

## The Unusual Reactivity of Benzene and Monosubstituted Benzenes towards Tetracyanoethylene Oxide: A Theoretical Study

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### Supporting Information

Table S1. B3LYP/6-31G(d) energies, enthalpies, free energies and entropies of the structures considered in this work.

Structure	$E_0$ (Hartree) <sup>[a]</sup>	H (Hartree) <sup>[a]</sup>	S (cal mol <sup>-1</sup> K <sup>-1</sup> ) <sup>[b]</sup>	$G_{298}$ (Hartree) <sup>[b]</sup>	low. freq. (cm <sup>-1</sup> )
1	-522.687806	-522.626868	98.2	-522.673535	82.3
ts1	-522.642317	-522.583048	96.5	-522.628875	-96.9
1'	-522.672262	-522.610955	101.0	-522.658950	33.8
ts1'	-522.652040	-522.592288	99.3	-522.639491	-215.7
2a	-232.248652	-232.142551	69.0	-232.175347	414.3
ts2a <i>endo</i>	-754.896344	-754.728311	127.6	-754.788917	-431.5
ts2a <i>exo</i>	-754.898051	-754.730082	125.4	-754.789655	-423.5
3a	-754.949345	-754.778663	120.6	-754.835944	30.3
ts3a	-754.886324	-754.720150	123.3	-754.778743	-309.3
6a	-455.925913	-455.793647	96.6	-455.839561	60.5
ts4a	-455.925510	-455.794530	95.2	-455.839771	-545.0
4a	-456.024789	-455.888491	100.0	-455.935992	6.3
2b	-271.566650	-271.431182	79.2	-271.468811	44.5
ts2bi <i>endo</i>	-794.213091	-794.015937	129.5	-794.077483	-406.0
ts2bi <i>exo</i>	-794.215158	-794.017927	129.2	-794.079302	-379.6
ts2bo <i>endo</i>	-794.215820	-794.018479	132.5	-794.081439	-418.3
ts2bo <i>exo</i>	-794.218013	-794.020533	132.4	-794.083428	-412.0
ts2bm <i>endo</i>	-794.216921	-794.019515	134.2	-794.083278	-417.4
ts2bm <i>exo</i>	-794.218799	-794.021410	133.6	-794.084897	-406.5
3bi	-794.264474	-794.064486	125.4	-794.124068	38.3
3bo	-794.270354	-794.070164	127.8	-794.130890	33.8

<b>3bm</b>	-794.270460	-794.070293	128.1	-794.131160	31.3
<b>ts3bo</b>	-794.203032	-794.007098	130.1	-794.074114	-329.7
<b>ts3bm</b>	-794.207393	-794.011771	131.0	-794.076437	-301.0
<b>ts3bp</b>	-794.209600	-794.013926	131.6	-271.468811	-304.5
<b>2c</b>	-331.482299	-331.383616	73.5	-331.418517	242.2
<b>ts2ci endo</b>	-854.126378	-853.966204	127.2	-854.026650	-419.7
<b>ts2ci exo</b>	-854.127447	-853.967204	127.2	-854.027651	-418.7
<b>ts2co endo</b>	-854.127659	-853.967071	128.9	-854.028296	-437.5
<b>ts2co exo</b>	-854.129899	-853.969265	128.5	-854.030330	-418.7
<b>ts2cm endo</b>	-854.128510	-853.967931	130.1	-854.029757	-429.5
<b>ts2cm exo</b>	-854.130408	-853.969796	129.1	-854.031112	-414.6
<b>3ci</b>	-854.176755	-854.013783	124.5	-854.072951	27.8
<b>3co</b>	-854.179730	-854.016268	125.5	-854.075882	27.8
<b>3cm</b>	-854.181103	-854.017752	125.0	-854.077160	29.6
<b>ts3co</b>	-854.115453	-853.956361	127.8	-854.016868	-302.4
<b>ts3cm</b>	-854.115719	-853.957093	127.7	-854.021543	-301.0
<b>ts3cp</b>	-854.119940	-853.960945	127.5	-331.418517	-302.2
<b>2d</b>	-691.844974	-691.747316	76.2	-691.783537	190.2
<b>ts2di endo</b>	-1214.483331	-1214.324291	129.5	-1214.385824	-412.8
<b>ts2di exo</b>	-1214.485583	-1214.326368	128.6	-1214.387474	-378.7
<b>ts2do endo</b>	-1214.488071	-1214.328687	131.1	-1214.390966	-437.6
<b>ts2do exo</b>	-1214.490984	-1214.331449	130.6	-1214.393497	-426.5
<b>ts2dm endo</b>	-1214.489706	-1214.330208	132.6	-1214.393190	-433.9
<b>ts2dm exo</b>	-1214.491129	-1214.331638	132.1	-1214.394380	-421.7
<b>3di</b>	-1214.535340	-1214.373524	126.1	-1214.433443	39.8
<b>3do</b>	-1214.542237	-1214.379868	127.7	-1214.440540	31.5
<b>3dm</b>	-1214.542394	-1214.380157	127.8	-1214.440883	29.1
<b>ts3do</b>	-1214.471564	-1214.313719	130.5	-1214.380538	-299.7
<b>ts3dm</b>	-1214.476471	-1214.318978	130.6	-1214.384022	-302.5
<b>ts3dp</b>	-1214.479829	-1214.322039	130.5	-691.783537	-312.0
<b>2e</b>	-346.771321	-346.629898	81.7	-346.668720	93.9
<b>ts2ei_conf1 endo</b>	-869.424486	-869.221220	134.6	-869.285169	-383.8
<b>ts2ei_conf2 endo</b>	-869.417440	-869.214328	134.5	-869.278247	-390.0
<b>ts2ei_conf1 exo</b>	-869.425697	-869.222234	133.1	-869.285492	-319.0
<b>ts2ei_conf2 exo</b>	-869.419818	-869.216678	135.0	-869.280800	-360.7
<b>ts2eo_conf1 endo</b>	-869.424259	-869.220767	136.0	-869.285377	-410.9
<b>ts2eo_conf2 endo</b>	-869.418075	-869.215067	136.9	-869.280133	-410.5
<b>ts2eo_conf1 exo</b>	-869.427353	-869.223827	135.4	-869.288143	-372.4
<b>ts2eo_conf2 exo</b>	-869.419224	-869.215993	138.6	-869.281840	-406.9
<b>ts2em_conf1 endo</b>	-869.422083	-869.218799	139.0	-869.284846	-390.7
<b>ts2em_conf2 endo</b>	-869.427963	-869.224416	135.9	-869.289004	-379.2
<b>ts2em_conf1 exo</b>	-869.424624	-869.221142	138.5	-869.286942	-377.7
<b>ts2em_conf2 exo</b>	-869.429773	-869.226136	135.3	-869.290425	-367.2
<b>3ei_conf1</b>	-869.462658	-869.257319	133.3	-869.320646	27.6
<b>3ei_conf2</b>	-869.457862	-869.252733	131.1	-869.315017	47.4
<b>3eo_conf1</b>	-869.477902	-869.271539	128.9	-869.334834	29.9
<b>3eo_conf2</b>	-869.469533	-869.263515	133.5	-869.326927	33.7
<b>3em_conf1</b>	-869.470422	-869.264475	135.1	-869.328657	30.3

<b>3em_conf2</b>	-869.477563	-869.271344	132.8	-869.334420	30.1
<b>ts3eo_conf1</b>	-869.416261	-869.214044	136.0	-869.278642	-322.9
<b>ts3em_conf1</b>	-869.410364	-869.208926	136.2	-869.273616	-281.7
<b>ts3em_conf2</b>	-869.412368	-869.210851	135.9	-869.275417	-297.7
<b>ts3ep_conf1</b>	-869.420856	-869.218571	134.9	-869.282666	-338.7
<b>ts3ep_conf2</b>	-869.422304	-869.220056	135.9	-869.284616	-297.8
<b>6eo</b>	-570.454899	-570.285793	109.8	-570.337945	28.7
<b>6em_conf1</b>	-570.447563	-570.280214	109.6	-570.332286	48.1
<b>6em_conf2</b>	-570.450531	-570.282940	109.1	-570.334766	44.4
<b>6ep</b>	-570.457215	-570.288588	109.6	-570.340677	44.2
<b>ts4eo</b>	-570.449123	-570.282482	108.3	-570.333934	-883.0
<b>ts4em_conf1</b>	-570.447405	-570.281243	108.2	-570.332667	-452.0
<b>ts4em_conf2</b>	-570.449912	-570.283626	107.7	-570.334802	-595.3
<b>ts4ep</b>	-570.453669	-570.287030	107.9	-570.338284	-830.9
<b>4eo_conf1</b>	-570.548628	-570.376832	107.9	-570.428104	42.5
<b>4eo_conf2</b>	-570.549753	-570.377952	108.7	-570.429591	26.7
<b>4em_conf1</b>	-570.548002	-570.376346	111.0	-570.429087	10.7
<b>4em_conf2</b>	-570.548470	-570.376804	111.0	-570.429566	10.5
<b>4ep_conf1</b>	-570.548498	-570.376850	112.0	-570.430044	8.3
<b>4ep_conf2</b>	-570.548560	-570.376904	111.1	-570.429670	13.5
<b>2f</b>	-436.750584	-436.639287	83.2	-436.678815	62.3
<b>ts2fi_endo</b>	-959.383828	-959.211344	135.9	-959.275913	-428.5
<b>ts2fi_exo</b>	-959.389192	-959.216565	134.6	-959.280510	-381.2
<b>ts2fo_endo</b>	-959.391757	-959.218753	136.7	-959.283705	-443.3
<b>ts2fo_exo</b>	-959.394182	-959.221203	135.9	-959.285750	-426.9
<b>ts2fm_endo</b>	-959.390122	-959.217173	139.6	-959.283488	-444.0
<b>ts2fm_exo</b>	-959.391896	-959.218968	138.5	-959.284775	-435.7
<b>3fi</b>	-959.430863	-959.255896	134.3	-959.319725	29.5
<b>3fo</b>	-959.444753	-959.268974	134.8	-959.333044	21.7
<b>3fm</b>	-959.442381	-959.266722	135.3	-959.331006	27.7
<b>ts3fm</b>	-959.377298	-959.206457	137.6	-959.269389	-323.0
<b>ts3fp</b>	-959.377298	-959.206457	137.6	-959.271841	-323.0
<b>5</b>	-298.960827	-298.928927	75.0	-298.964568	128.5

[a] 1 Hartree = 627.5 kcal mol<sup>-1</sup>. [b] Thermal corrections at 298.15 K.

