-364,044229	-364,442261	-364,319048	-364,809811	-365,101704	-0,15548	0,171497	0,178921	-15,0	-364,912578	-364,905154	-257,4 (-191,0)
$Cl^-(H_2O)_2$	-613,111866	-612,13717	-612,135907	-612,101701	-612,176371	-612,141037	-612,347559	-612,295809	-612.846195	-613,093633	-0,08112	0,046746	0,055803	-281,5	-612,934710	-612,927419	-

[a] All single point energy calculations (values in Hartree) performed for B3LYP/6-31+G(d) optimized geometries. [b] ZPE (obtained from B3LYP/6-31+G(d) frequency calculation) is scaled by 0.9636 (according to Jeffrey P. Merrick, Damian Moran, and Leo Radom, An evaluation of harmonic vibrational frequency scale factors. *J. Phys. Chem. A* **2007**, *111*, 11683-11700.)
[c] CPCM/B3LYP/6-31+G(d), ε = 78.4 (water). [d] G3B3 (Enthalpy) = G3B3 (0K) + [(Thermal correction to enthalpy) – (Zero-point correction)]; at 298.15 K. [e] The most stable rotamer, where relevant. [f] Isoxazolidine structure related to **7** (see Table S4). [g] Oxazinane structure related to **8** (see Table S4).

Table S4. Relative energies ΔH (in kJ/mol; at 298.15 K) for stationary points in rearrangement processes of **4**, calculated at different levels of theory.[a]

	B3LYP/6-31+G(d)					MP4(FC)/6-31+G(d)		B2PLYP/ aug-def2tzvpp	
Structure [b]	H Hartree	Thermal correction	ZPE	ΔG_{solv} [c]	ΔH (+ ΔG_{solv}) [c]	H (Hartree)	ΔH (+ ΔG_{solv}) [c]	H (Hartree)	ΔH (+ ΔG_{solv}) [c]
4_{eee}	-1156,034577	0,270681	0,254977	-4.7	0 (0)	-1153,769999	0,0 (0,0)	-1156,029928	0,0 (0,0)
4_{aee}	-1156,032205	0,270509	0,254908	1.1	6.2 (12.0)	-1153,768055	4,7 (10,5)	-1156,027777	5,2 (11,0)
4_{aaa}	-1156,021875	0,270743	0,255253	-5.9	33.3 (32.1)	-1153,756489	35,6 (34,4)	-1156,017908	31,6 (30,4)
$OH^-(H_2O)$	-152,230106	0,036269	0,031079	-352.4	-	-151,859943	-	-152,259023	-
4_{NI}	-1156,015471	0,269106	0,253718	-0.2	50.2 (54.7)	-1153,745178	61,0 (65,5)	-1156,009504	53,6 (58,1)
4_{RI}	-1156,014055	0,269783	0,254636	-5.4	53.9 (53.2)	-1153,747126	57,7 (57,0)	-1156,008185	57,1 (56,4)
4-TS_{A1}	-1308,307939	0,306627	0,285391	-189.9	-113.6 (53.6)	-1305,670314	-106,8 (62,0)	-1308,322580	-88,3 (78,9)
4-TS_{B1}	-1308,300310	0,307296	0,286634	-177.5	-93.6 (86.0)	-1305,663545	-87,3 (92,3)	-1308,315840	-70,6 (109,0)
4-TS_{A2}	-1308,305648	0,306800	0,287096	-194.3	-107.6 (55.2)	-1305,667881	-100,0 (62,8)	-1308,320783	-83,6 (79,2)
4-TS_{B2}	-1308,309547	0,306760	0,286885	-183.8	-117.6 (56.2)	-1305,673658	-115,3 (58,0)	-1308,324240	-92,7 (80,6)
4-TS_{A3}	-1308,300925	0,307164	0,286255	-181.8	-95.7 (79.6)	-1305,667576	-98,2 (77,1)	-1308,318015	-76,3 (99,0)
4-TS_{B3}	-1308,300450	0,307216	0,286244	-183.2	-94.5 (79.4)	-1305,666369	-94,9 (79,0)	-1308,317230	-74,2 (99,7)
4A	-695,266674	0,254779	0,240449	-22.4	-298.9 (-245.7)	-693,562684	-276,9 (-223,7)	-695,308619	-287,9 (-234,7)
4B	-695,267948	0,254907	0,240685	-24.6	-302.2 (-251.2)	-693,564759	-282,1 (-231,1)	-695,309871	-290,9 (-239,9)
7-TS	-1308,292846	0,309913	0,288944	-209.6	-74.6 (72.9)	-1305,660368	-80,3 (67,2)	-1308,309148	-53,0 (94,5)
7	-695,217490	0,255578	0,242794	-14.6	-169.7 (-108.7)	-693,514764	-149,0 (-88,0)	-695,254420	-155,2 (-94,2)
8-TS	-847,523713	0,294605	0.276873	-210.6	-67.4 (99.0)[d]	-845,465046	-96,9 (69,5) [d]	-847,596822	-73,3 (93,1)[d]
8	-695,270843	0,257267	0,244726	-7.6	-309.8 (-241.8)	-693,572372	-295,9 (-227,9)	-695,314165	-296,0 (-228,0)
$Cl^-(H_2O)_2$	-613,111866	0,055803	0,048512	-281.5	-	-612,176371	-	-613,093633	-

[a] All energies have been calculated for B3LYP/6-31+G(d) geometries. [b] Only lower energy isomers were included. [c] Solvation energies (ΔG_{solv}) calculated with CPCM/B3LYP/6-31+G(d) method. Single point energy calculation with continuum model have been performed in the model solvent ε = 78.4 (water). [d] Sum of energies for **4_{eee}** and $OH^-(H_2O)$ set to zero. [e] Relative to sum of energies for reactants **4B** and $OH^-(H_2O)$.

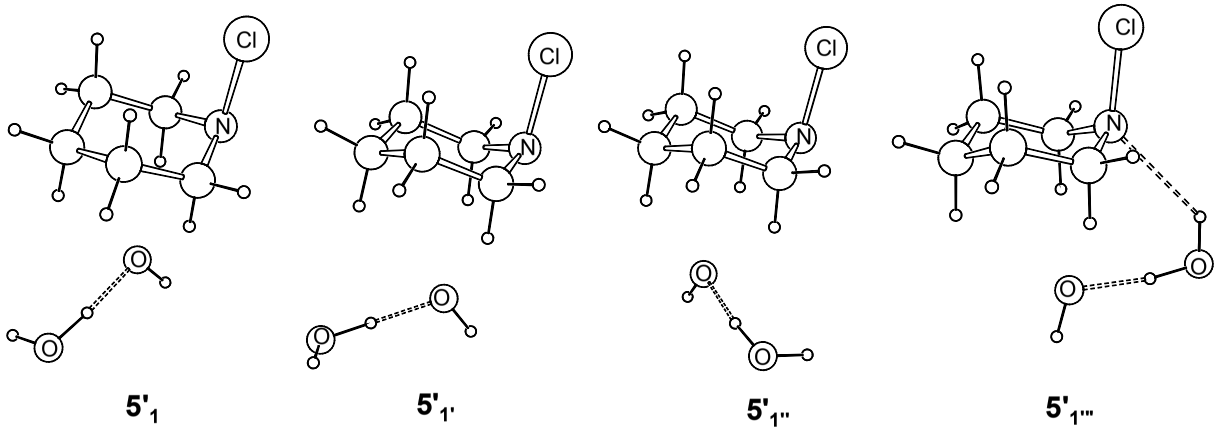

Figure S1. Four different minima of reactive complex **5'$_1$** located at the B3LYP/6-31+G(d) level of theory.

B3LYP/6-31+G(d) optimized geometry of **5-H_{eq}**

C,0,0.2212035831,0.6887212641,-1.266873409
C,0,-0.2079904224,-0.7824652441,-1.2185234213
C,0,-0.2079904224,-0.7824652441,1.2185234213
C,0,0.2212035831,0.6887212641,1.266873409
C,0,-0.2354681929,1.4312205755,0.
H,0,-1.3153613298,-0.8351718848,-1.2727839453
H,0,0.1885296878,-1.3263517115,-2.0840020079
H,0,1.3157533877,0.7327350698,-1.3475400948
H,0,-0.194257727,1.1667160357,-2.1639270776
H,0,-1.3153613298,-0.8351718848,1.2727839453
H,0,0.1885296878,-1.3263517114,2.0840020079
H,0,-0.194257727,1.1667160357,2.1639270776
H,0,1.3157533877,0.7327350698,1.3475400948
H,0,-1.3341144428,1.5022623154,0.
H,0,0.1451116344,2.4609973597,0.
N,0,0.312469182,-1.4093595662,0.
H,0,0.1086353105,-2.4060663326,0.

B3LYP/6-31+G(d) optimized geometry of **5-H_{ax}**

C,0,-0.0072802161,0.7795503533,1.2664202627
C,0,-0.0347815215,-0.7591446076,1.2202112135
C,0,-0.0347815215,-0.7591446076,-1.2202112135
C,0,-0.0072802161,0.7795503533,-1.2664202627
C,0,0.6522882741,1.3510644194,0.
H,0,0.9944563455,-1.1435671394,1.2809116925
H,0,-0.5754884275,-1.1665219546,2.0830829696
H,0,-1.0388501056,1.1564140529,1.3451223067
H,0,0.5237376478,1.1199539355,2.1666274028
H,0,0.9944563455,-1.1435671394,-1.2809116925
H,0,-0.5754884275,-1.1665219546,-2.0830829696
H,0,0.5237376478,1.1199539355,-2.1666274028
H,0,-1.0388501056,1.1564140529,-1.3451223067
H,0,1.7211155567,1.0865242104,0.
H,0,0.6026098011,2.4478335205,0.
N,0,-0.6351969741,-1.3126286935,0.
H,0,-1.6382579529,-1.1289785272,0.

B3LYP/6-31+G(d) optimized geometry of **5-H_{ni}**

C,0,0.2384219131,0.7188767764,-1.2709406063
C,0,-0.1923883362,-0.7587668507,-1.242257657
C,0,-0.1923883362,-0.7587668507,1.242257657
C,0,0.2384219131,0.7188767764,1.2709406063
C,0,-0.2385578458,1.4441023905,0.
H,0,-1.290259488,-0.8066998752,-1.3877192776
H,0,0.2605128668,-1.3113036365,-2.0731937771
H,0,1.3348695083,0.770370234,-1.3328575221
H,0,-0.1660591955,1.2110093835,-2.1666756664
H,0,-1.290259488,-0.8066998752,1.3877192776
H,0,0.2605128668,-1.3113036365,2.0731937771
H,0,-0.1660591955,1.2110093835,2.1666756664
H,0,1.3348695083,0.770370234,1.3328575221
H,0,-1.3394732724,1.4839032329,0.
H,0,0.1105172476,2.4850353643,0.
N,0,0.1829684408,-1.3934416007,0.
H,0,0.761982482,-2.2148432274,0.

