Supplementary Information

Unraveling polar Diels-Alder reactions with conceptual DFT analysis and the distortion/interaction model

Ariel M. Sarotti*

Instituto de Química Rosario (CONICET), Facultad de Ciencias Bioquímicas y Farmacéuticas, Universidad Nacional de Rosario, Suipacha 531, Rosario (2000), Argentina
sarotti@iquir-conicet.gov.ar

List of contents:

Computational methods

All calculations were performed using Gaussian 09.[1] Density functional theory (DFT) calculations were carried out with the B3LYP[2] and M06-2X[3] functionals with the standard 6-31G* basis set.[4] High accuracy CBS calculations were carried out with the CBS-QB3 method.[5] Geometries for all structures were fully optimized and normal coordinate analyses were used to confirm the nature of the stationary points. All transition structures were confirmed to have only one imaginary frequency corresponding to the formation of the expected bonds. Intrinsic Reaction Coordinate (IRC) calculations were performed to determine the connections between stationary points. The electronic structures of TSs and ground states were analyzed in terms of the Wiberg bond indices (WBI) and the natural charges obtained from the Natural Bond Orbital (NBO) program as implemented in Gaussian 09.[6] Reported thermochemical properties include zero-point energies (ZPEs) without scaling and were calculated at 1 atm and 298.15 K. Distortion energies were computed by performing a single point energy calculation using B3LYP/6-31G* on each of the separated, distorted fragments. The global electrophilicity index, ω, which measures the energy stabilization when the system acquires an additional electronic charge ΔN from the environment,[7] has been given by the following expression, $\omega = \mu^2/2\eta$, in terms of the electronic chemical potential μ and the chemical hardness η. Both quantities may be approached in terms of the one-electron energies fo the frontier molecular orbitals HOMO and LUMO, ε_H and ε_L, as $\mu \approx (\varepsilon_H + \varepsilon_L)/2$ and $\eta \approx (\varepsilon_L - \varepsilon_H)$, respectively.[8] The nucleophilicity index, N, was computed as $N = E_{HOMO(diene)} - E_{HOMO(TCE)}$ (eV),[9] where TCE accounts for tetracyanoethylene. The local electrophilic indices, ω_k,[10] were computed according to the following expression: $\omega_k = \omega.P^+_k$, where P^+_k is the electrophilic Parr function of atom k,[11] that was computed using the Mulliken atomic spin density (ASD) computed by single-point UB3LYP/6-31G* level of the anion resulting from adding one electron to the optimized neutral B3LYP/6-31G* geometry. The analysis of ANOVA were carried out using the Historical Data Response Surface Method (RSM) implemented in the software Design-Expert™.

[1] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y. Kitao, O.; Nakai, H. Vreven, T.; Montgomery, J. A., Jr.,; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J. and Fox, D. J. Gaussian 09, Gaussian, Inc., Wallingford CT, 2009.

[2] (a) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789. (b) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 1372-1377. (c) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648-5652.

[3] Zhao, Y.; Truhlar, D.G. *Acc. Chem. Res.* **2008**, *41*, 157.

[4] Hehre, W.J.; Radom, L.; Schleyer, R.v.R.; Pople, J.A. *Ab initio Molecular Orbital Theory*, Wiley: New York, 1986.

[5] (a) Montgomery, J.A.; Frisch, M.J.; Ochterski, J.W.; Petersson, G.A. *J. Chem. Phys.* **2000**, *112*, 6532. (b) Montgomery, J.A.; Frisch, M.J.; Ochterski, J.W.; Petersson, G.A. *J. Chem. Phys.* **1999**, *110*, 2822. (b) Petersson, G.A.; Malick, D.K.; Wilson, W.G.; Ochterski, J.W.; Montgomery, J.A.; Frisch, M.J. *J. Chem. Phys.* **1998**, *109*, 10570.

[6] NBO Version 3.1, Glendening, E. D.; Reed, A. E.; Carpenter, J. E.; Weinhold, F. For some original literature references, see: (a) Reed, A. E.; Weinstock, R. B.; Weinhold, F. *J. Chem. Phys.* **1985**, *83*, 735-746. (b) Reed, A. E.; Curtiss, L. A.; Weinhold, F. *Chem. Rev.* **1988**, *88*, 899-926.

[7] Parr, R.G.; von Szentpaly, L.; Liu, S. *J. Am. Chem. Soc.* **1999**, *121*, 1922-1924.

[8] a) Parr, R.G.; Pearson, R.G. *J. Am. Chem. Soc.* **1983**, *105*, 7512-7516. b) Parr, R.G.; Yang, W. *Density Functional Theory of Atoms and Molecules*; Oxford University Press: New York, 1989.

[9] Domingo, L.R.; Chamorro, E.; Pérez, P. *J. Org. Chem.* **2008**, *73*, 4615-4624.

[10] Domingo, L.R.; Aurell, M.J.; Pérez, P.; Contreras, R. *J. Phys. Chem. A* **2002**, *106*, 6871.

[11] Domingo, L.R.; Pérez, P.; Sáez, J.A. *RSC Adv.* **2013**, *3*, 1486.

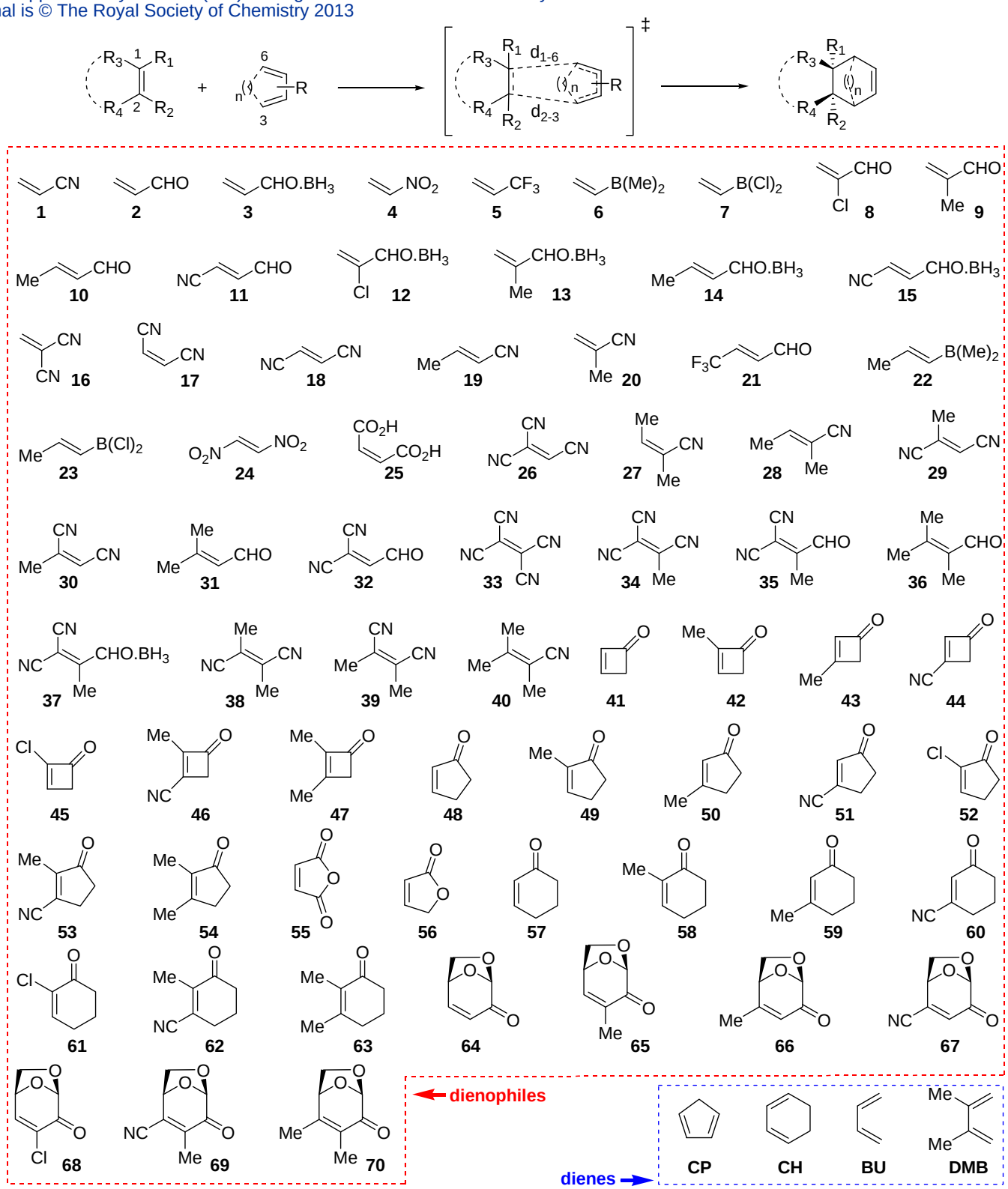


Figure S1. Set of dienophiles and dienes used in this study.

Table S1. Global reactivity indices and FMO energies for all reactants calculated at the B3LYP/6-31G* level.

