

Deciphering the curly arrows representation and electron flow for the 1,3-dipolar rearrangement between acetonitrile oxide and (1*S*,2*R*,4*S*)-2-cyano-7-oxabicyclo[2.2.1]hept-5-en-2-yl acetate derivatives

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Table S1: Electronic energies (a.u.) of species with ω B97X-D/6311G(d).

Species	2a, R=H	2b, R=Cl	2c, R=Br	2a, R=H	2a, R=Cl	2a, R=Br
	In vacuo			In benzene		
1	-207.87438	-207.87438	-207.87438	-207.87802	-207.87802	-207.87802
2	-628.67994	-1088.28794	-3202.25515	-628.68596	-1088.29364	-3202.26088
TS-PS	-836.54177	-1296.14790	-3410.11485	-836.54939	-1296.15551	-3410.12244
TS-PA	-836.52943	-1296.13292	-3410.09944	-836.53766	-1296.14133	-3410.10787
TS-MS	-836.53922	-1296.14618	-3410.11349	-836.54746	-1296.15357	-3410.12086
TS-MA	-836.52938	-1296.13179	-3410.09892	-836.53720	-1296.13903	-3410.10612
3	-836.64659	-1296.25560	-3410.22114	-836.65485	-1296.26330	-3410.22870
4	-836.64161	-1296.25191	-3410.21714	-836.64912	-1296.25916	-3410.22435
5	-836.64399	-1296.25074	-3410.21702	-836.65264	-1296.25813	-3410.22440
6	-836.64275	-1296.24906	-3410.21535	-836.65024	-1296.25586	-3410.22213

Table S2: Electronic thermodynamic parameters (H, G in a.u.; S in cal/mol·K) of species computed at 25°C in benzene with ω B97X-D/6311G(d).

Species	Case a, R=H			Case b, R=Cl			Case c, R=Br		
	H	G	S	H	G	S	H	G	S
1	-207.82227	-207.85410	66.988	-207.82227	-207.85410	66.988	-207.82227	-207.85410	66.988
2	-628.50311	-628.55271	104.392	-1088.11882	-1088.17191	111.735	-3202.08624	-3202.14007	113.302
TS-PS	-836.31026	-836.37110	128.036	-1295.92270	-1295.98660	134.494	-3409.89163	-3409.95715	137.890
TS-PA	-836.29827	-836.35641	122.363	-1295.91033	-1295.97243	130.696	-3409.87715	-3409.94044	133.212
TS-MS	-836.30837	-836.36963	128.940	-1295.92453	-1295.98875	135.170	-3409.89023	-3409.95611	138.663
TS-MA	-836.29809	-836.35827	126.642	-1295.90812	-1295.97050	131.308	-3409.87550	-3409.93933	134.351
3	-836.41132	-836.46929	122.021	-1296.02841	-1296.08874	126.981	-3409.99433	-3410.05617	130.143
4	-836.40525	-836.46209	119.638	-1296.02443	-1296.08487	127.216	-3409.98986	-3410.05151	129.736
5	-836.40920	-836.46728	122.249	-1296.02298	-1296.08324	126.823	-3409.98980	-3410.05183	130.557
6	-836.40655	-836.46324	119.314	-1296.02082	-1296.08037	125.333	-3409.98736	-3410.04795	127.535

Table S3: Relative (to the separate reactants) enthalpy (ΔH° , in kcal/mol), Gibbs energy (ΔG° , in kcal/mol) and entropy (ΔS° , in cal/mol.K) of species computed at 25°C in benzene with ω B97X-D/6311G(d). In parentheses are given syn-to-anti differences.

Species	Case a, R=H			Case b, R=Cl			Case c, R=Br		
	ΔH°	ΔG°	ΔS°	ΔH°	ΔG°	ΔS°	ΔH°	ΔG°	ΔS°
TS-PS	9.48	22.41	-43.34	11.54	24.72	-44.23	10.59	23.23	-42.40
TS-PA	17.01 (7.53)	31.62 (9.21)	-49.02 (-5.68)	19.3 (7.76)	33.62 (8.90)	-48.03 (-3.80)	19.68 (9.09)	33.72 (10.49)	-47.08 (-4.68)
TS-MS	10.67	23.33	-42.44	10.39	23.37	-43.55	11.47	23.88	-41.63
TS-MA	17.12 (6.45)	30.46 (7.13)	44.74 (-2.30)	20.69 (10.30)	34.82 (11.45)	-47.42 (-3.87)	20.71 (9.24)	34.41 (10.53)	-45.94 (-4.31)
3	-53.93	-39.21	-49.36	-54.80	-39.37	-51.74	-53.85	-38.9	-50.15
4	-50.12 (3.81)	-34.69 (4.52)	-51.74 (-2.38)	-52.3 (2.50)	-36.94 (2.43)	-51.51 (0.23)	-51.05 (2.80)	-35.98 (2.92)	-50.55 (-0.40)
5	-52.60	-37.95	-49.13	-51.39	-35.92	-51.90	-51.01	-36.18	-49.73
6	-50.93 (1.67)	-35.41 (2.54)	-52.07 (-2.94)	-50.03 (1.36)	-34.11 (1.81)	-53.39 (-1.49)	-49.48 (1.53)	-33.75 (2.43)	-52.76 (-3.03)

Table S4: Basin Populations in $|e|$ and IRC coordinates (RX, amu^{1/2} Bohr) along the **TS-PSa** reaction pathway.

	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V	
V(N2,C3)	6.12	6.26	4.71	4.53	4.10	3.71	3.65	3.45	3.40	3.27
V(C4,C5)	3.41	3.32	3.32	3.22	2.94	2.64	2.39	2.14	2.11	1.91
V(O1)	5.77	5.76	5.72	5.72	5.72	5.67	5.68	5.67	5.32	4.95
V(N2)	-	-	1.62	1.98	2.09	2.38	2.45	2.67	2.70	2.84
V(C3)	-	-	-	-	0.37	0.61	-	-	-	-
V(C4)	-	-	-	-	0.31	0.63	-	-	-	-
V(C5)	-	-	-	-	-	-	0.19	0.31	-	-
V(C3,C4)	-	-	-	-	-	-	1.43	1.73	1.79	2.02
V(O1,C5)	-	-	-	-	-	-	-	-	0.35	1.34
IRC	-24.604	-1.263	-0.947	0.000	0.316	1.578	1.894	3.156	3.472	10.712

Table S5: Basin Populations in $|e|$ and IRC coordinates (RX, amu^{1/2} Bohr) along the **TS-PSb** reaction pathway.

	SSD-I		SSD-II		SSD-III	SSD-IV		SSD-V	SSD-VI		SSD-VII		SSD-VIII	
V(N2,C3)	6.09	6.24	4.71	4.58	4.30	4.12	3.80	3.72	3.66	3.45	3.41	3.32	3.29	3.21
V(C4,C5)	3.59	3.50	3.48	3.45	3.47	3.13	2.90	2.54	2.44	2.21	2.17	2.09	2.08	2.01
V(O1)	5.72	5.67	5.66	5.65	5.63	5.63	5.59	5.58	5.58	5.60	5.34	5.17	5.13	4.88
V(N2)	-	-	1.59	1.82	1.93	2.02	2.29	2.36	2.41	2.60	2.65	2.74	2.77	2.86
V(C3)	-	-	-	-	0.23	0.36	0.60	0.66	-	-	-	-	-	-
V(C4)	-	-	-	-	-	0.37	0.63	0.69	-	-	-	-	-	-
V(C5)	-	-	-	-	-	-	-	0.31	0.36	0.47	0.48	0.52	-	-
V'(O1)	-	-	-	-	-	-	-	-	-	-	0.26	0.47	-	-
V(C3,C4)	-	-	-	-	-	-	-	-	1.45	1.76	1.81	1.93	1.93	2.04
V(O1,C5)	-	-	-	-	-	-	-	-	-	-	-	-	1.02	1.42
IRC	-15.134	-1.263	-0.947	-0.316	0.00	0.316	1.263	1.578	1.894	3.156	3.472	4.418	4.734	10.713

Table S6: Basin Populations in $|e|$ and IRC coordinates (RX, amu^{1/2} Bohr) along the **TS-PSc** reaction pathway.

	SSD-I		SSD-II		SSD-III	SSD-IV		SSD-V	SSD-VI		SSD-VII		SSD-VIII	
V(N2,C3)	6.15	6.27	4.75	4.53	4.25	4.10	3.81	3.72	3.67	3.46	3.45	3.30	3.28	3.21
V(C4,C5)	3.53	3.46	3.46	3.41	3.44	3.13	2.89	2.53	2.43	2.21	2.16	2.06	2.05	2.00
V(O1)	5.71	5.72	5.70	5.67	5.65	5.64	5.64	5.60	5.65	5.64	5.36	5.17	5.13	4.88
V(N2)	-	-	1.58	1.84	1.93	2.02	2.30	2.36	2.42	2.60	2.64	2.76	2.78	2.87
V(C3)	-	-	-	-	0.27	0.38	0.62	0.68	-	-	-	-	-	-
V(C4)	-	-	-	-	-	0.35	0.62	0.68	-	-	-	-	-	-
V(C5)	-	-	-	-	-	-	-	0.31	0.35	0.45	0.47	0.52	-	-
V'(O1)	-	-	-	-	-	-	-	-	-	-	0.24	0.50	-	-
V(C3,C4)	-	-	-	-	-	-	-	-	1.45	1.77	1.82	1.96	1.98	2.05
V(O1,C5)	-	-	-	-	-	-	-	-	-	-	-	-	1.09	1.41
IRC	-15.443	-1.261	-0.946	-0.315	0.000	0.315	1.261	1.576	1.892	3.152	3.467	4.727	5.043	10.698

Table S7: Basin Populations in $|e|$ and IRC coordinates (RX, amu^{1/2} Bohr) along the **TS-MSa** reaction pathway.

	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V		SSD-VI	
V(N2,C3)	6.12	6.32	4.80	4.61	4.23	4.12	3.74	3.66	3.42	3.38	3.26	
V(C4,C5)	3.43	3.30	3.32	3.27	3.23	2.97	2.62	2.40	2.08	2.05	1.93	
V(O1)	5.76	5.69	5.70	5.64	5.63	5.60	5.64	5.65	5.25	5.23	4.99	
V(N2)	-	-	1.59	1.84	1.95	2.02	2.37	2.43	2.68	2.69	2.84	
V(C3)	-	-	-	-	0.31	0.43	0.73	-	-	-	-	
V(C4)	-	-	-	-	-	-	-	0.19	0.37	-	-	
V(C5)	-	-	-	-	-	0.31	0.60	-	-	-	-	
V(C3,C5)	-	-	-	-	-	-	-	-	-	0.85	1.31	
V(O1,C4)	-	-	-	-	-	-	-	1.44	1.84	2.05	2.04	
IRC	-22.249	-1.254	-0.940	-0.314	0.000	0.314	1.567	1.881	3.761	4.075	10.010	

Table S8: Basin Populations in $|e|$ and IRC coordinates (RX, amu^{1/2} Bohr) along the **TS-MSb** reaction pathway.

	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V		SSD-VI	
V(N2,C3)	6.07	6.29	4.63	4.58	4.19	3.74	3.66	3.61	3.45	3.40	3.22	
V(C4,C5)	3.60	3.59	3.60	3.56	3.07	2.67	2.48	2.39	2.18	2.15	2.00	
V(O1)	5.66	5.71	5.71	5.71	5.66	5.62	5.60	5.62	5.39	5.33	4.91	
V(N2)	-	-	1.73	1.84	1.95	2.34	2.43	2.47	2.69	2.71	2.83	
V(C3)	-	-	-	-	0.33	0.61	0.65	-	-	-	-	
V(C4)	-	-	-	-	-	-	0.20	0.25	0.25	-	-	
V(C5)	-	-	-	-	0.50	0.88	0.88	-	-	-	-	
V(C3,C5)	-	-	-	-	-	-	-	1.61	1.87	1.91	2.11	
V(O1,C4)	-	-	-	-	-	-	-	-	-	0.75	1.36	
IRC	-10.975	-0.969	-0.646	-0.323	0.000	1.292	1.615	1.937	3.229	3.553	9.667	

Table S9: Basin Populations in $|e|$ and IRC coordinates (RX, amu^{1/2} Bohr) along the **TS-MSc** reaction pathway.

	SSD-I		SSD-II		SSD-III		SSD-IV	SSD-V		SSD-VI	
V(N2,C3)	6.09	6.25	4.72	4.55	4.19	3.75	3.68	3.61	3.43	3.40	3.23
V(C4,C5)	3,57	3.56	3.56	3.54	3.03	2.71	2.47	2.39	2.18	2.14	2.00
V(O1)	5,72	5.67	5.65	5.64	5.64	5.60	5.59	5.60	5.30	5,19	4.87
V(N2)	-	-	1.59	1.86	1.96	2.33	2.39	2.46	2.65	2,69	2.82
V(C3)	-	-	-	-	0.30	0.60	0.64	-	-	-	-
V(C4)	-	-	-	-	-	-	0.20	0.25	0.25	-	-
V(C5)	-	-	-	-	0.51	0.84	0.88	-	-	-	-
V(C3,C5)	-	-	-	-	-	-	-	1.60	1.85	1.90	2.10
V(O1,C4)	-	-	-	-	-	-	-	-	-	0.82	1.34
IRC	-10.973	-1.291	-0.968	-0.323	0.000	1.292	1.615	1.937	3.228	3.552	9.988

CDFT Analysis of the processes

The analysis of the reactivity indices defined in the framework of Conceptual DFT (CDFT) constitute a powerful tool to understand the reactivity of the different reagents engaged in the process of polar cycloaddition reactions, such as Diels-Alder and 32CA reactions.^{1,2} These indices are reported in Table S10 for the reactants of the studied process.

Table S10: ω B97X-D/6-311G(d) electronic chemical potential, μ ; chemical hardness, η ; electrophilicity, ω ; and nucleophilicity, N in eV, for the reagents involved in the studied reaction.

Species	μ	η	ω	N
1	-3.07	11.85	0.40	2.40
Ethylene	-3.71	11.99	0.57	1.69
2a	-4.16	10.92	0.79	1.78
2b	-4.24	10.52	0.86	1.89
2c	-4.20	10.34	0.85	2.02

From the results listed in table S10, it can be seen that the electronic chemical potential (μ) of dipole **1**, $\mu = -3.07$ eV is higher than those of dipolarophiles, **2a-c** ($\mu = -4.16$ - 4.24 eV) suggesting that along the polar reaction cycloaddition, the global electron density transfer (GEDT)³ will take place from the dipole **1** to dipolarophiles, **2a-c**.

Ethylene presents a nucleophilicity (N) index of 1.69 eV and an electrophilicity ω index of 0.57 eV, whereas the compound **2a** resulting from the substitution of the two hydrogen atoms within the ethylene molecule, possesses as nucleophilicity and electrophilicity indices 1.78 and 0.79 eV

respectively. The substitution of a hydrogen atom in compound **2a** by a halogen atom, either Cl or Br, also increases the N and ω indices of **2b** and **2c** to 1.89 and 2.02 eV and 0.86 and 0.85 eV, respectively. Then the different dipolarophiles **2a**, **2b**, and **2c** are considered strong nucleophiles participating in a polar reaction.