**Table S2. UB3LYP/6–31G(d) energies and spin contamination at different spin states (singlet and triplet) and enthalpies, free energies and entropies at singlet state of the partially biradical structures discussed on this work.**

Structure	Singlet							Triplet		
	$E_0$ (Hartree) <sup>[a]</sup>	$\langle S^2 \rangle$ <sup>[b]</sup>	$\langle S^2 \rangle$ <sup>[c]</sup>	H (Hartree) <sup>[a]</sup>	S (cal mol <sup>-1</sup> K <sup>-1</sup> ) <sup>[d]</sup>	G <sub>298</sub> (Hartree) <sup>[d]</sup>	low. freq. (cm <sup>-1</sup> )	$E_0$ (Hartree) <sup>[a]</sup>	$\langle S^2 \rangle$ <sup>[b]</sup>	$\langle S^2 \rangle$ <sup>[c]</sup>
ts1	-522.650287	0.716	0.141	-522.592261	101.2	-522.640349	-332.1	-522.638775	2.046	2.001
1'	-522.673381	0.352	0.024	-522.612715	102.0	-522.661181	24.7	-522.649475	2.040	2.001
ts2a'I	-754.889021	0.693	0.142	-754.722659	129.8	-754.784350	-454.6	-754.878950	2.053	2.002
3a'I	-754.893553	0.647	0.124	-754.726548	128.9	-754.787798	25.7	-754.881590	2.060	2.002
3a'II	-754.893788	1.059	0.476	-754.726624	129.9	-754.788354	21.9	-754.893795	2.059	2.002
ts2a'II	-754.890205	0.887	0.282	-754.723969	122.6	-754.782232	-24.6	-754.886061	2.060	2.002

[a] 1 Hartree = 627.5 kcal mol<sup>-1</sup>. [b] Expectation value of the S<sup>2</sup> operator *before* annihilation of the first spin contaminant (the theoretical values for a pure singlet and triplet are 0.000 and 2.000, respectively). [c] Expectation value of the S<sup>2</sup> operator *after* annihilation of the first spin contaminant (the theoretical values for a pure singlet and triplet are 0.000 and 2.000, respectively). [d] Thermal corrections at 298.15 K.

**Table S3. Single-point energies calculated on (U)B3LYP/6–31G(d) geometries.**

Structure	(U)B3LYP/6–311++G(2p,d)	CAS(n,n)/6–31G(d)			CCSD(T)/cc–pVTZ	
	$E_0$ (Hartree) <sup>[a]</sup>	n,n	$E_0$ (Hartree) <sup>[a]</sup>	$\mu_H$ <sup>[b]</sup>	$E_0$ (Hartree) <sup>[a]</sup>	$T_1$ -diagnostic <sup>[c]</sup>
1	-522.841453	6,6	-519.802590	1.9325	-521.860219	0.015
ts1	-522.796399	6,6	-519.745021	1.5178	-521.804002	0.016
1'	-522.825023	6,6	-519.764639	1.6393	-521.825578	0.014
ts1'	-522.804386	6,6	-519.768524	1.9280	-521.800142	0.015
2a	-232.317342	12,12	-230.702515	1.9578		
ts2a <i>endo</i>	-755.114553	12,12	-750.521867	1.8391		
ts2a <i>exo</i>	-755.116063	12,12	-750.526458	1.8919		
3a	-755.166790	12,12	-750.600839	1.8831		
ts2a'I	-755.107155	12,12	-750.503690	1.2765		
3a'I	-755.112258	12,12	-750.517076	1.2746		
3a'II	-755.111720	12,12	-750.557211	1.0059		
ts2a'II	-755.108198	12,12	-750.519076	1.1544		
ts3a	-755.107770					
6a	-456.060572					
ts4a	-456.060111					
4a	-456.156673					
2b	-271.645930					
ts2bi <i>endo</i>	-794.442197					
ts2bi <i>exo</i>	-794.443872					
ts2bo <i>endo</i>	-794.444773					
ts2bo <i>exo</i>	-794.446477					
ts2bm <i>endo</i>	-794.446201					
ts2bm <i>exo</i>	-794.447815					
3bi	-794.492618					
3bo	-794.498259					
3bm	-794.498832					

ts3bo	-794.434912
ts3bm	-794.439665
ts3bp	-794.441969
2c	-331.588844
ts2ci <i>endo</i>	-854.380604
ts2ci <i>exo</i>	-854.382381
ts2co <i>endo</i>	-854.382687
ts2co <i>exo</i>	-854.385041
ts2cm <i>endo</i>	-854.384443
ts2cm <i>exo</i>	-854.386061
3ci	-854.431278
3co	-854.434340
3cm	-854.436043
ts3co	-854.372205
ts3cm	-854.374607
ts3cp	-854.378243
2d	-691.942624
ts2di <i>endo</i>	-1214.731637
ts2di <i>exo</i>	-1214.733495
ts2do <i>endo</i>	-1214.735855
ts2do <i>exo</i>	-1214.738394
ts2dm <i>endo</i>	-1214.737517
ts2dm <i>exo</i>	-1214.738903
3di	-1214.781867
3do	-1214.788946
3dm	-1214.789338
ts3do	-1214.722619
ts3dm	-1214.727612
ts3dp	-1214.731198
2e	-346.876973
ts2ei_conf1 <i>endo</i>	-869.679426
ts2ei_conf2 <i>endo</i>	-869.672137
ts2ei_conf1 <i>exo</i>	-869.680747
ts2ei_conf2 <i>exo</i>	-869.674600
ts2eo_conf1 <i>endo</i>	-869.678976
ts2eo_conf2 <i>endo</i>	-869.673179
ts2eo_conf1 <i>exo</i>	-869.682030
ts2eo_conf2 <i>exo</i>	-869.673774
ts2em_conf1 <i>endo</i>	-869.678079
ts2em_conf2 <i>endo</i>	-869.683347
ts2em_conf1 <i>exo</i>	-869.680344
ts2em_conf2 <i>exo</i>	-869.684914
3ei_conf1	-869.716591
3ei_conf2	-869.711437
3eo_conf1	-869.732209
3eo_conf2	-869.723615
3em_conf1	-869.724912
3em_conf2	-869.732262

<b>ts3eo_conf1</b>	-869.673792
<b>ts3em_conf1</b>	-869.668923
<b>ts3em_conf2</b>	-869.671106
<b>ts3ep_conf1</b>	-869.678952
<b>ts3ep_conf2</b>	-869.680753
<b>6eo</b>	-570.626032
<b>6em_conf1</b>	-570.619472
<b>6em_conf2</b>	-570.622505
<b>6ep</b>	-570.629242
<b>ts4eo</b>	-570.619828
<b>ts4em_conf1</b>	-570.619251
<b>ts4em_conf2</b>	-570.621751
<b>ts4ep</b>	-570.625301
<b>4eo_conf1</b>	-570.716992
<b>4eo_conf2</b>	-570.718166
<b>4em_conf1</b>	-570.716930
<b>4em_conf2</b>	-570.717445
<b>4ep_conf1</b>	-570.717411
<b>4ep_conf2</b>	-570.717435
<b>2f</b>	-436.887126
<b>ts2fi endo</b>	-959.668880
<b>ts2fi exo</b>	-959.673993
<b>ts2fo endo</b>	-959.677159
<b>ts2fo exo</b>	-959.679212
<b>ts2fm endo</b>	-959.676194
<b>ts2fm exo</b>	-959.677811
<b>3fi</b>	-959.715571
<b>3fo</b>	-959.729537
<b>3fm</b>	-959.727766
<b>ts3fm</b>	-959.666370
<b>ts3fp</b>	-959.666370
<b>5</b>	-299.053889

[a] 1 Hartree = 627.5 kcal mol<sup>-1</sup>. [b] Occupation of the HOMO natural orbital. [c] Threshold for reasonable CCSD wave functions  $T_1$ -diagnostic = 0.020

**Cartesian coordinates for the minimum energy conformers of the structures considered in this work  
 (coordinates for all geometries can be obtained from the authors upon request).**

Structure 1 (B3LYP/6-31G(d))				C	-2.26520100	-1.11715500	-0.00041000
C	0.13367800	0.77579900	0.00000000	N	-3.15311400	-1.87252900	0.00023500
C	-0.49740100	-0.61026200	0.00000000	C	-1.47719600	1.21193800	0.00009600
O	-1.28111600	0.58329100	0.00000000	N	-1.77602600	2.33992300	0.00007600
C	-0.50027400	-1.39024100	1.22617100	Structure 1' (UB3LYP/6-31G(d))			
N	-0.50027400	-2.02602600	2.19629200	C	-1.21539400	-0.17765900	0.00013200
C	-0.50027400	-1.39024100	-1.22617100	O	-0.00000100	-0.72573000	-0.00032700
N	-0.50027400	-2.02602600	-2.19629200	C	1.21539300	-0.17765900	-0.00053700
C	0.72011100	1.29008400	-1.22615500	C	2.27564700	-1.10852100	-0.00014700
N	1.19979000	1.70762100	-2.19617000	N	3.17166700	-1.85561000	0.00038900
C	0.72011100	1.29008400	1.22615500	C	1.46931200	1.20720900	0.00014100
N	1.19979000	1.70762100	2.19617000	N	1.76162900	2.33800100	0.00025700
Structure ts1 (B3LYP/6-31G(d))				C	-2.27564700	-1.10852000	-0.00004400
C	0.00000000	1.05421600	0.30540500	N	-3.17166700	-1.85560900	0.00011300
C	0.00000000	-1.05421600	0.30540500	C	-1.46931100	1.20721000	0.00023400
O	0.00000000	0.00000000	1.19192900	N	-1.76162700	2.33800200	-0.00019500
C	1.07415000	-1.26306800	-0.58696500	Structure 2a (B3LYP/6-31G(d))			
N	1.95560500	-1.50412400	-1.31391200	C	1.06283000	-0.90589700	-0.00000500
C	-1.04487100	-1.99292000	0.42064800	C	-0.25325600	-1.37325100	-0.00006800
N	-1.91324200	-2.76763600	0.51359200	C	-1.31598900	-0.46746200	-0.00005500
C	-1.07415000	1.26306800	-0.58696500	C	-1.06275300	0.90598500	-0.00000800
N	-1.95560500	1.50412400	-1.31391200	C	0.25314000	1.37326900	-0.00006100
C	1.04487100	1.99292000	0.42064800	C	1.31602900	0.46735700	0.00005700
N	1.91324200	2.76763600	0.51359200	H	1.88971600	-1.61099600	0.00006600
Structure ts1 (UB3LYP/6-31G(d))				H	-0.45013100	-2.44198600	-0.00007700
C	0.61763300	-0.86287700	0.30907900	H	-2.34003000	-0.83109700	0.00015300
C	-0.61763300	0.86287700	0.30907900	H	-1.88981100	1.61087200	-0.00000700
O	0.00000000	0.00000000	1.21883300	H	0.45026200	2.44195100	-0.00001900
C	-1.88933000	0.53288200	-0.19453600	H	2.33998700	0.83124600	0.00006400
N	-2.94901100	0.26477400	-0.60897800	Structure 2b (B3LYP/6-31G(d))			
C	0.00000000	2.09318300	0.02614700	C	-1.20113600	-1.20545600	0.00216400
N	0.51590200	3.11603200	-0.20808900	C	-1.90508700	-0.00007900	0.00853100
C	1.88933000	-0.53288200	-0.19453600	C	-1.20134800	1.20534400	0.00216500
N	2.94901100	-0.26477400	-0.60897800	C	0.19418400	1.20237900	-0.00901200
C	0.00000000	-2.09318300	0.02614700	C	0.91387800	0.00012300	-0.01125500
N	-0.51590200	-3.11603200	-0.20808900	C	0.19432600	-1.20230700	-0.00901000
Structure ts1' (B3LYP/6-31G(d))				H	-1.73859700	-2.15043000	0.00146700
C	1.29540000	-0.00051700	-0.00434300	H	-2.99186000	-0.00017900	0.01407100
C	-1.29530800	-0.00047900	-0.00076300	H	-1.73890600	2.15026200	0.00147100
O	0.00005300	-0.00138700	-0.00048800	H	0.73435400	2.14686700	-0.01805300
C	-1.98178200	1.23993100	-0.00757900	H	0.73463100	-2.14672600	-0.01805900
N	-2.55798300	2.25302000	-0.00520400	C	2.42554200	0.00005400	0.00937300
C	-1.98292400	-1.24048300	0.00513000	H	2.83407700	0.88970100	-0.48225500
N	-2.56335300	-2.25111900	0.00915400	H	2.80992000	-0.00734400	1.03845300
C	1.98299100	-1.24051600	-0.00471900	H	2.83422400	-0.88250600	-0.49483400
N	2.56298800	-2.25140700	-0.00558000	Structure 2c (B3LYP/6-31G(d))			
C	1.98181300	1.23994600	0.00043200	C	1.13553300	-1.20862100	0.00000200
N	2.55812500	2.25290500	0.01233800	C	1.83592600	-0.00000100	-0.00000700
Structure 1' (B3LYP/6-31G(d))				C	1.13554300	1.20861300	0.00000300
C	-1.21313700	-0.17362200	-0.00072200	C	-0.26042100	1.21759400	-0.00000700
O	0.00000000	-0.69968500	0.00026400	C	-0.93162900	0.00000700	-0.00001800
C	1.21313800	-0.17362200	0.00083600	C	-0.26042000	-1.21759000	-0.00000100
C	2.26520200	-1.11715400	-0.00000700	H	1.67506900	-2.15175900	0.00000900
N	3.15311500	-1.87252700	-0.00036200	H	2.92195300	-0.00001000	-0.00000700
C	1.47719600	1.21193900	0.00053500	H	1.67507100	2.15175600	0.00000900
N	1.77602400	2.33992400	-0.00053100	H	-0.82866100	2.14202200	-0.00000200