	HOMO (eV)	LUMO (eV)	ω (eV)	μ (au)	η (au)	N (eV)
CP	-5.76	-0.27	0.83	-0.1107	0.2016	3.37
CH	-5.59	-0.47	0.89	-0.1113	0.1884	3.53
BU (*s-cis*)	-6.29	-0.62	1.05	-0.1270	0.2083	2.83
DMB(*s-cis*)	-6.14	-0.10	0.81	-0.1147	0.2221	2.98
1	-7.87	-1.53	1.74	-0.1728	0.2329	1.25
2	-7.00	-1.77	1.84	-0.1611	0.1921	2.12
3	-7.20	-3.07	3.20	-0.1887	0.1516	1.92
4	-8.05	-2.60	2.61	-0.1958	0.2002	1.07
5	-8.13	-0.55	1.24	-0.1594	0.2784	0.99
6	-7.46	-1.20	1.50	-0.1590	0.2300	1.66
7	-8.08	-2.21	2.25	-0.1891	0.2159	1.04
8	-7.52	-2.17	2.19	-0.1779	0.1967	1.60
9	-6.95	-1.59	1.70	-0.1569	0.1970	2.17
10	-6.79	-1.59	1.69	-0.1539	0.1910	2.33
11	-7.73	-3.10	3.17	-0.1990	0.1701	1.39
12	-7.42	-3.37	3.59	-0.1982	0.1489	1.70
13	-7.15	-2.88	2.95	-0.1844	0.1567	1.97
14	-6.98	-2.77	2.82	-0.1791	0.1547	2.14
15	-7.61	-4.14	4.98	-0.2160	0.1275	1.51
16	-8.47	-2.82	2.82	-0.2074	0.2076	0.65
17	-8.32	-2.99	3.01	-0.2078	0.1956	0.80
18	-8.36	-3.06	3.08	-0.2099	0.1946	0.76
19	-7.42	-1.22	1.50	-0.1586	0.2279	1.70
20	-7.54	-1.23	1.52	-0.1611	0.2320	1.58
21	-7.51	-2.48	2.48	-0.1835	0.1847	1.61
22	-7.04	-1.00	1.34	-0.1477	0.2222	2.08
23	-7.64	-1.96	2.03	-0.1764	0.2085	1.48
24	-8.82	-4.16	4.52	-0.2385	0.1711	0.30
25	-7.47	-2.84	2.87	-0.1893	0.1701	1.65
26	-8.79	-4.07	4.39	-0.2364	0.1733	0.33
27	-7.12	-0.97	1.33	-0.1485	0.2260	2.00
28	-7.10	-0.92	1.30	-0.1475	0.2272	2.02
29	-8.02	-2.73	2.73	-0.1976	0.1942	1.10
30	-7.97	-2.66	2.66	-0.1953	0.1952	1.15
31	-6.61	-1.42	1.55	-0.1475	0.1906	2.51
32	-8.22	-4.05	4.51	-0.2253	0.1532	0.90
33	-9.12	-4.96	5.95	-0.2587	0.1531	0.00
34	-8.43	-3.71	3.90	-0.2231	0.1735	0.69
35	-8.13	-3.76	4.05	-0.2185	0.1604	0.99
36	-6.60	-1.35	1.51	-0.1462	0.1931	2.52
37	-7.85	-4.67	6.15	-0.2300	0.1170	1.27
38	-7.69	-2.45	2.45	-0.1864	0.1927	1.43
39	-7.64	-2.32	2.33	-0.1830	0.1954	1.48
40	-6.84	-0.82	1.22	-0.1407	0.2213	2.28
41	-6.77	-1.35	1.52	-0.1493	0.1990	2.35
42	-6.60	-1.13	1.36	-0.1420	0.2012	2.52
43	-6.53	-1.08	1.33	-0.1398	0.2003	2.59
44	-7.51	-2.89	2.92	-0.1910	0.1700	1.61
45	-7.20	-1.76	1.85	-0.1646	0.1997	1.92
46	-7.33	-2.61	2.61	-0.1825	0.1734	1.79
47	-6.40	-0.89	1.21	-0.1339	0.2024	2.72
48	-6.46	-1.20	1.40	-0.1409	0.1933	2.66
49	-6.41	-1.04	1.30	-0.1370	0.1973	2.71
50	-6.31	-1.04	1.28	-0.1351	0.1939	2.81
51	-7.19	-2.62	2.63	-0.1801	0.1680	1.93
52	-6.92	-1.58	1.69	-0.1562	0.1963	2.20
53	-7.12	-2.39	2.39	-0.1747	0.1738	2.00
54	-6.29	-0.90	1.20	-0.1321	0.1979	2.83
55	-8.14	-3.19	3.24	-0.2082	0.1822	0.98
56	-7.39	-1.30	1.55	-0.1597	0.2239	1.73
57	-6.43	-1.31	1.46	-0.1423	0.1880	2.69
58	-6.42	-1.20	1.39	-0.1399	0.1918	2.70
59	-6.30	-1.16	1.35	-0.1370	0.1886	2.82
60	-7.12	-2.60	2.61	-0.1786	0.1661	2.00
61	-6.91	-1.70	1.78	-0.1582	0.1917	2.21
62	-7.08	-2.41	2.42	-0.1745	0.1715	2.04
63	-6.32	-1.10	1.32	-0.1364	0.1917	2.80
64	-6.47	-1.80	1.83	-0.1519	0.1718	2.65
65	-6.42	-1.65	1.70	-0.1482	0.1754	2.70
66	-6.35	-1.59	1.66	-0.1459	0.1748	2.77
67	-7.10	-3.03	3.15	-0.1861	0.1499	2.02
68	-6.86	-2.13	2.14	-0.1653	0.1739	2.26
69	-7.03	-2.81	2.87	-0.1808	0.1550	2.09
70	-6.33	-1.51	1.60	-0.1441	0.1771	2.79

Table S2. Local reactivity indices for all reactants calculated at the B3LYP/6-31G* level.

	P^{+}_{C1}	P^{+}_{C2}	ω_{C1}	ω_{C2}	$\Delta\omega_k$
1	0.630	0.198	1.10	0.35	0.75
2	0.524	0.040	0.96	0.07	0.89
3	0.543	-0.080	1.73	-0.25	1.99
4	0.442	0.006	1.15	0.02	1.13
5	0.637	0.380	0.79	0.47	0.32
6	0.501	-0.058	0.75	-0.09	0.84
7	0.511	-0.112	1.15	-0.25	1.40
8	0.537	0.044	1.17	0.10	1.08
9	0.514	0.034	0.87	0.06	0.82
10	0.507	0.006	0.86	0.01	0.85
11	0.304	0.203	0.96	0.64	0.32
12	0.550	-0.067	1.97	-0.24	2.21
13	0.527	-0.079	1.55	-0.23	1.79
14	0.522	-0.095	1.47	-0.27	1.74
15	0.366	0.059	1.82	0.29	1.53
16	0.740	0.097	2.09	0.27	1.81
17	0.348	0.348	1.04	1.04	0.00
18	0.334	0.334	1.03	1.03	0.00
19	0.594	0.186	0.89	0.28	0.61
20	0.620	0.201	0.94	0.31	0.64
21	0.404	0.131	1.00	0.32	0.68
22	0.478	-0.069	0.64	-0.09	0.73
23	0.492	-0.125	1.00	-0.25	1.25
24	0.179	0.179	0.81	0.81	0.00
25	0.404	0.132	1.16	0.38	0.78
26	0.463	0.215	2.03	0.94	1.09
27	0.595	0.181	0.79	0.24	0.55
28	0.585	0.188	0.76	0.24	0.52
29	0.340	0.311	0.93	0.85	0.08
30	0.352	0.334	0.94	0.89	0.05
31	0.452	0.028	0.70	0.04	0.66
32	0.367	0.196	1.66	0.88	0.77
33	0.322	0.322	1.91	1.91	0.00
34	0.473	0.190	1.85	0.74	1.10
35	0.360	0.179	1.46	0.73	0.73
36	0.461	0.013	0.69	0.02	0.67
37	0.244	0.202	1.50	1.24	0.26
38	0.317	0.317	0.78	0.78	0.00
39	0.339	0.339	0.79	0.79	0.00
40	0.535	0.183	0.65	0.22	0.43
41	0.633	0.049	0.96	0.07	0.89
42	0.616	0.037	0.84	0.05	0.79
43	0.577	0.046	0.77	0.06	0.70
44	0.356	0.205	1.04	0.60	0.44
45	0.626	0.040	1.16	0.07	1.08
46	0.335	0.196	0.87	0.51	0.36
47	0.561	0.035	0.68	0.04	0.63
48	0.552	0.028	0.77	0.04	0.73
49	0.533	0.017	0.69	0.02	0.67
50	0.497	0.029	0.64	0.04	0.60
51	0.326	0.191	0.86	0.50	0.35
52	0.558	0.028	0.94	0.05	0.89
53	0.305	0.181	0.73	0.43	0.30
54	0.482	0.017	0.58	0.02	0.56
55	0.258	0.258	0.84	0.84	0.00
56	0.550	0.159	0.85	0.25	0.61
57	0.495	0.031	0.72	0.05	0.68
58	0.484	0.024	0.67	0.03	0.64
59	0.458	0.030	0.62	0.04	0.58
60	0.300	0.198	0.78	0.52	0.27
61	0.510	0.035	0.91	0.06	0.84
62	0.285	0.190	0.69	0.46	0.23
63	0.461	0.014	0.61	0.02	0.59
64	0.463	0.069	0.85	0.13	0.72
65	0.447	0.059	0.76	0.10	0.66
66	0.442	0.055	0.73	0.09	0.64
67	0.276	0.234	0.87	0.74	0.13
68	0.474	0.070	1.01	0.15	0.86
69	0.256	0.226	0.74	0.65	0.09
70	0.438	0.039	0.70	0.06	0.64