In order to determine the most electrophilic and nucleophilic centers among the species, the analysis of the nucleophilic P_k^- and electrophilic P_k^+ Parr functions, coming from the changes of spin electron density for the nucleophile/electrophile interaction, is a powerful tool that makes possible to study the local reactivity in polar processes.⁴ The analysis of the nucleophilic Parr functions at dipole indicates that the O1 oxygen atom is the most nucleophilic center with a maximum value of $P_k^- = 0.70$, holding 1.68 eV of local nucleophilicity N_k index, compared with the C3 carbon which has $P_k^- = 0.39$ (see figure 1).

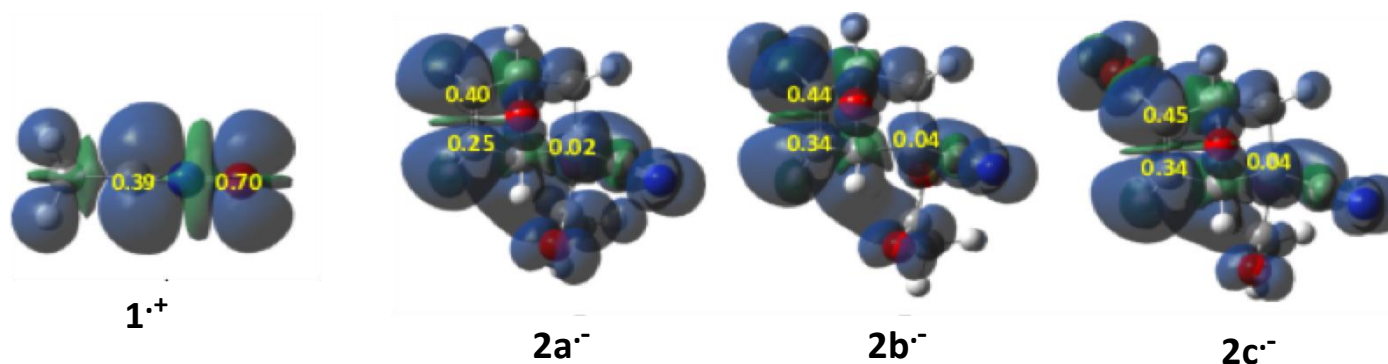


Figure S1: Figure 1: Three-dimensional representations of the atomic spin density of radical cation **1**^{•+} and radical anions **2a-c**^{•-}, together with the nucleophilic P_k^- Parr functions of **1** and the electrophilic P_k^+ of **2a-c**.

On the other hand, analysis of the electrophilic Parr functions of **2a** shows that the C5 carbon of these species is the most electrophilic center, $P_k^+ = 0.40$, with local electrophilicity ω_k value 0.316 eV, while the adjacent alkene C4 carbon is poorly electrophilically activated, $P_k^+ = 0.25$. The substitution of the C5 hydrogen atom by chlorine and bromine atoms in order to form dipolarophiles **2b-c**, increase the electrophilic P_k^+ Parr functions of these two species. Their C5 atoms present the values of 0.44 and 0.45, respectively, with local electrophilicity ω_k values of 0.34 eV each. However, this atomic substitution also increases the value of P_k^+ at the C4 atom position, that becomes 0.34 compared to 0.25 for **2a**. Therefore, the most favorable electrophile-nucleophile interaction along the nucleophilic attack of nitrile oxide **1** to compounds **2a**, **2b** and **2c** will take place between the most nucleophilic center of nitrile oxide **1**, the O1 oxygen, and the C5 carbon atom of dipolarophiles **2a**, **2b** and **2c**, which is the most electrophilic center in the three cases as we can see in figure S1. Therefore, the activation barriers along the para channels (in which the O1-C5 bonds are formed) should be lower than the corresponding barriers along the meta channels, in which the O1-C4 bonds are formed instead, as we have found.

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3. Domingo, L. R. A New C-C Bond Formation Model Based on the Quantum Chemical Topology of Electron Density. *RSC Adv.* **2014**, *4*, 32415–32428
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BET Analysis for the syn attack along the meta channel

The mechanism of the reaction between 1 and 2a.

As in the case of the para-*syn* reactive channel, a BET analysis associated with the formation of C3-C5 and O1-C4 bonds was also performed along the meta-*syn* attack of **1** over the C-C double bond of **2a**. The formation of two new sigma bonds takes place along six structural stability domains (SSDs) in accordance with Figure S2, which shows the evolution of the ELF basins engaged in the process.

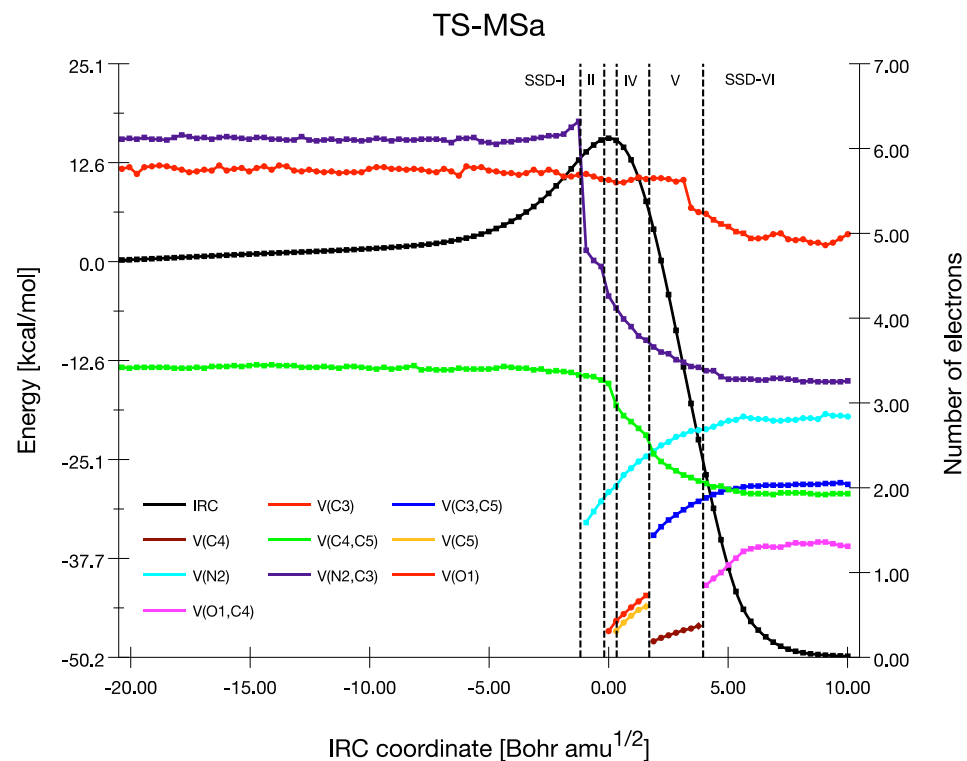


Figure S2: Population (in electrons) evolution of selected basins along the **TS-MSa** pathway for the 1,3-dipolar rearrangement between **1** and **2a**. The relative energy (in kcal/mol) along the reaction coordinate is represented by black lines with dots.

In SSD-I, the three main basins associated with the topology of reactants are: one disynaptic basin $V(N2,C3)$ associated with the N-C triple bond, one $V(O1)$ monosynaptic basin of oxygen atom for **1**, and one $V(C4,C5)$ for the double C-C bond of **2a**. At the first point of the second SSD-II domain, the initial $V(N2,C3)$ disynaptic basin has undergone a drop in population with a loss of 1.52 $|e|$. This drop corresponds to the formation of the $V(N2)$ monosynaptic basin with a population of 1.59 $|e|$, which illustrates the lone pair around the N2 atom of acetonitrile oxide (see Figure S3).

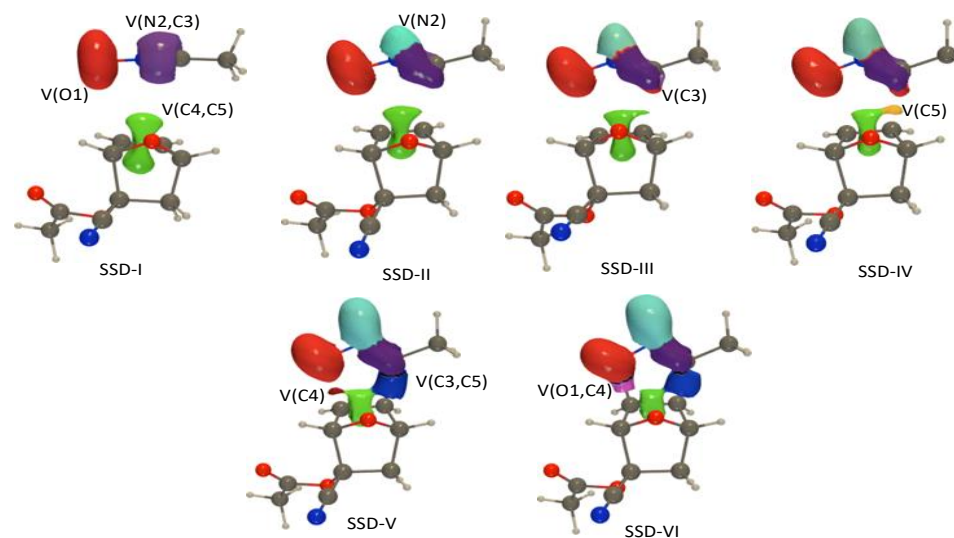
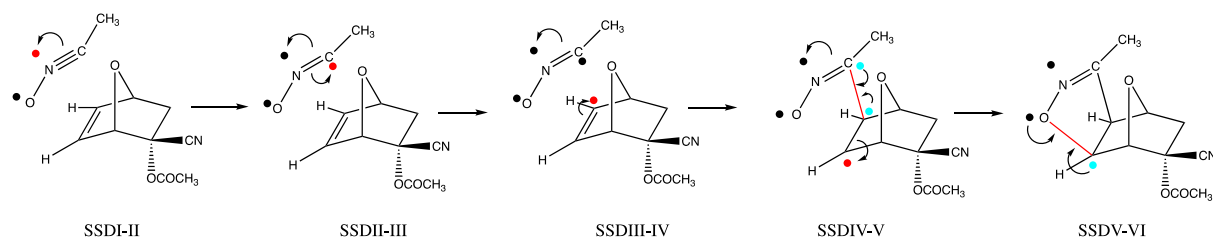


Figure S3: ELF basin isosurfaces ($\eta=0.7$) for selected points that are representative of each of the SSDs found along the IRC associated with the **TS-MSa** regioisomeric channel.

The SSD-III and SSD-IV domains correspond to the formation of the pseudo radical centers around the C3 and C5 atoms, which are involved in the formation of the C3-C5 bond. The V(C3) basin starts with a population of $0.31 |e|$ in the SSD-III domain but quickly reaches a value of $0.73 |e|$ at the end of the SSD-IV domain, while that of V(C5) is equal to $0.60 |e|$ (see Figure S2). The last two turning points are identical to those observed during the *para-syn* attack, namely a simultaneous appearance of V(C3,C5) and V(C4) basins in the SSD-V domain (concomitantly with the reduction of the initial V(C4,C5) basin, which loses a population of $0.22 |e|$) and finally the appearance of the V(O1,C4) basin.

The electronic flows, obtained from the analysis of the evolution of the populations of the different basins along the process, are depicted by using curly arrows in Scheme S1 for the path along **TS-MSa**.



Scheme S1: Curly arrows describing the electronic flows observed along the meta-*syn* path of the reaction between **1** and **2a**. The turning points between SSDs are indicated.

In this case, S_y is calculated to be 0.92 and $S_y^{\text{abs}}=0.87$, both values being slightly lower than those obtained for the para-*syn* case. This value implies that the topological changes also take place in a very synchronous way, at 87% of the maximum absolute synchronicity. The Cossío synchronicity is also slightly lower than in the para-*syn* case: 0.82. The TS can also be found slightly displaced to the products along the IRC (at approximately 67%), and therefore it has a product-like character in terms of its position along the IRC pathway.

The mechanism of the reaction between 1 and 2b-c.

In this case, the substitution of halogen atoms on **2a** does not affect the number of SSDs recorded, of which there are also six along the meta reactive path. However, the catastrophes taking place in the turning points between the SSDs are different. The first two SSD domains are identical, but the SSD-III and IV domains present notable changes: the two monosynaptic basins $V(C3)$ and $V(C5)$ appear in the SSD-III domain (see Figures S4 to S7) while the $V(C4)$ monosynaptic basin appears at the SSD-IV domain.

The calculated synchronicities ($S_y=0.90$ for **TS-MSb** and $S_y=0.89$ for **TS-MSc**) are slightly lower than that of **TS-MSa**, with the absolute synchronicity values around 83% in both cases. In these cases, the Cossío et al synchronicities are slightly greater than that of **TS-MSa**: 0.87 and 0.88 for **TS-MSb** and **TS-MSc**, respectively. All and all, the differences between the synchronicity values obtained with the two approaches are

always very small, as can be seen. Although they are calculated from different parameters (topological changes vs bond order evolution), both are intimately related with the modifications of the bonding scheme and therefore is not surprising that the values obtained are so similar.

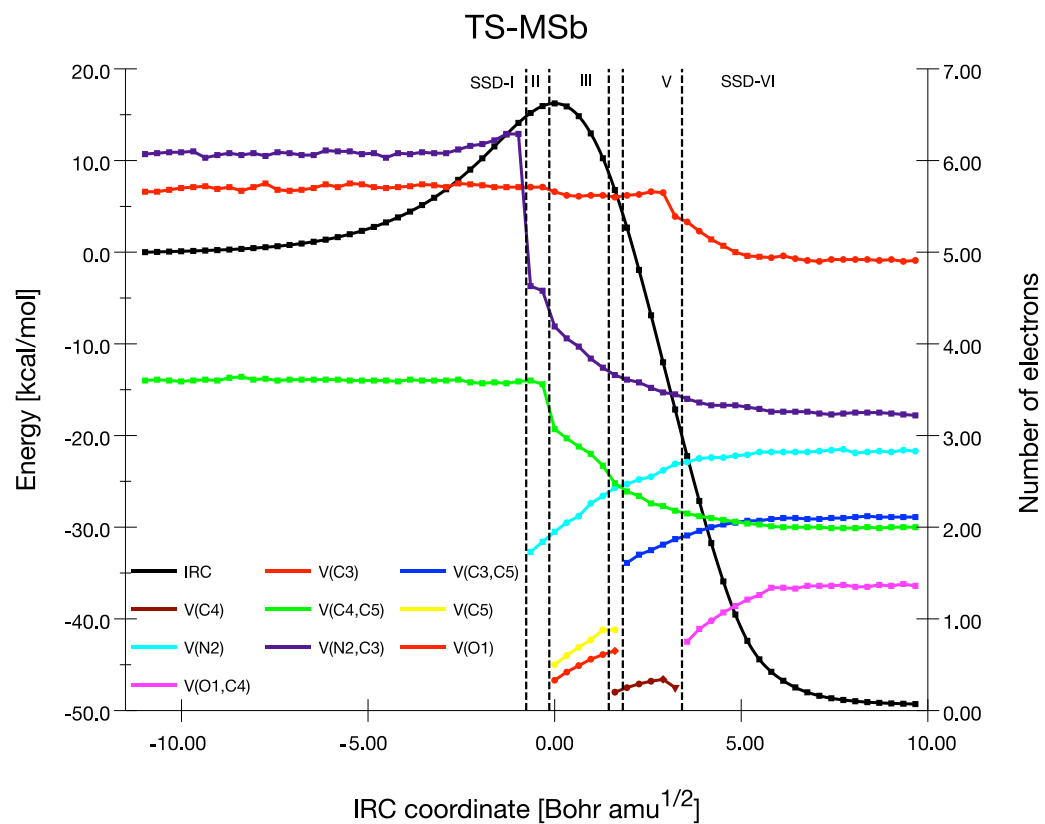


Figure S4: Population (in electrons) evolution of selected basins along the **TS-MSb** pathway of the reaction between **1** and **2b**.