B3LYP/6-31+G(d) optimized geometry of **5-H_{ri}**

N,0,0.395097707,-0.6413270934,1.2481385659
C,0,-0.1446849195,0.7186860542,1.2360724806
C,0,0.2269193894,1.4997039744,-0.033899088
C,0,0.0820615888,0.6759925854,-1.3496085867
C,0,-0.3295473547,-0.8261181398,-1.2165272416
C,0,-0.2390699197,-1.4563865078,0.2094549741
H,0,1.4057348418,-0.6116740632,1.112070535
H,0,0.2083151668,1.2544612022,2.1261899566
H,0,-1.236092744,0.6287555276,1.333150611
H,0,1.2715328739,1.8252957082,0.0698040855
H,0,-0.369506812,2.4202530446,-0.0909878106
H,0,1.0349133281,0.7271890868,-1.8885410988
H,0,-0.6435282717,1.1702998481,-2.0055708639
H,0,0.2887042186,-1.4111069677,-1.9082950056

H,0,-1.3596090215,-0.9448398845,-1.5746061676
H,0,-1.2530589099,-1.6771068058,0.5698945192
H,0,0.2875402133,-2.4165432425,0.1677711013

B3LYP/6-31+G(d) optimized geometry of **5-Cl$_{eq}$**

C,0,0.1987771976,1.5025277907,-1.2591162447
C,0,-0.1440383377,0.0058562979,-1.2186715057
C,0,-0.1440383377,0.0058562977,1.2186715057
C,0,0.1987771976,1.5025277904,1.259116245
C,0,-0.3058973988,2.2207834956,0.0000000002
H,0,-1.2392678286,-0.1368041119,-1.2417594791
H,0,0.2847965114,-0.5129394142,-2.0804778183
H,0,1.287386579,1.615464813,-1.3440146714
H,0,-0.2451661621,1.9366356052,-2.164177686
H,0,-1.2392678286,-0.1368041121,1.241759479
H,0,0.2847965114,-0.5129394146,2.0804778182
H,0,-0.2451661622,1.9366356048,2.1641776863
H,0,1.287386579,1.6154648127,1.3440146717
H,0,-1.4059239757,2.2284231231,0.0000000002
H,0,0.0179416344,3.2691167212,0.0000000003
N,0,0.4446142987,-0.5750287207,-0.0000000001
Cl,0,0.1137757524,-2.3417571703,-0.0000000002

B3LYP/6-31+G(d) optimized geometry of **5-Cl$_{ax}$**

C,0,-3.9272522355,-1.2744232397,-0.0320254146
C,0,-2.3957622466,-1.2818782384,0.0728876915
C,0,-2.3937372276,0.8835095465,1.2056937842
C,0,-3.925156558,0.9676878278,1.1409258682
C,0,-4.5495636792,-0.4366556398,1.0970710247
H,0,-2.0871430516,-1.7891557081,0.9997081748
H,0,-1.9310833805,-1.8169711439,-0.7599943917
H,0,-4.2220750069,-0.866440693,-1.0074233017
H,0,-4.2928597479,-2.3092343028,0.0041420056
H,0,-2.0850842691,0.4109824012,2.1506927765
H,0,-1.927636081,1.8721526149,1.1699426805
H,0,-4.2892663804,1.5286087193,2.0119043361
H,0,-4.2198357465,1.5367335594,0.2497908909
H,0,-4.3790611767,-0.9410936347,2.0610048319
H,0,-5.637132768,-0.3684035178,0.9685515337
N,0,-1.7556466621,0.0467873002,0.1679676073
Cl,0,-1.9004475826,0.8840057088,-1.4321618381

B3LYP/6-31+G(d) optimized geometry of **5-Cl$_{ni}$**

C,0,-3.9996596974,-1.2872683393,-0.0092861115
C,0,-2.461473079,-1.2709569653,-0.031648034
C,0,-2.4593229529,0.9632027362,1.1371927377
C,0,-3.9974993534,0.9564545655,1.1645702468
C,0,-4.5401067857,-0.4819407574,1.1836634313
H,0,-2.0738202372,-1.8959263934,0.7959256161
H,0,-2.0814322459,-1.7003567473,-0.9617588117
H,0,-4.375639577,-0.8531633334,-0.9459945932
H,0,-4.3502367696,-2.3275673376,0.0361605253
H,0,-2.0713713603,0.6391288863,2.122183006
H,0,-2.0779065154,1.9715591072,0.9592816262
H,0,-4.3465351569,1.5128391126,2.045367137
H,0,-4.3734009028,1.4789970967,0.2741332013
H,0,-4.2383222967,-0.9732518223,2.1222033595
H,0,-5.6373294919,-0.4750149129,1.172445065
N,0,-1.9537234195,0.0818055458,0.1013366467
Cl,0,-0.8809639585,0.7076711185,-1.0970967885

B3LYP/6-31+G(d) optimized geometry of **5-Cl$_{ri}$**

N,0,-0.3975831146,-1.3804596315,-0.3518347788
C,0,0.9245976009,-1.1114912688,0.2310519898
C,0,1.4786424765,0.3212164431,0.0700582406
C,0,0.4145229623,1.4401905873,-0.1450335344
C,0,-1.0878473662,1.06315738,0.0319903733
C,0,-1.3875371094,-0.4428361253,0.1972937864
H,0,1.6257428923,-1.8497143796,-0.1689518634
H,0,0.7793009735,-1.3510156198,1.2936963557
H,0,2.1681278499,0.3348901684,-0.7805334787
H,0,2.0879639256,0.542933567,0.9550307064

H,0,0.5386722779,1.8174173095,-1.1646445117
H,0,0.6486943245,2.2836988887,0.5135593199
H,0,-1.6398248027,1.434834099,-0.8376304741
H,0,-1.5094887097,1.5832966774,0.9010423623
H,0,-1.4198409653,-0.7140337831,1.2617633332
H,0,-2.3636786259,-0.6969037761,-0.2260098589
Cl,0,-0.3110924495,-1.1751912361,-2.1502767976

B3LYP/6-31+G(d) optimized geometry of **5**$_0$

C,0,0.6421123667,0.137296512,-1.1963799272
N,0,1.0926130241,-0.5733185428,0.
C,0,0.6421123667,0.137296512,1.1963799272
C,0,-0.8606904568,0.4477766954,1.2651009533
C,0,-1.3063844871,1.2027106852,0.
C,0,-0.8606904568,0.4477766954,-1.2651009533
H,0,0.9973812054,-0.4059301743,2.0799139548
H,0,1.1822824104,1.1111927694,-1.0833473935
H,0,0.9973812054,-0.4059301743,-2.0799139548
H,0,-1.4290075115,-0.4871043834,1.3861914522
H,0,-1.0475333454,1.0630361261,2.1571484408
H,0,-2.3990529937,1.3425978308,0.
H,0,-0.8183421523,2.186093936,0.
H,0,-1.4290075115,-0.4871043834,-1.3861914522
H,0,-1.0475333454,1.0630361261,-2.1571484408
H,0,1.1822824104,1.1111927694,1.0833473935
Cl,0,0.3217510935,-2.3552904096,0.
O,0,1.3694166514,2.8017613666,0.
H,0,2.2025083869,3.3016339085,0.

B3LYP/6-31+G(d) optimized geometry of **5'**$_1$

C,0,-0.4562936088,-1.1483214815,1.1725756716
C,0,-0.6566134638,-1.2149502734,-0.3485629911
C,0,-1.0494537203,1.1550113318,-0.5015421485
C,0,-0.8677660714,1.3470938929,1.010905119
C,0,0.0405104558,0.2474327962,1.5882541202
H,0,0.2792745451,-1.9133700753,1.4597739236
H,0,-1.3982273482,-1.3939076912,1.6859697174
H,0,-1.0313870157,-2.1919717126,-0.67491881
H,0,0.3172928269,-0.9912153696,-0.8385943185
H,0,-1.7161955618,1.907637156,-0.9372857402
H,0,-1.8498764014,1.3388879504,1.5066753501
H,0,1.05235002,0.393574807,1.1946701356
H,0,0.087199157,0.3281439117,2.684832108
N,0,-1.519125123,-0.1746407791,-0.923063863
H,0,-0.0546488776,1.204410091,-0.9871814098
O,0,1.9133917619,0.2433182178,-1.1820992219
H,0,-0.4194025404,2.3346444902,1.1856053268
H,0,2.8092224944,1.2726022871,-0.4619017266
H,0,2.2433188561,0.1857323196,-2.0927905149
O,0,3.439151697,1.9072335524,0.0821932135
H,0,4.0321346198,1.2902149014,0.5352599028
Cl,0,-3.2911537016,-0.4216973228,-0.2983858442

B3LYP/6-31+G(d) optimized geometry of **5'**$_1$,

C,0,-0.047989,0.01941,-1.212794
H,0,1.009099,0.344204,-1.157751
O,0,2.577408,1.007513,-0.006807
C,0,-0.940483,1.256088,1.268594
C,0,-0.042371,0.012362,1.209713
C,0,-0.946172,1.263517,-1.260259
C,0,-0.748235,2.114719,0.006216
H,0,-0.67547,1.833765,2.166018
H,0,-1.994082,0.957637,1.374675
H,0,-0.180544,-0.638992,2.079326
H,0,1.014235,0.337646,1.151836
H,0,-0.190341,-0.626713,-2.08564
H,0,-2.000284,0.96575,-1.36328
H,0,0.279303,2.500758,0.005069
H,0,-1.441624,2.969686,0.010339
Cl,0,-1.884053,-1.607878,-0.001906
N,0,-0.180909,-0.812271,-0.003737
H,0,-0.685323,1.84641,-2.155536
H,0,3.377223,1.556141,-0.007506
H,0,2.239068,-1.897793,0.002296

O,0,3.155832,-1.578368,0.003295
H,0,3.029583,-0.558411,-0.002008

B3LYP/6-31+G(d) optimized geometry of **5'$_2$**

C,0,-0.5045666125,0.9885158922,-1.2427547139
C,0,-0.1461102615,-0.5022395217,-1.1578726083
C,0,-0.1557122326,-0.4603409704,1.2597666497
C,0,-0.5336346606,1.0268493696,1.2910652737
C,0,-1.2843204084,1.4255836426,0.0090407061
H,0,-1.1100737028,1.1522455464,-2.1456398199
H,0,0.4119437644,1.5862539679,-1.355573325
H,0,0.4335046489,-0.8383528566,-2.0249416401
H,0,-1.0828419166,-1.0892701024,-1.0840276896
H,0,0.4246568103,-0.7557364949,2.1402210506
H,0,0.3746775592,1.6356970696,1.4100095457
H,0,-2.2625211139,0.9313553527,0.0091971876
H,0,-1.4597263197,2.5112549016,-0.0076669967
N,0,0.5731325548,-0.9137311199,0.0590518371
H,0,-1.0757017306,-1.0636124862,1.2169926012
O,0,-2.9588684768,-1.6303743562,-0.2232546371
H,0,-4.0034301215,-1.107027737,-1.3321207148
H,0,-1.1698072242,1.2012971074,2.1681253207
H,0,-3.5570512365,-1.0545666428,1.1542883636
H,0,-3.0645020113,-2.5942501472,-0.201936995
O,0,-3.9573096213,-0.6191444651,1.9917557992
H,0,-4.7693926435,-0.2092042511,1.6597619246
O,0,-4.6166245511,-0.7404040661,-2.069857915
H,0,-3.996690666,-0.4093163541,-2.7359232628
Cl,0,2.2727603638,-0.1310489381,0.0591633483

B3LYP/6-31+G(d) optimized geometry of **5'$_2$'**

C,0,0.2300262032,-0.1425084277,-1.113271532
H,0,-0.847242729,-0.0298142429,-0.934715709
O,0,-2.4456967119,0.3416954223,0.9886284914
C,0,1.0480364327,-1.2229257371,1.4673780434
C,0,0.6366889723,0.2397117237,1.2509129619
C,0,0.6091743404,-1.6240591072,-0.9919276074
C,0,0.3593494151,-2.1342330385,0.4372603219
H,0,0.7625333816,-1.5160726942,2.487776632
H,0,2.1413854451,-1.3227189706,1.3963892103
H,0,1.1415368144,0.918289994,1.9468493292
H,0,-0.4616634954,0.3353342237,1.3858846652
H,0,0.4550966145,0.2585518825,-2.1066171103
H,0,1.6649905182,-1.7606801491,-1.2675041858
H,0,-0.7213605587,-2.1321306695,0.6270052867
H,0,0.7135879881,-3.1704982298,0.540699432
Cl,0,2.6654305206,0.8789020599,-0.4633229544
N,0,0.8361214279,0.7597603577,-0.1125055361
H,0,0.0039005713,-2.1932425957,-1.7095902688
H,0,-3.0964837087,0.414207474,1.7028719519
H,0,-0.8281564808,2.5488096451,-0.151658953
H,0,-3.0247887771,-0.5765951909,-0.1557156593
O,0,-1.7740434962,2.7368697373,-0.0301315621
H,0,-2.1188966429,1.8744498075,0.3735296234
O,0,-3.3505437789,-1.1032886427,-0.9814937476
H,0,-3.6709832659,-0.406086632,-1.5723641235

B3LYP/6-31+G(d) optimized geometry of **5'$_2$''**

C,0,0.166480318,-1.187463838,-1.362288155
C,0,-0.3628659298,0.2267662822,-1.0906268677
C,0,-0.8350582649,-0.2893480121,1.2171017563
C,0,-0.3332310682,-1.7307631795,1.0645828655
C,0,0.7012005865,-1.8308553891,-0.0704052558
H,0,0.9681559884,-1.1184513451,-2.1109122441
H,0,-0.632738896,-1.8040003645,-1.8001032883
H,0,-0.7799833854,0.6968689628,-1.9878342428
H,0,0.4655315433,0.8459192369,-0.6780662283
H,0,-1.5929504268,-0.1899954345,2.0015476963
H,0,-1.18415751,-2.4021438924,0.8757156132
H,0,1.613055988,-1.3092771263,0.2405901458
H,0,0.9641777988,-2.8835511883,-0.2514452563
N,0,-1.3592052292,0.3233591739,-0.013028343
H,0,0.0363467678,0.3696108236,1.4328494364

O,0,1.8127577016,1.1962633939,0.8070864928
H,0,0.1220912306,-2.0406509018,2.0148338143
H,0,3.0649501328,0.3922389259,1.2386383891
H,0,1.9318609512,2.1101183582,1.1098952426
O,0,3.9179332631,-0.174614797,1.4359994718
H,0,4.4389429603,-0.0771774912,0.6257464906
Cl,0,-2.9405072918,-0.595444834,-0.5435359454
H,0,-2.2146083978,2.0871932176,0.2055247688
O,0,-2.8921477236,2.8044616909,0.229025547
H,0,-3.7010271067,2.3355657278,-0.0252739041