H	-0.82868500	-2.14200300	0.00000800
F	-2.28243700	-0.00000200	0.00001700

Structure **2d** (B3LYP/6-31G(d))

C	-1.20769100	-1.57458500	0.00000000
C	0.00000600	-2.27467500	0.00000000
C	1.20769800	-1.57458100	0.00000000
C	1.21639400	-0.17871000	0.00000000
C	0.00000000	0.50300400	0.00000000
C	-1.21639300	-0.17871700	0.00000000
H	-2.15125600	-2.11333600	0.00000000
H	0.00000700	-3.36089500	0.00000000
H	2.15126800	-2.11332500	0.00000000
H	2.14934900	0.37489000	0.00000000
H	-2.14934900	0.37488200	0.00000000
Cl	-0.00000600	2.26513900	0.00000000

Structure **2e** (B3LYP/6-31G(d))

C	1.85198200	-1.00034700	-0.00004600
C	2.28344700	0.33078800	-0.00003600
C	1.33598600	1.35170100	-0.00005200
C	-0.03289200	1.06355900	-0.00000900
C	-0.45467400	-0.27121200	0.00003800
C	0.49514500	-1.30360700	-0.00002300
H	2.57836100	-1.80896000	-0.00006900
H	3.34395000	0.56520400	-0.00005900
H	1.65568100	2.39073000	-0.00009000
H	-0.75064700	1.87609900	-0.00004200
H	0.14319800	-2.33060700	-0.00003100
O	-1.76120200	-0.67221300	-0.00000700
C	-2.76892900	0.32510300	0.00011400
H	-2.71022000	0.95966700	-0.89452700
H	-3.72082600	-0.20974900	0.00002200
H	-2.71026700	0.95941800	0.89493400

Structure **2f** (B3LYP/6-31G(d))

C	-1.82084300	1.21227600	-0.00000400
C	-2.51646200	-0.00000200	-0.00000600
C	-1.82085800	-1.21227000	0.00001100
C	-0.42742400	-1.22079700	0.00003000
C	0.24430300	-0.00000600	0.00003100
C	-0.42742400	1.22080000	0.00001300
H	-2.36275400	2.15330000	-0.00001600
H	-3.60279400	0.00001300	-0.00001900
H	-2.36274900	-2.15330600	0.00000800
H	0.14021500	-2.14314600	0.00004600
H	0.14024000	2.14313400	0.00001200
N	1.71809800	-0.00000100	0.00005200
O	2.28959100	-1.08986100	-0.00001100
O	2.28958500	1.08986200	-0.00009400

Structure **ts2a (endo)** (B3LYP/6-31G(d))

C	-2.73389500	-1.25863500	-0.31964200
C	-3.00600300	0.14641900	-0.35009900
C	-2.07958200	1.02612800	-0.83722600
C	-0.77782300	0.56889400	-1.23136200
C	-0.50262500	-0.85701300	-1.20731000
C	-1.54424600	-1.74968600	-0.77972000
C	0.99297900	-1.01133100	0.41359300
O	0.66662200	0.12484400	1.08171000
C	0.51902300	1.31080000	0.43580700
C	-0.24451400	2.24791400	1.20284000
N	-0.91894400	3.01257500	1.76308600
C	1.59743700	1.86532400	-0.33187200

N	2.40906100	2.36108700	-1.00345200
C	0.69090300	-2.18640700	1.17685000
N	0.39986700	-3.16534500	1.73350000
C	2.19729900	-1.07683000	-0.36802400
N	3.13163600	-1.19741100	-1.05165100
H	0.22952100	-1.23294700	-1.91536500
H	-0.21463100	1.17368500	-1.93501900
H	-3.50471800	-1.93990000	0.02860700
H	-3.97788800	0.50513000	-0.02421000
H	-2.30744000	2.08493300	-0.91026700
H	-1.36287300	-2.81946800	-0.81079700

Structure **ts2a (exo)** (B3LYP/6-31G(d))

C	-0.71574300	2.80183700	-0.35744000
C	0.71575800	2.80183300	-0.35743900
C	1.41411600	1.74535400	-0.87462500
C	0.72698900	0.56823400	-1.31632700
C	-0.72698400	0.56823800	-1.31632700
C	-1.41410500	1.74536100	-0.87462700
C	1.18411100	-0.96708900	0.22248000
O	-0.00000400	-1.63104700	0.13748600
C	-1.18411700	-0.96708300	0.22248000
C	-2.26921000	-1.72832400	-0.32235900
N	-3.16255700	-2.28063300	-0.82329000
C	-1.49335700	-0.17438100	1.37553900
N	-1.80112000	0.52104500	2.25669100
C	2.26920000	-1.72833500	-0.32235900
N	3.16254500	-2.28064700	-0.82329100
C	1.49335500	-0.17439300	1.37554100
N	1.80112000	0.52103300	2.25669500
H	-1.22457000	-0.07702400	-2.03360200
H	1.22457200	-0.07702900	-2.03360300
H	-1.24456500	3.67422900	0.01434100
H	1.24458400	3.67422300	0.01434300
H	2.49856300	1.77042700	-0.92811300
H	-2.49855200	1.77044000	-0.92811600

Structure **ts2a'I** (UB3LYP/6-31G(d))

C	-2.50855100	-1.83314500	-0.44674600
C	-3.52252500	-0.87169000	-0.64243000
C	-3.18574800	0.44628100	-1.00335200
C	-1.86575400	0.82295000	-1.13083000
C	-0.79236400	-0.10647500	-0.81642100
C	-1.18315200	-1.48676300	-0.56887900
C	2.22465300	-0.36055700	0.01160700
O	1.20549700	-0.28088800	0.91460900
C	0.07455300	0.51381100	0.74428900
C	-0.81990800	0.27255000	1.86459500
N	-1.58142700	0.07121900	2.71715000
C	0.31651600	1.93718400	0.54823500
N	0.43582800	3.07970000	0.37501300
C	2.96082100	-1.55762500	0.07340200
N	3.56888400	-2.55545000	0.10385500
C	2.61559300	0.68459000	-0.84157300
N	2.96020200	1.50762900	-1.59931700
H	0.11727900	0.00520600	-1.42019500
H	-1.60767900	1.83536000	-1.42598900
H	-2.77944500	-2.86033300	-0.22084700
H	-4.56495700	-1.15567300	-0.53756400
H	-3.97330200	1.16729100	-1.20203700
H	-0.40508700	-2.23309300	-0.43852400