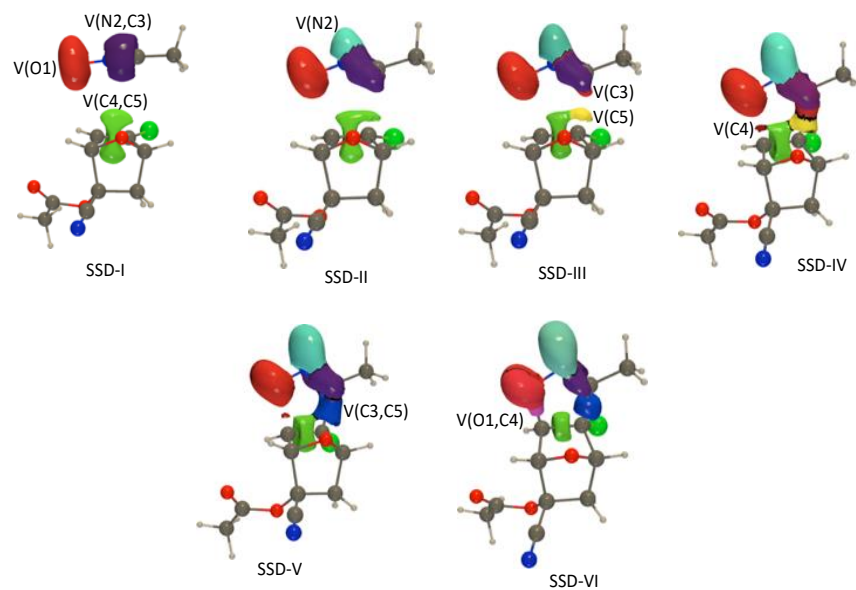


Figure S5: ELF basin isosurfaces ($\eta=0.7$) for selected points that are representative of each of the SSDs found along the IRC associated with the **TS-MSb** regioisomeric channel.

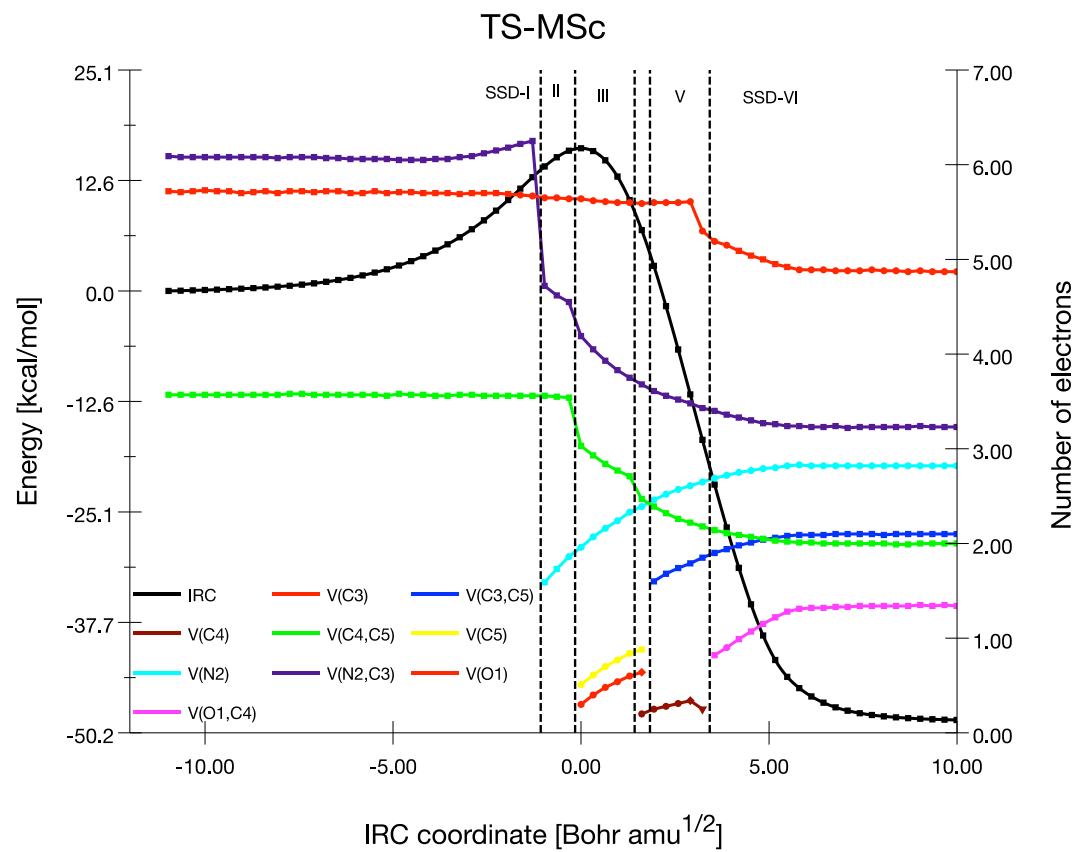


Figure S6: Population (in electrons) evolution of selected basins along the **TS-MSc** pathway of the reaction between **1** and **2c**.

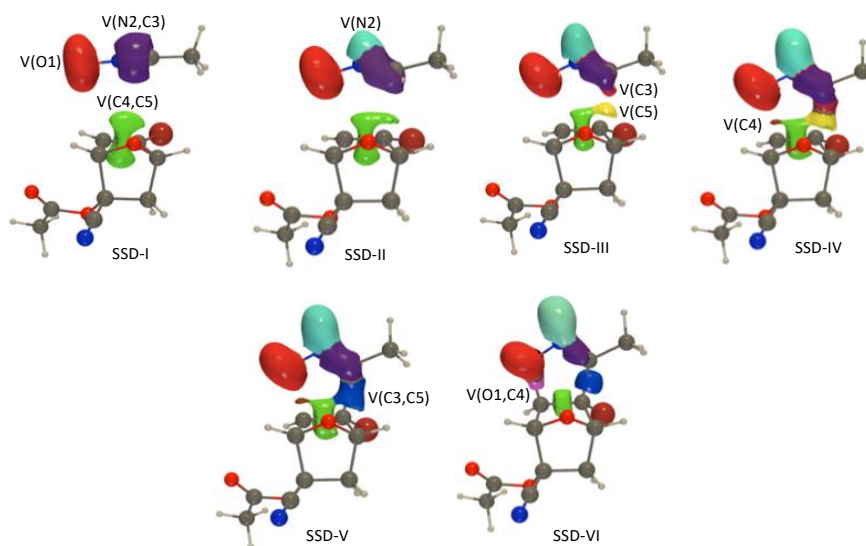
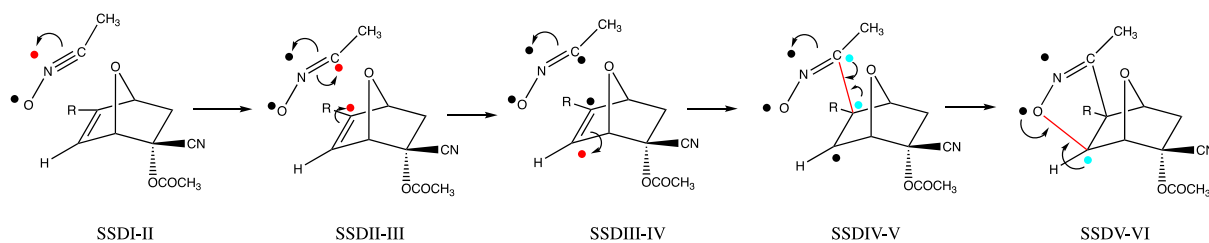


Figure S7: ELF basin isosurfaces ($\eta=0.7$) for selected points that are representative of each of the SSDs found along the IRC associated with the **TS-MSc** regioisomeric channel.

The electronic flows, obtained from the analysis of the evolution of the populations of the different basins along the process, are depicted by using curly arrows in Scheme S2 for the path along **TS-MSb** and **TS-MSc**.



Scheme S2: Curly arrows describing the electronic flows observed along the meta-*syn* path of the reaction between **1** and **2b** (R=Cl) or **2c** (R=Br). The turning points between SSDs are indicated.

It is worth noting that in the case of the *syn* attack along the meta channel for these halogenated compounds, the O-C bond is formed from some electron-density of the nitrile oxygen lone pairs and the V(C4) monosynaptic basin, i.e., there is no formation of a second monosynaptic basin on the O1 atom. The halogen atoms are in these cases far from the place where the O-C bond forms, and therefore they have no noticeable influence in the intimate mechanism by which the bond is formed.

Cartesian coordinates of the stationary points found *in vacuo*

Reactants

1

N	-0.73265500	-0.00004200	-0.00014600
O	-1.93587900	0.00014500	0.00039900
C	0.42248400	-0.00043600	-0.00124900
C	1.88102500	0.00014500	0.00042700
H	2.26366300	0.83211000	0.59517300
H	2.26447200	-0.93033800	0.42406200
H	2.26643200	0.09910100	-1.01647500

2a

C	0.12826700	0.52768100	0.28249900
C	1.26469300	0.38466000	1.32840800
C	2.35572900	-0.31086900	0.46612500
C	1.87751300	-1.72279600	0.17310000
C	0.92017200	-1.58964500	-0.73814500
C	0.82987200	-0.09787200	-0.99728800
O	2.15593500	0.34260300	-0.78370200
O	-1.01805600	-0.17037800	0.77075000
C	-0.21926600	1.93245100	0.03836100
H	0.92455200	-0.19717300	2.18393300

H	1.61380400	1.35840400	1.66987800
H	3.37791400	-0.17976400	0.81169100
H	0.43864500	0.24963200	-1.94551700
C	-2.03405300	-0.41142100	-0.09325900
N	-0.47483800	3.03871400	-0.13930300
C	-3.16974200	-1.08922700	0.61546400
O	-1.99746200	-0.11412000	-1.25283200
H	-2.81087100	-1.97351200	1.14493300
H	-3.93483300	-1.36546900	-0.10636400
H	-3.59240100	-0.40938800	1.35849200
H	0.26295100	-2.33928900	-1.15548100
H	2.20166500	-2.61706100	0.68824000

2b

C	0.71154000	-0.65852800	0.31538800
C	-0.44793900	-1.07516900	1.25822000
C	-1.59924700	-1.24077800	0.23163300
C	-1.93638700	0.14805700	-0.28862900
C	-0.95939300	0.49611000	-1.11492800
C	-0.02676000	-0.70028100	-1.09055500
O	-0.90286900	-1.79284300	-0.87432200
O	1.18177000	0.62240600	0.73102100
C	1.81733800	-1.62290800	0.34138100
H	-0.62439000	-0.30851000	2.01174400
H	-0.24137400	-2.02515400	1.74878000
H	-2.42932600	-1.87184800	0.53735800
H	0.62058300	-0.86837200	-1.94222800
C	1.99661800	1.30684200	-0.11086300
N	2.67011500	-2.39245700	0.37292700
C	2.44484800	2.58819600	0.52580800
O	2.28981700	0.91349800	-1.20332800
H	1.57907800	3.17529600	0.83804000

H	3.04827900	3.15385600	-0.18021500
H	3.03088300	2.36724000	1.42035400
H	-0.78346800	1.43722200	-1.61360200
Cl	-3.26144300	1.07610200	0.29044600

2c

C	1.30961200	-0.61441700	0.32583000
C	0.20026700	-1.19943400	1.23859000
C	-0.86527600	-1.57920800	0.17666600
C	-1.41006900	-0.27766700	-0.39486300
C	-0.47049100	0.20817600	-1.19579400
C	0.64745300	-0.81399300	-1.10345200
O	-0.04191800	-2.03195500	-0.88751700
O	1.53922700	0.73808700	0.71666400
C	2.55982400	-1.37709700	0.42123600
H	-0.13281600	-0.45736900	1.96298500
H	0.54449000	-2.08975100	1.76262200
H	-1.58839000	-2.33475600	0.47085000
H	1.34868400	-0.88962000	-1.92528100
C	2.27044200	1.52423000	-0.11304100
N	3.52689600	-1.99155000	0.50866200
C	2.45602200	2.88501200	0.48895000
O	2.68281300	1.15139600	-1.17376200
H	1.48336300	3.34995000	0.66297100
H	3.04918900	3.50163000	-0.18230600
H	2.95548700	2.79758400	1.45556400
H	-0.43022800	1.15374300	-1.71546800
Br	-3.01559200	0.50044600	0.16113200

Transition States

TS-PSa

C	-1.22017900	-0.80894500	0.07980500
C	-0.67662300	-2.01306000	-0.73470100
C	0.85259000	-1.81051400	-0.55870400
C	1.24192600	-0.57490800	-1.33940400
C	0.81699300	0.47893200	-0.58000100
C	0.13192000	-0.18041200	0.60882500
O	0.90001700	-1.35016000	0.79192600
O	-1.98961000	0.01651700	-0.79780200
C	-2.06099200	-1.23634600	1.20450900
H	-1.02398300	-1.96210300	-1.76609100
H	-0.98881800	-2.96021100	-0.29586100
H	1.46655200	-2.69761400	-0.68282300
H	0.03164800	0.37562200	1.53371600
C	-2.31374700	1.26341800	-0.38329000
N	-2.71087700	-1.58670900	2.08530500
C	-3.18206000	1.94039600	-1.40274000
O	-1.94255700	1.73310400	0.65513300
H	-2.72060000	1.88379000	-2.39002800
H	-3.33960000	2.97791700	-1.11697500
H	-4.14386200	1.42596400	-1.45994700
H	0.57839600	1.46773200	-0.94852400
H	3.46114900	2.68302700	1.63919500
H	1.79104000	2.93673800	1.09740300
C	2.67690200	1.14512300	0.41978800
C	2.50863900	2.18900000	1.43859500
N	3.42409300	0.37293200	-0.09975000
O	3.48520200	-0.54645700	-0.89969400
H	2.13368600	1.75707700	2.36940800
H	1.48525400	-0.57163400	-2.39094600