Table S3. C1 and C2 LUMO *pz* coefficients of compounds **1-70** computed at the B3LYP/6-31G* level.*

	pz_{C1}	pz_{C2}	Δ_{Cpz}
1	0.41	0.32	0.09
2	0.38	0.22	0.16
3	0.37	0.16	0.21
4	0.32	0.17	0.14
5	0.42	0.39	0.03
6	0.37	0.20	0.17
7	0.36	0.16	0.20
8	0.37	0.22	0.15
9	0.36	0.21	0.16
10	0.38	0.18	0.19
11	0.34	0.28	0.06
12	0.37	0.17	0.20
13	0.37	0.16	0.21
14	0.39	0.15	0.24
15	0.34	0.22	0.12
16	0.43	0.30	0.13
17	0.35	0.35	0.00
18	0.35	0.35	0.00
19	0.43	0.30	0.13
20	0.40	0.33	0.07
21	0.38	0.25	0.13
22	0.38	0.18	0.20
23	0.37	0.14	0.23
24	0.27	0.27	0.00
25	0.35	0.27	0.08
26	0.37	0.33	0.05
27	0.42	0.31	0.11
28	0.42	0.32	0.10
29	0.36	0.33	0.03
30	0.36	0.34	0.03
31	0.39	0.19	0.21
32	0.32	0.32	0.00
33	0.34	0.34	0.00
34	0.39	0.31	0.08
35	0.32	0.30	0.02
36	0.38	0.18	0.20
37	0.31	0.26	0.04
38	0.34	0.34	0.00
39	0.35	0.35	0.00
40	0.43	0.30	0.12
41	0.42	0.23	0.18
42	0.40	0.23	0.17
43	0.43	0.22	0.21
44	0.35	0.29	0.06
45	0.40	0.24	0.17
46	0.33	0.28	0.05
47	0.41	0.21	0.20
48	0.40	0.21	0.18
49	0.39	0.21	0.17
50	0.42	0.20	0.21
51	0.35	0.28	0.07
52	0.39	0.22	0.17
53	0.33	0.27	0.05
54	0.40	0.20	0.20
55	0.30	0.30	0.00
56	0.41	0.29	0.12
57	0.38	0.21	0.17
58	0.36	0.20	0.16
59	0.39	0.20	0.19
60	0.34	0.27	0.07
61	0.37	0.22	0.16
62	0.32	0.27	0.05
63	0.38	0.19	0.19
64	0.34	0.21	0.13
65	0.34	0.21	0.13
66	0.36	0.20	0.16
67	0.31	0.28	0.04
68	0.36	0.23	0.12
69	0.30	0.28	0.02
70	0.36	0.20	0.16

* Here, C1 is arbitarily defined as the atom with highest $2p_z$ value.

Table S4. C1-C6 and C2-C3 bond forming distances (see Figure S1), asynchronicity (Δd) and charge transfer for all transition structures computed for the DA reactions between **1-70** and **CP** at the B3LYP/6-31G* level.

	d_{C1C6} (Å)	d_{C2C3} (Å)	Δd (Å)	CT (e)
TS-1+CP	2.07	2.47	0.40	0.15
TS-2+CP	2.07	2.46	0.39	0.15
TS-3+CP	2.01	2.66	0.65	0.26
TS-4+CP	2.05	2.56	0.51	0.20
TS-5+CP	2.20	2.31	0.11	0.11
TS-6+CP	2.07	2.51	0.44	0.13
TS-7+CP	2.03	2.62	0.59	0.21
TS-8+CP	2.00	2.61	0.60	0.19
TS-9+CP	2.02	2.53	0.51	0.14
TS-10+CP	2.09	2.41	0.32	0.14
TS-11+CP	2.20	2.24	0.04	0.23
TS-12+CP	1.98	2.85	0.88	0.30
TS-13+CP	1.97	2.73	0.76	0.25
TS-14+CP	2.00	2.60	0.60	0.26
TS-15+CP	2.06	2.41	0.35	0.32
TS-16+CP	1.99	2.80	0.81	0.28
TS-17+CP	2.23	2.23	0.00	0.24
TS-18+CP	2.22	2.25	0.03	0.25
TS-19+CP	2.10	2.42	0.32	0.14
TS-20+CP	2.05	2.52	0.48	0.14
TS-21+CP	2.15	2.38	0.23	0.20
TS-22+CP	2.07	2.47	0.40	0.13
TS-23+CP	2.03	2.58	0.55	0.20
TS-24+CP	2.25	2.29	0.03	0.28
TS-25+CP	2.05	2.45	0.40	0.24
TS-26+CP	2.00	2.61	0.61	0.36
TS-27+CP	2.06	2.47	0.41	0.13
TS-28+CP	2.08	2.46	0.38	0.13
TS-29+CP	2.17	2.30	0.14	0.23
TS-30+CP	2.19	2.28	0.09	0.23
TS-31+CP	2.13	2.35	0.22	0.13
TS-32+CP	1.96	2.60	0.64	0.34
TS-33+CP	2.20	2.20	0.00	0.43
TS-34+CP	2.00	2.55	0.55	0.36
TS-35+CP	1.97	2.49	0.52	0.33
TS-36+CP	2.06	2.46	0.41	0.12
TS-37+CP	2.08	2.27	0.19	0.37
TS-38+CP	2.20	2.26	0.06	0.22
TS-39+CP	2.23	2.23	0.00	0.22
TS-40+CP	2.10	2.42	0.32	0.13
TS-41+CP	2.10	2.44	0.34	0.13
TS-42+CP	2.07	2.51	0.45	0.12
TS-43+CP	2.13	2.38	0.25	0.13
TS-44+CP	2.18	2.30	0.12	0.22
TS-45+CP	2.02	2.64	0.62	0.18
TS-46+CP	2.23	2.25	0.02	0.21
TS-47+CP	2.10	2.44	0.35	0.12
TS-48+CP	2.07	2.40	0.33	0.12
TS-49+CP	2.03	2.48	0.45	0.11
TS-50+CP	2.10	2.34	0.24	0.12
TS-51+CP	2.14	2.27	0.12	0.21
TS-52+CP	2.00	2.53	0.53	0.17
TS-53+CP	2.20	2.21	0.01	0.20
TS-54+CP	2.06	2.41	0.35	0.11
TS-55+CP	2.22	2.22	0.00	0.23
TS-56+CP	2.11	2.35	0.24	0.13
TS-57+CP	2.08	2.37	0.28	0.12
TS-58+CP	2.04	2.43	0.39	0.12
TS-59+CP	2.13	2.31	0.18	0.12
TS-60+CP	2.11	2.29	0.18	0.21
TS-61+CP	2.01	2.50	0.48	0.17
TS-62+CP	2.15	2.26	0.12	0.20
TS-63+CP	2.09	2.37	0.28	0.11
TS-64+CP	2.08	2.43	0.36	0.17
TS-65+CP	2.03	2.50	0.47	0.16
TS-66+CP	2.10	2.36	0.27	0.17
TS-67+CP	2.15	2.29	0.15	0.25
TS-68+CP	2.00	2.59	0.59	0.22
TS-69+CP	2.18	2.24	0.06	0.24
TS-70+CP	2.06	2.44	0.38	0.16

Table S5. C1-C6 and C2-C3 bond forming distances (see Figure S1), asynchronicity (Δd) and charge transfer for all transition structures computed for the DA reactions between **1-70** and **CH** at the B3LYP/6-31G* level.

	d_{C1C6} (Å)	d_{C2C3} (Å)	Δd (Å)	CT (e)
TS-1+CH	2.11	2.50	0.39	0.14
TS-2+CH	2.10	2.52	0.43	0.14
TS-3+CH	2.01	2.78	0.77	0.28
TS-4+CH	2.08	2.56	0.48	0.20
TS-5+CH	2.23	2.35	0.12	0.10
TS-6+CH	2.09	2.60	0.51	0.13
TS-7+CH	2.05	2.70	0.66	0.21
TS-8+CH	1.99	2.80	0.81	0.20
TS-9+CH	2.04	2.64	0.60	0.14
TS-10+CH	2.02	2.67	0.65	0.17
TS-11+CH	2.24	2.29	0.05	0.23
TS-12+CH	1.97	3.10	1.13	0.33
TS-13+CH	1.98	2.91	0.94	0.27
TS-14+CH	1.99	2.76	0.77	0.29
TS-15+CH	2.10	2.49	0.40	0.34
TS-16+CH	1.95	3.07	1.12	0.30
TS-17+CH	2.27	2.27	0.00	0.24
TS-18+CH	2.21	2.35	0.14	0.25
TS-19+CH	2.16	2.42	0.26	0.14
TS-20+CH	2.05	2.61	0.55	0.14
TS-21+CH	2.22	2.38	0.16	0.20
TS-22+CH	2.09	2.58	0.49	0.13
TS-23+CH	2.04	2.68	0.64	0.21
TS-24+CH	2.26	2.37	0.11	0.30
TS-25+CH	2.09	2.46	0.37	0.24
TS-26+CH	1.98	2.83	0.85	0.39
TS-27+CH	2.07	2.56	0.50	0.13
TS-28+CH	2.10	2.52	0.42	0.13
TS-29+CH	2.18	2.39	0.21	0.23
TS-30+CH	2.19	2.36	0.17	0.23
TS-31+CH	2.10	2.49	0.39	0.15
TS-32+CH	1.96	2.75	0.79	0.36
TS-33+CH	2.26	2.26	0.00	0.46
TS-34+CH	2.00	2.71	0.71	0.39
TS-35+CH	2.03	2.54	0.52	0.34
TS-36+CH	2.07	2.56	0.49	0.13
TS-37+CH	2.23	2.24	0.01	0.40
TS-38+CH	2.25	2.30	0.05	0.23
TS-39+CH	2.28	2.28	0.00	0.23
TS-40+CH	2.13	2.47	0.34	0.13
TS-41+CH	2.14	2.47	0.34	0.12
TS-42+CH	2.07	2.62	0.55	0.12
TS-43+CH	2.18	2.41	0.23	0.12
TS-44+CH	2.21	2.37	0.15	0.22
TS-45+CH	2.00	2.86	0.86	0.18
TS-46+CH	2.25	2.32	0.07	0.21
TS-47+CH	2.10	2.55	0.45	0.12
TS-48+CH	2.11	2.43	0.32	0.12
TS-49+CH	2.04	2.57	0.53	0.11
TS-50+CH	2.18	2.35	0.17	0.11
TS-51+CH	2.17	2.36	0.19	0.21
TS-52+CH	1.98	2.74	0.76	0.17
TS-53+CH	2.22	2.29	0.07	0.20
TS-54+CH	2.08	2.52	0.44	0.11
TS-55+CH	2.27	2.27	0.00	0.23
TS-56+CH	2.16	2.38	0.21	0.13
TS-57+CH	2.11	2.43	0.31	0.12
TS-58+CH	2.04	2.57	0.52	0.12
TS-59+CH	2.20	2.32	0.12	0.12
TS-60+CH	2.15	2.37	0.21	0.21
TS-61+CH	1.98	2.73	0.76	0.18
TS-62+CH	2.24	2.27	0.03	0.21
TS-63+CH	2.08	2.53	0.45	0.12
TS-64+CH	2.11	2.47	0.36	0.16
TS-65+CH	2.03	2.63	0.59	0.16
TS-66+CH	2.18	2.36	0.18	0.16
TS-67+CH	2.16	2.38	0.22	0.26
TS-68+CH	1.94	2.88	0.94	0.23
TS-69+CH	2.23	2.29	0.06	0.25
TS-70+CH	2.05	2.58	0.53	0.17