Structure <b>3a'I</b> (UB3LYP/6-31G(d))				C	2.83781300	0.28547900	0.84835700
C	2.62515500	1.65247700	0.00435700	N	3.45442500	0.77273500	1.71529000
C	3.47188800	0.85657100	-0.80233600	C	2.49044900	-1.57458600	-0.70666000
C	2.96515700	-0.29649100	-1.43505700	N	2.77314500	-2.62869900	-1.12876100
C	1.65314800	-0.66978500	-1.27947400	H	-0.16636400	-1.99834500	-0.89108200
C	0.70873500	0.12498900	-0.45964300	H	-1.09273300	0.06411400	-1.99533600
C	1.31181200	1.31878000	0.19282000	H	-3.75501000	-1.98710400	1.47408600
C	-2.03867400	0.60432300	0.08887400	H	-4.31949700	0.30451600	0.67670900
O	-1.25165300	-0.00408000	1.04409200	H	-2.80491300	1.52094600	-0.82602800
C	-0.11754600	-0.76311200	0.59559300	H	-1.71470800	-3.13866200	0.62878200
C	0.68509700	-1.04618300	1.79960900	Structure <b>ts2bi (exo)</b> (B3LYP/6-31G(d))			
N	1.34514100	-1.26247400	2.72751600	C	1.50028800	2.40729100	-0.47349100
C	-0.53467900	-2.04768900	-0.01209000	C	0.14118600	2.84048700	-0.39280100
N	-0.83468200	-3.05429100	-0.50397500	C	-0.86930900	2.01908100	-0.79500200
C	-2.14364800	2.00366600	0.18766400	C	-0.60030200	0.65487900	-1.20649200
N	-2.17861200	3.17054800	0.26790900	C	0.80190000	0.24188400	-1.33168200
C	-2.90494600	-0.14065600	-0.73472000	C	1.81279500	1.16988900	-0.99158200
N	-3.61969500	-0.73479000	-1.44491300	C	1.11220900	-0.96212000	-2.18277400
H	-0.16467800	0.46490200	-1.08667200	H	2.29338400	3.08579500	-0.17579000
H	1.27378600	-1.55647300	-1.77798600	H	-0.07642000	3.84458800	-0.04170800
H	3.02467200	2.54044000	0.48544200	H	-1.89931000	2.36317700	-0.78300900
H	4.51378700	1.13215300	-0.92998100	H	-1.25669600	0.25857300	-1.98079400
H	3.62150000	-0.89976200	-2.05550900	H	2.85129700	0.87249200	-1.11057400
H	0.67008800	1.93708900	0.81262600	H	1.00571400	-0.69522700	-3.24357600
Structure <b>3a'II</b> (UB3LYP/6-31G(d))				H	0.42121100	-1.78962200	-1.99097300
C	3.61010000	0.51490000	0.14280000	H	2.13360900	-1.32021600	-2.02956600
C	3.83430000	-0.73960000	-0.47790000	C	-1.43400600	-0.57571500	0.18861000
C	2.84060000	-1.74620000	-0.39480000	O	-0.44570400	-1.46851000	0.50332100
C	1.65170000	-1.53060000	0.24450000	C	0.80459200	-1.03550400	0.83012500
C	1.31880000	-0.20330000	0.86640000	C	1.80149700	-2.03620100	0.70663700
C	2.44180000	0.79430000	0.79390000	N	2.64900000	-2.82239900	0.55344600
C	-2.30800000	-0.45660000	0.05210000	C	1.04058400	0.06000200	1.68742000
O	-1.02180000	-0.60500000	0.48170000	N	1.32277700	1.02380600	2.28541600
C	-0.01590000	0.39680000	0.21260000	C	-2.51479900	-1.25972300	-0.49099200
C	-0.37030000	1.66460000	0.88190000	N	-3.36789400	-1.74733000	-1.11119400
N	-0.59680000	2.63780000	1.47130000	C	-1.90311500	0.29538900	1.24870200
C	0.15930000	0.59610000	-1.23820000	N	-2.32792200	1.00459200	2.06509600
N	0.32940000	0.72300000	-2.37820000	Structure <b>ts2bo (exo)</b> (B3LYP/6-31G(d))			
C	-3.14950000	-1.54380000	0.34550000	C	-0.31581800	-2.81929000	-0.19060100
N	-3.85570000	-2.44390000	0.58520000	C	-1.61307000	-2.22571500	-0.09984400
C	-2.79510000	0.67300000	-0.61840000	C	-1.87986200	-0.98713900	-0.62726100
N	-3.23900000	1.60000000	-1.18020000	C	-0.78402300	-0.22448600	-1.17154500
H	1.00350000	-0.34570000	1.91470000	C	0.52915000	-0.83563300	-1.29032700
H	0.90880000	-2.31780000	0.31720000	C	0.71130200	-2.17358100	-0.82336900
H	4.39230000	1.26890000	0.11300000	C	-0.41146600	1.37739300	0.31120200
H	4.76670000	-0.93340000	-0.99690000	O	0.92214100	1.50943100	0.08193700
H	3.03430000	-2.72000000	-0.83710000	C	1.74977900	0.43046500	0.10640900
H	2.29660000	1.75240000	1.28440000	C	2.97787400	0.67469200	-0.58734300
Structure <b>ts2a'II</b> (UB3LYP/6-31G(d))				N	3.95458500	0.80820900	-1.20610100
C	-3.07909900	-1.46668700	0.80368800	C	1.83549100	-0.40036700	1.26836400
C	-3.38817600	-0.15755900	0.36096300	N	1.92839100	-1.14724100	2.15659900
C	-2.54889400	0.52522800	-0.47593400	C	-1.14798200	2.51290000	-0.16365900
C	-1.23554600	-0.04798300	-0.90884800	N	-1.78658100	3.38208900	-0.60039800
C	-1.02838300	-1.47205200	-0.49534000	C	-0.88243700	0.79786800	1.53594900
C	-1.90802600	-2.10974700	0.33787500	N	-1.34477900	0.30656000	2.48437600
C	2.12255000	-0.31446800	-0.20287100	H	1.17804800	-0.46898800	-2.07939000
O	1.19919200	0.38187500	-0.93332700	H	-1.02582800	0.55670600	-1.88720700
C	-0.02570800	0.87391800	-0.34297600	H	-0.16942800	-3.82127500	0.20170000
C	-0.03879800	0.86559600	1.13050000	H	-2.41862000	-2.79922300	0.35048400
N	-0.12244400	0.84924400	2.28706100	H	1.67664900	-2.65343300	-0.95268700
C	-0.18882700	2.25543700	-0.83495600	C	-3.26616800	-0.39751300	-0.63618800
N	-0.36176100	3.32158800	-1.25691900	H	-3.33962800	0.48258900	0.01481600

H -3.55038400 -0.07177300 -1.64442600  
 H -4.00586000 -1.12491900 -0.29084800

Structure **ts2bm** (*exo*) (B3LYP/6-31G(d))

C -2.57169500 -0.45435900 -0.44094100  
 C -1.96829400 -1.76056000 -0.40668400  
 C -0.70658900 -1.97954100 -0.87617900  
 C 0.11391400 -0.87922400 -1.31053100  
 C -0.49948700 0.43547700 -1.37408800  
 C -1.85519100 0.59166100 -0.97569600  
 C -3.98130000 -0.28367900 0.05705100  
 H -2.55939700 -2.59487400 -0.03822000  
 H -0.28898800 -2.98234000 -0.89061200  
 H 0.90252100 -1.08879700 -2.02753000  
 H -0.06898100 1.16440300 -2.05235700  
 H -2.31699100 1.57046400 -1.07266400  
 H -4.02701100 -0.44921900 1.14054500  
 H -4.65749500 -1.01036300 -0.40988200  
 H -4.36099900 0.72162800 -0.14461600  
 C 1.61729900 -0.66987900 0.21729200  
 O 1.78889800 0.67872300 0.17114400  
 C 0.72759600 1.52631800 0.26396400  
 C 1.00580000 2.81893800 -0.27068500  
 N 1.17340300 3.86065700 -0.76404500  
 C -0.19431500 1.45027700 1.34745200  
 N -1.03182300 1.40504600 2.15664300  
 C 2.76530400 -1.36555900 -0.29972200  
 N 3.63711000 -1.96654000 -0.78053600  
 C 1.02338800 -1.27282300 1.38176400  
 N 0.53667900 -1.82815700 2.28053900

Structure **ts2ci** (*exo*) (B3LYP/6-31G(d))

C 1.90844500 2.09120600 -0.51341500  
 C 0.64398800 2.74837500 -0.38853200  
 C -0.51128100 2.12627300 -0.76471100  
 C -0.50853600 0.74192600 -1.18893900  
 C 0.79758400 0.12114200 -1.29032800  
 C 1.99223700 0.82060300 -1.03329200  
 H 2.81438400 2.62199100 -0.23990500  
 H 0.61738800 3.77356500 -0.03319800  
 H -1.45779400 2.65705200 -0.74347900  
 H -1.20327100 0.45709000 -1.97690400  
 H 2.93870900 0.31474300 -1.19290500  
 C -1.53405600 -0.39762200 0.18568200  
 O -0.64952100 -1.39762400 0.46890300  
 C 0.64601600 -1.11627500 0.77645300  
 C 1.52111100 -2.22086300 0.59440400  
 N 2.27956100 -3.08615100 0.41203600  
 C 1.01706000 -0.10582400 1.69576700  
 N 1.42668800 0.77748400 2.34066600  
 C -2.68692200 -0.92362700 -0.50957000  
 N -3.59716200 -1.27935300 -1.13833400  
 C -1.87692400 0.52900500 1.24312500  
 N -2.19342100 1.30206300 2.05109100  
 F 0.84719600 -1.01418300 -2.00699000

Structure **ts2co** (*exo*) (B3LYP/6-31G(d))

C -0.31678800 -2.83404300 -0.27616000  
 C -1.60558900 -2.23859200 -0.12186500  
 C -1.81184900 -0.98789300 -0.61510100  
 C -0.76193300 -0.18721400 -1.17826300  
 C 0.53239800 -0.82710300 -1.33923200  
 C 0.70537100 -2.17063900 -0.91104900  
 C -0.45785300 1.35537700 0.24838800

O 0.88474800 1.51506300 0.10455000  
 C 1.73857100 0.45981200 0.19324900  
 C 2.99406600 0.71059300 -0.43416300  
 N 4.00286800 0.85610000 -0.99767800  
 C 1.72283000 -0.42696200 1.30653000  
 N 1.72323400 -1.23948000 2.14220100  
 C -1.17804900 2.49177700 -0.26497600  
 N -1.79179600 3.35898300 -0.73666500  
 C -0.97764500 0.82699800 1.48518000  
 N -1.45594800 0.39413700 2.45241500  
 H 1.20711400 -0.41722300 -2.08270900  
 H -1.05888000 0.55245500 -1.91624400  
 H -0.16639600 -3.84701200 0.08369500  
 H -2.42186200 -2.77815500 0.34530900  
 H 1.66272800 -2.65667200 -1.06924400  
 F -3.01670800 -0.39941600 -0.53048300

Structure **ts2cm** (*exo*) (B3LYP/6-31G(d))

C -2.59710000 -0.17012200 -0.39234100  
 C -2.19863000 -1.53949300 -0.39748200  
 C -0.97551300 -1.87494900 -0.89858000  
 C -0.04006800 -0.85286700 -1.30090800  
 C -0.50043500 0.52670200 -1.33362700  
 C -1.81446800 0.83469500 -0.89344600  
 H -2.90049900 -2.28514300 -0.03973200  
 H -0.67022400 -2.91568400 -0.95301800  
 H 0.71563500 -1.12992000 -2.03023300  
 H -0.01493000 1.20868500 -2.02220800  
 H -2.19981500 1.84699100 -0.94491200  
 C 1.43925200 -0.86969900 0.22785000  
 O 1.84897800 0.42302000 0.15087300  
 C 0.95767300 1.45171000 0.23452500  
 C 1.44636500 2.65203900 -0.35918600  
 N 1.78243500 3.62583400 -0.90282500  
 C 0.06830900 1.57708800 1.33917700  
 N -0.73712900 1.70473500 2.17190600  
 C 2.45034400 -1.77382800 -0.25586300  
 N 3.20379200 -2.53510100 -0.70822600  
 C 0.74244900 -1.32835800 1.40331000  
 N 0.16030700 -1.77058300 2.30760900  
 F -3.82854300 0.10213300 0.05147600

Structure **ts2di** (*exo*) (B3LYP/6-31G(d))

C 0.93389800 2.61738000 -0.71985100  
 C -0.48134300 2.72724600 -0.87741000  
 C -1.23272700 1.63408300 -1.18571500  
 C -0.64381200 0.30286500 -1.25155900  
 C 0.81465700 0.25441500 -1.14898700  
 C 1.57659100 1.41477100 -0.93832200  
 H 1.51812800 3.50377600 -0.49629000  
 H -0.94933800 3.70213000 -0.78485000  
 H -2.29997300 1.72729700 -1.36199600  
 H -1.05723600 -0.35263400 -2.01663600  
 H 2.65818900 1.33883700 -0.90404400  
 C -1.37461000 -0.77720000 0.23458600  
 O -0.29460200 -1.30941900 0.89050900  
 C 0.73522800 -0.52025200 1.29599400  
 C 1.93311100 -1.22963900 1.55650800  
 N 2.94376400 -1.78197700 1.73704100  
 C 0.57048000 0.76856100 1.83509300  
 N 0.53833400 1.89204500 2.16110600  
 C -2.13882200 -1.84668500 -0.38322800  
 N -2.74978500 -2.65040800 -0.95721800  
 C -2.22136500 0.11755000 1.00836500