B3LYP/6-31+G(d) optimized geometry of **5'**$_3$

C,0,0.9832024095,-1.0513734108,-0.1191014195
H,0,0.0160497079,-0.8586675792,-0.6146857776
O,0,-1.6077696312,0.6191571862,-1.2189894469
C,0,1.4319788529,1.6521463876,0.8661505179
C,0,1.546157019,1.249771462,-0.6113919687
C,0,0.8430054159,-0.7544365402,1.3809844445
C,0,0.4587513417,0.7183245361,1.6066677332
H,0,1.0819010558,2.6925562172,0.9210146148
H,0,2.4246848545,1.6211271325,1.3376065129
H,0,2.2597945486,1.8774897018,-1.1553433186
H,0,0.5514124189,1.3300989346,-1.082753136
H,0,1.2903575378,-2.0854882585,-0.3073910484
H,0,1.7864712982,-0.986354032,1.8955687565
H,0,-0.5528420653,0.8822789817,1.2155931278
H,0,0.4443050449,0.9516196059,2.6807491513
Cl,0,3.6381180388,-0.4630176869,-0.2792747134
N,0,1.896136598,-0.1609312193,-0.8590637408
H,0,-3.108225151,-0.9545339263,0.8348139282
O,0,-3.5119937249,-0.6896834985,-0.0045337148
H,0,-1.6972194437,0.4362764509,-2.1676616017
H,0,-2.0570634696,3.3547751824,-0.0963918408
O,0,-2.6149524706,2.9904388396,-0.7990268504
H,0,-2.2042468453,2.0651186305,-1.0058450866
H,0,0.0754305385,-1.4197921712,1.8006786147
H,0,-2.7572610526,-0.2034945202,-0.5160394637
O,0,-4.9069937202,1.7980827723,0.5164357912
H,0,-4.2261469899,2.3378637347,0.0576765671
H,0,-4.5809708065,0.8826701472,0.3711879877

B3LYP/6-31+G(d) optimized geometry of **5'**$_{3a}$

C,0,1.0706251482,-1.2845251375,-0.1965128457
H,0,0.1015816327,-1.1136784501,-0.7055616459
O,0,-1.683564344,-0.2345996689,-1.4182261943
C,0,1.4111088099,1.4011957659,0.8879712489
C,0,1.5866534041,1.051285128,-0.5954693115
C,0,0.8939832433,-1.0435616103,1.3095848738
C,0,0.4608426619,0.4081919201,1.5782072012
H,0,1.007724606,2.4196260273,0.9573598709
H,0,2.3929990758,1.3996771571,1.3829585725
H,0,2.3108931048,1.7089542593,-1.0877006146
H,0,0.6210815707,1.1527428767,-1.1099745091
H,0,1.4148036959,-2.3017543919,-0.4132608287
H,0,1.832544405,-1.2680464936,1.8371454294
H,0,-0.5528091904,0.5597992232,1.1889526416
H,0,0.4252066142,0.6051582338,2.6589081281
Cl,0,3.71374284,-0.6124188324,-0.2811944697
N,0,1.9710447053,-0.3448192479,-0.887828475
H,0,-3.4374061135,-1.6874791695,0.4940678833
O,0,-3.8000232962,-1.1311495912,-0.2106774127
H,0,-1.7277755018,-0.4139582483,-2.3697284082
H,0,-1.8218467628,1.2703026352,-1.0929043395
O,0,-1.9258219973,2.2555687615,-0.7814431872
H,0,-2.4301906431,2.6887491714,-1.4853201926
H,0,0.1363190955,-1.7437056306,1.6886522865
H,0,-2.9692579657,-0.8098517652,-0.7377605078
O,0,-4.1739372015,1.5014971201,0.9199998131
H,0,-3.3877229797,1.8755545891,0.4665161916
H,0,-4.1964869632,0.5789020611,0.5806473714

B3LYP/6-31+G(d) optimized geometry of **5'**$_{3b}$

C,0,-0.5430002588,-1.1525603626,1.1317938389
C,0,-1.0349634474,-0.8423386529,-0.2888986537

C,0,-1.2354427199,1.528126254,0.2112832228
C,0,-0.7378044599,1.3192648724,1.6480379448
C,0,0.1587633574,0.0733710893,1.7393538982
H,0,0.1523174138,-2.0013333883,1.0801012958
H,0,-1.3894391124,-1.4615586417,1.7626502651
H,0,-1.5820704319,-1.6848139404,-0.7260274296
H,0,-0.1592944685,-0.6199292776,-0.9316728678
H,0,-1.9293306569,2.3721138294,0.1386521928
H,0,-1.5990502395,1.2218755272,2.3246414412
H,0,1.0854259939,0.2652123082,1.185339721
H,0,0.4342674988,-0.1217726248,2.7859644723
N,0,-1.8772132457,0.3590620163,-0.4232725784
H,0,-0.3757893652,1.7384259116,-0.4393794176
O,0,1.7263478487,-0.1284035354,-1.7156609592
H,0,2.795014387,-1.1284517909,-1.4816269174
H,0,-0.1782839638,2.2137081095,1.9518507341
H,0,1.9620777576,1.3246658218,-1.0940399022
H,0,1.6169798558,-0.0225106049,-2.6732630369
O,0,2.0975408416,2.2402892674,-0.6535343022
H,0,3.0271923183,2.236775697,-0.3838989962
O,0,3.5423354349,-1.8634467145,-1.3251578209
H,0,3.0603944988,-2.7030496456,-1.3149418092
Cl,0,-3.5060490029,0.0568130937,0.4335278929
O,0,5.3661992039,-1.6786854118,-3.3709504707
H,0,4.7381260146,-1.8001574531,-2.6070076443
H,0,5.1310278076,-0.8058138733,-3.7180012537

B3LYP/6-31+G(d) optimized geometry of **5'**$_3$,,

C,0,-0.5260538535,-1.2052762881,1.163925951
C,0,-0.662271003,-1.2218077839,-0.3636642349
C,0,-0.7993307809,1.1953690293,-0.4692828697
C,0,-0.6535482912,1.3295236357,1.050947777
C,0,0.0929506033,0.1201639487,1.6399807061
H,0,0.1101425736,-2.0492803551,1.4640878488
H,0,-1.5111454908,-1.3628067275,1.6272774575
H,0,-1.1296294766,-2.1410987754,-0.732596289
H,0,0.3443066248,-1.1021318885,-0.8143218778
H,0,-1.3735017883,2.0181086207,-0.9068991453
H,0,-1.6479485753,1.4319559358,1.5094948645
H,0,1.1370318429,0.1625531501,1.312372833
H,0,0.0874730626,0.1698657587,2.73835522
N,0,-1.3902871293,-0.0758784525,-0.9374829238
H,0,0.2026694433,1.1666669391,-0.9268474833
O,0,2.1646631262,-0.0979203284,-1.0943548107
H,0,3.1782296066,-1.0865224887,-0.3145549735
H,0,-0.0929247371,2.2493802398,1.2571851786
H,0,2.5517170293,1.3434161144,-0.4770118213
H,0,2.4558478457,-0.0973148427,-2.0195113504
O,0,2.790539309,2.2237712536,-0.0128350472
H,0,3.570372423,1.9945705391,0.5134089353
O,0,3.7697499097,-1.7506636854,0.1949619486
H,0,3.2305710746,-2.553857544,0.2343860787
Cl,0,-3.1831680411,-0.1470060434,-0.3911532777
H,0,-1.748274723,-0.2208711654,-2.8687010763
O,0,-2.1952605589,-0.3164246139,-3.7428761212
H,0,-3.1332900455,-0.3446406922,-3.5024390668

B3LYP/6-31+G(d) partially optimized geometry of **5TS**$_0$

NImag=1 (767*i* cm^{-1})

C 0.54046 0.07456 -1.35351
N 1.1905 -0.28179 -0.09768
C 0.70014 0.29059 1.01076
C -0.78281 0.62996 1.17414
C -1.37021 1.18826 -0.12789
C -0.97875 0.28314 -1.30491
H 1.18995 -0.06837 1.92254
H 1.03894 1.01668 -1.64899
H 0.81723 -0.68838 -2.08525
H -1.28818 -0.3064 1.45516
H -0.89683 1.34519 1.99699
H -2.46428 1.26783 -0.05071
H -0.97648 2.20145 -0.28426
H -1.44629 -0.70277 -1.19734

H-1.31477 0.71471 -2.25966
H 1.22961 1.45864 0.88183
Cl 0.27444 -2.76016 -0.04169
O 1.50137 3.01016 0.94957
H 2.46757 2.96544 1.06089

B3LYP/6-31+G(d) optimized geometry of **5TS$_{1\ (anti)}$**

NImag=1 (231*i* cm^{-1})

C,0,-0.1198213101,-1.604386505,1.2562345607
C,0,0.4500612158,-0.1788967569,1.2994752995
C,0,0.0014946489,0.1693379094,-1.0221864649
C,0,-0.5922219701,-1.2351209891,-1.1954457609
C,0,-1.1648392504,-1.7444043204,0.1373453792
H,0,-0.5664868918,-1.8385837546,2.2339400367
H,0,0.7062931455,-2.3102498865,1.0964555836
H,0,1.2538484949,-0.0849486788,2.0361510617
H,0,-0.3546309733,0.5275225724,1.5616995269
H,0,0.4009570033,0.5790277983,-1.9569445505
H,0,0.1897587054,-1.9166545956,-1.564700224
H,0,-2.0499999096,-1.1468331708,0.3877629609
H,0,-1.4862230048,-2.7927265978,0.0463362555
Cl,0,2.6677657506,-0.715266814,-0.36706266
N,0,0.9368295905,0.365017748,0.0242078435
H,0,-0.8939873934,0.8572280565,-0.6701613415
H,0,-3.8370174103,1.1414555908,-0.1071037685
O,0,-2.265471264,1.5091450092,-0.1195332148
O,0,-4.8212206182,0.8742080087,-0.1991959952
H,0,-2.1589519126,2.4705908395,-0.2006873864
H,0,-1.3823731635,-1.1910727443,-1.9569670863
H,0,-4.8789894829,0.577388281,-1.1188970551

B3LYP/6-31+G(d) optimized geometry of **5TS$_{1\ (syn)}$**

NImag=1 (472*i* cm^{-1})

C,0,2.3897328854,-1.2877441513,-0.6058237646
C,0,2.3567699091,0.0910233602,0.0615323592
C,0,0.0072214561,-0.202232553,0.6949290158
C,0,0.0600361806,-1.6604530776,0.2146556356
C,0,1.4751301332,-2.2529362783,0.1598692016
H,0,2.7894596029,-0.0032215023,1.0757653881
H,0,2.9645924232,0.821977742,-0.478382981
H,0,2.0486500464,-1.1926577943,-1.6451594697
H,0,3.4290041782,-1.6506903011,-0.6314486789
H,0,-0.1125376628,-0.0815671077,1.7859731097
H,0,-1.0776482171,0.2233172401,0.3603468629
H,0,-0.6022344248,-2.2618739635,0.8507126415
H,0,-0.3784960688,-1.6969195771,-0.7928594687
H,0,1.8690243582,-2.3925494141,1.1806507273
H,0,1.4681504709,-3.2456280341,-0.3146733466
N,0,1.0413749982,0.682816751,0.3245480785
O,0,-2.4629909753,0.554752679,-0.0443883671
H,0,-2.3094233334,1.0627443502,-0.8575834839
O,0,-4.3124564194,-1.3181074479,-0.2493351343
H,0,-4.975959877,-0.9081969135,0.324187444
H,0,-3.5520882294,-0.6356571786,-0.2357852345
Cl,0,0.6037902156,1.5126027118,-1.5671005148

B3LYP/6-31+G(d) optimized geometry of **5TS$_2$**

NImag=1 (384*i* cm^{-1})

C,0,0.339012074,0.0935924741,-1.0075558339
H,0,-0.6720550084,0.6801072007,-0.6351656955
O,0,-2.0256326773,1.2371509749,-0.2950813649
C,0,0.4627607983,-1.8506904775,1.1198039007
C,0,0.8474667668,-0.372964963,1.2801559976
C,0,-0.0995361707,-1.3490220335,-1.2870161789
C,0,-0.5755078016,-2.0351863531,0.0019490252
H,0,0.0766211383,-2.2272732144,2.0789433979
H,0,1.3705753546,-2.4211827329,0.8861991049
H,0,1.6668009462,-0.2456444912,1.9926603449
H,0,-0.0170418705,0.1998162222,1.655733532
H,0,0.668670281,0.6232565647,-1.9082583391
H,0,0.7541424358,-1.8966345929,-1.7150536337