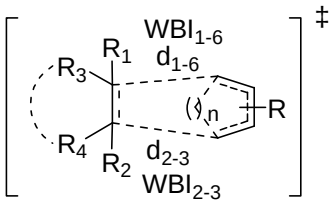
Table S6. C1-C6 and C2-C3 bond forming distances (see Figure S1), asynchronicity (Δd) and charge transfer for all transition structures computed for the DA reactions between **1-70** and **BU** at the B3LYP/6-31G* level.

	d_{C1C6} (Å)	d_{C2C3} (Å)	Δd (Å)	CT (e)
TS-1+BU	2.11	2.49	0.38	0.12
TS-2+BU	2.09	2.52	0.43	0.12
TS-3+BU	2.02	2.75	0.73	0.23
TS-4+BU	2.10	2.52	0.42	0.16
TS-5+BU	2.23	2.34	0.11	0.08
TS-6+BU	2.10	2.59	0.49	0.11
TS-7+BU	2.07	2.68	0.61	0.17
TS-8+BU	2.00	2.74	0.74	0.16
TS-9+BU	2.04	2.64	0.60	0.10
TS-10+BU	2.13	2.44	0.31	0.10
TS-11+BU	2.23	2.28	0.06	0.19
TS-12+BU	2.02	2.91	0.89	0.26
TS-13+BU	2.02	2.83	0.81	0.22
TS-14+BU	2.01	2.70	0.69	0.23
TS-15+BU	2.10	2.47	0.37	0.29
TS-16+BU	1.98	2.86	0.88	0.24
TS-17+BU	2.26	2.26	0.00	0.21
TS-18+BU	2.21	2.33	0.12	0.21
TS-19+BU	2.14	2.41	0.26	0.10
TS-20+BU	2.06	2.57	0.52	0.11
TS-21+BU	2.20	2.38	0.17	0.16
TS-22+BU	2.10	2.56	0.47	0.10
TS-23+BU	2.06	2.63	0.58	0.17
TS-24+BU	2.25	2.35	0.10	0.24
TS-25+BU	2.09	2.45	0.36	0.20
TS-26+BU	2.00	2.67	0.67	0.32
TS-27+BU	2.07	2.53	0.46	0.09
TS-28+BU	2.09	2.49	0.39	0.10
TS-29+BU	2.19	2.35	0.16	0.19
TS-30+BU	2.20	2.33	0.13	0.20
TS-31+BU	2.15	2.41	0.26	0.10
TS-32+BU	2.00	2.62	0.62	0.29
TS-33+BU	2.25	2.25	0.00	0.39
TS-34+BU	2.03	2.57	0.54	0.32
TS-35+BU	2.05	2.46	0.42	0.28
TS-36+BU	2.06	2.56	0.51	0.09
TS-37+BU	2.17	2.28	0.11	0.34
TS-38+BU	2.25	2.27	0.01	0.18
TS-39+BU	2.26	2.26	0.00	0.19
TS-40+BU	2.10	2.48	0.38	0.09
TS-41+BU	2.13	2.50	0.37	0.10
TS-42+BU	2.06	2.63	0.57	0.09
TS-43+BU	2.18	2.40	0.22	0.10
TS-44+BU	2.23	2.33	0.10	0.18
TS-45+BU	2.02	2.75	0.73	0.14
TS-46+BU	2.22	2.34	0.12	0.17
TS-47+BU	2.09	2.55	0.46	0.09
TS-48+BU	2.11	2.43	0.33	0.09
TS-49+BU	2.02	2.58	0.56	0.08
TS-50+BU	2.16	2.36	0.20	0.09
TS-51+BU	2.18	2.32	0.15	0.17
TS-52+BU	1.98	2.66	0.67	0.14
TS-53+BU	2.19	2.30	0.11	0.16
TS-54+BU	2.05	2.52	0.46	0.08
TS-55+BU	2.27	2.27	0.00	0.20
TS-56+BU	2.15	2.38	0.22	0.10
TS-57+BU	2.09	2.45	0.36	0.10
TS-58+BU	2.01	2.61	0.60	0.09
TS-59+BU	2.16	2.36	0.20	0.09
TS-60+BU	2.17	2.32	0.16	0.17
TS-61+BU	1.95	2.70	0.76	0.14
TS-62+BU	2.16	2.32	0.15	0.16
TS-63+BU	2.02	2.57	0.55	0.09
TS-64+BU	2.10	2.48	0.39	0.14
TS-65+BU	2.02	2.63	0.61	0.13
TS-66+BU	2.15	2.39	0.24	0.13
TS-67+BU	2.19	2.33	0.13	0.22
TS-68+BU	2.00	2.75	0.75	0.19
TS-69+BU	2.18	2.31	0.13	0.21
TS-70+BU	2.02	2.58	0.56	0.14

Table S7. C1-C6 and C2-C3 bond forming distances (Figure S1), asynchronicity (Δd) and charge transfer for all transition structures computed for the DA reactions between **1-70** and **DMB** at the B3LYP/6-31G* level.*

	d_{C1C6} (Å)	d_{C2C3} (Å)	Δd (Å)	CT (e)
TS-1+DMB	2.07	2.52	0.44	0.15
TS-2+DMB	2.07	2.55	0.49	0.14
TS-3+DMB	2.01	2.81	0.81	0.27
TS-4+DMB	2.04	2.64	0.61	0.21
TS-5+DMB	2.21	2.35	0.14	0.10
TS-6+DMB	2.08	2.60	0.52	0.13
TS-7+DMB	2.05	2.71	0.66	0.20
TS-8+DMB	1.99	2.76	0.77	0.19
TS-9+DMB	2.02	2.67	0.66	0.13
TS-10+DMB	2.10	2.47	0.37	0.13
TS-11+DMB	2.24	2.26	0.02	0.22
TS-12+DMB	2.03	2.93	0.90	0.29
TS-13+DMB	2.02	2.86	0.84	0.25
TS-14+DMB	2.00	2.76	0.76	0.28
TS-15+DMB	2.06	2.54	0.48	0.34
TS-16+DMB	1.98	2.89	0.91	0.28
TS-17+DMB	2.25	2.25	0.00	0.24
TS-18+DMB	2.21	2.31	0.11	0.24
TS-19+DMB	2.11	2.43	0.33	0.13
TS-20+DMB	2.04	2.59	0.55	0.14
TS-21+DMB	2.17	2.40	0.23	0.19
TS-22+DMB	2.08	2.57	0.49	0.12
TS-23+DMB	2.04	2.67	0.63	0.20
TS-24+DMB	2.25	2.34	0.09	0.28
TS-25+DMB	2.05	2.51	0.47	0.25
TS-26+DMB	1.99	2.73	0.74	0.37
TS-27+DMB	2.06	2.54	0.48	0.12
TS-28+DMB	2.07	2.51	0.44	0.13
TS-29+DMB	2.17	2.34	0.17	0.22
TS-30+DMB	2.19	2.32	0.13	0.23
TS-31+DMB	2.13	2.42	0.29	0.12
TS-32+DMB	1.97	2.69	0.72	0.35
TS-33+DMB	2.24	2.24	0.00	0.44
TS-34+DMB	1.99	2.65	0.66	0.37
TS-35+DMB	2.00	2.52	0.52	0.33
TS-36+DMB	2.04	2.58	0.53	0.12
TS-37+DMB	2.14	2.31	0.17	0.39
TS-38+DMB	2.23	2.27	0.04	0.21
TS-39+DMB	2.25	2.25	0.00	0.22
TS-40+DMB	2.09	2.48	0.39	0.12
TS-41+DMB	2.10	2.52	0.42	0.13
TS-42+DMB	2.04	2.68	0.64	0.12
TS-43+DMB	2.16	2.41	0.25	0.12
TS-44+DMB	2.20	2.34	0.14	0.21
TS-45+DMB	2.01	2.81	0.79	0.17
TS-46+DMB	2.21	2.34	0.13	0.20
TS-47+DMB	2.07	2.58	0.51	0.12
TS-48+DMB	2.08	2.46	0.37	0.12
TS-49+DMB	2.01	2.60	0.60	0.11
TS-50+DMB	2.14	2.37	0.23	0.11
TS-51+DMB	2.16	2.33	0.18	0.20
TS-52+DMB	1.96	2.70	0.74	0.17
TS-53+DMB	2.19	2.29	0.10	0.19
TS-54+DMB	2.04	2.53	0.50	0.11
TS-55+DMB	2.25	2.25	0.00	0.23
TS-56+DMB	2.13	2.39	0.27	0.13
TS-57+DMB	2.08	2.46	0.38	0.12
TS-58+DMB	1.99	2.64	0.65	0.11
TS-59+DMB	2.15	2.36	0.21	0.11
TS-60+DMB	2.14	2.34	0.20	0.20
TS-61+DMB	1.94	2.74	0.80	0.17
TS-62+DMB	2.17	2.31	0.14	0.19
TS-63+DMB	2.02	2.57	0.55	0.11
TS-64+DMB	2.08	2.50	0.42	0.17
TS-65+DMB	2.01	2.64	0.63	0.16
TS-66+DMB	2.13	2.40	0.27	0.16
TS-67+DMB	2.17	2.34	0.17	0.24
TS-68+DMB	1.97	2.77	0.80	0.22
TS-69+DMB	2.18	2.31	0.12	0.23
TS-70+DMB	2.02	2.58	0.56	0.16