N -2.93744200 0.82083000 1.59277400  
 Cl 1.59383700 -1.18741500 -1.75582500

Structure **ts2do (exo)** (B3LYP/6-31G(d))

C -0.20669100 -2.80110700 -0.15280300  
 C -1.47798200 -2.16917300 0.00941900  
 C -1.68697900 -0.92510300 -0.51560900  
 C -0.61754500 -0.16883400 -1.10682200  
 C 0.65763900 -0.84224900 -1.29197200  
 C 0.80842800 -2.18584500 -0.83673300  
 O -0.14500600 1.38584500 0.33916300  
 C 1.18423000 1.48125000 0.06798800  
 C 1.98924700 0.38648100 0.07251100  
 C 3.19370500 0.59245500 -0.67041700  
 N 4.14873700 0.69592600 -1.32778900  
 C 2.08389900 -0.46026400 1.21983400  
 N 2.17929400 -1.22872800 2.08954600  
 C -0.85124600 2.55934800 -0.09537300  
 N -1.44845600 3.47279200 -0.49675200  
 C -0.57864000 0.82573700 1.58985100  
 N -0.99003700 0.35302100 2.56979100  
 H 1.28923200 -0.49205800 -2.10165500  
 H -0.88774400 0.59980400 -1.82363700  
 H -0.07517800 -3.80781600 0.23151400  
 H -2.28788100 -2.69776700 0.49997500  
 H 1.74651500 -2.70166300 -1.01629400  
 Cl -3.26461800 -0.17560700 -0.44374500

Structure **ts2dm (exo)** (B3LYP/6-31G(d))

C -2.30589400 -0.30504600 -0.46048100  
 C -1.82305000 -1.65303000 -0.45598000  
 C -0.57266600 -1.92670200 -0.92833500  
 C 0.31725800 -0.86518300 -1.31853800  
 C -0.20421600 0.48983400 -1.34981500  
 C -1.54734500 0.73076300 -0.94046500  
 H -2.48012200 -2.44582100 -0.11630300  
 H -0.21827600 -2.95231900 -0.97341600  
 H 1.10636500 -1.10429600 -2.02519500  
 H 0.25041800 1.19301800 -2.03905700  
 H -1.96121500 1.73090700 -1.00767600  
 C 1.79057900 -0.79534100 0.25037500  
 O 2.10185300 0.52480700 0.16902700  
 C 1.13624700 1.48267900 0.23143400  
 C 1.55282900 2.71805900 -0.35088500  
 N 1.82936500 3.71471300 -0.88570800  
 C 0.23961800 1.55752800 1.33910800  
 N -0.55938700 1.64892200 2.18173200  
 C 2.86603300 -1.62484800 -0.22170800  
 N 3.67728000 -2.33001400 -0.66557700  
 C 1.09722400 -1.30138100 1.40491000  
 N 0.51706200 -1.78483600 2.28953800  
 Cl -3.94364300 -0.02385000 0.06893100

Structure **ts2ei (conf1, exo)** (B3LYP/6-31G(d))

C 0.74103200 2.62587000 -0.64463800  
 C -0.67053700 2.68794900 -0.83519500  
 C -1.36583100 1.57683000 -1.20861700  
 C -0.71255800 0.28172200 -1.31461500  
 C 0.75248600 0.29203900 -1.23245700  
 C 1.45094700 1.46453300 -0.90328400  
 H 1.27797700 3.52126000 -0.35025900  
 H -1.18136900 3.63547400 -0.69870700  
 H -2.43443300 1.62671800 -1.39184900  
 H -1.07574200 -0.36230100 -2.11521900

H 2.53085200 1.45257900 -0.81520300  
 C -1.32088700 -0.90643900 0.11122800  
 O -0.24458300 -1.32934000 0.84282600  
 C 0.63136100 -0.44720100 1.41902500  
 C 1.86216300 -1.03248100 1.78839200  
 N 2.90255400 -1.48744500 2.06188700  
 C 0.28968600 0.82990500 1.86945600  
 N 0.10431200 1.95655800 2.13977000  
 C -1.89700600 -2.05660500 -0.57094400  
 N -2.35569800 -2.92612900 -1.18870800  
 C -2.33549200 -0.15452600 0.83947300  
 N -3.18092700 0.42624500 1.38384700  
 O 1.29834200 -0.86109500 -1.62722900  
 C 2.72985200 -0.99364200 -1.66464700  
 H 2.91384600 -2.00593100 -2.02273900  
 H 3.15951100 -0.26589800 -2.36105500  
 H 3.15631800 -0.87074500 -0.66637200

Structure **ts2eo (conf1, exo)** (B3LYP/6-31G(d))

C -0.43742100 -2.73444400 -0.35169500  
 C -1.61770400 -1.97120100 -0.15920800  
 C -1.67417100 -0.67990800 -0.63019200  
 C -0.49702500 -0.05035600 -1.20642100  
 C 0.66932500 -0.88393100 -1.42723900  
 C 0.66178700 -2.22609200 -1.02195200  
 C 0.02224800 1.38933400 0.17808400  
 O 1.38050800 1.38758600 0.12144000  
 C 2.10742800 0.24842300 0.29860200  
 C 3.41143500 0.31679400 -0.25138600  
 N 4.46855800 0.32673600 -0.74400200  
 C 1.82542100 -0.69384600 1.30979500  
 N 1.58043000 -1.56268500 2.05190200  
 C -0.50130000 2.62688100 -0.35743200  
 N -0.95316900 3.58146700 -0.84153000  
 C -0.61532300 0.99800700 1.41989600  
 N -1.18160800 0.71172700 2.39343700  
 H 1.43535000 -0.52191200 -2.10364100  
 H -0.70327000 0.71246100 -1.95312900  
 H -0.42363800 -3.76074000 0.00246600  
 H -2.47010400 -2.42683500 0.32966400  
 H 1.52981000 -2.85023900 -1.20665700  
 O -2.73485800 0.14992600 -0.56393600  
 C -3.90664000 -0.29097300 0.12712800  
 H -3.67385200 -0.51341800 1.17378300  
 H -4.60919000 0.54052600 0.07126600  
 H -4.33813600 -1.17278500 -0.36032800

Structure **ts2em (conf2, exo)** (B3LYP/6-31G(d))

C -2.24975600 -0.57833500 -0.51965000  
 C -1.68478400 -1.89839300 -0.57092700  
 C -0.41081700 -2.08147100 -1.00797800  
 C 0.43237600 -0.94244200 -1.31930600  
 C -0.22241400 0.34627400 -1.45186200  
 C -1.54810500 0.50909800 -1.03672300  
 H -2.31016400 -2.72693100 -0.25563000  
 H 0.02051400 -3.07755300 -1.04863600  
 H 1.27392900 -1.12162600 -1.98382100  
 H 0.24248200 1.10921400 -2.06347300  
 H -2.01768000 1.48115300 -1.12146500  
 C 1.63825600 -0.77545800 0.32236300  
 O 2.08771900 0.50589100 0.25979700  
 C 1.22596500 1.57205300 0.24182900  
 C 1.75557100 2.71340100 -0.40620100  
 N 2.14236400 3.64558100 -0.99208100

C	0.16582100	1.72404300	1.15854600
N	-0.79233500	1.86737400	1.81337200
C	2.71283000	-1.70733700	0.05537000
N	3.52155400	-2.49198000	-0.22852300
C	0.81993600	-1.16132000	1.45514500
N	0.16581400	-1.53608000	2.33948800
O	-3.48586100	-0.52346000	-0.01273100
C	-4.06862800	0.76033100	0.24765300
H	-4.99735800	0.55476100	0.77967900
H	-3.39526100	1.35977600	0.87009500
H	-4.29061200	1.28483400	-0.68861600

Structure **ts2fi** (*exo*) (B3LYP/6-31G(d))

C	-0.03302900	2.90098200	-0.47815400
C	-1.38055500	2.56505600	-0.81051000
C	-1.70197500	1.30722300	-1.22966600
C	-0.71352400	0.24087600	-1.23567600
C	0.65214000	0.65393400	-0.95074000
C	0.98147800	1.97766200	-0.62616300
H	0.20463700	3.91396500	-0.17084200
H	-2.14348200	3.33593500	-0.76736300
H	-2.71563300	1.06695400	-1.53590000
H	-0.79377100	-0.50092000	-2.02702200
H	2.02160300	2.23473500	-0.46658100
C	-1.25691900	-1.05311700	0.16353500
O	-0.09438100	-1.42165200	0.78891300
C	0.74864900	-0.50647700	1.31581900
C	2.05411700	-0.99705300	1.57084400
N	3.14521400	-1.35802200	1.76355500
C	0.31585300	0.66399900	1.97484100
N	0.02887900	1.70792200	2.41511900
C	-1.81339400	-2.18711900	-0.54985200
N	-2.28760900	-3.03709900	-1.18284900
C	-2.25183400	-0.38960200	0.99055000
N	-3.08730700	0.11882800	1.61687800
O	2.87651300	0.14631600	-1.34958900
O	1.36781200	-1.38807400	-1.74445400
N	1.71811400	-0.26042300	-1.38416200

Structure **ts2fo** (*exo*) (B3LYP/6-31G(d))

C	0.00010600	-2.81412300	-0.36157300
C	-1.25190800	-2.19768000	-0.07958800
C	-1.48090900	-0.91248000	-0.48641700
C	-0.47262600	-0.09762300	-1.10542700
C	0.79696200	-0.74741500	-1.36511500
C	0.96985200	-2.12638700	-1.04732900
C	0.05816100	1.48799100	0.26737800
O	1.41439100	1.43456800	0.12344900
C	2.09980000	0.27259500	0.21187300
C	3.39767300	0.34365900	-0.38224000
N	4.43237400	0.34104800	-0.91527300
C	1.94143100	-0.61474200	1.31876400
N	1.82112300	-1.42981100	2.14228700
C	-0.45552700	2.71408000	-0.28130100
N	-0.86342100	3.68316200	-0.77646300
C	-0.52867600	1.05781500	1.50751100
N	-1.04080700	0.68758100	2.48378400
H	1.44289600	-0.30319400	-2.11528100
H	-0.81009200	0.66874900	-1.79372000
H	0.15706900	-3.84707800	-0.06990600
H	-2.04722800	-2.74544200	0.41214900
H	1.90333100	-2.61114000	-1.31761800
O	-3.72147500	-1.06283400	0.07660400
O	-2.92456700	0.87543500	-0.54283500

N	-2.81195600	-0.32960700	-0.29898900
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Structure **ts2fm** (*exo*) (B3LYP/6-31G(d))