H,0,-1.5320297974,-1.5882676051,0.3042376718
H,0,-0.7620080609,-3.1044175496,-0.1737522473
Cl,0,3.1649960872,-0.506783882,-0.4041267976
N,0,1.2081016008,0.3446377927,0.050897074
H,0,-4.8202222609,0.4462239237,-0.3222351435
O,0,-4.505386109,0.4879271842,-1.240898581
H,0,-1.896120517,2.195396029,-0.3822701215
H,0,-3.3321301918,-0.2251773126,2.0476139867
O,0,-3.6036796925,0.668565552,1.7926566811
H,0,-2.9506602764,0.9321669006,1.0682363367
H,0,-0.9018690685,-1.3398736898,-2.035409324
H,0,-3.5605919802,0.7665570787,-1.1032207926

B3LYP/6-31+G(d) optimized geometry of **5TS$_2$'**

NImag=1 (387*i* cm^{-1})

C,0,0.0278016154,-0.6882579325,0.0338225052
H,0,-1.0871746224,-0.1913166632,0.1510908982
O,0,-2.5066881894,0.2719890323,0.2672317958
C,0,1.6533515155,1.4387791106,1.1179430842
C,0,0.983424424,1.4878427157,-0.2622954575
C,0,0.616373909,-0.8371223891,1.4408103838
C,0,0.8679634634,0.5360062634,2.0818837636
H,0,1.7332577887,2.461410928,1.5157823427
H,0,2.6736113706,1.0546234909,0.9947880175
H,0,1.5908888316,2.0383478807,-0.9851737613
H,0,0.0094159034,2.000347151,-0.1930308366
H,0,-0.1692400797,-1.650284911,-0.4506685832
H,0,1.5619327056,-1.3966596947,1.3716837401
H,0,-0.0988195201,1.0047579541,2.3183155313
H,0,1.4091938218,0.4286828949,3.0330769754
Cl,0,2.5725319488,-0.5771278659,-1.4267712354
N,0,0.6363815226,0.1925249282,-0.862675073
H,0,-0.0748399875,-1.4297527377,2.0538518371
H,0,-2.5626818473,0.9922630737,0.9155217353
H,0,-1.1660102143,0.8497597008,-2.343003282
H,0,-3.6917885865,-0.8827989948,0.612935698
O,0,-2.0704060024,1.2048560553,-2.2896695483
H,0,-2.362571391,0.9133146954,-1.3833820757
O,0,-4.4324702964,-1.5541379557,0.7273631343
H,0,-4.8137870833,-1.6180617305,-0.1603085896

B3LYP/6-31+G(d) optimized geometry of **5TS$_2$''**

NImag=1 (173*i* cm^{-1})

C,0,-0.2389365228,-1.590156575,1.1895275124
C,0,0.3816651013,-0.1908912115,1.298350178
C,0,0.0994134623,0.220112924,-1.0474679388
C,0,-0.5318501448,-1.1571310597,-1.2863136313
C,0,-1.2059834548,-1.6727937638,-0.0038588501
H,0,-0.7683546686,-1.8119532839,2.1268766357
H,0,0.5656079939,-2.3312611898,1.0860270627
H,0,1.1232754345,-0.1279569843,2.1004973379
H,0,-0.4174733531,0.5479356141,1.4805290977
H,0,0.5790644443,0.6308365881,-1.9425087538
H,0,0.2427081042,-1.860999942,-1.6280283829
H,0,-2.0870348852,-1.0548046101,0.2030764578
H,0,-1.5494267715,-2.7089230901,-0.1396717674
Cl,0,2.6381398379,-0.8038705322,-0.2550173508
N,0,0.9948059398,0.3280370478,0.0653566429
H,0,-0.7626787281,0.9224974547,-0.7107715757
H,0,-3.6310674784,1.0389374397,0.377844315
O,0,-2.1642869721,1.5376281564,-0.0101380557
O,0,-4.5776438997,0.6709353556,0.5317890382
H,0,-2.1266807775,2.507232758,-0.0162167916
H,0,2.0470511742,1.97471146,0.2519479093
O,0,2.7919292098,2.6186761203,0.3151501603
H,0,3.5616777616,2.0534178629,0.1495191497
H,0,-1.2722623116,-1.0645757442,-2.0918578789
H,0,-4.9018924959,0.5198662048,-0.3677935206

B3LYP/6-31+G(d) optimized geometry of **5TS$_3$**

NImag=1 (314*i* cm^{-1})

C,0,0.4375710173,-0.9603762575,-0.5506813379
H,0,-0.669859763,-0.6160120545,-0.8934575866
O,0,-2.156900668,-0.2845918181,-1.1198291661
C,0,0.9646259972,1.1767653766,1.3264236551
C,0,0.9917899894,1.3496860445,-0.1972868418
C,0,0.3436395375,-1.2446521272,0.9524338214
C,0,0.0193809424,0.0363586059,1.7351660799
H,0,0.6473434723,2.1250982626,1.782063223
H,0,1.9845687088,0.9676747647,1.6740434619
H,0,1.7372391842,2.0844430199,-0.5120219363
H,0,0.0058522375,1.6969282114,-0.5464767213
H,0,0.6700993388,-1.8506569081,-1.1446157471
H,0,1.3036241614,-1.6653682652,1.2889289019
H,0,-1.0164266264,0.3289484906,1.5217241684
H,0,0.0880290549,-0.1467242669,2.8170506081
Cl,0,3.2981043952,-0.3093882704,-0.5954722077
N,0,1.2156995135,0.1224887485,-0.9745232694
H,0,-4.7781854195,-1.2196208093,0.03686637
O,0,-3.9960104039,-1.77573271,0.1640673927
H,0,-2.2635035964,-0.3937509209,-2.0786803188
H,0,-3.1728161153,1.9899363284,0.5749217101
O,0,-2.7652281237,2.1878464143,-0.2805778073
H,0,-2.5401174168,1.2804226784,-0.6584145578
H,0,-0.4309165674,-2.0029023153,1.1206761326
H,0,-3.2673791021,-1.2751314772,-0.3180497644
H,0,1.6397301422,0.2772776535,-2.8941258081
O,0,2.0947090264,0.285902368,-3.7677269291
H,0,3.0037211734,0.0613088933,-3.5151170052

B3LYP/6-31+G(d) optimized geometry of **5TS$_3$**,

NImag=1 (544*i* cm^{-1})

C,0,1.0295222317,-1.0416337366,-0.1009848693
H,0,-0.1078944543,-0.8277013326,-0.5931291452
O,0,-1.4834957257,-0.6513316221,-0.9913429329
C,0,1.5873474036,1.6158592722,0.8670505498
C,0,1.6418024704,1.2094976338,-0.6124617047
C,0,0.8968697996,-0.7490033369,1.3978756153
C,0,0.5982259076,0.7365205193,1.6479320463
H,0,1.3076195292,2.6772385735,0.9395905303
H,0,2.5939949844,1.5119176193,1.2902006462
H,0,2.4299028403,1.7456073498,-1.146714598
H,0,0.6833479022,1.4503479149,-1.1028611478
H,0,1.2237449782,-2.0974364252,-0.3201166224
H,0,1.8420961362,-1.0310372584,1.8863960746
H,0,-0.4287068301,0.9535079674,1.3225127015
H,0,0.6473104241,0.9661056068,2.7217925337
Cl,0,3.9532212799,-0.5045584014,-0.3283825785
N,0,1.8114092501,-0.2220243495,-0.8896751248
H,0,-3.0752782088,-2.0368195487,1.2527714949
O,0,-3.4262627883,-1.9290964583,0.356876256
H,0,-1.4760071721,-0.9752394242,-1.9070766658
H,0,-2.329026236,2.2139602167,-0.2283224046
O,0,-2.7699089663,1.7096325006,-0.9275128016
H,0,-2.2569712528,0.8450498217,-0.9877348655
H,0,0.1054888864,-1.3814758622,1.8219685491
H,0,-2.678832216,-1.4988736649,-0.163562919
O,0,-5.0812286275,0.472186371,0.3607308386
H,0,-4.4151247146,1.0061417226,-0.1211508332
H,0,-4.6681268315,-0.4166526687,0.3886873772

B3LYP/6-31+G(d) optimized geometry of **5A**

C -4.5569991683 -0.1976926612 -0.0362549068
C -3.0245010522 -0.2389135254 0.0354807954
C -2.4351475072 1.1028799345 0.4229178428
C -4.4992908377 2.0468266848 1.095099544
C -5.0956238988 0.6334690792 1.1344014173
H -1.3521972061 1.2081024311 0.2936681673
H -2.6881793497 -0.985896317 0.7723052946
H -2.5853100009 -0.5516875158 -0.9219299438
H -4.8671307393 0.2658885949 -0.9834742855
H -4.9714725696 -1.213014162 -0.0296997824
H -4.7090712241 2.5817376483 2.0294826083
H -4.9705858452 2.6407888352 0.2976291194

H -4.8234936877 0.1478877119 2.0829660124
H -6.1914009515 0.6915269439 1.1100271567
N -3.0500983217 2.1228059877 0.8768369602

B3LYP/6-31+G(d) optimized geometry of **6_{eq}**

H,0,2.0683121081,1.8564322688,-0.1526687305
H,0,-0.1103737654,3.0130417761,0.3221630637
H,0,1.2868917391,1.2285458825,1.3185239677
C,0,1.1983576409,1.3091328168,0.2203772834
C,0,-0.1040681786,2.0265274764,-0.158559044
H,0,-0.1165525456,2.1939573607,-1.2432219701
H,0,-1.3863138667,1.1654196578,1.3602243013
N,0,1.19390622,-0.0197464697,-0.4140435659
C,0,-1.3328317899,1.2095319636,0.2608859806
H,0,0.1640902958,-0.9895887813,1.1882469693
C,0,0.0996281955,-0.863926803,0.0918194097
C,0,-1.2460619756,-0.2211669647,-0.2941356345
H,0,-1.2941813816,-0.1770563611,-1.39103643
H,0,0.2003630527,-1.8510469776,-0.3691613594
C,0,-2.3984221828,-1.1070744289,0.1784570651
H,0,-2.2614164213,-2.1315070985,-0.2008593306
H,0,-2.41540762,-1.1489449515,1.2793449099
H,0,-2.2552379658,1.6876428408,-0.0838848585
Cl,0,2.7499931403,-0.8347401717,-0.0300456368
O,0,-3.6185856145,-0.5513609565,-0.3184428169
H,0,-4.3606816446,-1.0994976091,-0.0223707534

B3LYP/6-31+G(d) optimized geometry of **$6TS_{A1}$**

NImag=1 (633i cm^{-1})

O,0,1.8990556404,-0.3732207777,0.1626438658
C,0,1.2845668335,-0.2426834078,1.4185416398
C,0,-0.2099300751,0.1095775379,1.1759584334
C,0,-0.5563680379,-0.7896669371,-0.0296299486
H,0,0.573057069,-0.6760742762,-0.517486387
H,0,-2.541693105,1.0853782319,-1.8481011209
H,0,-1.6507397679,2.9192024652,-0.3456228752
H,0,-0.7732702459,1.1987327742,-1.9054314862
C,0,-1.6330771302,0.9573019838,-1.2547237404
C,0,-1.6203566224,1.8679473705,-0.0227944416
H,0,-2.5328973694,1.6700847029,0.552103188
H,0,0.5170360561,1.9247581546,0.2639029728
N,0,-1.4869339668,-0.4756164781,-0.9820191393
C,0,-0.3712315675,1.6008168866,0.8243144296
H,0,-0.8420408825,-0.1479426295,2.0378664618
H,0,1.7703484541,0.5457524643,2.0214190309
H,0,1.3542949289,-1.1844372072,1.996302147
H,0,-0.3959342198,2.1966278778,1.7479130584
H,0,-0.5915157607,-1.8559631742,0.2193095698
Cl,0,-3.5845884878,-0.9030569192,-0.0883989866
H,0,3.5085390161,-1.279159439,0.0446225383
H,0,3.447114783,1.4230978261,-1.7498671437
O,0,3.5942293668,1.4795665606,-0.7944653572
H,0,2.9000926074,0.868370815,-0.4032368486
O,0,4.4766571418,-1.4171500034,-0.1000807213
H,0,4.7609828117,-0.5119265621,-0.3141792189

B3LYP/6-31+G(d) optimized geometry of **$6TS_{A2}$**

NImag=1 (382i cm^{-1})

C,0,-0.947124521,0.2602727241,1.855161686
C,0,-1.4857205239,1.2865574316,0.8509189647
C,0,-0.4630692401,0.1280259863,-0.9703297457
C,0,0.1574898548,-0.9483780652,-0.0578375684
C,0,0.360284172,-0.3715270562,1.3533652264
H,0,-1.7118429519,-0.5126783203,2.0055055974
H,0,-2.4644442872,1.674962704,1.1459852384
H,0,-0.7898353589,2.1418140509,0.7937586376
H,0,-0.6026832824,-0.2127856148,-2.0032295908
H,0,-0.5728131888,-1.769493116,0.0215167991
H,0,1.1504285854,0.3889669515,1.3314365271
H,0,0.6971045677,-1.1599727605,2.0366720462