The synchronicity[12] of a concerted reaction can be quantified in different manners:



a) Using the difference in the lengths of the two bonds forming ($\Delta d = d_{2\text{-}3} - d_{1\text{-}6}$).

b) Using the difference in the Wiberg bond indices (WBI) of the two bonds forming ($\Delta_{WBI} = WBI_{1\text{-}6} - WBI_{2\text{-}3}$).

c) Using the method developed by Moyano and co-workers,[13] as follows:

$$Sy = 1 - \frac{\sum_{i=1}^{n} \frac{|\delta B_i - \delta B_{av}|}{\delta B_{av}}}{2n-2}$$

Where n is the number of bonds directly involved in the reaction (in this case, n = 6) and δB_i stands for the relative variation of a given bond index B_i at the transition structure (TS) according to

$$\delta B_i = \frac{B_i^{TS} - B_i^{R}}{B_i^{P} - B_i^{R}}$$

where the superscripts R and P refer to the reactants and the product, respectively. The average value of δB_i, denoted as δB_{av} is therefore

$$\delta B_{av} = n^{-1} \sum_{i=1}^{n} \delta B_i$$

12 a) Dewar, M. J. S. *J. Am. Chem. Soc.* **1984**, *106*, 209. b) Borden, W. T.; Loncharich, R. J.; Houk, K. N. *Annu. Rev. Phys. Chem.* **1988**, *39*, 213. c) Leroy, G.; Sana, M. *Tetrahedron* **1975**, *31*, 2091.

13 Moyano, A.; Pericás, M. A.; Valentí, E. *J. Org. Chem.* **1989**, *54*, 573.

Table S8. Different measurements of asynchronicity all transition structures computed for the DA reactions between **1-70** and **CP** at the B3LYP/6-31G* level.

	Δd (Å)	Δ_{WBI}	Sy
TS-1+CP	0.40	0.19	0.89
TS-2+CP	0.39	0.21	0.88
TS-3+CP	0.65	0.33	0.82
TS-4+CP	0.51	0.25	0.83
TS-5+CP	0.11	0.06	0.93
TS-6+CP	0.44	0.22	0.88
TS-7+CP	0.59	0.29	0.84
TS-8+CP	0.60	0.30	0.84
TS-9+CP	0.51	0.26	0.87
TS-10+CP	0.32	0.18	0.90
TS-11+CP	0.04	0.00	0.92
TS-12+CP	0.88	0.41	0.78
TS-13+CP	0.76	0.38	0.81
TS-14+CP	0.60	0.32	0.84
TS-15+CP	0.35	0.21	0.90
TS-16+CP	0.81	0.36	0.79
TS-17+CP	0.00	0.00	0.93
TS-18+CP	0.03	0.01	0.92
TS-19+CP	0.32	0.16	0.91
TS-20+CP	0.48	0.22	0.88
TS-21+CP	0.23	0.14	0.91
TS-22+CP	0.40	0.21	0.90
TS-23+CP	0.55	0.28	0.86
TS-24+CP	0.03	0.01	0.90
TS-25+CP	0.40	0.20	0.89
TS-26+CP	0.61	0.29	0.85
TS-27+CP	0.41	0.20	0.89
TS-28+CP	0.38	0.19	0.90
TS-29+CP	0.14	0.06	0.93
TS-30+CP	0.09	0.04	0.93
TS-31+CP	0.22	0.13	0.92
TS-32+CP	0.64	0.30	0.84
TS-33+CP	0.00	0.00	0.92
TS-34+CP	0.55	0.28	0.86
TS-35+CP	0.52	0.27	0.87
TS-36+CP	0.41	0.21	0.90
TS-37+CP	0.19	0.10	0.92
TS-38+CP	0.06	0.02	0.93
TS-39+CP	0.00	0.00	0.93
TS-40+CP	0.32	0.16	0.91
TS-41+CP	0.34	0.18	0.88
TS-42+CP	0.45	0.23	0.86
TS-43+CP	0.25	0.14	0.90
TS-44+CP	0.12	0.04	0.92
TS-45+CP	0.62	0.30	0.81
TS-46+CP	0.02	0.01	0.92
TS-47+CP	0.35	0.19	0.88
TS-48+CP	0.33	0.18	0.89
TS-49+CP	0.45	0.23	0.87
TS-50+CP	0.24	0.14	0.92
TS-51+CP	0.12	0.04	0.93
TS-52+CP	0.53	0.27	0.85
TS-53+CP	0.01	0.01	0.93
TS-54+CP	0.35	0.19	0.90
TS-55+CP	0.00	0.00	0.92
TS-56+CP	0.24	0.13	0.91
TS-57+CP	0.28	0.17	0.90
TS-58+CP	0.39	0.22	0.88
TS-59+CP	0.18	0.12	0.92
TS-60+CP	0.18	0.07	0.93
TS-61+CP	0.48	0.26	0.86
TS-62+CP	0.12	0.04	0.93
TS-63+CP	0.28	0.16	0.91
TS-64+CP	0.36	0.19	0.88
TS-65+CP	0.47	0.24	0.86
TS-66+CP	0.27	0.16	0.90
TS-67+CP	0.15	0.06	0.92
TS-68+CP	0.59	0.30	0.83
TS-69+CP	0.06	0.02	0.93
TS-70+CP	0.38	0.21	0.88

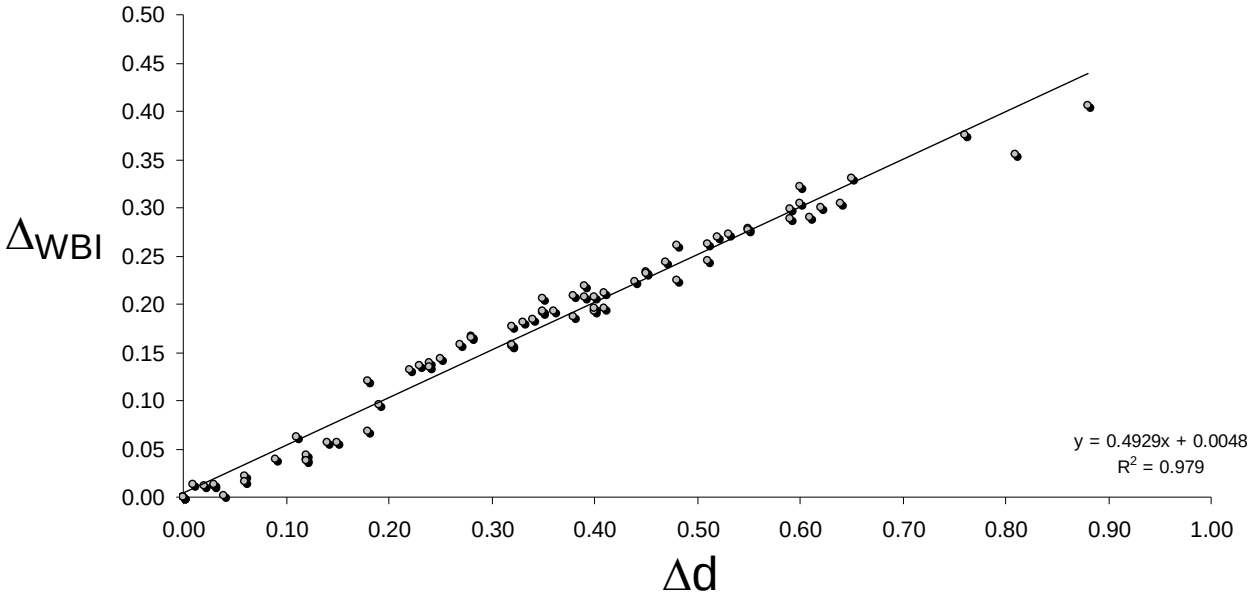


Figure S2. Plot of Δ_{WBI} versus Δd correspondig to the reactions between **1-70** and **CP**.