TS-PSb

C	1.41131400	-0.55633800	-0.62052400
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C	0.70057700	-1.93128700	-0.72929700
C	-0.76534400	-1.47911000	-0.94568000
C	-1.24419400	-0.84556000	0.34615400
C	-0.65661700	0.38642500	0.41480200
C	0.18995800	0.42434500	-0.84872600
O	-0.57990700	-0.33105800	-1.76322100
O	2.03433800	-0.47609600	0.66236000
C	2.42350700	-0.36868400	-1.66666800
H	0.85997900	-2.51582600	0.17631100
H	1.05448000	-2.49568000	-1.59100700
H	-1.43169100	-2.19546700	-1.41622300
H	0.46060800	1.38649600	-1.26775200
C	2.45627100	0.73543800	1.09597000
N	3.20631400	-0.23276600	-2.49696700
C	3.16100100	0.60029000	2.41280300
O	2.27393800	1.75338500	0.48935100
H	2.57393900	-0.01238500	3.09839700
H	3.33577200	1.58692100	2.83599500
H	4.11823700	0.09695300	2.25791600
H	-0.41389100	0.90769400	1.33042600
H	-2.52174900	3.79799600	-0.75097200
H	-2.01953600	3.58551300	0.93980700
C	-2.24495100	1.78791000	-0.15968500
C	-1.89350900	3.21108700	-0.07859000
N	-3.07643800	0.97537300	-0.42987500
O	-3.30996300	-0.21723300	-0.47173700
H	-0.85010200	3.35473700	-0.36538600
Cl	-1.80297000	-1.78319300	1.68135300

TS-PSc

C	-1.65163300	-0.24485200	0.82034300
C	-0.72718400	-1.14854000	1.67860100

C	0.57398200	-0.30813700	1.67866700
C	1.13550100	-0.32976000	0.26886900
C	0.34820800	0.50844700	-0.47093600
C	-0.68815700	0.97866700	0.54008700
O	0.04681700	1.01098900	1.74732200
O	-2.05658900	-0.98591300	-0.33161900
C	-2.83963300	0.19549200	1.56127400
H	-0.62393100	-2.13268500	1.22277000
H	-1.10856000	-1.25812200	2.69302300
H	1.27343100	-0.49496400	2.48757000
H	-1.19673000	1.91978300	0.36680800
C	-2.62181400	-0.31071900	-1.36032900
N	-3.75965400	0.53851900	2.15837200
C	-3.04351100	-1.26345900	-2.43881600
O	-2.74327000	0.88190300	-1.37841000
H	-2.19273600	-1.86953000	-2.75646700
H	-3.44433800	-0.70569100	-3.28198900
H	-3.80319900	-1.94506100	-2.05076300
H	0.16652300	0.41477700	-1.53272400
H	1.40756100	4.34961600	-1.31609800
H	1.06794800	3.14476200	-2.57545900
C	1.52735500	2.34240300	-0.67021000
C	0.93732900	3.38567200	-1.51817500
N	2.44159000	2.01984800	0.02649400
O	2.88890100	1.11991000	0.70996000
H	-0.13253800	3.47285100	-1.31957100
Br	2.14352800	-1.76716300	-0.39272600

TS-MSa

C	-1.22073300	0.78480300	0.14198800
C	-0.36701400	1.58891200	1.15817900
C	1.06100800	1.25207500	0.66034900

C	1.35834100	-0.21005300	0.98170800
C	0.57940100	-0.90953000	0.10243800
C	-0.08286200	0.14405400	-0.75495400
O	0.85854900	1.20250900	-0.74636800
O	-2.02645100	-0.14387800	0.86896200
C	-2.07800300	1.66568200	-0.66056300
H	-0.57570600	1.25965200	2.17550700
H	-0.56159700	2.65804400	1.07882200
H	1.81860800	1.99235600	0.90960800
H	-0.37888400	-0.11740700	-1.76286400
C	-2.68587700	-1.09594800	0.16212300
N	-2.73465300	2.38280600	-1.27318400
C	-3.52321200	-1.93963300	1.07781200
O	-2.59060000	-1.21713500	-1.02477600
H	-2.91326500	-2.33404200	1.89247700
H	-3.96990200	-2.75443800	0.51271300
H	-4.30932100	-1.32562200	1.52262300
H	0.24455000	-1.93165700	0.18156600
H	4.32007900	1.38114800	0.66203400
H	4.52367200	0.04083600	1.80181800
C	3.38076700	-0.42132500	0.08149200
C	4.47371400	0.30257800	0.74316900
N	3.07123300	-1.09361000	-0.85601500
O	2.13013900	-1.63582800	-1.40615100
H	5.42921900	0.05506000	0.27715200
H	1.67020700	-0.56334300	1.95715800

TS-MSb

C	1.44558900	0.68062300	-0.46672400
C	0.52079600	0.85178900	-1.70025800
C	-0.85600000	0.97734500	-1.01024200
C	-1.23096700	-0.37939100	-0.41269200

C	-0.38326000	-0.54994000	0.64737600
C	0.38567500	0.74729300	0.70957800
O	-0.52587400	1.69378900	0.16828500
O	2.13424300	-0.56176400	-0.59860300
C	2.41160600	1.78004000	-0.35216200
H	0.60626300	-0.00727800	-2.36501900
H	0.75722000	1.76049700	-2.25242500
H	-1.62250100	1.49548800	-1.58231400
H	0.77340500	1.07137600	1.66686400
C	2.83010400	-1.01738100	0.47520100
N	3.15047200	2.65773200	-0.28734900
C	3.54577300	-2.28915800	0.13013300
O	2.84337300	-0.45542800	1.53182800
H	2.84500300	-3.01625400	-0.28421100
H	4.02245800	-2.69026500	1.02149400
H	4.30037100	-2.08758500	-0.63320600
H	-0.05403900	-1.48187500	1.07731800
H	-4.08622800	1.56596800	-0.62942000
H	-4.35755000	-0.14208300	-1.02772000
C	-3.11911700	0.18408800	0.64365900
C	-4.24725600	0.57080600	-0.20873900
N	-2.71007100	0.03471400	1.75430400
O	-1.71325900	-0.26180500	2.39335100
H	-5.17172900	0.58219000	0.37137700
Cl	-1.81300100	-1.67954800	-1.43065300

TS-MSc

C	-1.71756700	-0.45649400	-0.69368000
C	-0.71556100	-0.21101800	-1.85190400
C	0.57626500	-0.79941500	-1.24256700
C	1.04716900	0.11043800	-0.10536400
C	0.13447600	-0.07532200	0.89812300

C	-0.77537000	-1.15832400	0.36923100
O	0.07108300	-1.89812700	-0.50008600
O	-2.25344400	0.80483400	-0.29749600
C	-2.80307800	-1.35970800	-1.09463500
H	-0.65165500	0.85192900	-2.08208400
H	-1.00097800	-0.75814800	-2.74950700
H	1.32682500	-1.12411700	-1.95967300
H	-1.27541100	-1.80292000	1.08080100
C	-2.98308300	0.85223200	0.84699700
N	-3.63573900	-2.07327600	-1.43810300
C	-3.52985300	2.23236300	1.05860400
O	-3.14481300	-0.09625100	1.55880800
H	-2.73262400	2.97356800	0.98164700
H	-4.00644300	2.28857000	2.03453500
H	-4.26244500	2.45525200	0.27965200
Br	1.90687000	1.76769200	-0.46454100
H	-0.12825400	0.61763400	1.68084300
H	3.66557000	-2.01994300	-1.02766700
H	4.13683900	-0.33221900	-0.74054400
C	2.76498900	-1.11260800	0.65331000
C	3.90116000	-1.28192800	-0.25744900
N	2.27672300	-1.39441200	1.70460100
O	1.26766800	-1.25619700	2.37842100
H	4.77998700	-1.62037200	0.29427900

TS-MAa

C	-0.91747000	-0.66375900	-0.38052200
C	0.25539000	-1.34295500	-1.13898600
C	1.03326500	-1.97336400	0.03923000
C	1.72168800	-0.89967600	0.89162800
C	0.69471700	-0.32100600	1.58671300
C	-0.55565900	-1.04496000	1.10842300

O	-0.05992800	-2.36239300	0.87894700
O	-0.95176200	0.70926700	-0.73225500
C	-2.20489100	-1.28623600	-0.73053200
H	0.80056700	-0.60027900	-1.71846800
H	-0.10664500	-2.12198700	-1.80842300
H	1.63751400	-2.84023700	-0.21847400
H	-1.40214600	-1.05403600	1.78373400
C	-1.72560500	1.53199000	0.02503500
N	-3.19524800	-1.78590100	-1.03054800
C	-1.68145100	2.93233500	-0.50348300
O	-2.34220600	1.14861600	0.97711700
H	-2.45588100	3.52414900	-0.02028300
H	-1.81583100	2.93967600	-1.58594000
H	-0.70067200	3.35287600	-0.27563000
H	3.27831500	-0.53289200	-1.93444600
H	3.97234300	1.09487500	-1.82566300
C	2.51865200	0.65801600	-0.35500400
C	3.61513100	0.24357600	-1.24407000
N	1.90518300	1.60801300	0.04405200
O	1.02661900	1.92952900	0.82793300
H	4.44841700	-0.15723100	-0.66251000
H	0.74083500	0.25551600	2.49471200
H	2.72926900	-1.01912900	1.27233100

TS-MAb

C	1.20718500	-0.76215900	0.41990400
C	0.06758300	-1.11062800	1.41654200
C	-1.01465300	-1.63240000	0.44625200
C	-1.59736500	-0.49609600	-0.40854900
C	-0.62086800	-0.21642000	-1.32430900
C	0.52227800	-1.15395000	-0.94312100
O	-0.18999100	-2.31277300	-0.50574600

O	1.58431400	0.59080900	0.61316900
C	2.37715500	-1.62991800	0.63349600
H	-0.19850600	-0.23251200	2.00034400
H	0.36696300	-1.90891200	2.09402700
H	-1.74638600	-2.31042300	0.87775200
H	1.21803600	-1.39536700	-1.73717000
C	2.39119700	1.15211800	-0.32896700
N	3.27630400	-2.31627500	0.83486500
C	2.72558000	2.56734100	0.02805300
O	2.75719400	0.55971400	-1.30235600
H	3.62392300	2.86971300	-0.50648500
H	2.86203400	2.68140200	1.10326400
H	1.89317300	3.20077000	-0.28439900
H	-2.32144300	0.58434400	2.65501700
H	-2.55812100	2.32938600	2.44548700
C	-1.69048100	1.35915000	0.78848000
C	-2.60081900	1.36228900	1.94199800
N	-0.99086100	2.03682300	0.09419600
O	-0.28230500	1.99276200	-0.89944800
H	-3.62474500	1.17548900	1.61490800
H	-0.74724600	0.18344200	-2.31618900
Cl	-3.31295400	-0.50007200	-0.80668300

TS-MAc

C	1.60902100	-0.78687200	0.42294500
C	0.53030300	-1.02488300	1.51464200
C	-0.65415500	-1.51079300	0.65013500
C	-1.23527600	-0.36596700	-0.19707400
C	-0.31417600	-0.17572200	-1.19154400
C	0.79601300	-1.17375500	-0.86832600
O	0.05098300	-2.27030100	-0.33747700
O	2.08809200	0.54203700	0.53883400

C	2.73172900	-1.72665200	0.57809500
H	0.36416100	-0.10913100	2.07681700
H	0.83101900	-1.81409200	2.20206200
H	-1.38442100	-2.13032600	1.16366800
H	1.40943800	-1.48282600	-1.70578400
C	2.84926800	1.02276000	-0.48217300
N	3.59600400	-2.46730500	0.73489200
C	3.28945300	2.42657700	-0.20365700
O	3.10226200	0.37941400	-1.45917200
H	4.17955000	2.64805600	-0.78940600
H	3.48046100	2.57771100	0.85842200
H	2.48442300	3.09761600	-0.50952300
H	-1.63275600	0.86059900	2.88933800
H	-1.79817400	2.60673600	2.62779900
C	-1.13133300	1.52952400	0.94416100
C	-1.93460800	1.62524400	2.17092900
N	-0.43876500	2.13738800	0.18152400
O	0.18821900	2.01983600	-0.86020700
H	-2.99150600	1.48159400	1.94260300
H	-0.48500100	0.20767300	-2.18323800
Br	-3.12033600	-0.28682400	-0.51635100

TS-PAa

C	-1.07918300	-0.13730000	0.18657400
C	-0.90677100	-0.79102300	-1.21373400
C	-0.43996500	-2.20870300	-0.80187700
C	1.00888000	-2.17527600	-0.33770400
C	0.97596000	-1.52942400	0.86854900
C	-0.51885400	-1.27782800	1.10562600
O	-1.12727500	-2.38258400	0.45019300
O	-0.37117200	1.07629000	0.41045300
C	-2.49561500	0.06836200	0.53032100

H	-0.17439000	-0.26555900	-1.82022500
H	-1.85459700	-0.82170000	-1.74686400
H	-0.70658600	-3.00393900	-1.49238200
H	-0.84254400	-1.21019000	2.14144800
C	-0.62645400	2.11688500	-0.42605400
N	-3.59094700	0.21613500	0.84436700
C	0.27182600	3.27641700	-0.10718000
O	-1.44153400	2.07149600	-1.29858100
H	0.32125800	3.45023900	0.96838300
H	-0.09163900	4.16593300	-0.61665000
H	1.28119900	3.04929800	-0.46131800
C	2.51198700	1.07667800	1.65808700
C	2.22543200	0.24889700	0.48038700
O	2.13238600	-0.63585500	-1.63027300
N	2.41559800	0.10480500	-0.69197900
H	1.57453800	1.39244500	2.11742900
H	3.08423700	1.96155300	1.37253400
H	3.08936700	0.51195000	2.39328800
H	1.65156900	-1.71338000	1.69383500
H	1.79233200	-2.80411100	-0.72848400

TS-PAb

C	-0.99191100	-0.94213800	0.19919900
C	-0.23697300	-1.25320100	-1.12510500
C	1.14575200	-1.65749800	-0.56822900
C	1.90223800	-0.43276800	-0.05861800
C	1.26124200	-0.04836300	1.08539100
C	0.16878800	-1.11682300	1.23611700
O	0.78188400	-2.27472900	0.67705900
O	-1.55919100	0.35539400	0.31583100
C	-2.02488300	-1.94772600	0.49576800
H	-0.19862200	-0.39227700	-1.78496800

H	-0.70180800	-2.08622800	-1.64826600
H	1.72503000	-2.33861400	-1.18484600
H	-0.16721800	-1.30588500	2.25257800
C	-2.46686300	0.73355300	-0.62472800
N	-2.81656800	-2.73201300	0.77535200
C	-2.87823300	2.15978000	-0.40544800
O	-2.83952800	0.01139900	-1.50029100
H	-3.08889400	2.34742800	0.64820900
H	-3.75428700	2.38183600	-1.01054400
H	-2.05747600	2.81523500	-0.70935200
C	0.05469400	2.73632100	1.80936500
C	0.59592700	2.00588000	0.65902200
O	1.23605300	1.34221000	-1.43806400
N	0.82599100	2.02912700	-0.51256100
H	-0.81584600	2.20659100	2.20031400
H	-0.24520100	3.74302300	1.51208000
H	0.80124000	2.81658600	2.60189500
H	1.75790600	0.36460900	1.95329900
Cl	3.56157700	-0.14873000	-0.43074300