Cl,0,-3.3081081522,-0.4785358846,-0.477638291
N,0,-1.5810713471,0.8433322397,-0.5453354448
H,0,0.3886305284,1.001426016,-1.0452155
H,0,2.8419172306,1.2608932513,-0.24083749
O,0,1.6881216635,1.8084359376,-1.1013040235
O,0,3.6051657041,0.7869023541,0.2818595875
H,0,1.4596483587,2.7321955315,-0.910906507
H,0,4.3615709702,0.8101534355,-0.3220002109
H,0,-0.7895997063,0.7570063262,2.8246428785
C,0,1.4589584114,-1.4942888584,-0.7171777226
H,0,1.2287138579,-2.4224052055,-1.255970563
H,0,1.8204461938,-0.7644157872,-1.4542522928
O,0,2.5137904438,-1.8078105741,0.1889265697
H,0,2.9820230173,-0.9576226974,0.3663021921

B3LYP/6-31+G(d) optimized geometry of **6TS$_{A3}$**

NImag=1 (270*i* cm^{-1})

C,0,-0.5185066542,-0.5968740658,1.7948002973
C,0,-0.7312388122,-1.619821097,0.6723340297
C,0,-0.3537233889,0.0340017901,-1.0169121057
C,0,-0.0819831482,1.1499060508,0.012994378
C,0,0.4110235645,0.5363774536,1.3352588455
H,0,-1.4941309245,-0.1927693976,2.0948020458
H,0,-1.4612439275,-2.3852790412,0.9509615411
H,0,0.2240782762,-2.1231323909,0.4515361563
H,0,-0.7216692629,0.4299332694,-1.9713085501
H,0,-1.0278926596,1.6853509337,0.1931700869
H,0,1.4202844285,0.1315400764,1.1794377028
H,0,0.4827275133,1.3149484634,2.1053092876
Cl,0,-3.129284526,-0.4489708228,-0.3133030618
N,0,-1.1298226614,-1.0719620696,-0.6305568955
H,0,0.714244426,-0.4587536883,-1.2458934262
H,0,2.8125010236,-1.7795679121,-0.266480381
O,0,2.2483122482,-0.7846644145,-1.4043877518
O,0,3.1939401835,-2.3443221669,0.4967593106
H,0,2.315507529,-1.235280138,-2.2619138072
H,0,3.9147434303,-1.8000550395,0.8447564431
C,0,0.9196396109,2.1353990788,-0.5779980924
H,0,0.5640346072,2.4805970292,-1.5624409403
H,0,1.8840563542,1.6324671028,-0.719373772
O,0,1.0524674787,3.2761363878,0.3024416286
H,0,1.867185203,3.7410873663,0.0628044362
H,0,-0.0906879117,-1.110983758,2.6673165943

B3LYP/6-31+G(d) optimized geometry of **6TS$_{B1}$**

NImag=1 (524*i* cm^{-1})

N,0,-1.3788924898,-0.8812809049,-0.5713897964
C,0,-1.0726708471,-1.0601526463,0.8668201604
C,0,-0.2980994564,0.093518949,1.5449081323
C,0,-0.8573344546,1.4426599663,1.0501457444
C,0,1.2375534655,-0.0624718655,1.3695043908
C,0,-0.6757616535,0.1688599431,-1.132690952
C,0,-0.7683858151,1.5606241131,-0.4858966816
Cl,0,-3.5457561366,-0.364561024,-0.5961368528
H,0,-0.4547055925,-1.9735745901,0.8891514774
H,0,-2.0075526888,-1.294825495,1.3789381022
H,0,-0.4801441436,0.025736879,2.6293022007
H,0,-0.3215998937,2.2696044383,1.5360132264
H,0,-1.9085611438,1.5133311677,1.356214279
H,0,1.5390234727,-0.9505000856,1.9631857222
H,0,1.7175280686,0.8131057821,1.8530520267
H,0,-0.7843626865,0.1935016183,-2.2226324819
H,0,0.1123590894,2.141273761,-0.7872683779
H,0,-1.6591601178,2.0665569947,-0.8820579233
O,0,1.6766600133,-0.208811122,0.0452452233
H,0,0.4642927391,-0.1560265198,-0.7974095491
H,0,2.9049016391,0.8368673033,-0.4183241892
H,0,3.0374890119,-1.404185132,-0.2552268836
O,0,3.9466541769,-1.7392368156,-0.4573048698
H,0,4.4225200586,-0.9021946678,-0.5948848055
O,0,3.7061810446,1.3468054095,-0.7539758655
H,0,3.5102943401,1.5088275433,-1.6882724573

B3LYP/6-31+G(d) optimized geometry of **$6TS_{B2}$**

NImag=1 (367*i* cm^{-1})

```
 C,0,-0.9438871475,1.504251406,0.1761752119
 C,0,1.1198363841,-2.2737608124,0.1849278065
 C,0,0.0152806927,-1.2249521648,0.420238406
 C,0,-0.3896472353,-0.5501413852,-0.9029239773
 N,0,-1.2905932977,0.6010858461,-0.8287957063
 H,0,-1.6496240406,2.3422806589,0.1983040554
 H,0,1.4647985124,-2.6433538118,1.1691287962
 H,0,0.6960383603,-3.1338174674,-0.3517253533
 H,0,-0.8672833758,-1.7714733541,0.7852498331
 H,0,-0.8230899389,-1.2755011889,-1.5976050907
 H,0,0.5066183553,-0.1301325426,-1.3851049018
 C,0,-0.6261029615,0.9524034346,1.5700968707
 C,0,0.4030763799,-0.1836065306,1.4902544605
 H,0,-1.5640193898,0.5920621624,2.0194974176
 H,0,1.3863650187,0.2412461922,1.2649451064
 H,0,0.4925835646,-0.6887537477,2.4644633258
 H,0,-0.2454110899,1.7673627322,2.2000250361
 O,0,1.5072848502,2.4873190638,-0.5639474586
 O,0,2.2220374823,-1.8493432343,-0.6031955415
 O,0,3.2615666117,0.6819396343,-0.0744901256
 H,0,2.5734913796,1.4387046246,-0.3043854591
 H,0,2.5682282953,-0.9672364656,-0.315401151
 H,0,0.1072605821,1.9520143276,-0.2483966964
 Cl,0,-3.2057128597,-0.3159467832,-0.3280415359
 H,0,4.0317452667,0.8461510958,-0.6368295684
 H,0,1.4391416008,2.7135313102,-1.5058257604
```

B3LYP/6-31+G(d) optimized geometry of **$6TS_{B3}$**

NImag=1 (286*i* cm^{-1})

```
 C,0,-0.492043233,1.971776317,0.714662589
 C,0,-0.1307520577,1.1738882473,-0.5542011015
 C,0,0.181418109,-0.8583279223,0.6587212948
 C,0,-0.1294614881,-0.1884740438,2.0013794388
 C,0,-1.043993431,1.0296708883,1.801660695
 H,0,0.4252929166,2.4488180687,1.0860015434
 H,0,0.3795825379,1.8070538017,-1.2867684428
 H,0,-1.0562159651,0.7934321588,-1.0177894991
 H,0,0.8101753864,-1.7497945138,0.7625338613
 H,0,0.815931552,0.1153971255,2.476180932
 H,0,-2.0416016875,0.6826404364,1.5024177096
 H,0,-1.1472066537,1.5758242714,2.7516506953
 Cl,0,2.5890507467,0.6803593184,0.1174396491
 N,0,0.6649489242,-0.0455016485,-0.3823307013
 H,0,-0.8766218057,-1.2175643305,0.2216431468
 H,0,-3.3589901815,-0.3581136244,-0.2637427505
 O,0,-2.3711871813,-1.5810504145,-0.105957094
 O,0,-4.0021138273,0.4463640699,-0.2931500873
 H,0,-2.3193091915,-2.0952631942,-0.9279487502
 H,0,-0.614535534,-0.9213041025,2.6596658084
 H,0,-4.82072636,0.1039549429,0.0933126115
 C,0,-1.4935177326,3.0706465949,0.335932745
 H,0,-1.0501395757,3.7482357564,-0.4033046573
 H,0,-2.3954253851,2.6184593597,-0.0999962967
 O,0,-1.8609438188,3.9211635629,1.4390642367
 H,0,-2.3978892167,3.3868641914,2.0439729469
```

B3LYP/6-31+G(d) optimized geometry of **6A**

```
 N,0,-1.1704645562,-1.48044341,-0.0341328102
 C,0,0.00325147,-1.1672393376,0.3503690595
 C,0,0.5656738339,0.2182363837,0.6237495742
 C,0,-0.5412187814,1.2888075046,0.6139970274
 C,0,-1.5651645277,0.9844215015,-0.4862187271
 C,0,-2.1495638486,-0.4188553659,-0.2898761872
 H,0,0.6958370945,-2.0008370407,0.5169437895
 H,0,-0.0963494794,2.2821266687,0.4916197291
 H,0,-1.049921426,1.2863931439,1.5878691606
 H,0,-1.0850850534,1.043816918,-1.473549378
 H,0,-2.8520046574,-0.4281959037,0.5571843744
 H,0,-2.7329896091,-0.7272387368,-1.1659345907
```

H,0,-2.3726539663,1.7276196152,-0.486290131
H,0,1.0337588187,0.1815057334,1.6191981406
C,0,1.7082844832,0.5161989825,-0.3567129758
H,0,1.3068153405,0.6938761596,-1.3657523493
H,0,2.38834016,-0.3477398972,-0.4096487206
O,0,2.4051162459,1.6711103666,0.1187080116
H,0,3.1069519588,1.8999110142,-0.5092223771

B3LYP/6-31+G(d) optimized geometry of **6B**

N,0,-1.5539003344,-1.3167637808,-0.1178113881
C,0,-2.2225973086,-0.2321305474,-0.1450165032
C,0,-1.6924043693,1.1800911317,-0.0217767836
C,0,-0.1669897213,1.2358976401,-0.1682622076
C,0,0.4658362286,0.0690820668,0.6023658747
C,0,-0.1020999941,-1.2612378977,0.0771543608
H,0,-3.3053562462,-0.3352932492,-0.2762703677
H,0,-2.1904279639,1.8101836363,-0.7715670498
H,0,-2.0053523832,1.5813452214,0.9554016532
H,0,0.2274326312,2.1926687967,0.1879970966
H,0,0.1027897424,1.1511579667,-1.231914665
H,0,0.1921315292,0.167199565,1.6641355549
H,0,0.3563914574,-1.5187821617,-0.8907110319
H,0,0.1569473626,-2.0821299909,0.7581383742
C,0,1.9894286971,0.0667918488,0.5296142967
H,0,2.3859927114,-0.8343671734,1.0232318087
H,0,2.3129727102,0.04791739,-0.5239200471
O,0,2.4778151418,1.2447980908,1.179594182
H,0,3.4454796991,1.2564411068,1.1307305519

B3LYP/6-31+G(d) optimized geometry of **"7"**

C,0,-1.6160468385,-0.9984995315,0.2757821695
C,0,-0.1934070685,-2.8204418594,1.424266059
C,0,0.3417111666,-2.1489707327,-0.8599951284
C,0,-1.117249134,-1.674200562,-1.0314043517
C,0,-1.7679845665,-3.0425192577,-1.2595679828
H,0,0.699055282,-2.9101418358,2.0560594933
H,0,0.7694145711,-2.5092413552,-1.8015793132
H,0,1.0180369076,-1.4040374652,-0.4311383954
H,0,-1.2588378354,-1.0207428773,-1.8987546143
H,0,-1.7414667621,-3.3373247209,-2.3168421091
H,0,-2.8010908544,-3.1000716583,-0.8975581007
H,0,-0.9222231271,-3.5488616028,1.7894330252
O,0,-0.9575036829,-3.9855729447,-0.5095226721
N,0,0.190876417,-3.2844996733,0.0599854115
C,0,-0.7378217758,-1.3764449332,1.4910463791
H,0,0.1118366564,-0.683898505,1.5423032523
H,0,-1.2940769397,-1.2347253836,2.4256238129
H,0,-2.6594686815,-1.2874313855,0.4552524435
H,0,-1.6146637343,0.092406284,0.1606406214