C	-2.07242900	-0.40995700	-0.49482000
C	-1.52340400	-1.72541600	-0.43693000
C	-0.25604300	-1.93799600	-0.89934500
C	0.56668000	-0.84328200	-1.33198600
C	-0.00840900	0.49042500	-1.35053100
C	-1.38128600	0.65901400	-0.98746600
H	-2.14613600	-2.53421300	-0.07631500
H	0.15132000	-2.94392200	-0.92562700
H	1.35910100	-1.05276600	-2.04342200
H	0.42487600	1.21797800	-2.02925300
H	-1.86395400	1.62567600	-1.07065100
C	2.14285200	-0.63942900	0.20060500
O	2.20961000	0.72055200	0.18186700
C	1.09583900	1.48435400	0.30007800
C	1.30573900	2.82758400	-0.15243100
N	1.41856200	3.90474800	-0.57708000
C	0.21017200	1.32029600	1.41458500
N	-0.57857600	1.20954600	2.26321100
C	3.31010800	-1.23940100	-0.37740700
N	4.20219800	-1.76431900	-0.90839600
C	1.58734700	-1.32205100	1.33271800
N	1.12210000	-1.94627700	2.19755200
O	-3.95241800	0.91082300	-0.18524200
O	-4.08049400	-1.20654100	0.32820500
N	-3.47882500	-0.21745100	-0.08325800

Structure **3a** (B3LYP/6-31G(d))

C	-1.39431800	-2.46683600	-0.37045900
C	-2.33966600	-1.58381800	-1.05644800
C	-2.00864500	-0.32215400	-1.37443300
C	-0.65471900	0.21908500	-1.00522200
C	0.43358100	-0.86069100	-0.82394800
C	-0.10204400	-2.13575000	-0.21816300
C	1.47842800	-0.08483100	0.04945300
O	0.73206600	0.81172200	0.88544400
C	-0.60407400	0.98803300	0.38580700
C	-1.55155600	0.47038500	1.39733500
N	-2.29100700	0.08975700	2.20515100
C	-0.86183100	2.42932600	0.19187600
N	-1.07478100	3.55281700	-0.00144500
C	2.29161700	-0.95610200	0.91916500
N	2.92670000	-1.66735800	1.57854800
C	2.38451100	0.70407600	-0.82432900
N	3.05657800	1.32407200	-1.53786100
H	-1.75809900	-3.41749600	0.00851200
H	-3.32853300	-1.96677900	-1.29165100
H	-2.70976200	0.34980500	-1.85979300
H	-0.31663300	0.94579300	-1.75008900
H	0.90663300	-1.09369600	-1.78769200
H	0.59973200	-2.81075300	0.26259900

Structure **3bi** (B3LYP/6-31G(d))

C	2.15437000	-1.89212800	-0.80980200
C	1.21101200	-2.50543800	0.12565300
C	-0.02623100	-2.01286600	0.29984200
C	-0.52130600	-0.84903600	-0.54045800
C	0.66053000	0.06208700	-0.95925700
C	1.90641900	-0.68652600	-1.34689500
C	0.83727100	1.02009700	0.30175900
O	-0.41506900	0.98986300	1.01040600
C	-1.36408300	0.17654900	0.31170600

C	-2.23632400	-0.46836900	1.31158800
N	-2.92684600	-1.01018300	2.06910100
C	-2.20624800	1.04984700	-0.54803500
N	-2.83472100	1.74739100	-1.22913700
C	1.89551500	0.60229200	1.24527400
N	2.72963000	0.30982300	1.99545300
C	1.12373900	2.40250400	-0.13767500
N	1.35168000	3.47301600	-0.52149700
H	0.33359700	0.70747300	-1.78098200
H	3.06894800	-2.42583900	-1.05202700
H	1.52472800	-3.39006000	0.67236000
H	-0.73421000	-2.50041400	0.96388800
H	2.60257500	-0.20609600	-2.02738200
C	-1.30610300	-1.40952300	-1.74284700
H	-0.64891200	-2.06141900	-2.32455300
H	-2.15838400	-2.00625900	-1.40117500
H	-1.67736300	-0.61354700	-2.39593100

Structure **3bo** (B3LYP/6-31G(d))

C	-0.92658800	-2.62151400	-0.17590300
C	-2.06645100	-1.83316600	-0.64160100
C	-1.95874700	-0.52509600	-0.94117000
C	-0.61136700	0.14220000	-0.76048900
C	0.60525200	-0.80420300	-0.83896200
C	0.33110200	-2.15507600	-0.22664500
C	1.69223100	0.05158500	-0.10582900
O	1.00870000	0.77835500	0.92506600
C	-0.40164900	0.84314300	0.65391000
C	-1.11813400	0.18421300	1.76765000
N	-1.68322200	-0.30213800	2.65558000
C	-0.81705400	2.26040400	0.60275000
N	-1.15925500	3.36612800	0.52744200
C	2.75648200	-0.74985000	0.52743600
N	3.58957200	-1.40348500	0.99930300
C	2.31319800	1.01089400	-1.05578400
N	2.75558300	1.76143400	-1.82147100
H	-1.11724000	-3.62167200	0.20290700
H	-3.03014300	-2.32829000	-0.72854900
H	-0.48764200	0.94116100	-1.49857300
H	0.92330500	-0.93444600	-1.88255300
H	1.17489100	-2.76301500	0.08494200
C	-3.10455000	0.33374800	-1.39685500
H	-4.02885600	-0.24647200	-1.46636100
H	-3.28221300	1.17087400	-0.70822100
H	-2.90280300	0.77775600	-2.38115900

Structure **3bm** (B3LYP/6-31G(d))

C	-1.87378400	-1.78248100	0.05740700
C	-2.57157200	-0.67087100	-0.61095900
C	-1.85612500	0.36898800	-1.07818300
C	-0.36543500	0.43069000	-0.89866600
C	0.31466500	-0.94339000	-0.73376100
C	-0.53940900	-1.91717100	0.03931400
C	1.65976800	-0.53288400	-0.04331500
O	1.36812300	0.60317100	0.78409100
C	0.11743200	1.20348900	0.40647500
C	-0.81628000	1.09357800	1.54892700
N	-1.53602500	1.02857900	2.45562300
C	0.33664100	2.63380500	0.11202900
N	0.49082500	3.75110700	-0.15794400
C	2.23710100	-1.58852600	0.81082200
N	2.67468700	-2.44297200	1.46081700
C	2.66060500	-0.14374700	-1.06988100
N	3.40759200	0.17466100	-1.89803200

H	-2.48127500	-2.52714900	0.56587700
H	0.09789200	0.96121000	-1.73598600
H	0.55597200	-1.37436600	-1.71491700
H	-0.05453900	-2.76789400	0.50906100
C	-4.06964400	-0.74832800	-0.72620400
H	-4.48039800	0.12169100	-1.24568400
H	-4.37665600	-1.65109700	-1.26964800
H	-4.52974200	-0.80192400	0.26871600
H	-2.33957000	1.21562400	-1.55741700

Structure **3ci** (B3LYP/6-31G(d))

C	-1.19053600	-2.58800100	-0.55392200
C	-2.22929900	-1.69628500	-1.07483900
C	-2.00304800	-0.38444200	-1.24638500
C	-0.68773300	0.20241400	-0.84776400
C	0.48843500	-0.78423400	-0.82057600
C	0.07751200	-2.17589300	-0.40030700
C	1.50664000	-0.04286700	0.12051400
O	0.73228400	0.77519500	1.01396500
C	-0.64274200	0.83082900	0.61553700
C	-1.45783400	0.08255600	1.59765100
N	-2.08791800	-0.48506000	2.38829000
C	-1.08922500	2.23607800	0.60084700
N	-1.47062000	3.33054900	0.59984600
C	2.32717300	-0.96596700	0.93013800
N	2.96740800	-1.71210700	1.54461100
C	2.41572200	0.82918900	-0.66256000
N	3.13540700	1.49758800	-1.27841300
H	-1.46068600	-3.61228000	-0.31603100
H	0.92394700	-0.83002200	-1.82765500
H	0.85705300	-2.85538800	-0.07052300
H	-2.75305100	0.30643200	-1.61841600
H	-3.20028300	-2.11770100	-1.31783300
F	-0.34728600	1.24781600	-1.69906700

Structure **3co** (B3LYP/6-31G(d))

C	-1.03147900	-2.60325500	-0.17062800
C	-2.14770100	-1.79133600	-0.65615400
C	-1.93725100	-0.50478700	-0.95036800
C	-0.60768800	0.16107800	-0.78539000
C	0.57476900	-0.83147100	-0.81387900
C	0.23849500	-2.16738200	-0.19419600
C	1.67309800	0.00419700	-0.07055600
O	0.99131300	0.80031300	0.90867100
C	-0.40829200	0.91108000	0.60366600
C	-1.17263600	0.31464600	1.72062500
N	-1.77131300	-0.13542900	2.60554300
C	-0.77045800	2.33769200	0.48624700
N	-1.06051200	3.45371700	0.36412900
C	2.67621700	-0.82172600	0.62738000
N	3.46154300	-1.49413200	1.15173500
C	2.36791400	0.89863900	-1.03193400
N	2.86908600	1.59968600	-1.80815500
H	-1.25662300	-3.59520700	0.20923000
H	-3.13941500	-2.21942100	-0.75194900
H	-0.48136900	0.91876000	-1.56403800
H	0.91334800	-0.98923000	-1.84687700
H	1.05613500	-2.79708900	0.14137700
F	-2.91601500	0.31872600	-1.35986000

Structure **3cm** (B3LYP/6-31G(d))

C	-1.88305200	-1.82523400	0.02991000
C	-2.53608100	-0.69981200	-0.63021600
C	-1.87820000	0.36840900	-1.09825300

C	-0.39218000	0.43681000	-0.89985400
C	0.29734300	-0.93535500	-0.72862300
C	-0.54655200	-1.93238300	0.03071000
C	1.63611000	-0.51332200	-0.03224700
O	1.33613700	0.62893500	0.78343700
C	0.07875600	1.21530800	0.40733700
C	-0.85629500	1.08535800	1.54575700
N	-1.57725600	0.99390500	2.44918300
C	0.28036300	2.64800000	0.11559100
N	0.42126500	3.76713900	-0.15381900
C	2.21093300	-1.56067500	0.83359800
N	2.64414400	-2.40954800	1.49373300
C	2.64106800	-0.12892600	-1.05619500
N	3.39171000	0.18583200	-1.88236900
H	-2.51775000	-2.56462200	0.50778000
H	0.07686000	0.96538100	-1.73493200
H	0.54671700	-1.36274500	-1.70923200
H	-0.05270300	-2.77844300	0.49869100
H	-2.40093800	1.19599000	-1.56390600
F	-3.86817900	-0.79971100	-0.74645400

Structure **3di** (B3LYP/6-31G(d))

C	1.70777100	-2.35521900	-0.59789400
C	0.76696500	-2.60812400	0.49064100
C	-0.31191500	-1.83139800	0.69916900
C	-0.60650800	-0.68728500	-0.22190200
C	0.66223800	-0.15051200	-0.91687400
C	1.66290900	-1.20605500	-1.29054400
C	1.19470600	0.90090300	0.15758700
O	0.06984000	1.23879900	0.99572900
C	-1.11957000	0.61083800	0.51071000
C	-1.98719100	0.32474400	1.66748900
N	-2.67460900	0.07549100	2.56677100
C	-1.82505900	1.54396500	-0.40412600
N	-2.32844700	2.32514400	-1.09763200
C	2.25856500	0.38179500	1.04149200
N	3.10191100	0.00417800	1.74151300
C	1.69812200	2.11536800	-0.51757100
N	2.09390400	3.05095200	-1.07705800
H	0.36288400	0.42897900	-1.79418000
H	2.44889000	-3.11365600	-0.83097000
H	0.93573700	-3.46935500	1.13042600
H	-1.03936300	-2.06170800	1.47061300
H	2.35439500	-0.98945100	-2.09829600
Cl	-1.85745800	-1.24292200	-1.44045000