TS-PAc

C	-1.42041900	-0.94767400	0.19189500
C	-0.60075000	-1.24555800	-1.09633700
C	0.76127800	-1.62994200	-0.47646400
C	1.47800800	-0.39094600	0.05922600
C	0.77821300	-0.01310600	1.17149500
C	-0.30416800	-1.09797800	1.28016000
O	0.35075600	-2.24739600	0.75415800
O	-2.02351900	0.33618900	0.27861400
C	-2.44363700	-1.97531400	0.44515300
H	-0.54407500	-0.38226600	-1.75196600
H	-1.02929500	-2.08344500	-1.64211000

H	1.37298700	-2.30816800	-1.06396900
H	-0.68229200	-1.28782300	2.28163600
C	-2.90039300	0.68596000	-0.70155900
N	-3.23111400	-2.77492700	0.69123100
C	-3.38320500	2.09079000	-0.49055300
O	-3.20563900	-0.04511200	-1.59564400
H	-3.76407200	2.21765000	0.52432500
H	-4.16434800	2.31608900	-1.21273500
H	-2.55034400	2.78502000	-0.62845700
C	-0.53501600	2.72969200	1.83623400
C	0.08455600	2.01701100	0.71397200
O	0.84262000	1.38541000	-1.35389900
N	0.36858800	2.05254000	-0.44579800
H	-1.43838600	2.20204500	2.14767600
H	-0.79852500	3.74722500	1.54150000
H	0.15068900	2.78195200	2.68410500
H	1.22503700	0.41398300	2.05951300
Br	3.29885000	-0.06045400	-0.25493500

Products

3a

C	-1.11183600	-0.81048800	-0.00899400
C	-0.47545400	-1.92808500	-0.88171800
C	1.00426300	-1.81264600	-0.48087900
C	1.60557200	-0.56130600	-1.13261200
C	1.00074800	0.55355400	-0.26003100
C	0.15476700	-0.26920400	0.73469800
O	0.91286200	-1.44763800	0.89582800
O	-1.76891900	0.11509100	-0.87672100
C	-2.07956000	-1.35637400	0.95198400
H	-0.67520400	-1.73785700	-1.93648200

H	-0.87164600	-2.90774000	-0.62016800
H	1.60131400	-2.71415100	-0.58891100
H	-0.04871500	0.19322200	1.69404200
C	-2.22693500	1.27293100	-0.33035100
N	-2.83073700	-1.81466200	1.69075100
C	-3.00908900	2.05682500	-1.34087500
O	-2.01700500	1.58532300	0.80591700
H	-2.47968600	2.10076700	-2.29360500
H	-3.19245300	3.05848000	-0.95877300
H	-3.96454200	1.55686300	-1.51725500
H	0.43750700	1.32128600	-0.78985900
H	1.80912900	3.12265900	0.90948800
H	1.72300900	1.97325200	2.24127600
C	2.25492400	1.10680800	0.35993300
C	2.27935400	2.23131300	1.33528100
N	3.31678300	0.52398300	-0.02501900
O	3.01875300	-0.47909800	-0.93584800
H	3.30634900	2.46820400	1.61123700
H	1.40657000	-0.48962800	-2.20312700

3b

C	1.29591000	-0.77251500	-0.29953700
C	0.48334600	-2.02749100	0.12451300
C	-0.89636300	-1.71013200	-0.46598400
C	-1.61905000	-0.59689900	0.31691700
C	-0.78011100	0.64294100	-0.03193400
C	0.19694000	0.03838500	-1.06239400
O	-0.56075100	-1.00072100	-1.65504800
O	1.82009500	-0.16020500	0.87706000
C	2.39749900	-1.11654000	-1.20878300
H	0.50417700	-2.14397000	1.20593500
H	0.88306300	-2.92912700	-0.33633800

H	-1.53150100	-2.56068600	-0.69709200
H	0.57585600	0.71592600	-1.81897600
C	2.37715500	1.07399200	0.75170000
N	3.24938900	-1.41652500	-1.91880300
C	2.97028200	1.51415800	2.05530600
O	2.35953400	1.69405800	-0.27264200
H	2.20590700	1.51001800	2.83508300
H	3.38903500	2.51160600	1.94508700
H	3.75038600	0.81377500	2.35971200
H	-0.29467800	1.11588200	0.81912900
H	-1.29689900	3.53911800	-0.25439000
H	-0.83023700	2.95346300	-1.84819200
C	-1.83963000	1.51225700	-0.63995900
C	-1.61844800	2.91252700	-1.09123500
N	-2.97259900	0.94276700	-0.72790200
O	-2.88515300	-0.36402900	-0.23257500
H	-2.53486300	3.32492300	-1.51156000
Cl	-1.79016300	-0.92420900	2.08250100

3c

C	-1.52171800	-0.36750800	0.77198000
C	-0.51285500	-1.30755800	1.48775800
C	0.66865000	-0.35919000	1.72823100
C	1.42849000	-0.02572300	0.42914500
C	0.40774200	0.83845800	-0.33093900
C	-0.70075100	0.96341600	0.73727200
O	0.01380900	0.88598500	1.95691300
O	-1.84291700	-0.93898900	-0.49495700
C	-2.75210800	-0.18595800	1.55397200
H	-0.28920500	-2.16823100	0.86134400
H	-0.90640100	-1.65574300	2.44120200
H	1.32261000	-0.60379900	2.56042100

H	-1.30014200	1.86594200	0.70158500
C	-2.52715500	-0.16883500	-1.38195200
N	-3.70310500	-0.06239700	2.18658100
C	-2.89196900	-0.96911500	-2.59504200
O	-2.77609100	0.98591400	-1.18453500
H	-2.01611500	-1.48949000	-2.98620300
H	-3.31276500	-0.31055800	-3.35132100
H	-3.62800000	-1.72719600	-2.31827200
H	0.06711600	0.42609700	-1.27783000
H	0.56299700	3.01149900	-2.32236000
H	-0.17945900	3.67290400	-0.86893700
C	1.21070200	2.09279000	-0.50846500
C	0.75510400	3.28060800	-1.27985400
N	2.34678000	2.05149100	0.06030900
O	2.50650700	0.82080800	0.70821000
H	1.51156100	4.06376100	-1.24942100
Br	2.08762400	-1.59391200	-0.55646100

4a

C	-0.52446200	-1.00331400	-0.25215000
C	0.58552500	-1.49749100	-1.21881300
C	1.77867800	-1.59538400	-0.26450600
C	2.35799300	-0.19223900	0.02195600
C	1.31870300	0.37450000	1.00305000
C	0.29387300	-0.79420900	1.06560100
O	1.16635500	-1.91048200	0.99079100
O	-1.15217500	0.13316400	-0.83328700
C	-1.52730800	-2.05753900	-0.02651500
H	0.73131500	-0.77372300	-2.01821600
H	0.34061900	-2.46718700	-1.64821100
H	2.51147000	-2.35869200	-0.51163600
H	-0.30736100	-0.83922400	1.96697500

C	-2.07939100	0.79272000	-0.09968600
N	-2.29039600	-2.90448600	0.11586900
C	-2.67814200	1.90610600	-0.90362700
O	-2.34240500	0.50351600	1.03384200
H	-1.88683700	2.50700300	-1.35511300
H	-3.30950100	2.51988200	-0.26518600
H	-3.27628100	1.48670300	-1.71573500
C	0.23821200	2.79963500	0.95305600
C	1.01812300	1.68664900	0.33845300
O	2.35648100	0.70345600	-1.09165400
N	1.58338900	1.82345800	-0.79516500
H	-0.71195900	2.45362000	1.36326300
H	0.05921700	3.58829900	0.22223500
H	0.80486700	3.22813200	1.78600200
H	1.70273600	0.51499000	2.01526700
H	3.37388400	-0.24644300	0.41698500

4b

C	0.97869700	-1.07254000	0.23910700
C	-0.07008400	-1.60130000	1.25527700
C	-1.34360600	-1.55838700	0.40651400
C	-1.81333000	-0.09270100	0.23302800
C	-0.87934800	0.41908300	-0.86859500
C	0.07719100	-0.79995200	-1.01398900
O	-0.85478100	-1.86246800	-0.89951000
O	1.63844600	0.04165000	0.82513400
C	1.96349600	-2.11275100	-0.09633500
H	-0.09945800	-0.96303700	2.13495900
H	0.14601500	-2.62595800	1.55249000
H	-2.12485300	-2.25727200	0.68779900
H	0.60595000	-0.85441300	-1.95879000
C	2.47147700	0.76872300	0.04268400

N	2.71430800	-2.94981300	-0.33153500
C	3.08209600	1.88405300	0.83280300
O	2.64358500	0.53053700	-1.12004200
H	2.29268000	2.46941300	1.30898500
H	3.68194200	2.51148200	0.17764400
H	3.70936400	1.47301900	1.62652600
C	0.19628000	2.84168300	-1.01383100
C	-0.48332700	1.73711300	-0.27895300
O	-1.58044300	0.73815500	1.33178000
N	-0.88369900	1.88903400	0.92157500
H	1.10055700	2.49266000	-1.51496200
H	0.44340600	3.65563100	-0.33248600
H	-0.47395400	3.23136300	-1.78602600
H	-1.37914900	0.53432400	-1.83037400
Cl	-3.56285200	-0.01781800	-0.21889400

4c

C	1.42647300	-1.07404200	0.23521300
C	0.40310400	-1.60887100	1.27371900
C	-0.89097600	-1.56414900	0.45585200
C	-1.36352700	-0.09587400	0.29846900
C	-0.46054400	0.41538800	-0.83012500
C	0.49530800	-0.80212100	-0.99661800
O	-0.43247500	-1.86572400	-0.86114500
O	2.09497700	0.04116400	0.80926900
C	2.40725900	-2.10951500	-0.12559600
H	0.39512800	-0.97575600	2.15748500
H	0.62678500	-2.63520000	1.55959100
H	-1.66189400	-2.26707800	0.75413900
H	1.00176600	-0.85615400	-1.95357400
C	2.90709400	0.77435600	0.01094200
N	3.15550400	-2.94306600	-0.38065000

C	3.52859700	1.89110100	0.79057400
O	3.05553300	0.53998400	-1.15584700
H	2.74633000	2.47106500	1.28485100
H	4.11122500	2.52319900	0.12445000
H	4.17485400	1.48174200	1.56981300
C	0.60711000	2.83939500	-1.00735700
C	-0.04929100	1.73430600	-0.25257400
O	-1.09494100	0.73300900	1.38966800
N	-0.41222700	1.88527700	0.95995100
H	1.49884900	2.49187700	-1.53155900
H	0.86996900	3.65540500	-0.33441000
H	-0.08481400	3.22538400	-1.76208800
H	-0.97772600	0.53002700	-1.78231700
Br	-3.28433800	-0.00649400	-0.13463000

5a

C	-1.11613900	0.76203100	0.19483400
C	-0.20426200	1.49647900	1.21819800
C	1.17495300	1.30655700	0.56895400
C	1.64449100	-0.15252400	0.76153500
C	0.73465400	-0.89088600	-0.23838400
C	-0.05559600	0.27714800	-0.84840700
O	0.86923000	1.34921800	-0.81902800
O	-1.82039000	-0.26977400	0.88741300
C	-2.06955400	1.69127000	-0.42627000
H	-0.30604400	1.04100600	2.20321900
H	-0.45903500	2.55276600	1.28902900
H	1.90894000	2.07303500	0.80879600
H	-0.42934600	0.11177000	-1.85211500
C	-2.57673600	-1.12038900	0.13885800
N	-2.79705500	2.45488000	-0.88192700
C	-3.32053700	-2.07462700	1.02427800

O	-2.61060000	-1.07816600	-1.05540900
H	-2.62157400	-2.63385400	1.64958500
H	-3.90047400	-2.75937900	0.41014300
H	-3.98369300	-1.51781400	1.68920200
H	0.11939900	-1.68815200	0.17427800
H	4.31744200	1.13689400	0.70973100
H	4.43093900	-0.30480600	1.72016600
C	2.98735000	-0.44282600	0.14786400
C	4.28545100	0.04305900	0.69287000
N	2.92756300	-1.14444600	-0.91039300
O	1.61402500	-1.47039800	-1.20544300
H	5.11012100	-0.31693100	0.07856800
H	1.57719400	-0.48636200	1.79940000

5b

C	1.34141500	0.70900600	-0.39195800
C	0.36415300	1.02271400	-1.55786200
C	-0.95669700	1.19757200	-0.79898900
C	-1.51019100	-0.15507900	-0.28463100
C	-0.50693600	-0.49775700	0.83104400
C	0.36781400	0.76346400	0.83066100
O	-0.53526400	1.78409300	0.42371800
O	1.94228400	-0.55863500	-0.64714000
C	2.37850300	1.74252000	-0.26837000
H	0.37236500	0.21526900	-2.28700100
H	0.62893200	1.95352600	-2.05658700
H	-1.69498700	1.82933400	-1.28746600
H	0.82421000	1.00508200	1.78317200
C	2.71208900	-1.09736800	0.33958600
N	3.16984500	2.57321200	-0.20933800
C	3.34384000	-2.37249300	-0.12918200
O	2.83385100	-0.58837000	1.41493500

H	2.59035300	-3.03923500	-0.55191800
H	3.84909500	-2.85310500	0.70529700
H	4.06648900	-2.14998100	-0.91739900
H	0.02629100	-1.43585400	0.70109800
H	-4.04736400	1.37221600	-0.47402000
H	-4.41838600	-0.32511200	-0.79135800
C	-2.76880800	-0.01440000	0.53079000
C	-4.09441200	0.37780700	-0.02016000
N	-2.59296000	-0.25275300	1.76759000
O	-1.27821200	-0.58339900	2.02742200
H	-4.83532200	0.39583700	0.77784100
Cl	-1.71328000	-1.39391900	-1.57332200

5c

C	-1.60237100	-0.48466700	-0.64965900
C	-0.54977600	-0.34693800	-1.78384800
C	0.66779500	-1.02505300	-1.14370300
C	1.30520200	-0.15527700	-0.03087000
C	0.22683300	-0.21381600	1.06613500
C	-0.75888000	-1.21577800	0.44547600
O	0.07286100	-2.04629900	-0.35535500
O	-2.05908500	0.82290500	-0.30975200
C	-2.73605900	-1.32052500	-1.06790500
H	-0.40771400	0.70046600	-2.04163800
H	-0.85315100	-0.89362600	-2.67514400
H	1.38302700	-1.45290300	-1.84241800
H	-1.32363200	-1.80494900	1.15807300
C	-2.87027100	0.94106700	0.77842400
N	-3.60211500	-1.97870300	-1.43739600
C	-3.34483300	2.35459600	0.92539300
O	-3.14002700	0.01655900	1.48749700
H	-2.51288300	3.05351700	0.82732800

H	-3.83144200	2.47456900	1.89054000
H	-4.05849600	2.57770000	0.12870700
Br	1.84307000	1.62986700	-0.62037300
H	-0.20782700	0.74060700	1.35008500
H	3.62897600	-1.89684600	-0.74357400
H	4.23321900	-0.28682900	-0.33717800
C	2.43760000	-0.84471800	0.68347600
C	3.75330000	-1.17843800	0.07250300
N	2.15756600	-1.15318800	1.88558100
O	0.87336000	-0.76506000	2.21074300
H	4.40618600	-1.62138400	0.82340000