B3LYP/6-31+G(d) optimized geometry of **"8"**

C,0,3.0699741695,0.8569600866,0.5947828226
C,0,1.6049747574,0.5134983895,0.9037910243
C,0,2.5512661522,-0.9124221353,-0.9232019953
H,0,3.7055942557,0.70073441,1.4783719125
H,0,3.1714514291,1.9070800104,0.2853879263
C,0,1.5329326315,-0.9784365041,1.2752851763
H,0,0.493922151,-1.2734277704,1.4793174203
H,0,2.1122619013,-1.1660537728,2.1898045634
H,0,3.0537228336,-1.5195157653,-1.6787207157
H,0,1.2461118267,1.1313402733,1.7363202047
C,0,1.3719600802,-0.1241529699,-1.5051195246
H,0,0.635559711,-0.8252312336,-1.9118992519
H,0,1.7380125557,0.494774159,-2.3310262186
C,0,0.7665851746,0.7494559971,-0.3672866202
H,0,0.7841495785,1.8125814829,-0.6366881785
N,0,2.0773584943,-1.7738639287,0.1435123017
O,0,3.5636683032,0.018996874,-0.4686261059
H,0,-0.2805310166,0.483556984,-0.178467041
H,0,2.8335950111,-2.3763545868,0.4560322994

B3LYP/6-31+G(d) optimized geometry of $\mathbf{4}_{eee}$

C,0,-0.8760734424,0.6755228207,-0.7097445372

C,0,-2.3980117765,0.7217149917,-0.4674083735
C,0,-2.341796661,-1.2658102393,0.924159035
C,0,-0.8257765626,-1.3948848118,0.7393281138
C,0,-0.1569773278,-0.0294624793,0.4714934252
H,0,-2.6251986678,1.3534713197,0.4051830868
H,0,-2.8989182971,1.1511899891,-1.3403012876
H,0,-0.7042873648,0.0899959224,-1.6246020652
H,0,-2.5739095961,-0.6660098661,1.8215569141
H,0,-2.7971988595,-2.2524640318,1.0462747651
H,0,-0.3980602603,-1.8486434823,1.6420789967
H,0,-0.628339244,-2.0828564194,-0.0918908867
H,0,-0.3138980794,0.5980536184,1.3579904497
C,0,-0.3384818355,2.0809822635,-0.9872990044
H,0,-0.8807598126,2.5179493812,-1.8399794236
H,0,0.7257817186,2.0201591601,-1.2526432219
O,0,-0.5167432315,2.88851992,0.1821350751
C,0,1.3448711076,-0.1623999374,0.2682129425
C,0,2.2380758125,0.4966829695,1.125802023
C,0,1.8831892329,-0.9460574196,-0.766317266
C,0,3.6229388674,0.3830032798,0.9700868535
H,0,1.84517799,1.115274313,1.9290886245
C,0,3.2628505572,-1.0735752367,-0.9429810275
H,0,1.2221684528,-1.4722862527,-1.4508762836
C,0,4.1071340529,-0.4031441411,-0.0662310548
H,0,4.3149845875,0.8909914848,1.6346306745
H,0,3.681309165,-1.6799037934,-1.7403794082
F,0,5.453501758,-0.5226662508,-0.2300894386
N,0,-2.8985666617,-0.6517966776,-0.2908569242
Cl,0,-4.6867420904,-0.5760936389,-0.115463689
H,0,-0.1528900516,3.7708827141,0.0165153725

B3LYP/6-31+G(d) optimized geometry of **4**$_{aee}$

C,0,-1.07003066,0.7736102718,-0.5326591466
C,0,-2.5518760844,0.9815649151,-0.159735228
C,0,-2.4654016468,-0.7187838383,1.574360863
C,0,-0.9890795374,-1.0038082284,1.2785068016
C,0,-0.2744193125,0.2346728287,0.6898944726
H,0,-2.6317985038,1.775445018,0.5943387234
H,0,-3.1328014864,1.3012351073,-1.0304094803
H,0,-1.0240109372,0.0271681735,-1.338310797
H,0,-2.5527657927,0.0521784052,2.3543067703
H,0,-2.9831528573,-1.6104129004,1.9386543543
H,0,-0.4888407431,-1.3122202388,2.2057661907
H,0,-0.9166815769,-1.8504890792,0.5853678372
H,0,-0.2951938086,1.0229602149,1.4543059429
Cl,0,-3.4459010619,-1.4644412021,-0.8098230507
C,0,-0.4842854207,2.0631779511,-1.1090770782
H,0,-1.0780965837,2.3742143813,-1.9827094875
H,0,0.5481852152,1.8897931917,-1.4406478854
O,0,-0.5198432594,3.0807176989,-0.0989867087
C,0,1.1862560488,-0.0462708533,0.3702299948
C,0,2.2047842802,0.6973063091,0.9844307448
C,0,1.5609750897,-1.0485262057,-0.5404636835
C,0,3.5548594918,0.4583179099,0.7095588672
H,0,1.939467974,1.4835002501,1.6872830932
C,0,2.9026484545,-1.3043941345,-0.8327348741
H,0,0.7989542178,-1.6463885774,-1.0345331585
C,0,3.8753723518,-0.5413582405,-0.1983428632
H,0,4.3440138433,1.032646446,1.1849751839
H,0,3.1948315481,-2.0789103163,-1.5351465194
F,0,5.1861374351,-0.7836513033,-0.4771621809
N,0,-3.2407094107,-0.1705685118,0.4449266611
H,0,-0.1293144167,3.8929378374,-0.4539505089

B3LYP/6-31+G(d) optimized geometry of **4**$_{aaa}$

C,0,1.0321455917,-0.772790492,-1.3419687157
C,0,1.5491405906,-1.7724349427,-0.2967650032
C,0,1.5540812551,-0.0443007842,1.4110287197
C,0,0.9899213626,1.0295459574,0.4578036299
C,0,0.2139653882,0.3937282253,-0.7426559123
H,0,0.7188101047,-2.2974201474,0.1930125034
H,0,2.184636204,-2.5343078016,-0.7565862363
H,0,1.8959671531,-0.3561795338,-1.8740200923
H,0,0.7096342275,-0.5282568449,1.9226411091

H,0,2.1819939185,0.4043202415,2.1868638885
H,0,0.278798275,1.6070851247,1.0622949086
H,0,0.1573301278,1.1768298277,-1.5091926398
N,0,2.2912807867,-1.1802620785,0.8309635051
Cl,0,3.9258165085,-0.6441883744,0.2605205758
H,0,0.4436703112,-1.3070614652,-2.0983228455
C,0,2.0214936616,2.0616742532,-0.0121601186
H,0,2.6609646281,2.3593449325,0.8315414348
H,0,2.6691313478,1.6639585479,-0.8021425362
O,0,1.28038254,3.1927920535,-0.4953857179
C,0,-1.2399910347,0.0698376746,-0.381673989
C,0,-1.8055727665,-1.2116890724,-0.4417840585
C,0,-2.0853509383,1.1340509355,-0.0127476753
C,0,-3.150845431,-1.438591224,-0.1250905455
H,0,-1.2103839677,-2.0642574067,-0.7507345159
C,0,-3.4281265726,0.9337882438,0.3053486622
H,0,-1.6875741193,2.1460027784,0.0119001423
C,0,-3.9354228415,-0.3593069784,0.248578703
H,0,-3.5826802346,-2.433549388,-0.1708881899
H,0,-4.0758418873,1.7589506746,0.5850765693
F,0,-5.2442303526,-0.5683571167,0.5604004299
H,0,1.8952070636,3.8307624002,-0.8878094798

B3LYP/6-31+G(d) optimized geometry of **4**$_{ni}$

NImag=1 (272*i* cm^{-1})

C,0,-0.9309224494,0.7464939604,-0.5949182091
C,0,-2.4290861088,0.9134803965,-0.2474960494
C,0,-2.3593343758,-1.0892120212,1.2572766575
C,0,-0.8725258317,-1.2902481045,0.9279606321
C,0,-0.17871265,0.0463284777,0.5722188658
H,0,-2.5372986744,1.6889748744,0.5290379163
H,0,-2.9788933655,1.2563369047,-1.1280574946
H,0,-0.8662875475,0.1013003967,-1.4841054487
H,0,-2.4586837257,-0.5582855788,2.2233469282
H,0,-2.862349627,-2.0529997295,1.366726339
H,0,-0.3648668243,-1.7489565728,1.7871900451
H,0,-0.7882557807,-1.9902724842,0.0863296122
H,0,-0.2630297271,0.7064617746,1.4461103503
N,0,-3.0104161648,-0.3316910726,0.2103905265
Cl,0,-4.3906949356,-0.9813080565,-0.5930347025
C,0,-0.313232863,2.0914488527,-0.9851354056
H,0,-0.8976449102,2.5364453908,-1.8061019532
H,0,0.7147272532,1.9402376391,-1.3414347709
O,0,-0.3226086047,2.9599879423,0.1551188286
C,0,1.3047509719,-0.1490093381,0.2952030708
C,0,2.2661941516,0.4994818563,1.0843497387
C,0,1.7583307834,-0.982833123,-0.7406092365
C,0,3.6357015052,0.3274512539,0.860900973
H,0,1.9394740167,1.1569998403,1.8863016638
C,0,3.1211657247,-1.1685356904,-0.9850817419
H,0,1.0423730012,-1.5027408979,-1.3725730061
C,0,4.0348935023,-0.5062957406,-0.174422693
H,0,4.3804146535,0.8272873468,1.4726461753
H,0,3.474018585,-1.8132915485,-1.7841261758
F,0,5.3659564311,-0.6820370585,-0.4043540182

B3LYP/6-31+G(d) optimized geometry of **4**$_{ri}$

NImag=1 (149*i* cm^{-1})

N,0,-2.8644481678,-1.0610520281,0.2323831684
C,0,-2.1967900661,-1.1305529963,1.5527425533
C,0,-1.0803371854,-0.0915222921,1.8699798743
C,0,-0.4867045335,0.7817930851,0.7078954786
C,0,-1.3475679038,0.7848987362,-0.5954445245
C,0,-2.7777711226,0.2817288191,-0.3524264577
Cl,0,-2.124837478,-2.2584827656,-0.9177968265
H,0,-1.8424192965,-2.1531602466,1.6896277347
H,0,-3.016662133,-0.9921100364,2.2704561507
H,0,-0.2584454325,-0.6087630248,2.3753750078
H,0,-1.4907921028,0.6040020012,2.6101293077
H,0,-0.5081346495,1.8102681699,1.0813039015
H,0,-0.8930517739,0.1010385186,-1.3222690217
H,0,-3.3039480121,0.9320665714,0.3590393556
H,0,-3.3523109528,0.2841980119,-1.284653601

C,0,0.9729209434,0.4598790486,0.414054725
C,0,1.3752360778,-0.8152813596,-0.0209068588
C,0,1.9624128665,1.439741467,0.5789665138
C,0,2.7152951888,-1.105982205,-0.2815708348
H,0,0.6323396382,-1.5960620204,-0.1636256077
C,0,3.3117311157,1.1724381788,0.321280377
H,0,1.679139785,2.4329237908,0.920857649
C,0,3.6594737463,-0.1007368547,-0.105080755
H,0,3.0291404654,-2.0899660255,-0.6163321148
H,0,4.0781596753,1.9304638332,0.4499803779
F,0,4.9689693763,-0.3773695669,-0.3582628844
C,0,-1.3530199686,2.1577638917,-1.2660266587
H,0,-0.3197637007,2.4760582783,-1.468779861
H,0,-1.8865033954,2.095698749,-2.2269083844
O,0,-2.0049415451,3.0949455363,-0.3981165325
H,0,-1.9896025987,3.9728967848,-0.8069235517

B3LYP/6-31+G(d) optimized geometry of **4-TS$_{A1}$**

NImag=1 (749*i* cm^{-1})

O,0,-1.7680228744,2.0942628651,-0.236145489
C,0,-0.9064406424,1.4415862441,-1.1427074094
C,0,-0.8571176612,-0.0515664436,-0.7217077769
C,0,-2.3431092262,-0.3250100644,-0.4080889495
H,0,-2.50177214,0.8255820709,0.0568278132
H,0,-2.2335427748,-2.3744989193,2.1408983816
H,0,0.1707025665,-1.5934972995,2.2445585116
H,0,-2.1102834951,-0.6155769561,2.3152366039
C,0,-1.9011975003,-1.4631929611,1.6386854095
C,0,-0.4064602528,-1.5115051972,1.3126839652
H,0,-0.218425685,-2.4161804373,0.7238745271
H,0,-0.186796287,0.6077924397,1.2020200798
N,0,-2.7887820893,-1.2430222743,0.4944847992
C,0,0.0202050499,-0.2455509573,0.5448901011
H,0,-0.5054624264,-0.7036335348,-1.5328830702
H,0,0.0971404318,1.8941784336,-1.1240496713
H,0,-1.2857103694,1.5210502143,-2.1780711044
H,0,-2.980499667,-0.2975306775,-1.2990131434
Cl,0,-2.6192505269,-3.345805561,-0.5087842741
O,0,-3.414131431,4.044075958,-1.1821993356
H,0,-2.7740146446,3.3518517331,-0.8542242913
H,0,-4.2800276742,3.6172872974,-1.1091990923
H,0,-0.4751421911,4.1896482605,1.6462931285
O,0,-0.2449155484,3.2496598829,1.6676895438
H,0,-0.8536550151,2.8287034092,0.991719661
C,0,1.5068242337,-0.2137179529,0.2329446146
C,0,2.2908646141,0.8774478953,0.6426635556
C,0,2.1370838768,-1.2550943129,-0.4688615898
C,0,3.6624213268,0.9314430953,0.3689051806
H,0,1.8163864958,1.7024918882,1.1706446374
C,0,3.5057758771,-1.2208923387,-0.7512220832
H,0,1.5543228352,-2.109840577,-0.8035799082
C,0,4.2404753725,-0.1233147645,-0.3220295221
H,0,4.2705072009,1.7755443832,0.6811151471
H,0,3.9961544752,-2.024786447,-1.2925467339
F,0,5.5845547662,-0.0822143945,-0.5935172165