Structure **3do** (B3LYP/6-31G(d))

C	-0.59894100	-2.70021400	-0.08815000
C	-1.82301100	-1.96654100	-0.40648900
C	-1.77223400	-0.65336700	-0.67812600
C	-0.47622000	0.10782500	-0.62745700
C	0.76805800	-0.78323600	-0.84637200
C	0.61973300	-2.16202600	-0.25216400
C	1.87890100	0.10793000	-0.19503500
O	1.26459000	0.76745600	0.91893800
C	-0.16597800	0.80472400	0.77219400
C	-0.76270600	0.10879900	1.93182700
N	-1.22814800	-0.42239400	2.85114900
C	-0.61185600	2.21277800	0.77678800
N	-0.96036700	3.31858100	0.75738800
C	3.03547700	-0.65702300	0.30745200
N	3.93860000	-1.28314500	0.67644900
C	2.35809700	1.11999200	-1.17183300
N	2.68876200	1.90988600	-1.95408100

H	-0.70027600	-3.71866700	0.27471100
H	-2.77221500	-2.49166300	-0.40511000
H	-0.48295500	0.91021200	-1.36952800
H	0.98803700	-0.87368600	-1.91875600
H	1.51990200	-2.73271600	-0.04650900
Cl	-3.20218000	0.28638400	-1.01991000

Structure **3dm** (B3LYP/6-31G(d))

C	-1.73125000	-1.61669800	0.23345400
C	-2.33915900	-0.45932600	-0.42843400
C	-1.60504700	0.53244300	-0.95568300
C	-0.10687600	0.47361700	-0.84742300
C	0.46951000	-0.94895000	-0.68788400
C	-0.41190700	-1.84243700	0.15023600
C	1.87882300	-0.63293200	-0.08074700
O	1.71993800	0.53450700	0.73809300
C	0.50598200	1.23158000	0.41182400
C	-0.37070900	1.22053000	1.60284900
N	-1.04336700	1.22630500	2.54717000
C	0.82671600	2.63154100	0.06946300
N	1.05913100	3.72540800	-0.23766300
C	2.41967200	-1.71676500	0.76131700
N	2.82287300	-2.59366600	1.40354000
C	2.84565600	-0.33911300	-1.16950200
N	3.56549300	-0.09158900	-2.04453300
H	-2.38040600	-2.29066100	0.78200100
H	0.34827300	0.94739900	-1.72221800
H	0.62018800	-1.41663800	-1.67013600
H	0.03187200	-2.71615700	0.61800700
H	-2.06159200	1.39624400	-1.42569900
Cl	-4.08442500	-0.42719900	-0.50135900

Structure **3ei (conf1)** (B3LYP/6-31G(d))

C	-1.32318500	2.59437600	-0.64587700
C	-0.31347500	2.69408200	0.40812300
C	0.60385800	1.73330900	0.61528000
C	0.67106000	0.54084200	-0.31196200
C	-0.70685200	0.22652900	-0.93928600
C	-1.52210700	1.43771500	-1.29567500
C	-1.38871700	-0.72142500	0.12276000
O	-0.32219700	-1.33154500	0.87588700
C	0.95166300	-0.83676500	0.45872700
C	1.79298200	-0.68674500	1.65957700
N	2.47277500	-0.53184300	2.58656500
C	1.59087400	-1.81448000	-0.45492100
N	2.06563100	-2.60365600	-1.15956600
C	-2.27059100	-0.01969100	1.08263000
N	-2.97040800	0.50096400	1.84634000
C	-2.17551100	-1.77831900	-0.54742100
N	-2.79024000	-2.58952300	-1.10318200
H	-0.51297600	-0.38064900	-1.82933000
H	-1.92460400	3.46913700	-0.87452900
H	-0.31696400	3.57848700	1.03973600
H	1.34729700	1.82993700	1.39991200
H	-2.28378500	1.33109000	-2.06190700
O	1.56884200	0.70737000	-1.38527700
C	2.86598700	1.23589200	-1.09405900
H	3.40976600	0.61372100	-0.37204400
H	3.40122500	1.22430400	-2.04441100
H	2.80665700	2.26386800	-0.72079400

Structure **3eo (conf1)** (B3LYP/6-31G(d))

C	-0.75795200	-2.59620400	0.00730200
C	-1.92446700	-1.78991900	-0.33975400

C	-1.76858500	-0.48999200	-0.66577200
C	-0.40526400	0.14907700	-0.65649800
C	0.76659700	-0.84010000	-0.82029000
C	0.50535500	-2.17127600	-0.16156000
C	1.93919900	-0.00344200	-0.20357000
O	1.37100100	0.77522100	0.85891900
C	-0.05236700	0.89693600	0.70065500
C	-0.70147600	0.31321000	1.89518000
N	-1.21619000	-0.11778000	2.84040100
C	-0.41083700	2.32830500	0.62461200
N	-0.69534800	3.44961500	0.54522000
C	3.02390400	-0.82675300	0.36321000
N	3.87320600	-1.49424100	0.78389300
C	2.51206600	0.90696000	-1.22899400
N	2.91555200	1.61972000	-2.05025100
H	-0.93928200	-3.58787600	0.41241800
H	-2.90535200	-2.24746900	-0.29203700
H	-0.36559700	0.90980800	-1.44084100
H	0.98592400	-0.99349900	-1.88591400
H	1.35297000	-2.80479800	0.07821900
O	-2.72341600	0.41985600	-0.95838800
C	-4.08543000	-0.00317500	-0.89264200
H	-4.68194200	0.87580600	-1.13697700
H	-4.27980400	-0.79978600	-1.62066600
H	-4.33258500	-0.35576900	0.11543000

Structure **3em** (conf2) (B3LYP/6-31G(d))

C	-1.51224600	-1.87262500	0.24197600
C	-2.28523200	-0.76878600	-0.34205500
C	-1.67289900	0.31599000	-0.86698100
C	-0.17838000	0.41876000	-0.80135700
C	0.56412200	-0.93133500	-0.71528600
C	-0.18218800	-1.95137000	0.10934200
C	1.94862600	-0.48228000	-0.13709200
O	1.69345200	0.63461700	0.72812900
C	0.39553800	1.19462200	0.46974400
C	-0.43351300	1.03970100	1.68437100
N	-1.07281600	0.93724200	2.64629400
C	0.53772400	2.63405600	0.17435700
N	0.62532100	3.75776100	-0.09919400
C	2.63325900	-1.52614500	0.64969200
N	3.15361000	-2.37169500	1.24832000
C	2.84330700	-0.04832800	-1.24094200
N	3.50536600	0.30428300	-2.12556300
H	-2.07463600	-2.63292900	0.77480000
H	0.20021300	0.97317200	-1.66548600
H	0.73378000	-1.34018600	-1.72040600
H	0.37179000	-2.78974500	0.52090100
H	-2.21930800	1.15086100	-1.28741300
O	-3.61598000	-0.99364800	-0.28073000
C	-4.48436900	0.02672800	-0.76565800
H	-5.49792000	-0.34142300	-0.60414700
H	-4.33522500	0.96101700	-0.21121000
H	-4.32133000	0.20443300	-1.83589600

Structure **3fi** (B3LYP/6-31G(d))

C	-1.37313900	2.62343700	-0.39475100
C	-0.40034300	2.65936700	0.69671800
C	0.51530300	1.69269800	0.88315000
C	0.59965000	0.54250500	-0.08209800
C	-0.70510400	0.29293800	-0.85728800
C	-1.52342700	1.52138400	-1.14333500
C	-1.44631000	-0.76191000	0.07206300
O	-0.43576900	-1.36760700	0.90153300

C	0.86357400	-0.86802900	0.58474100
C	1.63754500	-0.80255700	1.83673700
N	2.23356800	-0.74637900	2.82898300
C	1.52582600	-1.80560500	-0.35769200
N	1.99097000	-2.55155700	-1.11376300
C	-2.45049200	-0.16034500	0.97544200
N	-3.24343900	0.28933900	1.69154600
C	-2.10669200	-1.80096000	-0.74501000
N	-2.62076800	-2.59684200	-1.41363700
H	-0.45718900	-0.21925000	-1.79084500
H	-1.97986700	3.50465800	-0.57780800
H	-0.41669400	3.50928600	1.37299100
H	1.26369400	1.75006700	1.66537600
H	-2.24949500	1.46420100	-1.94788100
O	1.54741600	1.05304000	-2.20554400
O	2.88535300	0.87977100	-0.48299700
N	1.78898300	0.84427900	-1.02710500

Structure **3fo** (B3LYP/6-31G(d))

C	-0.50424000	-2.74207000	0.03441500
C	-1.71756000	-1.98294500	-0.22958300
C	-1.64670700	-0.67457700	-0.52702400
C	-0.35355500	0.08317500	-0.57199100
C	0.85800500	-0.84779800	-0.82529100
C	0.70882800	-2.22032300	-0.21512800
C	2.01861100	0.00828800	-0.21744500
O	1.46590900	0.63713100	0.93950300
C	0.04656800	0.83670400	0.78010200
C	-0.61261700	0.27499500	1.97601800
N	-1.13759900	-0.17712800	2.90549500
C	-0.22272800	2.28716300	0.70822200
N	-0.39063500	3.43324500	0.65970900
C	3.18325200	-0.78732300	0.21295400
N	4.08677900	-1.44393900	0.52307200
C	2.46907400	1.02651800	-1.20205300
N	2.78208200	1.81760000	-1.99025700
H	-0.60194600	-3.75530400	0.41045700
H	-2.68882300	-2.46282100	-0.18117300
H	-0.40286400	0.85142100	-1.34539000
H	1.03793100	-0.96059200	-1.90291500
H	1.60957300	-2.80654900	-0.05850900
O	-3.93277000	-0.51451100	-0.84532300
O	-2.73496200	1.31670700	-0.82902600
N	-2.86932300	0.09142200	-0.75271600

Structure **3fm** (B3LYP/6-31G(d))

C	-1.56230900	-1.61035600	0.20491500
C	-2.14255300	-0.40246000	-0.37090800
C	-1.41147300	0.60931700	-0.85762700
C	0.08560800	0.51631100	-0.80260300
C	0.63616200	-0.92464800	-0.72162900
C	-0.24839000	-1.84864100	0.08136900
C	2.05919100	-0.66196500	-0.12014200
O	1.92341200	0.45582500	0.76816800
C	0.73738400	1.20996600	0.47570200
C	-0.13063100	1.18873400	1.67278600
N	-0.80486600	1.18226300	2.61594800
C	1.10503000	2.60853500	0.17635100
N	1.37621000	3.70321700	-0.09358500
C	2.59769500	-1.79843300	0.64974500
C	2.99944100	-2.71558600	1.23390200
N	3.01198200	-0.31584400	-1.20579600
N	3.71843100	-0.02402400	-2.07806300
H	-2.22388100	-2.30015200	0.71339600