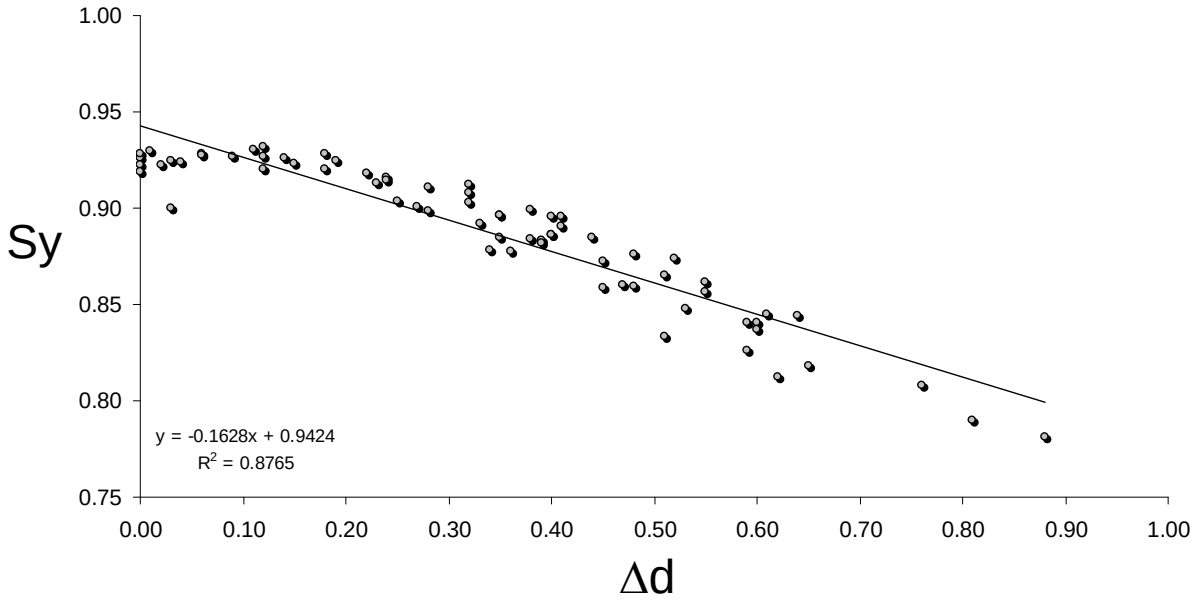


Figure S3. Plot of Sy versus Δd correspondig to the reactions between **1-70** and **CP**.

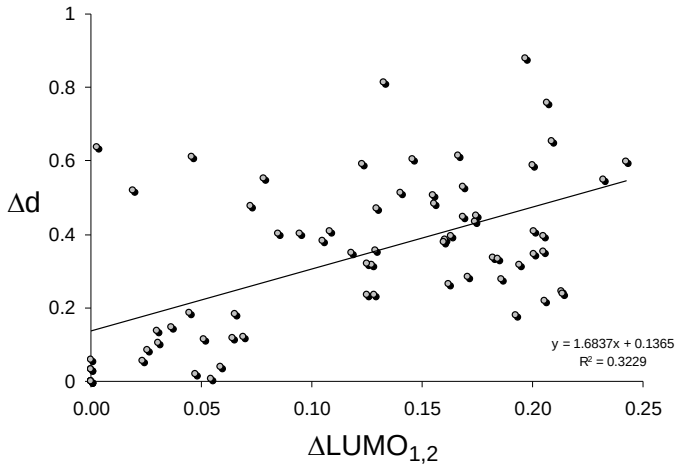


Figure S4. Plot of Δd versus $\Delta LUMO_{1,2}$ correspondig to the reactions between **1-70** and **CP**.

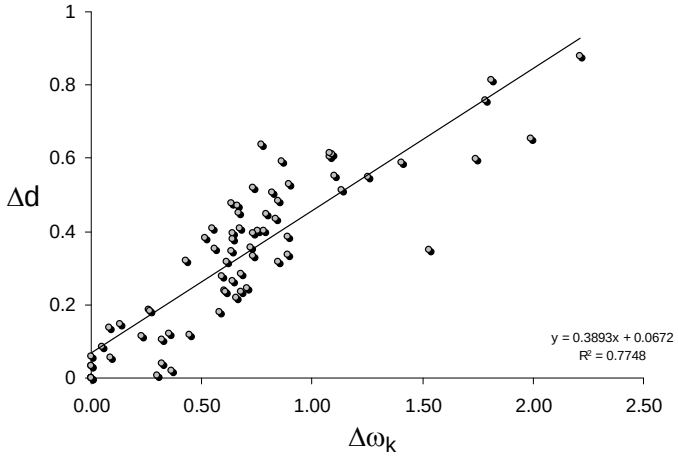


Figure S5. Plot of Δd versus $\Delta\omega_k$ correspondig to the reactions between **1-70** and **CP**.

Table S9. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for compounds **CP**, **CH**, **BU** and **DMB** (in au).

	E	ZPE	H	G
CP	-194.101058	-194.008165	-194.003079	-194.034762
CH	-233.418936	-233.296106	-233.289989	-233.324356
BU	-155.992144	-155.906655	-155.901065	-155.933101
DMB	-234.626780	-234.484039	-234.476042	-234.514358

Table S10. Δd values computed for the DA reactions between **1-70** and **CP** at the B3LYP/6-31G* level, Δd values estimated from $\Delta\omega_k$ (0.39* $\Delta\omega_k$+0.07), and difference between both values.

	Δd (Å)	0.39.$\Delta\omega_k$+0.07	Difference
TS-1+CP	0.40	0.36	0.04
TS-2+CP	0.39	0.42	-0.03
TS-3+CP	0.65	0.85	-0.20
TS-4+CP	0.51	0.51	0.00
TS-5+CP	0.11	0.19	-0.08
TS-6+CP	0.44	0.40	0.04
TS-7+CP	0.59	0.62	-0.03
TS-8+CP	0.60	0.49	0.11
TS-9+CP	0.51	0.39	0.12
TS-10+CP	0.32	0.40	-0.08
TS-11+CP	0.04	0.19	-0.15
TS-12+CP	0.88	0.93	-0.05
TS-13+CP	0.76	0.77	-0.01
TS-14+CP	0.60	0.75	-0.15
TS-15+CP	0.35	0.67	-0.32
TS-16+CP	0.81	0.78	0.03
TS-17+CP	0.00	0.07	-0.07
TS-18+CP	0.03	0.07	-0.04
TS-19+CP	0.32	0.31	0.01
TS-20+CP	0.48	0.32	0.16
TS-21+CP	0.23	0.34	-0.11
TS-22+CP	0.40	0.35	0.05
TS-23+CP	0.55	0.56	-0.01
TS-24+CP	0.03	0.07	-0.04
TS-25+CP	0.40	0.37	0.03
TS-26+CP	0.61	0.50	0.11
TS-27+CP	0.41	0.28	0.13
TS-28+CP	0.38	0.27	0.11
TS-29+CP	0.14	0.10	0.04
TS-30+CP	0.09	0.09	0.00
TS-31+CP	0.22	0.33	-0.11
TS-32+CP	0.64	0.37	0.27
TS-33+CP	0.00	0.07	-0.07
TS-34+CP	0.55	0.50	0.05
TS-35+CP	0.52	0.35	0.17
TS-36+CP	0.41	0.33	0.08
TS-37+CP	0.19	0.17	0.02
TS-38+CP	0.06	0.07	-0.01
TS-39+CP	0.00	0.07	-0.07
TS-40+CP	0.32	0.24	0.08
TS-41+CP	0.34	0.42	-0.08
TS-42+CP	0.45	0.38	0.07
TS-43+CP	0.25	0.34	-0.09
TS-44+CP	0.12	0.24	-0.12
TS-45+CP	0.62	0.49	0.13
TS-46+CP	0.02	0.21	-0.19
TS-47+CP	0.35	0.32	0.03
TS-48+CP	0.33	0.35	-0.02
TS-49+CP	0.45	0.33	0.12
TS-50+CP	0.24	0.30	-0.06
TS-51+CP	0.12	0.21	-0.09
TS-52+CP	0.53	0.42	0.11
TS-53+CP	0.01	0.19	-0.18
TS-54+CP	0.35	0.29	0.06
TS-55+CP	0.00	0.07	-0.07
TS-56+CP	0.24	0.31	-0.07
TS-57+CP	0.28	0.34	-0.06
TS-58+CP	0.39	0.32	0.07
TS-59+CP	0.18	0.30	-0.12
TS-60+CP	0.18	0.18	0.00
TS-61+CP	0.48	0.40	0.08
TS-62+CP	0.12	0.16	-0.04
TS-63+CP	0.28	0.30	-0.02
TS-64+CP	0.36	0.35	0.01
TS-65+CP	0.47	0.33	0.14
TS-66+CP	0.27	0.32	-0.05
TS-67+CP	0.15	0.12	0.03
TS-68+CP	0.59	0.41	0.18
TS-69+CP	0.06	0.11	-0.05
TS-70+CP	0.38	0.32	0.06

Table S11. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for compounds **1**-**70** (in au).