B3LYP/6-31+G(d) optimized geometry of **4-TS$_{B1}$**

NImag=1 (427*i* cm^{-1})

```
 N,0,1.2908225576,2.1811742248,-0.2427458556
 C,0,0.698182759,1.3634948804,-1.3398854733
 C,0,0.6981617288,-0.1607093263,-1.099122379
 C,0,0.058322044,-0.5451861397,0.2754686937
 C,0,2.1003577819,-0.8155500165,-1.2751613045
 C,0,1.5816701538,1.419586221,0.8811184078
 C,0,0.523299668,0.4385746525,1.3921792665
 Cl,0,-0.2841404044,3.6039026804,0.2753929152
 H,0,1.2981462677,1.5909130392,-2.2340538471
 H,0,-0.3103281022,1.72699508,-1.5449774769
 H,0,0.0798767789,-0.5934897006,-1.8999039147
 H,0,0.4601583168,-1.5352282356,0.519854603
 H,0,2.4684029785,-0.5184677723,-2.2791878099
 H,0,1.9343418734,-1.9115526493,-1.3176667403
 H,0,2.0296271261,2.0300634253,1.6716884927
 H,0,0.9389898839,-0.1278499169,2.2342820451
 H,0,-0.3191099962,1.0243472311,1.7814017588
 O,0,3.0365772839,-0.498595625,-0.2882513501
 H,0,2.4347804511,0.6953639865,0.4066002188
 H,0,3.2808112503,-1.7359090645,0.8094794828
 H,0,4.7833355611,-0.9365107891,-0.6574360298
 O,0,5.6374139787,-1.435826693,-0.6315085755
 H,0,5.4155343929,-2.147899342,-0.0076355427
 O,0,3.5428797784,-2.4772381933,1.4407217447
 H,0,3.8094198847,-2.0193414766,2.2511181681
 C,0,-1.452745727,-0.705006648,0.1804470444
 C,0,-2.332936696,0.3923347587,0.1617000593
 C,0,-2.0094141025,-1.9900168069,0.0696009031
 C,0,-3.7136455202,0.2151131087,0.0286977136
 H,0,-1.9446268788,1.403378226,0.2555910781
 C,0,-3.3876795305,-2.1903102866,-0.0615387006
 H,0,-1.351395498,-2.8563604645,0.0896005449
 C,0,-4.2128847625,-1.0753811668,-0.081361918
 H,0,-4.3913356059,1.0637351043,0.013454994
 H,0,-3.8146783294,-3.185828296,-0.1413816988
 F,0,-5.5665063458,-1.256142009,-0.2061265177
```

B3LYP/6-31+G(d) optimized geometry of **4-TS$_{A2}$**

NImag=1 (364*i* cm^{-1})

```
 C,0,-1.044380226,0.0555229733,1.8297208651
 C,0,-1.4470724486,1.1469538627,0.8308066103
 C,0,-0.0139761711,0.270835136,-0.8433838704
 C,0,0.4545808592,-0.9105638581,0.028584008
 C,0,0.3520593806,-0.5385313163,1.5305211127
 H,0,-1.8047020568,-0.7323340982,1.7925796907
 H,0,-2.4847119552,1.4556625175,0.9852335696
 H,0,-0.8083788241,2.0375837153,0.9544930469
 H,0,0.0927666539,0.0497832907,-1.9126156396
 H,0,-0.2576109132,-1.7289790456,-0.1735653526
 H,0,1.1045070495,0.2395122418,1.7080203118
 Cl,0,-2.8044981542,-0.6394861085,-0.937724717
 N,0,-1.2713140058,0.825556421,-0.5868799592
 H,0,0.677748573,1.2543055002,-0.6370309398
 H,0,2.760681044,1.9258417185,-1.1754509219
 O,0,1.5683999787,2.48453133,-0.4617677001
 O,0,3.5410142643,1.3764502256,-1.6167374053
 H,0,1.83497132,2.5525898004,0.469706199
 H,0,3.3119499899,1.3028964392,-2.5544353155
 H,0,-1.0606974759,0.4706809335,2.8483605134
 C,0,1.8422764604,-1.4560234908,-0.3672344749
 H,0,1.9506008695,-2.4624332861,0.0580002361
 H,0,1.873601099,-1.5674116409,-1.4648745911
 O,0,2.9537315769,-0.708743485,0.094165558
 H,0,3.1813797087,0.000950061,-0.5574449395
 C,0,0.6787677158,-1.701451156,2.4559745561
 C,0,1.8565392595,-1.6969058603,3.2189619134
 C,0,-0.1718689739,-2.8141366043,2.5722629872
 C,0,2.1774642451,-2.7500685802,4.0818796628
 H,0,2.5475256402,-0.8648899596,3.114614023
 C,0,0.1282331416,-3.8795862257,3.4264357925
 H,0,-1.0848043806,-2.8582173167,1.983869355
```

C,0,1.3000866077,-3.8209690538,4.168615829
H,0,3.0919111995,-2.7470741469,4.6678844628
H,0,-0.5292426523,-4.7394889979,3.5163753208
F,0,1.6011238608,-4.8595553659,5.0127407428

B3LYP/6-31+G(d) optimized geometry of **4-TS$_{B2}$**

NImag=1 (413*i* cm^{-1})

C,0,-0.984807005,1.4885341912,0.1336511195
C,0,1.0782364122,-2.283896215,0.0685554074
C,0,-0.0384996247,-1.2514686029,0.3312830289
C,0,-0.39580905,-0.5262819467,-0.9805287857
N,0,-1.2937141988,0.6235124658,-0.9113141238
H,0,-1.6771376455,2.3372533094,0.1549401159
H,0,1.3821240885,-2.7405277218,1.0249673433
H,0,0.673278253,-3.0892205741,-0.5587711912
H,0,-0.9277883771,-1.8182243592,0.6421271891
H,0,-0.8021028795,-1.2329961917,-1.7095173308
H,0,0.5215783606,-0.100097521,-1.4151578391
C,0,-0.7400055326,0.8874236062,1.5186100112
C,0,0.3123390077,-0.2416533101,1.4604995868
H,0,-1.6966110344,0.508269388,1.9065712529
H,0,1.2629688848,0.2319721867,1.2066273483
H,0,-0.3934270786,1.6747082053,2.2004750806
O,0,1.5256911679,2.4138349605,-0.3986499838
O,0,2.2117530737,-1.7963717691,-0.637475691
O,0,3.2772268947,0.6475254758,0.2376427943
H,0,2.6081915507,1.3965121622,-0.0568388174
H,0,2.5697420754,-0.9672052599,-0.2351243229
H,0,0.103799558,1.9322639915,-0.2191076771
Cl,0,-3.2278141944,-0.3145118764,-0.5109310519
H,0,4.104231021,0.8302001659,-0.2309866456
H,0,1.5528729647,2.6822813851,-1.3311835368
C,0,0.5001450334,-0.9069524449,2.8147304241
C,0,1.7383395751,-0.8311273271,3.47209721
C,0,-0.5440206528,-1.5946618608,3.4567453166
C,0,1.9390120761,-1.417472175,4.7269287206
H,0,2.5593899833,-0.3087827795,2.9861417513
C,0,-0.366097469,-2.1894381542,4.7091824714
H,0,-1.5154910256,-1.6689732965,2.9741044527
C,0,0.8776763215,-2.0864371204,5.3184437163
H,0,2.8974597773,-1.361205017,5.2349627228
H,0,-1.1716510316,-2.721772711,5.2068418445
F,0,1.0611472601,-2.6673606192,6.5483663386

B3LYP/6-31+G(d) optimized geometry of **4-TS$_{A3}$**

NImag=1 (368*i* cm^{-1})

C,0,0.883526982,0.5041338744,-1.6675564761
C,0,1.0889964391,1.5825757667,-0.599152594
C,0,0.3728587759,0.0971540295,1.1219863437
C,0,0.1322816639,-1.080480569,0.150725277
C,0,-0.2184885006,-0.4937637089,-1.2454781344
H,0,1.8346094421,-0.016691781,-1.8329576428
H,0,1.9255869625,2.2413479679,-0.8470619292
H,0,0.1779911607,2.1989479815,-0.5228795956
H,0,0.5635460935,-0.2452066789,2.145262762
H,0,1.0620421925,-1.6669845118,0.0877429804
H,0,-1.1413088486,0.079440785,-1.1074383055
Cl,0,3.2561568691,0.2991765333,0.7211539804
N,0,1.2783273809,1.1030106835,0.7731655685
H,0,-0.6871157828,0.6929323985,1.1403343349
H,0,-3.1650014512,0.8154525612,-0.2618367979
O,0,-2.1406829903,1.1315181812,0.9434967982
O,0,-3.7933487188,0.5005997796,-1.0024791196
H,0,-2.2519309045,1.9960633202,1.3694247866
H,0,-4.495105231,0.0345028953,-0.5256390172
C,0,-0.9604755596,-1.986953076,0.7385017923
H,0,-0.7584435065,-2.1507776937,1.8028569199
H,0,-1.9388783234,-1.4967787207,0.6595514519
O,0,-1.0042227656,-3.3087002411,0.1742546011
H,0,-1.2116095349,-3.22158116,-0.7692601354
H,0,0.6040562668,0.9853390852,-2.6157302361
C,0,-0.4927756347,-1.515849822,-2.3368600869

C,0,-1.7786548203,-1.5994655999,-2.9016340383
C,0,0.5069949334,-2.3715641987,-2.8332595174
C,0,-2.0610526535,-2.5067746122,-3.9306166714
H,0,-2.5638159015,-0.9469668488,-2.5197476858
C,0,0.2430897129,-3.2826437879,-3.8596287255
H,0,1.5066808654,-2.3350193302,-2.4076985556
C,0,-1.0409846463,-3.3277661109,-4.388466906
H,0,-3.0523482656,-2.5750509952,-4.3695210788
H,0,1.0113159285,-3.9482756246,-4.2423556785
F,0,-1.3065436497,-4.2180053212,-5.3978549691

B3LYP/6-31+G(d) optimized geometry of **4-TS$_{B3}$**

NImag=1 (358*i* cm^{-1})

C,0,0.2430943283,1.2743036426,-0.1712880801
C,0,0.6345891717,0.2412577399,-1.2525592908
C,0,0.7957352541,-1.5462298196,0.3114600985
C,0,0.4533679666,-0.6305702462,1.4877754076
C,0,-0.4369482911,0.5432527783,1.0179364811
H,0,1.1631762957,1.7713133691,0.1630701552
H,0,1.2157139557,0.7199857225,-2.0459320167
H,0,-0.2837365644,-0.1738635806,-1.701179373
H,0,1.3659232122,-2.4330944468,0.6083300541
H,0,1.3804975717,-0.2540975157,1.9450632127
H,0,-1.3562336711,0.0932281338,0.6268426572
Cl,0,3.2976207864,-0.2124131452,-0.3641767204
N,0,1.3559586483,-0.9600126852,-0.8294960324
H,0,-0.2858498177,-1.9173138744,-0.0897127038
H,0,-3.0694208744,-1.5799788672,0.5481697345
O,0,-1.7936033751,-2.1071951923,-0.2948809327
O,0,-3.8034325734,-1.2268697103,1.1621214348
H,0,-1.9424360473,-2.8728274509,-0.8715446227
H,0,-0.0845784574,-1.2098279923,2.2484721662
H,0,-3.8424540798,-1.883487006,1.8723216553
C,0,-0.6566662701,2.3287534314,-0.8372251227
H,0,-0.2296415826,2.616765044,-1.8051302612
H,0,-1.6525728993,1.8977396628,-1.0277768501
O,0,-0.7817383208,3.5624883395,-0.1199412959
H,0,-1.1096160781,3.3588876514,0.7706539007
C,0,-0.8339238919,1.4271733389,2.1905406901
C,0,-2.1563465723,1.3877027447,2.669692467
C,0,0.0912541935,2.2473746359,2.8614058522
C,0,-2.5494145059,2.152049221,3.774883144
H,0,-2.8755839537,0.7314466673,2.178944524
C,0,-0.2842336597,3.0173800992,3.9663747592
H,0,1.1199352542,2.2952284506,2.5130785243
C,0,-1.6027396239,2.9518920845,4.3986007617
H,0,-3.5696660797,2.1261672998,4.1469105856
H,0,0.4255395129,3.657384294,4.4823749608
F,0,-1.9790241514,3.7064277614,5.4807210556