H	0.52095100	1.02292200	-1.66857300
H	0.76680900	-1.34425500	-1.72813900
H	0.18887800	-2.75704600	0.48435500
H	-1.88573100	1.49996800	-1.25312800
O	-4.10685700	0.71662900	-0.90128700
O	-4.25244500	-1.23582300	0.06446000
N	-3.61865700	-0.29409600	-0.40557600

Structure **ts3a** (B3LYP/6-31G(d))

C	-1.55314600	-2.37272200	-0.29502300
C	-2.40795800	-1.46452400	-0.98764900
C	-1.91110400	-0.28114300	-1.51581200
C	-0.58243300	0.08339800	-1.30271700
C	0.39243200	-0.91146000	-0.76782200
C	-0.22630900	-2.11580500	-0.14693000
C	1.62087900	-0.32395300	-0.11130700
O	0.72347200	0.83493600	1.24080500
C	-0.45202400	1.22745100	0.92491400
C	-1.62368700	0.57376200	1.44665900
N	-2.58607900	0.03196300	1.81932100
C	-0.66331800	2.53318800	0.33474800
N	-0.83246200	3.57751300	-0.15090600
C	2.39241600	-1.16800900	0.73828800
N	2.98191000	-1.88263500	1.44471300
C	2.34366200	0.65667400	-0.85656800
N	2.88380800	1.47681200	-1.48343000
H	-1.97770300	-3.27475700	0.13443800
H	-3.45821300	-1.71083000	-1.10575400
H	-2.57280800	0.40842800	-2.03077300
H	-0.18050100	0.97390400	-1.77583400
H	0.87127600	-1.31377400	-1.69900800
H	0.42347000	-2.80917000	0.37792100

Structure **ts3b (p)** (B3LYP/6-31G(d))

C	-1.89388600	-1.76930400	0.02907900
C	-2.54382800	-0.67164500	-0.63140700
C	-1.76025000	0.28312000	-1.27914800
C	-0.37197100	0.24786200	-1.21309100
C	0.33157800	-0.96823600	-0.71164700
C	-0.54582000	-1.91461800	0.03219700
C	1.73332900	-0.74110500	-0.18441100
O	1.35614900	0.65223900	1.17245900
C	0.32459000	1.37541700	0.93809900
C	-0.93486900	1.10971500	1.57905700
N	-1.98035400	0.87831500	2.04037000
C	0.45182900	2.66431000	0.29428300
N	0.54869300	3.69591200	-0.23706600
C	2.30590700	-1.75671000	0.63522500
N	2.72783800	-2.59693200	1.32324100
C	2.63353900	-0.04131200	-1.04483600
N	3.32349300	0.56383100	-1.76262600
H	-2.50991400	-2.49418900	0.55426200
H	-2.24032800	1.12109000	-1.77635600
H	0.21407600	0.97263500	-1.76968600
H	0.57816500	-1.51764200	-1.65581500
H	-0.07715300	-2.75432100	0.53611000
C	-4.04008600	-0.58679500	-0.61429200
H	-4.39376000	-0.48575300	0.41930900
H	-4.40675500	0.26837800	-1.18712100
H	-4.49158600	-1.50019000	-1.02245700

Structure **ts3c (p)** (B3LYP/6-31G(d))

C	-1.93510200	-1.77089500	0.04901900
C	-2.52901300	-0.66780100	-0.62833600

C	-1.78945100	0.30512600	-1.28269500
C	-0.40361600	0.26075500	-1.20124400
C	0.29115100	-0.96510500	-0.69928400
C	-0.58624800	-1.90776700	0.05554600
C	1.69867900	-0.74784500	-0.18157500
O	1.34175000	0.65992500	1.17164300
C	0.31447000	1.38930300	0.94214600
C	-0.94369700	1.12506700	1.58591600
N	-1.98494800	0.88418400	2.05199600
C	0.44611800	2.67585900	0.29444500
C	0.54733500	3.70393600	-0.24265600
N	2.26483800	-1.76352800	0.64118300
N	2.67822700	-2.60555800	1.33226500
C	2.59742900	-0.06002400	-1.05211200
N	3.28487300	0.53729500	-1.77886200
H	-2.58340600	-2.47129600	0.56451800
H	-2.29869400	1.12648600	-1.77504700
H	0.18881700	0.98043100	-1.75694800
H	0.53007900	-1.52173500	-1.64068800
H	-0.11747500	-2.74282800	0.56640600
F	-3.85389800	-0.61425700	-0.66762500

Structure **ts3d (p)** (B3LYP/6-31G(d))

C	-1.73782200	-1.62865000	0.20346200
C	-2.31904900	-0.50938000	-0.47134900
C	-1.53679200	0.41105000	-1.15928600
C	-0.15153600	0.28612300	-1.14484200
C	0.49411200	-0.97155800	-0.66388100
C	-0.39948800	-1.84294600	0.15130800
C	1.93770200	-0.83422500	-0.22920800
O	1.73601200	0.61963200	1.10977400
C	0.73697000	1.39757900	0.92617700
C	-0.48779400	1.21964900	1.66153100
N	-1.50103400	1.05794800	2.21396300
C	0.89966900	2.66639900	0.24937500
N	1.02741300	3.68021200	-0.30844700
C	2.48745600	-1.86599900	0.58475300
N	2.88973700	-2.71778600	1.27028600
C	2.82865400	-0.21391600	-1.15688300
N	3.51234300	0.32897900	-1.92836200
H	-2.38318000	-2.29316100	0.76734200
H	-2.00043500	1.26149100	-1.64726400
H	0.44936800	0.96159100	-1.74550400
H	0.64961700	-1.55424100	-1.60783800
H	0.04130100	-2.69440200	0.66034400
Cl	-4.03861600	-0.33932700	-0.45554700

Structure **ts3e (p, conf2)** (B3LYP/6-31G(d))

C	-1.51602500	-1.92743600	0.16383800
C	-2.25391800	-0.83170800	-0.40635100
C	-1.58905700	0.18639400	-1.11123500
C	-0.20926300	0.20394500	-1.15256000
C	0.60078400	-0.97752300	-0.72014800
C	-0.17197600	-1.99053000	0.05852100
C	2.01029900	-0.66469700	-0.23691400
O	1.66446900	0.65393500	1.16227300
C	0.61471100	1.37812400	0.99096400
C	-0.62164900	1.07730200	1.64792500
N	-1.66439500	0.82454100	2.10823700
C	0.69209700	2.66511900	0.34405500
N	0.73448500	3.69576100	-0.19795800
C	2.68052800	-1.67565000	0.51316700
N	3.18143900	-2.51336400	1.14949100
C	2.82375200	0.08895500	-1.13907800



N	3.43488700	0.73771000	-1.88954800
H	-2.07971400	-2.67899000	0.70643900
H	-2.14174100	1.00887900	-1.54904900
H	0.29792600	0.97241000	-1.72750100
H	0.82896800	-1.48897100	-1.68592000
H	0.37793100	-2.81255800	0.50611700
O	-3.56778000	-0.91327500	-0.24366800
C	-4.39636200	0.20891300	-0.58690200
H	-5.40351300	-0.07483100	-0.28426000
H	-4.07021600	1.09370300	-0.03230400
H	-4.37159200	0.39530100	-1.66560500

Structure **ts3f (p)** (B3LYP/6-31G(d))

C	-1.55582100	-1.62331600	0.15715700
C	-2.11126400	-0.46137100	-0.44681400
C	-1.33977300	0.47756600	-1.11162100
C	0.04286400	0.32680800	-1.14012700
C	0.67355600	-0.95267500	-0.70434600
C	-0.22013300	-1.85437300	0.07653400
C	2.12023400	-0.84804500	-0.28301600
O	1.91687400	0.53635200	1.14350600
C	0.94131100	1.34331200	0.99567400
C	-0.29336600	1.16087600	1.71573000
N	-1.31219100	1.00106200	2.25766800
C	1.13851300	2.63979600	0.37940200
N	1.30290700	3.67650900	-0.12280300
C	2.67862800	-1.91877700	0.47311900
N	3.09297900	-2.80176500	1.10964500
C	3.00945200	-0.16638900	-1.16860600
N	3.69483700	0.42366900	-1.90255000
H	-2.21605900	-2.29691200	0.68917300
H	-1.81519000	1.35214400	-1.53979700
H	0.64542100	1.01599800	-1.72312100
H	0.83640700	-1.50513400	-1.66892300
H	0.21528400	-2.73765600	0.53264400
O	-4.02429300	0.74759500	-0.90986900
O	-4.22411600	-1.13530300	0.18430000
N	-3.56692900	-0.26491300	-0.38367300

Structure **4a** (B3LYP/6-31G(d))

C	2.00842900	0.02212000	-1.36156500
C	2.94601300	0.00449500	-0.32569200
C	2.51724400	-0.01633200	1.00129000
C	1.15210000	-0.01964000	1.29440500

C	0.21629500	-0.00209500	0.25844400
C	0.64520200	0.01889500	-1.07274100
C	-1.28288500	-0.00688800	0.59242600
C	-1.95968000	-1.21245600	0.07147400
N	-2.47007400	-2.17182600	-0.33362000
C	-1.96197300	1.20863800	0.09841600
N	-2.47443300	2.17557500	-0.28551600
H	2.33836100	0.03846700	-2.39620100
H	4.00800800	0.00710800	-0.55405000
H	3.24131500	-0.02997300	1.81077100
H	0.81936000	-0.03592400	2.32945500
H	-1.39703600	-0.01917400	1.68464300
H	-0.08292700	0.03282800	-1.87941400

Structure **4e (p, conf2)** (B3LYP/6-31G(d))

C	1.14659000	0.00690300	-1.33445400
C	2.08693000	0.00132700	-0.28945100
C	1.64558500	-0.00479500	1.03873100
C	0.27461600	-0.00579400	1.30878600
C	-0.65932700	-0.00071400	0.27571600
C	-0.21003700	0.00580300	-1.05322300
C	-2.15758800	-0.00234600	0.59773400
C	-2.83509900	-1.21130600	0.08325400
N	-3.34371900	-2.17369600	-0.31717200
C	-2.83595300	1.20984600	0.09209300
N	-3.34534500	2.17464300	-0.30149900
H	1.50877200	0.01204600	-2.35726300
H	2.34845400	-0.00854800	1.86331900
H	-0.05783500	-0.01062500	2.34418400
H	-2.27872500	-0.00639600	1.68937600
H	-0.92621900	0.01012100	-1.87062200
O	3.39041800	0.00298300	-0.67302900
C	4.39412400	-0.00187800	0.33326800
H	4.32972700	-0.90046000	0.96017800
H	5.34714800	0.00042400	-0.19767500
H	4.32973100	0.89066100	0.96869300

Structure **5** (B3LYP/6-31G(d))

C	0.00000000	0.48646800	0.00000000
O	-0.00008400	1.69561800	0.00000000
C	1.23363100	-0.30461100	0.00000000
C	-1.23352500	-0.30476600	0.00000000
N	-2.22117200	-0.91624500	0.00000000
N	2.22117700	-0.91625300	0.00000000