	E	ZPE	H	G
1	-170.831553	-170.780570	-170.775482	-170.806451
2	-191.911974	-191.850322	-191.845023	-191.876601
3	-218.557189	-218.462749	-218.455446	-218.491819
4	-283.087910	-283.032697	-283.027055	-283.060471
5	-415.626329	-415.568663	-415.562102	-415.598118
6	-182.689212	-182.569106	-182.560657	-182.600741
7	-1023.332753	-1023.283217	-1023.276526	-1023.313688
8	-651.505321	-651.452747	-651.446686	-651.481596
9	-231.233543	-231.143442	-231.136819	-231.172062
10	-231.232083	-231.141978	-231.135251	-231.170694
11	-284.151760	-284.091096	-284.084216	-284.120577
12	-678.146096	-678.061014	-678.052826	-678.092581
13	-257.878744	-257.755990	-257.747263	-257.787354
14	-257.881383	-257.758609	-257.749811	-257.790015
15	-310.793267	-310.700168	-310.691220	-310.732334
16	-263.062684	-263.012884	-263.006341	-263.042013
17	-263.068025	-263.017912	-263.011406	-263.047174
18	-263.069800	-263.019901	-263.013215	-263.048955
19	-210.153884	-210.074537	-210.068007	-210.102773
20	-210.151515	-210.072170	-210.065765	-210.100426
21	-528.946720	-528.879458	-528.870967	-528.912443
22	-222.011233	-221.862776	-221.852868	-221.896499
23	-1062.655991	-1062.578228	-1062.570000	-1062.610939
24	-487.574299	-487.516387	-487.508254	-487.549494
25	-455.726292	-455.642851	-455.634651	-455.675460
26	-355.295391	-355.246924	-355.238664	-355.279073
27	-249.472856	-249.365195	-249.357268	-249.395674
28	-249.470718	-249.363068	-249.355033	-249.393850
29	-302.392155	-302.313966	-302.305872	-302.345292
30	-302.389739	-302.311599	-302.303529	-302.342911
31	-270.550740	-270.432402	-270.424246	-270.463324
32	-376.378754	-376.319489	-376.310980	-376.352018
33	-447.518338	-447.471690	-447.461587	-447.506622
34	-394.619231	-394.542781	-394.532895	-394.576926
35	-415.703786	-415.616561	-415.606393	-415.651327
36	-309.865742	-309.719198	-309.709400	-309.752774
37	-442.342426	-442.222994	-442.210766	-442.260060
38	-341.712690	-341.606423	-341.596743	-341.639746
39	-341.707330	-341.601283	-341.591438	-341.635146
40	-288.789666	-288.654015	-288.644410	-288.687023
41	-229.991213	-229.922927	-229.917670	-229.949904
42	-269.315201	-269.218829	-269.211874	-269.248434
43	-269.316902	-269.220579	-269.213758	-269.249832
44	-322.232983	-322.165905	-322.158992	-322.195881
45	-689.588911	-689.529651	-689.523357	-689.559194
46	-361.559513	-361.464422	-361.455719	-361.497111
47	-308.640155	-308.515820	-308.507238	-308.547711
48	-269.349344	-269.250976	-269.244878	-269.279611
49	-308.671574	-308.545333	-308.537487	-308.576482
50	-308.672377	-308.546106	-308.538374	-308.576970
51	-361.590770	-361.493751	-361.485900	-361.525349
52	-728.943818	-728.854786	-728.847548	-728.885836
53	-400.915381	-400.790453	-400.780819	-400.824499
54	-347.993221	-347.839144	-347.829528	-347.873488
55	-379.289544	-379.233658	-379.227530	-379.262731
56	-305.264184	-305.189272	-305.183671	-305.217239
57	-308.666132	-308.538185	-308.531158	-308.568087
58	-347.986463	-347.830442	-347.821834	-347.862334
59	-347.987714	-347.831766	-347.823190	-347.863642
60	-400.907242	-400.780617	-400.771831	-400.813361
61	-768.259863	-768.141349	-768.133185	-768.173479
62	-440.228781	-440.074148	-440.063721	-440.108901
63	-387.303713	-387.119770	-387.109463	-387.154071
64	-457.864823	-457.749222	-457.741757	-457.780141
65	-497.186729	-497.043142	-497.034010	-497.076111
66	-497.187201	-497.043663	-497.034552	-497.076585
67	-550.104428	-549.990302	-549.980999	-550.024047
68	-917.458241	-917.352115	-917.343469	-917.385230
69	-589.428153	-589.286093	-589.275068	-589.321924
70	-536.505616	-536.334275	-536.323273	-536.370118

Table S12. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the transition structures of the reactions between compounds **1**-**70** and **CP** (in au).

	E	ZPE	H	G
TS-1+CP	-364.906426	-364.759340	-364.750581	-364.791783
TS-2+CP	-385.987063	-385.829218	-385.820285	-385.861855
TS-3+CP	-412.641803	-412.451192	-412.440028	-412.486949
TS-4+CP	-477.169715	-477.018370	-477.008956	-477.052078
TS-5+CP	-609.699523	-609.546029	-609.535726	-609.580883
TS-6+CP	-376.765456	-376.548622	-376.536733	-376.584761
TS-7+CP	-1217.413704	-1217.268011	-1217.257421	-1217.304245
TS-8+CP	-845.580778	-845.432210	-845.422188	-845.466788
TS-9+CP	-425.303090	-425.116957	-425.106529	-425.151318
TS-10+CP	-425.301209	-425.115073	-425.104662	-425.149444
TS-11+CP	-478.229048	-478.072427	-478.061752	-478.107740
TS-12+CP	-872.233198	-872.052113	-872.039764	-872.090020
TS-13+CP	-451.958563	-451.739781	-451.727061	-451.777313
TS-14+CP	-451.956519	-451.737460	-451.724874	-451.774750
TS-15+CP	-504.877327	-504.687963	-504.675109	-504.726095
TS-16+CP	-457.148958	-457.003225	-456.992590	-457.038548
TS-17+CP	-457.144764	-456.998847	-456.988402	-457.033827
TS-18+CP	-457.147576	-457.001631	-456.991198	-457.036551
TS-19+CP	-404.220632	-404.045343	-404.035094	-404.079507
TS-20+CP	-404.219948	-404.044733	-404.034431	-404.078872
TS-21+CP	-723.024629	-722.861535	-722.849201	-722.899490
TS-22+CP	-416.079952	-415.834845	-415.821497	-415.872511
TS-23+CP	-1256.728225	-1256.554392	-1256.542304	-1256.592164
TS-24+CP	-681.666483	-681.512275	-681.500365	-681.549860
TS-25+CP	-649.808119	-649.628677	-649.616622	-649.665888
TS-26+CP	-549.380189	-549.236027	-549.223651	-549.273659
TS-27+CP	-443.534400	-443.331066	-443.319285	-443.366796
TS-28+CP	-443.532743	-443.329374	-443.317515	-443.365254
TS-29+CP	-496.462771	-496.288796	-496.276820	-496.325258
TS-30+CP	-496.458095	-496.284290	-496.272275	-496.320777
TS-31+CP	-464.612139	-464.397630	-464.385932	-464.433097
TS-32+CP	-570.463973	-570.309043	-570.296395	-570.347065
TS-33+CP	-641.602697	-641.460499	-641.446286	-641.500238
TS-34+CP	-588.693444	-588.521292	-588.507437	-588.560137
TS-35+CP	-609.778034	-609.594788	-609.580813	-609.633798
TS-36+CP	-503.923760	-503.681216	-503.667998	-503.718320
TS-37+CP	-636.419447	-636.203715	-636.187505	-636.245416
TS-38+CP	-535.775108	-535.573055	-535.559606	-535.610777
TS-39+CP	-535.769292	-535.567527	-535.553985	-535.605364
TS-40+CP	-482.845239	-482.613875	-482.600730	-482.650779
TS-41+CP	-424.065243	-423.901307	-423.892259	-423.934329
TS-42+CP	-463.382932	-463.191024	-463.180221	-463.226197
TS-43+CP	-463.381763	-463.189746	-463.179216	-463.224212
TS-44+CP	-516.309986	-516.147401	-516.136542	-516.182897
TS-45+CP	-883.662454	-883.507743	-883.497441	-883.542962
TS-46+CP	-555.628426	-555.437803	-555.425244	-555.475061
TS-47+CP	-502.699380	-502.479569	-502.467208	-502.516201
TS-48+CP	-463.416227	-463.221973	-463.212099	-463.255990
TS-49+CP	-502.731753	-502.509526	-502.498002	-502.545306
TS-50+CP	-502.730687	-502.508335	-502.497044	-502.543544
TS-51+CP	-555.659635	-555.466726	-555.455020	-555.503152
TS-52+CP	-923.008526	-922.823647	-922.812551	-922.859489
TS-53+CP	-594.975425	-594.754577	-594.741252	-594.792503
TS-54+CP	-542.046169	-541.795889	-541.782953	-541.832763
TS-55+CP	-573.371214	-573.219581	-573.209448	-573.254352
TS-56+CP	-499.333965	-499.163059	-499.153582	-499.196769
TS-57+CP	-502.730142	-502.506271	-502.495374	-502.541543
TS-58+CP	-542.041507	-541.789731	-541.777236	-541.826644
TS-59+CP	-542.042950	-541.791098	-541.778750	-541.827618
TS-60+CP	-594.972989	-594.750670	-594.737908	-594.788297
TS-61+CP	-962.319755	-962.105478	-962.093313	-962.142605
TS-62+CP	-634.283591	-634.033274	-634.018978	-634.072291
TS-63+CP	-581.351861	-581.071957	-581.058090	-581.109910
TS-64+CP	-651.938101	-651.726871	-651.715362	-651.763206
TS-65+CP	-691.251544	-691.012247	-690.999147	-691.050137
TS-66+CP	-691.251060	-691.011688	-690.998707	-691.049216
TS-67+CP	-744.180062	-743.970210	-743.956851	-744.008802
TS-68+CP	-1111.528417	-1111.326705	-1111.313945	-1111.364787
TS-69+CP	-783.493158	-783.255331	-783.240391	-783.295323
TS-70+CP	-730.563085	-730.295671	-730.281186	-730.334510

Table S13. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the products of the reactions between compounds **1**-**70** and **CP** (in au).