6a

C	-0.88536700	-0.69794700	-0.39045000
C	0.27916500	-1.32672500	-1.20700400
C	1.21279500	-1.79918900	-0.08423800
C	1.95107200	-0.62116000	0.60460300
C	0.81911800	-0.01843600	1.45452700
C	-0.37661700	-0.93112500	1.07050000
O	0.28390000	-2.18010000	0.93180100
O	-1.05109600	0.64386900	-0.81585400
C	-2.13724300	-1.44571400	-0.59376000
H	0.69940900	-0.57867100	-1.87832500
H	-0.06193000	-2.17697300	-1.79566000
H	1.84169100	-2.64890000	-0.33912300
H	-1.16535900	-0.99856400	1.81007300
C	-1.78979500	1.46488600	-0.01960900
N	-3.09252200	-2.05612100	-0.78066300
C	-1.72808000	2.86885200	-0.53134200
O	-2.37475700	1.07234600	0.94771400
H	-0.70483500	3.23190000	-0.41074800
H	-2.41334200	3.49393300	0.03650600

H	-1.97309000	2.90144600	-1.59410600
H	4.35148100	0.35576300	-0.83599300
H	3.17574200	-0.16244600	-2.04039600
C	2.32117300	0.57630400	-0.22072900
C	3.37603800	0.59102800	-1.27233200
N	1.64431500	1.61925700	0.05709700
O	0.75842000	1.36108900	1.09667000
H	3.43014000	1.57091200	-1.74559900
H	0.97535100	-0.07412200	2.53136400
H	2.79690700	-0.99850600	1.18331600

6b

C	1.20641700	-0.78292700	0.42373900
C	0.09066300	-1.09401500	1.45959800
C	-1.09257800	-1.43105500	0.53890900
C	-1.66914100	-0.15665300	-0.12843000
C	-0.61209700	0.11937900	-1.20894500
C	0.42647100	-0.99873200	-0.91352700
O	-0.44322200	-2.06172000	-0.56109300
O	1.69823000	0.52115400	0.67944000
C	2.30056100	-1.76300900	0.51464200
H	-0.05418100	-0.23659800	2.11473300
H	0.34056300	-1.96291200	2.06631900
H	-1.84028500	-2.09444800	0.96413300
H	1.04790400	-1.27695700	-1.75602900
C	2.45134900	1.10586900	-0.29544100
N	3.13287900	-2.54784100	0.61991800
C	2.76292200	2.52106100	0.07296000
O	2.77602400	0.52750900	-1.29096800
H	1.82883300	3.08735000	0.08589200
H	3.44613900	2.94492500	-0.65929300
H	3.19918000	2.56940400	1.07197600

H	-3.49562200	1.43340500	1.60563900
H	-2.25291700	0.71151000	2.62347300
C	-1.62744400	1.14124700	0.62210700
C	-2.42812100	1.45275900	1.83802400
N	-0.82288600	1.98712200	0.10944700
O	-0.22730200	1.47439700	-1.03148700
H	-2.16553100	2.43955600	2.21702300
H	-0.97860200	-0.00293000	-2.22665200
Cl	-3.32525200	-0.47420800	-0.77186600

6c

C	1.60641300	-0.80689300	0.42515600
C	0.55485800	-1.02476700	1.54836700
C	-0.71181600	-1.31425400	0.72696200
C	-1.26022600	-0.02326300	0.06401200
C	-0.27373100	0.15756200	-1.10120900
C	0.71799400	-1.01222900	-0.84405300
O	-0.18257600	-2.01193400	-0.39607600
O	2.18803000	0.47277300	0.60391400
C	2.64787500	-1.84581800	0.46662100
H	0.51042400	-0.14502900	2.18840100
H	0.79851900	-1.89257600	2.15934200
H	-1.45912900	-1.92195800	1.22851900
H	1.25829900	-1.34979400	-1.72021600
C	2.89985900	0.98637900	-0.43952000
N	3.44050000	-2.67453700	0.53573700
C	3.31095000	2.39214800	-0.13898600
O	3.12038300	0.36347400	-1.43667800
H	2.41315400	3.01458700	-0.12012900
H	3.99157900	2.74539300	-0.91014600
H	3.78254300	2.45337000	0.84285500
H	-2.83373200	1.78311200	1.87730400

H	-1.61325300	0.92221200	2.81041300
C	-1.08134500	1.28703700	0.76895100
C	-1.75760000	1.68119000	2.03595500
N	-0.26833800	2.06783800	0.17239400
O	0.20113800	1.49168500	-0.99698500
H	-1.36084100	2.63132000	2.39154100
H	-0.71321100	0.03012200	-2.08862800
Br	-3.12899100	-0.26898300	-0.48237500

Cartesian coordinates of the stationary points found in benzene

Reactants

1

N	-0.72996200	0.00033400	0.00000000
O	-1.93944900	0.00000000	0.00000000
C	0.42368600	-0.00086500	0.00015400
C	1.88213700	0.00000000	0.00000000
H	2.26396100	-1.02071800	-0.05593200
H	2.26301000	0.55981500	-0.85621400
H	2.26341500	0.46299500	0.91195800

2a

C	0.12607000	0.51556100	0.28867200
C	1.26579900	0.37142000	1.33083400
C	2.36152700	-0.30368200	0.45913100
C	1.89607500	-1.71622800	0.15335300
C	0.93337000	-1.58487700	-0.75303600
C	0.82808800	-0.09226600	-0.99949900
O	2.15056200	0.36101600	-0.78644500
O	-1.01471800	-0.19465900	0.76783800
C	-0.22649000	1.92207600	0.05685600

H	0.93413300	-0.22510300	2.17920000
H	1.60711200	1.34284300	1.68604500
H	3.38237600	-0.16542600	0.80426800
H	0.43034700	0.25913600	-1.94376000
C	-2.04247800	-0.40520000	-0.09036600
N	-0.48082600	3.02992800	-0.11336800
C	-3.15905300	-1.12973900	0.59859900
O	-2.02411100	-0.04487600	-1.23397500
H	-2.78192000	-2.03448600	1.07810300
H	-3.93202600	-1.38001000	-0.12412200
H	-3.57830700	-0.49225300	1.37995800
H	0.28141300	-2.33762000	-1.17308700
H	2.23134800	-2.61081900	0.66036600

2b

C	-0.70595800	-0.64787600	-0.31804000
C	0.45386000	-1.06375200	-1.26073400
C	1.60299400	-1.23688900	-0.23357400
C	1.94330800	0.14892100	0.29138000
C	0.96567400	0.50117600	1.11532200
C	0.02962200	-0.69223300	1.08915800
O	0.90194800	-1.78853400	0.87289200
O	-1.17660900	0.63343800	-0.72637000
C	-1.80828100	-1.61755700	-0.34520100
H	0.63492600	-0.29430200	-2.00994700
H	0.24777900	-2.01019600	-1.75780200
H	2.42985500	-1.87071400	-0.54074700
H	-0.61854400	-0.85779100	1.94088600
C	-2.02249700	1.29525700	0.10331200
N	-2.65386500	-2.39514600	-0.37616900
C	-2.43955300	2.59858400	-0.50520300
O	-2.36057000	0.86115700	1.16863600

H	-1.55873400	3.19471600	-0.75086700
H	-3.07663600	3.13972700	0.19014800
H	-2.97988300	2.41262500	-1.43557000
H	0.79330000	1.44256300	1.61474200
Cl	3.27481400	1.07336000	-0.27985000

2c

C	-1.30364100	-0.60824300	-0.32695800
C	-0.19377300	-1.18901500	-1.24178500
C	0.87176300	-1.57248400	-0.18174400
C	1.41655200	-0.27290300	0.39331900
C	0.47710600	0.21432000	1.19389800
C	-0.64078100	-0.80756400	1.10201200
O	0.04732900	-2.02659800	0.88430100
O	-1.54020700	0.74316800	-0.71171200
C	-2.54909900	-1.38075600	-0.42029800
H	0.13996300	-0.44380100	-1.96227600
H	-0.53469200	-2.07676700	-1.77182000
H	1.59275400	-2.32822900	-0.47901200
H	-1.34017200	-0.88327300	1.92551400
C	-2.30100600	1.51362200	0.10655900
N	-3.50943800	-2.00637400	-0.50380200
C	-2.46973400	2.88436200	-0.47302100
O	-2.75056400	1.11340900	1.14354300
H	-1.49256400	3.34823200	-0.62126400
H	-3.07341700	3.49223900	0.19660800
H	-2.95255000	2.81476200	-1.44950500
H	0.43802200	1.15927100	1.71485100
Br	3.02548400	0.50383700	-0.15621200

Transition States

TS-PSa

C	-1.22130000	-0.80799100	0.06855300
C	-0.67810800	-2.01180000	-0.74630500
C	0.85041100	-1.817557000	-0.55880100
C	1.24921600	-0.58078400	-1.33166900
C	0.82321700	0.47308700	-0.57265100
C	0.13026200	-0.18673500	0.61085700
O	0.89119200	-1.36160900	0.79545800
O	-1.97762600	0.02623700	-0.80955300
C	-2.06917300	-1.23841600	1.18773600
H	-1.01604200	-1.95511600	-1.78021500
H	-0.99709400	-2.96035400	-0.31583500
H	1.45787200	-2.70880200	-0.68288700
H	0.02774500	0.36737600	1.53675000
C	-2.31919600	1.26340700	-0.37883700
N	-2.72022200	-1.59393000	2.06575200
C	-3.13345500	1.97331300	-1.41766100
O	-1.99564200	1.69777900	0.69192300
H	-2.61877400	1.95326300	-2.37961400
H	-3.30995200	2.99989900	-1.10526300
H	-4.08886100	1.45974900	-1.54496100
H	0.58655100	1.46207600	-0.94225100
H	3.45230800	2.68834500	1.64520200
H	1.80450100	2.96497700	1.04918800
C	2.67734900	1.14694900	0.42859200
C	2.49655700	2.20996500	1.42466500
N	3.43086000	0.37622300	-0.08314100
O	3.49593700	-0.55131500	-0.87939400
H	2.08653000	1.79921900	2.34979100
H	1.49517700	-0.57604400	-2.38252700

TS-PSb

C	1.40623900	-0.56633900	-0.60431000
C	0.69102100	-1.93932700	-0.70479200
C	-0.77103900	-1.48388100	-0.93483500
C	-1.25556100	-0.83578500	0.34725100
C	-0.66366000	0.39461000	0.41086000
C	0.19061800	0.41908100	-0.84777000
O	-0.57665800	-0.34168100	-1.76138800
O	2.02212300	-0.47513000	0.67912400
C	2.42031700	-0.39368600	-1.65253000
H	0.84215800	-2.51553100	0.20728100
H	1.04633200	-2.51600600	-1.55744700
H	-1.43438200	-2.20365000	-1.40381900
H	0.46642600	1.37751200	-1.27185500
C	2.48552200	0.73312900	1.08191200
N	3.20034800	-0.27194400	-2.48770800
C	3.15954000	0.61845400	2.41459500
O	2.35818600	1.73209900	0.42947500
H	2.55394000	0.02589800	3.10106000
H	3.33769900	1.61131900	2.82124600
H	4.11510300	0.10415100	2.28715100
H	-0.42508800	0.92159100	1.32429600
H	-2.65418100	3.82857000	-0.55503900
H	-1.77279200	3.51865400	0.95621400
C	-2.24830000	1.79534900	-0.17094900
C	-1.88392200	3.21420700	-0.08623900
N	-3.08313300	0.98644700	-0.43951500
O	-3.31658000	-0.21059100	-0.47813200
H	-0.93617400	3.39238700	-0.59733700
Cl	-1.82592700	-1.75993300	1.68864900

TS-PSc

C	1.64649700	-0.24746000	-0.81599600
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C	0.72131900	-1.14294900	-1.68138400
C	-0.57634200	-0.29829400	-1.68010000
C	-1.13939000	-0.32167600	-0.27113900
C	-0.35140000	0.51201200	0.47360300
C	0.68889300	0.98139500	-0.53347600
O	-0.04371800	1.02088800	-1.74301700
O	2.04181700	-0.99221200	0.33473100
C	2.83702200	0.19152100	-1.55533700
H	0.61402700	-2.12922600	-1.23168500
H	1.10193800	-1.24992200	-2.69613700
H	-1.27303100	-0.48161100	-2.49187600
H	1.20082600	1.91947000	-0.35378300
C	2.63812900	-0.32509400	1.35240300
N	3.75510900	0.53487100	-2.15534800
C	3.01542600	-1.27195700	2.44985700
O	2.81445700	0.86178800	1.33986800
H	2.13693400	-1.82896600	2.78092400
H	3.44341600	-0.71688800	3.28118500
H	3.74162900	-1.99658100	2.07605200
H	-0.17227800	0.41334600	1.53537600
H	-1.54406100	4.27757700	1.52159100
H	-0.80111100	3.02945800	2.54342400
C	-1.52954000	2.34335800	0.68262100
C	-0.91815700	3.38382000	1.51777400
N	-2.45028500	2.02396400	-0.00620800
O	-2.89945100	1.12080900	-0.69166900
H	0.06782400	3.64955000	1.13198900
Br	-2.14712800	-1.76332300	0.38518800

TS-MSa

C	-1.22126900	0.77564100	0.15704400
C	-0.36165200	1.57330800	1.17319600

C	1.06286500	1.25040100	0.65713600
C	1.36935100	-0.21281800	0.96209700
C	0.58695500	-0.90864100	0.08274300
C	-0.08975800	0.14832400	-0.75807200
O	0.84444900	1.21255400	-0.75038800
O	-2.01752600	-0.16444600	0.87700800
C	-2.08402900	1.66411000	-0.63264900
H	-0.55618200	1.23072900	2.18861300
H	-0.56189300	2.64234000	1.11090400
H	1.81788000	1.99254000	0.90531900
H	-0.39611800	-0.10513800	-1.76521300
C	-2.70268500	-1.09143000	0.16194700
N	-2.73909000	2.38835500	-1.23881600
C	-3.48692200	-1.98502900	1.07453900
O	-2.65472400	-1.15917900	-1.03380900
H	-2.80377300	-2.54821900	1.71417900
H	-4.08638500	-2.67231600	0.48231100
H	-4.12977300	-1.38772400	1.72300000
H	0.26032900	-1.93402600	0.15636400
H	4.27760900	1.33959300	0.84797500
H	4.56333900	-0.12637300	1.79947400
C	3.38378400	-0.41104300	0.06864700
C	4.47109900	0.26693700	0.78542500
N	3.08477600	-1.06435800	-0.88532600
O	2.14317900	-1.59676400	-1.45322600
H	5.41771300	0.11626600	0.26386700
H	1.68799200	-0.57152900	1.93320800