B3LYP/6-31+G(d) optimized geometry of **4A**

O,0,1.9738400179,1.4752031913,1.5506806064
C,0,1.3772590197,0.2565234458,1.9940925011
C,0,1.4323191237,-0.8770213548,0.9537476987
C,0,2.8734131209,-1.2810074961,0.6701979239
H,0,1.3408991417,1.9565492583,0.9974052767
H,0,2.8154099455,-2.6324826196,-2.167220719
H,0,0.4997119283,-1.5041683378,-2.3274300356
H,0,2.8478958445,-0.884144728,-2.2772260186
C,0,2.5413300739,-1.7175117079,-1.6279317955
C,0,1.0282349317,-1.6762806951,-1.3813701387
H,0,0.6863647936,-2.6486458964,-0.9996369765
H,0,1.084095497,0.3675635211,-0.7616703427
N,0,3.3857783628,-1.6507503022,-0.4342586365
C,0,0.6779490339,-0.572903094,-0.3614833589
H,0,0.9528936376,-1.7425428534,1.4438549888
H,0,0.3385769758,0.4237695189,2.308925586
H,0,1.9480698002,-0.0409573709,2.880719305
H,0,3.5486260276,-1.2454810756,1.5324716317
C,0,-0.8192380634,-0.3830643726,-0.1801064696
C,0,-1.4378678375,0.8100779567,-0.5825687491
C,0,-1.6316095122,-1.3915705952,0.3649084025
C,0,-2.8158231251,1.006446081,-0.4476163885
H,0,-0.8359855721,1.6031764183,-1.0224787493

C,0,-3.0093981055,-1.2192798624,0.5110031433
H,0,-1.190560031,-2.3339290663,0.680352358
C,0,-3.574777652,-0.017327872,0.1015602252
H,0,-3.2940440951,1.9295428636,-0.7599280332
H,0,-3.6390320478,-1.9971540243,0.9316656178
F,0,-4.9161922347,0.1587780696,0.2419051465

B3LYP/6-31+G(d) optimized geometry of **4B**

O,0,-1.3359761596,2.6718018184,0.2844071814
C,0,-1.2881188863,1.8713097945,-0.9005498299
C,0,-1.713948982,0.4118130959,-0.6744802216
H,0,-0.5134780768,2.5401578881,0.780281468
H,0,-1.0247016959,-2.2743962451,1.3933157392
C,0,-1.3834839367,-1.7874320541,0.4761110674
H,0,-0.9581039524,-2.373798569,-0.3532217851
H,0,-1.1489060138,0.141088007,1.3744212846
N,0,-3.718253892,-0.983404855,0.0863745482
C,0,-0.894377122,-0.3255947092,0.4127710332
H,0,-1.5618775914,-0.108405063,-1.6346039519
H,0,-0.2858647468,1.9118854446,-1.3468184275
H,0,-1.9815003328,2.3459917655,-1.6041865125
C,0,0.614843466,-0.2345978849,0.2502479362
C,0,1.4128266803,0.2588145387,1.293630523
C,0,1.2585727317,-0.6567890999,-0.9255126847
C,0,2.8049293007,0.3380951377,1.1803679092
H,0,0.9420701561,0.5772583672,2.2220603484
C,0,2.6458989093,-0.5864372409,-1.0628651481
H,0,0.6729668448,-1.0478626606,-1.7540696806
C,0,3.3932989764,-0.0872445682,-0.0020475716
H,0,3.4224516316,0.7170916625,1.9886917744
H,0,3.1456906127,-0.9102823406,-1.9705236625
F,0,4.7455279334,-0.0161852149,-0.1285251729
C,0,-3.2099972994,0.3271235717,-0.3186640624
H,0,-3.8121105537,0.6502644014,-1.1777626426
H,0,-3.439769078,1.0318989442,0.4923060197
C,0,-2.8923507121,-1.8935518186,0.4189053788
H,0,-3.3179092115,-2.8622991133,0.7020241422

B3LYP/6-31+G(d) optimized geometry of **7-TS**

NImag=1 (208*i* cm^{-1})

C,0,-0.3803393889,-0.2584111977,0.2823301109
C,0,1.6465034045,0.8382874543,1.3397232928
C,0,1.3024103472,1.1439373784,-1.0612186007
C,0,0.3861423901,-0.098396996,-1.0768801603
C,0,1.350752207,-1.2686537628,-1.3157793331
H,0,-0.1155192797,-1.2437751326,0.6839029687
H,0,1.9990830954,1.630140394,2.0035143087
H,0,1.8519882405,1.2390409921,-2.0030563388
H,0,0.6929913525,2.0441378557,-0.9385741509
H,0,-0.3305222954,0.0024700907,-1.9056492193
H,0,1.7067080432,-1.2333634714,-2.365692271
H,0,0.8111635862,-2.2314607696,-1.1940451657
H,0,2.0565643739,-0.1074410458,1.7056920746
O,0,2.3859403161,-1.1398907092,-0.4045936788
N,0,2.292507945,1.0549937067,0.0212034351
C,0,0.1177453859,0.7822391926,1.3189779979
H,0,-0.2862769883,1.7766303104,1.0871786697
H,0,-0.2548922274,0.518881864,2.3179918039
Cl,0,2.7119422498,3.3837109398,0.1858318486
C,0,-1.8910615122,-0.2213847829,0.1347594852
C,0,-2.6816906835,-1.2923739448,0.5778394959
C,0,-2.5497419891,0.8846793086,-0.4313132484
C,0,-4.0768601786,-1.2752930705,0.4657113179
H,0,-2.1975169107,-2.1614334584,1.0175957324
C,0,-3.9405044694,0.9260349547,-0.554399022
H,0,-1.9682415809,1.7321173077,-0.7863165661
C,0,-4.6771158511,-0.1609720928,-0.1004814039
H,0,-4.686184864,-2.1071480597,0.8066401569
H,0,-4.448248101,1.7802300517,-0.9926145856
F,0,-6.0415268117,-0.1300365822,-0.2183664777
H,0,2.4128000835,-2.277314934,0.8575250086
H,0,3.8777253824,-1.9987722332,-0.9335547068
O,0,4.5466077611,-2.7173726232,-1.0829876801

H,0,4.1827237454,-3.4440236383,-0.553282449
O,0,2.5351752726,-2.9667980885,1.5741814474
H,0,3.3732789496,-2.7182332078,1.991751903

B3LYP/6-31+G(d) optimized geometry of **7**

C,0,-1.6538924439,-1.0161851009,0.2946755783
C,0,-0.1862513822,-2.8129383748,1.431975758
C,0,0.3358546712,-2.164701671,-0.8510017544
C,0,-1.1148108168,-1.6660762086,-1.0251672368
C,0,-1.7672942249,-3.0255688755,-1.2860339432
H,0,-2.6327079172,-1.4676059904,0.5001139924
H,0,0.7199950677,-2.8945358667,2.0447993565
H,0,0.7530393759,-2.5270376231,-1.7966064082
H,0,1.0308968631,-1.438722728,-0.4212042173
H,0,-1.2409419012,-0.9933398921,-1.8789713119
H,0,-1.6788761947,-3.3206189992,-2.340222191
H,0,-2.8205603036,-3.0763665724,-0.9884172854
H,0,-0.9098343464,-3.5319638263,1.824579129
O,0,-1.0160872634,-3.967318203,-0.4785934449
N,0,0.1669257845,-3.2975545204,0.0675893595
C,0,-0.7224943399,-1.3663895381,1.4869687269
H,0,0.1227128038,-0.6669829484,1.4916808256
H,0,-1.2511017514,-1.1991442011,2.433092938
C,0,-1.8771357078,0.4836878321,0.1842735344
C,0,-3.1190497502,1.0448897944,0.5146670594
C,0,-0.85595566,1.3516366926,-0.2385223889
C,0,-3.3477579403,2.4221163787,0.4324353554
H,0,-3.9288064404,0.3963293644,0.8419746503
C,0,-1.0604173565,2.7296399229,-0.33114193
H,0,0.1197403838,0.9530002238,-0.506228679
C,0,-2.308439375,3.2379950352,0.0089529405
H,0,-4.3096292083,2.8563357643,0.6866974569
H,0,-0.2739556837,3.4016325342,-0.6604278232
F,0,-2.5168639425,4.5801895976,-0.0792560466

B3LYP/6-31+G(d) optimized geometry of **8-TS**

NImag=1 (188*i* cm^{-1})

C,0,1.894012958,-1.407568012,-0.9294063341
C,0,0.607206673,-0.5304434337,-0.9749847898
C,0,1.9100542672,0.259069715,1.0687397189
H,0,2.5777776839,-1.0516409172,-1.7300746044
H,0,1.6175856032,-2.4492046378,-1.1971604531
C,0,1.0101139275,0.9564521062,-0.9554467341
H,0,0.1195101088,1.6130258497,-0.8991924707
H,0,1.4935938591,1.2067109975,-1.9151807856
H,0,2.6706342144,0.3244996089,1.8477297984
H,0,0.028438885,-0.7673166479,-1.8803396334
C,0,0.5723850488,-0.3184228126,1.52061393
H,0,0.0138688284,0.4841071147,2.0259868757
H,0,0.7377300423,-1.1106675683,2.2575748053
C,0,-0.2197363374,-0.8753860242,0.2993011962
H,0,-0.225945714,-1.9702615083,0.3753290662
N,0,1.9686025621,1.197603706,0.1311291609
O,0,2.4942873268,-1.3854916407,0.3314289628
C,0,-1.6734156915,-0.4409428821,0.2055366514
C,0,-2.6399383934,-1.3600661021,-0.2392666745
C,0,-2.1159566184,0.858965383,0.5096783454
C,0,-3.9876679445,-1.0155960084,-0.380771075
H,0,-2.3292216274,-2.3751534473,-0.4788427323
C,0,-3.458289099,1.229698088,0.374983927
H,0,-1.406268048,1.6016642177,0.8602302894
C,0,-4.3685938083,0.2818874462,-0.0694623643
H,0,-4.7285597307,-1.7344646663,-0.7187579996
H,0,-3.7940413445,2.2355189803,0.6105634959
F,0,-5.687963992,0.635380366,-0.1982429249
H,0,4.5508229184,1.8442581441,-1.4171205041
H,0,4.282874159,-1.0869688072,0.291924627
O,0,4.4758174425,2.0236732635,-0.4682733903
H,0,3.5073965599,1.7739658658,-0.2344934269
O,0,5.222322948,-0.771125837,0.2572288792
H,0,5.1275103329,0.1925811007,0.1150631674

B3LYP/6-31+G(d) optimized geometry of **8**

C,0,3.0626728035,0.8651746049,0.5753156015
C,0,1.6057999899,0.4981544169,0.9050079601
C,0,2.5654894705,-0.9307600998,-0.9048920945
H,0,3.6941918877,0.8087560644,1.4716069678
H,0,3.1304715865,1.8875406264,0.1736965179
C,0,1.5865278219,-0.9849692082,1.3082631256
H,0,0.5882075715,-1.2943109546,1.6387196757
H,0,2.2721175449,-1.1337912153,2.1551711823
H,0,3.0642267091,-1.5495153009,-1.6532965856
H,0,1.240342857,1.1211860391,1.7299615755
C,0,1.4417380533,-0.0877966802,-1.5155435618
H,0,0.7294624919,-0.7437373814,-2.0243723839
H,0,1.8714157712,0.5792959779,-2.2706216019
C,0,0.7555759092,0.7383478196,-0.3793064482
H,0,0.8562192538,1.8047198074,-0.6179189906
N,0,2.0090870519,-1.7864186249,0.1304297156
O,0,3.597612077,-0.0570252927,-0.3934360224
C,0,-0.7303133667,0.473608759,-0.1890184645
C,0,-1.5957422005,1.5466012987,0.0764197078
C,0,-1.2830662593,-0.8170809744,-0.2482211609
C,0,-2.9653921994,1.3547606773,0.2783280965
H,0,-1.1963331213,2.5580013855,0.1190118163
C,0,-2.6491523643,-1.0325789481,-0.0496831167
H,0,-0.6396123907,-1.6698691399,-0.4490555269
C,0,-3.4644764375,0.0612701492,0.2109457835
H,0,-3.6350939435,2.1860178893,0.4758493802
H,0,-3.0787881666,-2.0285896461,-0.0964184467
F,0,-4.7980123394,-0.1412813883,0.4006824837
H,0,2.6917098085,-2.488926511,0.4018028149