TS-MSb

C	1.44227000	0.66944600	-0.47381700
C	0.51499800	0.83600600	-1.70604000
C	-0.85983200	0.97036800	-1.01429800

C	-1.23644200	-0.38100600	-0.40542800
C	-0.38647300	-0.54775100	0.65382700
C	0.38596500	0.74745300	0.70568300
O	-0.52319900	1.69366000	0.16103800
O	2.12705600	-0.57465000	-0.59477100
C	2.40804000	1.77100100	-0.36774800
H	0.59623200	-0.02715700	-2.36567100
H	0.75104500	1.73937400	-2.26658400
H	-1.62511100	1.48743200	-1.58772100
H	0.77769200	1.07697100	1.65967900
C	2.84673700	-1.00827200	0.47234700
N	3.14186400	2.65338900	-0.30815600
C	3.52952200	-2.30251300	0.15321400
O	2.89984400	-0.40572900	1.50699800
H	2.80615700	-3.02787400	-0.22295800
H	4.01837100	-2.68608800	1.04552100
H	4.27142800	-2.13904000	-0.63141000
H	-0.05704200	-1.47913600	1.08499400
H	-4.07217600	1.55487700	-0.65803800
H	-4.36454700	-0.15818300	-1.01790100
C	-3.12089300	0.19179000	0.64543600
C	-4.24454500	0.57153800	-0.21573300
N	-2.71435000	0.04934000	1.75774700
O	-1.71318800	-0.24466200	2.39815100
H	-5.16669100	0.60623200	0.36669600
Cl	-1.81930300	-1.68963700	-1.41233700

TS-MSc

C	-1.71429100	-0.45190300	-0.69141800
C	-0.71124400	-0.21468300	-1.85038400
C	0.57878500	-0.80464200	-1.23907400
C	1.05116700	0.10758400	-0.10433100

C	0.13677100	-0.06995800	0.89949200
C	-0.77518800	-1.15306400	0.37528900
O	0.06804900	-1.89975800	-0.49059300
O	-2.24720600	0.80976000	-0.29706400
C	-2.79936100	-1.35819900	-1.08961000
H	-0.64399200	0.84691900	-2.08488000
H	-0.99607600	-0.76278000	-2.74730700
H	1.32728800	-1.13441800	-1.95512400
H	-1.27792000	-1.79317400	1.08931600
C	-2.99808100	0.85619100	0.83361300
N	-3.62764600	-2.07835900	-1.43016900
C	-3.51301500	2.24357000	1.06386900
O	-3.19821600	-0.10591500	1.51963600
H	-2.69559600	2.96479400	1.01812500
H	-4.00701500	2.29324500	2.03129700
H	-4.22423800	2.50100200	0.27594400
Br	1.91231400	1.76334900	-0.46737800
H	-0.12694500	0.63074100	1.67501000
H	3.64161100	-2.01445500	-1.03570700
H	4.14539200	-0.33953500	-0.73026900
C	2.76402300	-1.11447100	0.65894900
C	3.89375700	-1.29029000	-0.25822800
N	2.27947800	-1.38779500	1.71403600
O	1.26702700	-1.24102100	2.38774500
H	4.76649900	-1.65179300	0.28794900

TS-MAa

C	-0.90980200	-0.66388300	-0.38024000
C	0.26435700	-1.33224700	-1.14581000
C	1.04901900	-1.96412400	0.02597300
C	1.73403300	-0.89366100	0.88369700
C	0.70728900	-0.32279100	1.58596700

C	-0.54147000	-1.04747900	1.10751100
O	-0.04392900	-2.36305700	0.86819200
O	-0.96098400	0.70846100	-0.73134200
C	-2.19428400	-1.29872000	-0.72253800
H	0.80510700	-0.58409800	-1.72178100
H	-0.09216900	-2.10898700	-1.82057100
H	1.65632400	-2.82591300	-0.23878200
H	-1.38547700	-1.06264100	1.78612500
C	-1.74556300	1.52376500	0.01917400
N	-3.18317800	-1.80833200	-1.01105400
C	-1.69983800	2.92674100	-0.49931300
O	-2.37606300	1.12973000	0.96013000
H	-2.46558900	3.52121800	-0.00593400
H	-1.84608000	2.94089500	-1.58017600
H	-0.71389000	3.34014500	-0.28140500
H	3.29783400	-0.52437100	-1.91381100
H	3.96134500	1.11761800	-1.82772000
C	2.51766600	0.67516700	-0.35194600
C	3.62098500	0.26734100	-1.23503900
N	1.89428400	1.61684100	0.05036200
O	1.01009000	1.92327300	0.83919100
H	4.45960700	-0.10915900	-0.64578700
H	0.75414500	0.23992800	2.50252600
H	2.74383200	-1.01210100	1.25816300

TS-MAb

C	1.20140600	-0.75745500	0.42128900
C	0.06302800	-1.09713500	1.42205800
C	-1.02092600	-1.62377600	0.45743900
C	-1.60331500	-0.49382800	-0.40485100
C	-0.62917800	-0.22008500	-1.32528800
C	0.51444600	-1.15399300	-0.94006900

O	-0.19564800	-2.31152600	-0.49382700
O	1.58822000	0.59279900	0.61026900
C	2.36744200	-1.63270000	0.63227500
H	-0.20228500	-0.21500800	1.99963600
H	0.35923200	-1.88992100	2.10693900
H	-1.75078300	-2.29837200	0.89622900
H	1.20738600	-1.40012700	-1.73526100
C	2.40887600	1.14554400	-0.32244400
N	3.26299600	-2.32609800	0.82604000
C	2.73467700	2.56414900	0.02404800
O	2.79367600	0.53953400	-1.28237100
H	3.62514800	2.87378300	-0.51904900
H	2.88039800	2.68255800	1.09754100
H	1.89308800	3.18936600	-0.28019900
H	-2.36052400	0.56575200	2.61657900
H	-2.50123400	2.32751600	2.46856000
C	-1.69156000	1.37147300	0.77794800
C	-2.59936300	1.38209700	1.93309700
N	-0.98660000	2.03734200	0.07839000
O	-0.27802300	1.97744600	-0.91762300
H	-3.63251600	1.26369400	1.60405700
H	-0.75879000	0.16405800	-2.32300600
Cl	-3.31958200	-0.50198700	-0.80280200

TS-MAc

C	1.60358700	-0.78214800	0.42524200
C	0.52671900	-1.01252300	1.52004900
C	-0.65910100	-1.50213700	0.66107900
C	-1.24063600	-0.36411600	-0.19367500
C	-0.32223400	-0.18010900	-1.19218400
C	0.78914300	-1.17389400	-0.86439200
O	0.04701400	-2.26922500	-0.32515200

O	2.09104700	0.54352200	0.53710100
C	2.72240800	-1.72829800	0.57856500
H	0.36140400	-0.09382400	2.07693600
H	0.82516100	-1.79646700	2.21406200
H	-1.38674500	-2.11842900	1.18116300
H	1.40008600	-1.48727800	-1.70211900
C	2.86605500	1.01596100	-0.47511100
N	3.58303000	-2.47484900	0.72815100
C	3.29840700	2.42263000	-0.20484100
O	3.13730700	0.35920900	-1.44042900
H	4.18133400	2.65138600	-0.79825100
H	3.49809700	2.57617800	0.85526700
H	2.48502000	3.08752400	-0.50182000
H	-1.64424000	0.87642900	2.87132900
H	-1.77330400	2.62689300	2.61741000
C	-1.12943000	1.54501000	0.93064700
C	-1.93081500	1.65033200	2.15728100
N	-0.43241600	2.13747700	0.16081500
O	0.19327800	2.00013400	-0.88247000
H	-2.99025800	1.53032700	1.92815600
H	-0.49787200	0.18595700	-2.18961700
Br	-3.12590800	-0.28829900	-0.51267500

TS-PAa

C	-1.06245900	-0.19720300	0.18723800
C	-0.85782400	-0.83935200	-1.21398200
C	-0.30762700	-2.22775900	-0.80592900
C	1.13724800	-2.11128600	-0.34576100
C	1.07244000	-1.46776400	0.86070300
C	-0.43206800	-1.30213700	1.10502400
O	-0.98140300	-2.44049600	0.45054300
O	-0.43226600	1.05678300	0.40902600

C	-2.48985300	-0.08382900	0.53334300
H	-0.15795400	-0.27027900	-1.81966900
H	-1.80241700	-0.92706200	-1.74648100
H	-0.53092300	-3.03562600	-1.49666200
H	-0.75202700	-1.25230900	2.14272700
C	-0.76236500	2.08477300	-0.41516400
N	-3.59342700	-0.01155700	0.84558700
C	0.07647900	3.29022200	-0.11478300
O	-1.59728400	1.99251300	-1.26800900
H	0.17252100	3.44497000	0.96001000
H	-0.36414600	4.16619600	-0.58530700
H	1.07724900	3.13226500	-0.52619200
C	2.45431300	1.19890900	1.66417300
C	2.20808600	0.37518800	0.47495000
O	2.16131000	-0.50531500	-1.64038100
N	2.40467900	0.25100700	-0.69845200
H	3.09303900	0.66615400	2.37147900
H	1.50652600	1.42744600	2.15224800
H	2.94552100	2.13225300	1.38365900
H	1.75935700	-1.61117900	1.68455000
H	1.95340400	-2.69543600	-0.73861000

TS-PAb

C	-0.99142800	-0.93374000	0.19843900
C	-0.23572400	-1.24494700	-1.12517400
C	1.14622700	-1.65213500	-0.56799500
C	1.90379000	-0.42845300	-0.05941000
C	1.26124200	-0.03769000	1.08170400
C	0.16819400	-1.10410600	1.23676000
O	0.77939400	-2.26644600	0.67994100
O	-1.56429600	0.35910700	0.31464800
C	-2.01864000	-1.94744600	0.49280200

H	-0.19473100	-0.38134100	-1.78155200
H	-0.69825400	-2.07617500	-1.65301800
H	1.72146500	-2.33610200	-1.18473600
H	-0.16614900	-1.28640200	2.25461600
C	-2.48719600	0.72924400	-0.61289100
N	-2.80269500	-2.74151200	0.76669100
C	-2.89494700	2.15561600	-0.40218400
O	-2.87412000	-0.00757900	-1.47282800
H	-3.09007500	2.35171600	0.65269400
H	-3.77897100	2.37453100	-0.99645400
H	-2.07746600	2.80758900	-0.72169600
C	0.05884800	2.74096900	1.79352200
C	0.59382700	2.00771000	0.64246700
O	1.26070900	1.33433100	-1.44463800
N	0.83598200	2.02844200	-0.52646200
H	0.82041500	2.85043700	2.56766200
H	-0.79010200	2.19673800	2.21000300
H	-0.27176100	3.73439200	1.48528000
H	1.75280000	0.37951600	1.95031700
Cl	3.57065700	-0.15816700	-0.42058400

TS-PAc

C	-1.41907900	-0.94587400	0.18929900
C	-0.59984600	-1.23637700	-1.10067000
C	0.76430400	-1.62024500	-0.48433800
C	1.47830900	-0.38176000	0.05475800
C	0.77626000	-0.00476200	1.16625200
C	-0.30178900	-1.09328500	1.27644300
O	0.35521600	-2.24197900	0.74662300
O	-2.02769300	0.33239000	0.28310500
C	-2.43472400	-1.98348200	0.43752300
H	-0.54552600	-0.36838000	-1.75053300

H	-1.02316900	-2.07274900	-1.65269700
H	1.37379100	-2.29636000	-1.07607600
H	-0.67605800	-1.28239100	2.27912700
C	-2.91763000	0.68377800	-0.68298700
N	-3.21232400	-2.79519400	0.67577900
C	-3.36929900	2.09898300	-0.48670200
O	-3.24785800	-0.05832900	-1.56179100
H	-3.60319700	2.29099300	0.56093400
H	-4.23847200	2.29498900	-1.11015200
H	-2.55907200	2.77173300	-0.78093100
C	-0.55582900	2.72068600	1.82294900
C	0.06744000	2.01313200	0.69986200
O	0.86018700	1.38299100	-1.35679300
N	0.36599000	2.05219900	-0.45588300
H	0.16657500	2.88218900	2.62491000
H	-1.38568200	2.12717800	2.20933300
H	-0.93561900	3.68890300	1.49215200
H	1.21615800	0.42626300	2.05576100
Br	3.30534600	-0.05962200	-0.24670300

Products

3a

C	-1.10722800	-0.80998700	-0.01782500
C	-0.46702000	-1.92415600	-0.89209200
C	1.01032700	-1.81216800	-0.48367000
C	1.61612700	-0.56137600	-1.13022900
C	1.00351300	0.55469800	-0.26509200
C	0.15628200	-0.26688000	0.72962800
O	0.91417300	-1.44588800	0.89478500
O	-1.76587300	0.11606200	-0.88032800
C	-2.07000000	-1.36357000	0.94528100

H	-0.65930200	-1.72841400	-1.94689200
H	-0.86406700	-2.90575300	-0.64029800
H	1.60326500	-2.71619200	-0.58991700
H	-0.04824000	0.19768900	1.68773300
C	-2.24220400	1.26386200	-0.32811000
N	-2.81234900	-1.82956000	1.68821600
C	-2.99409800	2.06586700	-1.34464300
O	-2.06568800	1.55042200	0.82214700
H	-2.43716500	2.12673000	-2.28033900
H	-3.18862100	3.06062900	-0.95069700
H	-3.94393600	1.56933000	-1.55684800
H	0.44104000	1.31797700	-0.80168300
H	1.79381900	3.13457400	0.88559800
H	1.68690000	1.99750600	2.22668600
C	2.24946400	1.11648900	0.36289400
C	2.25855800	2.24912900	1.32866000
N	3.31673200	0.53376700	-0.00800000
O	3.02925900	-0.47766500	-0.91691500
H	3.27970700	2.49164100	1.62089400
H	1.42863300	-0.49005900	-2.20207600

3b

C	1.29085400	-0.77507300	-0.28529200
C	0.47121800	-2.02474900	0.14090300
C	-0.90285100	-1.70834200	-0.46221100
C	-1.62928700	-0.59040700	0.30976400
C	-0.78164200	0.64583100	-0.02968200
C	0.19897500	0.03835200	-1.05549700
O	-0.55789000	-1.00059400	-1.65145300
O	1.81453600	-0.15900500	0.88709500
C	2.38987300	-1.13133400	-1.19468100
H	0.48378300	-2.13351700	1.22314400

H	0.86980000	-2.93258600	-0.30789600
H	-1.53475100	-2.56045000	-0.69515000
H	0.58152700	0.71557500	-1.81052600
C	2.40394200	1.05998900	0.75030700
N	3.23550700	-1.44321300	-1.90703900
C	2.97012600	1.51938700	2.05708200
O	2.42930000	1.64982300	-0.29289800
H	2.18598900	1.54646600	2.81624100
H	3.40985800	2.50638600	1.93665100
H	3.72963600	0.81246100	2.39635700
H	-0.29970500	1.11548900	0.82517300
H	-1.26932500	3.54047200	-0.24207800
H	-0.80118400	2.96031400	-1.83819200
C	-1.82985900	1.52449400	-0.64419400
C	-1.59356000	2.92491700	-1.08560500
N	-2.96536800	0.96163700	-0.74527000
O	-2.88837900	-0.35111500	-0.25451500
H	-2.50229600	3.35113300	-1.50852500
Cl	-1.8265640	-0.9154100	2.07410400

3c

C	-1.52080500	-0.39355700	0.75755400
C	-0.50628000	-1.33911300	1.45793000
C	0.66605900	-0.38639900	1.72206800
C	1.42828800	-0.02319300	0.43261800
C	0.40234400	0.84129300	-0.32033900
C	-0.71003300	0.94389800	0.74681500
O	0.00119500	0.85194000	1.96812800
O	-1.83511900	-0.94013400	-0.51966700
C	-2.75023300	-0.23351000	1.54738200
H	-0.27344900	-2.18440000	0.81440000
H	-0.89737000	-1.71297000	2.40227800

H	1.31569600	-0.64245100	2.55380200
H	-1.31405100	1.84377500	0.72211300
C	-2.55005100	-0.16596300	-1.37999300
N	-3.69553700	-0.12656500	2.19142300
C	-2.84261100	-0.91628200	-2.64120000
O	-2.86173800	0.96303700	-1.12448100
H	-1.90607000	-1.19159100	-3.13114300
H	-3.43986100	-0.29518100	-3.30421500
H	-3.37530000	-1.84021700	-2.41030400
H	0.06762700	0.43816000	-1.27352900
H	0.53498900	3.03180300	-2.28551600
H	-0.21210600	3.67485400	-0.82530600
C	1.19211500	2.10638800	-0.48107000
C	0.72538200	3.29620300	-1.24181800
N	2.32632500	2.07067900	0.09247600
O	2.49559200	0.83223600	0.72949700
H	1.47285200	4.08761300	-1.20676700
Br	2.11448700	-1.56724100	-0.57344600

4a

C	-0.51620800	-0.98050800	-0.25807400
C	0.59929100	-1.45598200	-1.22773600
C	1.78602200	-1.58327900	-0.26781000
C	2.37906100	-0.19306600	0.04686900
C	1.32560800	0.37876000	1.01013600
C	0.29745000	-0.78659200	1.06380900
O	1.16169800	-1.90916300	0.98110300
O	-1.15268900	0.16028600	-0.81899500
C	-1.50862300	-2.04928600	-0.04799100
H	0.75381600	-0.71375800	-2.00827100
H	0.35488400	-2.41200500	-1.68645000
H	2.51062200	-2.35101900	-0.52317000

H	-0.30507800	-0.83365800	1.96428400
C	-2.12041100	0.77114300	-0.09348000
N	-2.25802500	-2.91019400	0.08347500
C	-2.73243800	1.89033700	-0.87625500
O	-2.40914800	0.43040400	1.02050900
H	-1.95485100	2.49479500	-1.34495900
H	-3.35110100	2.50009400	-0.22184400
H	-3.35171800	1.47263200	-1.67360400
C	0.21545500	2.78712800	0.92405900
C	1.02808400	1.68530900	0.33367400
O	2.41734400	0.71336900	-1.05834500
N	1.62282000	1.82669800	-0.78424400
H	-0.73124600	2.42305000	1.32658100
H	0.02512600	3.56436300	0.18422100
H	0.76047900	3.23487600	1.76089700
H	1.69428500	0.52967300	2.02607800
H	3.38383400	-0.26751700	0.46424900

4b

C	0.96597700	-1.04985500	0.25079400
C	-0.08638400	-1.54437400	1.28034700
C	-1.35951300	-1.53008700	0.42825200
C	-1.84014500	-0.07274100	0.22837500
C	-0.88596500	0.43735600	-0.85760100
C	0.06329000	-0.78702100	-1.00107500
O	-0.86829600	-1.84909800	-0.87454400
O	1.64895600	0.06498400	0.80580000
C	1.92724600	-2.11767300	-0.07106800
H	-0.11917400	-0.87592100	2.13714800
H	0.12726500	-2.55636400	1.61857100
H	-2.13235200	-2.23231000	0.72295700
H	0.58570400	-0.84763600	-1.94890800

C	2.53309200	0.72485300	0.01690200
N	2.65404500	-2.97862700	-0.29522600
C	3.18151500	1.83805000	0.77660900
O	2.72187900	0.42690100	-1.13017200
H	2.42158200	2.44429200	1.27257800
H	3.77556000	2.44727400	0.09955900
H	3.82635100	1.42000300	1.55277700
C	0.24390100	2.83410400	-0.97014200
C	-0.48279700	1.74754900	-0.25519400
O	-1.64970200	0.77120200	1.32382200
N	-0.91974400	1.91067200	0.93097400
H	1.14883700	2.46018300	-1.45187200
H	0.49918700	3.64068600	-0.28357200
H	-0.39612300	3.23957700	-1.75910800
H	-1.36968000	0.56936800	-1.82536200
Cl	-3.58183900	-0.0250790	-0.26714400

4c

C	1.41544700	-1.05167300	0.24830300
C	0.39236500	-1.54841900	1.30574400
C	-0.90489300	-1.53160500	0.48991400
C	-1.38834400	-0.07122900	0.30711600
C	-0.46703400	0.43665000	-0.80939700
C	0.47796300	-0.78845400	-0.97806700
O	-0.45042000	-1.84987600	-0.82563000
O	2.11208300	0.06320400	0.78578500
C	2.36842200	-2.11807500	-0.10162000
H	0.38496000	-0.88340200	2.16574200
H	0.61422200	-2.56208500	1.63371900
H	-1.66634100	-2.23679800	0.80580400
H	0.97365500	-0.84992400	-1.94011800
C	2.97382600	0.72538900	-0.02544100

N	3.08924000	-2.97816600	-0.34742500
C	3.63779000	1.84064400	0.71773900
O	3.13395200	0.42813900	-1.17704800
H	2.88806300	2.44629500	1.22979100
H	4.21534000	2.44990900	0.02656800
H	4.30059200	1.42506100	1.47996600
C	0.65988800	2.83330600	-0.95767100
C	-0.04308100	1.74646800	-0.21982200
O	-1.15812200	0.77067700	1.39564800
N	-0.43958500	1.90938600	0.98052400
H	1.54929400	2.46051000	-1.46815800
H	0.93607500	3.64024900	-0.27966000
H	-0.00564400	3.23799200	-1.72566400
H	-0.97126800	0.57035900	-1.76596900
Br	-3.30287300	-0.01005300	-0.16813000

5a

C	-1.11256400	0.75644300	0.20279800
C	-0.19757100	1.48552500	1.22726700
C	1.17984600	1.29903900	0.57417800
C	1.65025500	-0.15986700	0.76006800
C	0.73576400	-0.89701800	-0.23540300
C	-0.05521200	0.27166500	-0.84336900
O	0.86954700	1.34404100	-0.81592500
O	-1.82134000	-0.27497100	0.88764000
C	-2.05897800	1.69343400	-0.41964700
H	-0.29511500	1.02475700	2.20982100
H	-0.45017700	2.54145100	1.30669000
H	1.91299200	2.06522900	0.81480100
H	-0.43124700	0.10703100	-1.84652200
C	-2.59457800	-1.10844700	0.13797400
N	-2.77634400	2.46390800	-0.87996600

C	-3.31555700	-2.08557400	1.01414100
O	-2.65568700	-1.03164100	-1.05533500
H	-2.60055100	-2.65814700	1.60805000
H	-3.90869000	-2.75654900	0.39767900
H	-3.96410100	-1.54720300	1.70790200
H	0.12311100	-1.69421200	0.18055400
H	4.30801000	1.14061600	0.70969000
H	4.43165400	-0.30634300	1.71033300
C	2.99117000	-0.44380300	0.14018900
C	4.28688600	0.04700500	0.68527600
N	2.92999400	-1.14462900	-0.91874700
O	1.61185300	-1.47534400	-1.20837300
H	5.11561900	-0.30214600	0.07028300
H	1.59120600	-0.49653500	1.79683700

5b

C	1.34089900	0.70203500	-0.39812200
C	0.36150300	1.01490900	-1.56234800
C	-0.95709300	1.19471600	-0.80170100
C	-1.51092300	-0.15552000	-0.28069100
C	-0.50545200	-0.49709500	0.83337100
C	0.37147200	0.76269800	0.82742900
O	-0.53092800	1.78369700	0.42081900
O	1.93734600	-0.56717500	-0.64630800
C	2.37756700	1.73774500	-0.27895000
H	0.36690500	0.20597700	-2.28961100
H	0.62462000	1.94306800	-2.06621400
H	-1.69414500	1.82642700	-1.29080300
H	0.83091400	1.00598500	1.77823100
C	2.72906200	-1.09132800	0.33083400
N	3.16301100	2.57416400	-0.22179900
C	3.30012500	-2.40381800	-0.10602000

O	2.89652100	-0.54482300	1.38314600
H	2.49328900	-3.12881100	-0.23670100
H	3.99796500	-2.76451300	0.64569500
H	3.80299100	-2.29370000	-1.06775100
H	0.02444700	-1.43747000	0.70661700
H	-4.03952400	1.37610100	-0.48067500
H	-4.41882700	-0.32117000	-0.78447600
C	-2.76934400	-0.00761700	0.53507500
C	-4.09315000	0.38633700	-0.01849200
N	-2.59236600	-0.24069800	1.77279300
O	-1.27525900	-0.57483600	2.03252800
H	-4.83600600	0.41413900	0.77728700
Cl	-1.71979800	-1.39962100	-1.56190300

5c

C	-1.60420400	-0.48446800	-0.64589000
C	-0.54948100	-0.37043000	-1.78066600
C	0.66390900	-1.04404400	-1.12877900
C	1.30221400	-0.15994200	-0.02740200
C	0.22172200	-0.19690100	1.06850200
C	-0.76735100	-1.20433100	0.46158600
O	0.06190500	-2.05121600	-0.32364500
O	-2.05137000	0.82795600	-0.32000400
C	-2.74002300	-1.32406700	-1.05379000
H	-0.40238400	0.67176700	-2.05546400
H	-0.85180100	-0.92870300	-2.66480600
H	1.37720400	-1.48555700	-1.81996500
H	-1.33654700	-1.77939500	1.18246000
C	-2.88122800	0.96132600	0.75226300
N	-3.60194700	-1.99182700	-1.41572400
C	-3.26830500	2.39478300	0.93907400
O	-3.21003500	0.02998400	1.42935300

H	-2.37712900	2.98953200	1.15224400
H	-3.97239700	2.47669600	1.76344700
H	-3.71346600	2.78585800	0.02289800
Br	1.84969600	1.61296700	-0.64002500
H	-0.20860600	0.76346600	1.33883200
H	3.61715200	-1.90812800	-0.72555500
H	4.23154800	-0.30190600	-0.32328800
C	2.43250300	-0.84448300	0.69646200
C	3.74673500	-1.18944200	0.08896100
N	2.15035600	-1.13585500	1.90240500
O	0.86468000	-0.73648000	2.22190500
H	4.39783800	-1.63364800	0.84050600

6a

C	-0.87667300	-0.69947000	-0.39086100
C	0.28929500	-1.31960600	-1.21149300
C	1.22711900	-1.79079400	-0.09217100
C	1.95758200	-0.61226500	0.60252200
C	0.82441700	-0.02049200	1.45716700
C	-0.36677900	-0.93618200	1.06985600
O	0.29731200	-2.18190600	0.92325600
O	-1.05480800	0.64238900	-0.81265200
C	-2.12616400	-1.45338400	-0.59239100
H	0.70522100	-0.56862800	-1.88184900
H	-0.04587200	-2.16954800	-1.80360800
H	1.86087300	-2.63457200	-0.35175000
H	-1.15396100	-1.01037000	1.81059100
C	-1.80595300	1.45437800	-0.02255600
N	-3.08114300	-2.06632000	-0.77310300
C	-1.75305900	2.86043000	-0.52710500
O	-2.39981300	1.05164200	0.93743400
H	-0.73410700	3.23247900	-0.39909000

H	-2.44695000	3.47883200	0.03739300
H	-1.99139500	2.89495300	-1.59120600
H	4.34881300	0.37266200	-0.83219500
H	3.17507000	-0.14006000	-2.04037900
C	2.32025500	0.58988600	-0.21930100
C	3.37518400	0.61085700	-1.27024600
N	1.63907200	1.62884700	0.06378700
O	0.75291100	1.36055000	1.10539000
H	3.43067900	1.59205200	-1.74047300
H	0.98245400	-0.08152600	2.53310500
H	2.80753000	-0.98551000	1.17672900

6b

C	1.20235100	-0.77908500	0.42651200
C	0.08742400	-1.08341400	1.46474700
C	-1.09647100	-1.42487200	0.54717400
C	-1.67193700	-0.15481700	-0.12890700
C	-0.61457400	0.11684900	-1.20972000
C	0.42264100	-1.00038600	-0.91030100
O	-0.44619700	-2.06202300	-0.55144500
O	1.70059200	0.52377300	0.67655100
C	2.29551900	-1.76155400	0.51735500
H	-0.05645200	-0.22298100	2.11571200
H	0.33399700	-1.94816400	2.07811600
H	-1.84251600	-2.08533200	0.97865500
H	1.04191000	-1.28196800	-1.75328900
C	2.46431000	1.09976400	-0.29272200
N	3.12830500	-2.54669200	0.61701400
C	2.77853800	2.51544900	0.06775000
O	2.79874900	0.51072100	-1.28081600
H	1.84648000	3.08487500	0.07707000
H	3.46431300	2.93529400	-0.66426600

H	3.21331900	2.56709000	1.06713400
H	-3.50511200	1.45992600	1.58651600
H	-2.28380700	0.70791400	2.60785700
C	-1.63395100	1.14611200	0.61753200
C	-2.43982500	1.45976100	1.82918200
N	-0.82660200	1.98938200	0.10456800
O	-0.22670700	1.47163400	-1.03463600
H	-2.16622500	2.43854300	2.22059100
H	-0.97864600	-0.00769400	-2.22777800
Cl	-3.32675500	-0.47658800	-0.77566100

6c

C	1.60247100	-0.80253000	0.42840700
C	0.55252300	-1.01596900	1.55349800
C	-0.71459000	-1.30855800	0.73497800
C	-1.26254200	-0.02184700	0.06368500
C	-0.27695800	0.15325400	-1.10283400
C	0.71450300	-1.01446800	-0.84056400
O	-0.18452000	-2.01280800	-0.38638300
O	2.18771800	0.47640900	0.60132900
C	2.64456300	-1.84202500	0.46997100
H	0.50833200	-0.13519900	2.19171500
H	0.79389300	-1.88091200	2.16888000
H	-1.45989500	-1.91320600	1.24212200
H	1.25318100	-1.35534600	-1.71643700
C	2.91147500	0.98075900	-0.43603600
N	3.43833400	-2.67014700	0.53376200
C	3.32278900	2.38729200	-0.14412300
O	3.14448100	0.34599700	-1.42494900
H	2.42633600	3.01158400	-0.13010800
H	4.00596400	2.73657900	-0.91464100
H	3.79234900	2.45310200	0.83830300

H	-2.83837400	1.80312400	1.86247100
H	-1.63124200	0.92935400	2.80039700
C	-1.08547400	1.29226600	0.76337500
C	-1.76428800	1.69103700	2.02730700
N	-0.27137200	2.06984800	0.16377800
O	0.20018700	1.48721200	-1.00416300
H	-1.36200900	2.63699000	2.38739500
H	-0.71483600	0.02127800	-2.09013000
Br	-3.13120500	-0.27071400	-0.48329700