	E	ZPE	H	G
P-1+CP	-364.967788	-364.815401	-364.807571	-364.846648
P-2+CP	-386.042653	-385.879965	-385.871791	-385.911927
P-3+CP	-412.688367	-412.492967	-412.482634	-412.527686
P-4+CP	-477.228078	-477.071625	-477.062988	-477.105226
P-5+CP	-609.767100	-609.608163	-609.598693	-609.642112
P-6+CP	-376.815521	-376.594901	-376.583590	-376.631158
P-7+CP	-1217.460196	-1217.310206	-1217.300413	-1217.346345
P-8+CP	-845.634290	-845.481303	-845.472073	-845.514769
P-9+CP	-425.355757	-425.165145	-425.155610	-425.198276
P-10+CP	-425.356791	-425.166026	-425.156365	-425.199743
P-11+CP	-478.279399	-478.118339	-478.108336	-478.153195
P-12+CP	-872.275528	-872.090089	-872.078630	-872.126308
P-13+CP	-452.001210	-451.777777	-451.766098	-451.813531
P-14+CP	-452.002822	-451.779360	-451.767533	-451.815819
P-15+CP	-504.921654	-504.727852	-504.715704	-504.765323
P-16+CP	-457.195379	-457.045108	-457.035425	-457.078794
P-17+CP	-457.200063	-457.049437	-457.039802	-457.083343
P-18+CP	-457.203369	-457.052636	-457.043002	-457.086619
P-19+CP	-404.282066	-404.101687	-404.092368	-404.134631
P-20+CP	-404.280237	-404.100063	-404.090785	-404.132663
P-21+CP	-723.080899	-722.913135	-722.901495	-722.950464
P-22+CP	-416.129298	-415.880612	-415.867826	-415.918402
P-23+CP	-1256.774049	-1256.595994	-1256.584703	-1256.633773
P-24+CP	-681.725152	-681.565997	-681.554844	-681.603301
P-25+CP	-649.853477	-649.669450	-649.658016	-649.706423
P-26+CP	-549.423909	-549.275584	-549.264039	-549.311859
P-27+CP	-443.593690	-443.385492	-443.374734	-443.419628
P-28+CP	-443.591238	-443.382878	-443.372155	-443.417017
P-29+CP	-496.516208	-496.337623	-496.326563	-496.372755
P-30+CP	-496.513058	-496.334606	-496.323505	-496.369783
P-31+CP	-464.666136	-464.447482	-464.436512	-464.482369
P-32+CP	-570.502888	-570.344013	-570.332127	-570.381204
P-33+CP	-641.640713	-641.494945	-641.481460	-641.533460
P-34+CP	-588.735715	-588.559566	-588.546592	-588.596927
P-35+CP	-609.814885	-609.627953	-609.614737	-609.666053
P-36+CP	-503.974341	-503.727315	-503.715117	-503.763018
P-37+CP	-636.454156	-636.234836	-636.219376	-636.275722
P-38+CP	-535.827109	-535.620768	-535.608277	-535.657016
P-39+CP	-535.821804	-535.615373	-535.602887	-535.651626
P-40+CP	-482.901119	-482.664952	-482.652913	-482.700161
P-41+CP	-424.126731	-423.958249	-423.950045	-423.990112
P-42+CP	-463.443188	-463.246753	-463.236962	-463.280121
P-43+CP	-463.441831	-463.245615	-463.235920	-463.278918
P-44+CP	-516.366950	-516.200180	-516.190161	-516.234444
P-45+CP	-883.722725	-883.563722	-883.554237	-883.597526
P-46+CP	-555.683949	-555.489321	-555.477657	-555.525103
P-47+CP	-502.757463	-502.533256	-502.521990	-502.567961
P-48+CP	-463.470770	-463.271998	-463.262856	-463.305149
P-49+CP	-502.785535	-502.558901	-502.548260	-502.593320
P-50+CP	-502.783550	-502.557034	-502.546444	-502.591534
P-51+CP	-555.709096	-555.512121	-555.501126	-555.547681
P-52+CP	-923.064442	-922.875389	-922.864912	-922.910511
P-53+CP	-595.023350	-594.798400	-594.785951	-594.835036
P-54+CP	-542.096140	-541.841436	-541.829481	-541.876906
P-55+CP	-573.424858	-573.268503	-573.259181	-573.302289
P-56+CP	-499.392560	-499.216748	-499.208007	-499.249565
P-57+CP	-502.787342	-502.559126	-502.548972	-502.593675
P-58+CP	-542.099662	-541.843585	-541.831957	-541.879253
P-59+CP	-542.097507	-541.841375	-541.829799	-541.877462
P-60+CP	-595.025228	-594.798905	-594.786877	-594.835933
P-61+CP	-962.382835	-962.164262	-962.152820	-962.200233
P-62+CP	-634.335937	-634.081718	-634.068256	-634.119553
P-63+CP	-581.405739	-581.121603	-581.108626	-581.158489
P-64+CP	-651.994367	-651.778513	-651.767758	-651.814000
P-65+CP	-691.307985	-691.064190	-691.051994	-691.100663
P-66+CP	-691.301901	-691.058090	-691.045959	-691.094675
P-67+CP	-744.228656	-744.014695	-744.002107	-744.052256
P-68+CP	-1111.585923	-1111.379870	-1111.367792	-1111.416998
P-69+CP	-783.541198	-783.299376	-783.285325	-783.337959
P-70+CP	-730.612413	-730.340451	-730.326920	-730.378014

Table S14. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the transition structures of the reactions between compounds **1**-**70** and **CH** (in au).

	E	ZPE	H	G
TS-1+CH	-404.216785	-404.040162	-404.030184	-404.074312
TS-2+CH	-425.298424	-425.110935	-425.100828	-425.145101
TS-3+CH	-451.953934	-451.733552	-451.721230	-451.770849
TS-4+CH	-516.480725	-516.299685	-516.289151	-516.334714
TS-5+CH	-649.009736	-648.826751	-648.815192	-648.863416
TS-6+CH	-416.077732	-415.831254	-415.818257	-415.868577
TS-7+CH	-1256.725432	-1256.550071	-1256.538320	-1256.587614
TS-8+CH	-884.892324	-884.714246	-884.702995	-884.750321
TS-9+CH	-464.614230	-464.398421	-464.386904	-464.433933
TS-10+CH	-464.613914	-464.397745	-464.386359	-464.433265
TS-11+CH	-517.540039	-517.353761	-517.341953	-517.390447
TS-12+CH	-911.546446	-911.335686	-911.322213	-911.374794
TS-13+CH	-491.270491	-491.022182	-491.008240	-491.061557
TS-14+CH	-491.267509	-491.018812	-491.005039	-491.057743
TS-15+CH	-544.188937	-543.969963	-543.955952	-544.009533
TS-16+CH	-496.460533	-496.285172	-496.273298	-496.322237
TS-17+CH	-496.455215	-496.279811	-496.268152	-496.316409
TS-18+CH	-496.458043	-496.282516	-496.270903	-496.318980
TS-19+CH	-443.529852	-443.324694	-443.313412	-443.360093
TS-20+CH	-443.529755	-443.324927	-443.313469	-443.360579
TS-21+CH	-762.333681	-762.141013	-762.127531	-762.180316
TS-22+CH	-455.391071	-455.116230	-455.101814	-455.155072
TS-23+CH	-1296.038618	-1295.835049	-1295.821805	-1295.874122
TS-24+CH	-720.977250	-720.793493	-720.780423	-720.832334
TS-25+CH	-689.118206	-688.909364	-688.896043	-688.948368
TS-26+CH	-588.691607	-588.517982	-588.504345	-588.557322
TS-27+CH	-482.844073	-482.610933	-482.598123	-482.647745
TS-28+CH	-482.840882	-482.607725	-482.594762	-482.645349
TS-29+CH	-535.772652	-535.569129	-535.555958	-535.607172
TS-30+CH	-535.767624	-535.563966	-535.550931	-535.601600
TS-31+CH	-503.923260	-503.679050	-503.666244	-503.716032
TS-32+CH	-609.775159	-609.590758	-609.576867	-609.630525
TS-33+CH	-680.914047	-680.742287	-680.726925	-680.783456
TS-34+CH	-628.003289	-627.801522	-627.786509	-627.841973
TS-35+CH	-649.087904	-648.875022	-648.859970	-648.915194
TS-36+CH	-543.233372	-542.960647	-542.946557	-542.998488
TS-37+CH	-675.730598	-675.485199	-675.467933	-675.528084
TS-38+CH	-575.084041	-574.852271	-574.837762	-574.891212
TS-39+CH	-575.077015	-574.845582	-574.830903	-574.885152
TS-40+CH	-522.152726	-521.891592	-521.877377	-521.929949
TS-41+CH	-463.377392	-463.183936	-463.173688	-463.218384
TS-42+CH	-502.694778	-502.473365	-502.461421	-502.509717
TS-43+CH	-502.691955	-502.470422	-502.458680	-502.506348
TS-44+CH	-555.621489	-555.429374	-555.417326	-555.466251
TS-45+CH	-922.974784	-922.790531	-922.778999	-922.827249
TS-46+CH	-594.939174	-594.718818	-594.705194	-594.757154
TS-47+CH	-542.009499	-541.759938	-541.746520	-541.797575
TS-48+CH	-502.728109	-502.504398	-502.493315	-502.539906
TS-49+CH	-542.042854	-541.791001	-541.778405	-541.827863
TS-50+CH	-542.040056	-541.788255	-541.775747	-541.825082
TS-51+CH	-594.970649	-594.748321	-594.735382	-594.786354
TS-52+CH	-962.319858	-962.105409	-962.093103	-962.142762
TS-53+CH	-634.285107	-634.034608	-634.020187	-634.073751
TS-54+CH	-581.354387	-581.074296	-581.060293	-581.112401
TS-55+CH	-612.683397	-612.502139	-612.490840	-612.538328
TS-56+CH	-538.645531	-538.445151	-538.434471	-538.480323
TS-57+CH	-542.042357	-541.788819	-541.776817	-541.825307
TS-58+CH	-581.353248	-581.071492	-581.058062	-581.109144
TS-59+CH	-581.352594	-581.071054	-581.057603	-581.108912
TS-60+CH	-634.283763	-634.031773	-634.017890	-634.070753
TS-61+CH	-1001.631379	-1001.387512	-1001.374206	-1001.425872
TS-62+CH	-673.593196	-673.312954	-673.297714	-673.352862
TS-63+CH	-620.660790	-620.351188	-620.336270	-620.390206
TS-64+CH	-691.249666	-691.008872	-690.996193	-691.046500
TS-65+CH	-730.562767	-730.293885	-730.279693	-730.332807
TS-66+CH	-730.560584	-730.291593	-730.277479	-730.330512
TS-67+CH	-783.490980	-783.251730	-783.237140	-783.291861
TS-68+CH	-1150.839937	-1150.608737	-1150.594755	-1150.648298
TS-69+CH	-822.802968	-822.535510	-822.519523	-822.576622
TS-70+CH	-769.871737	-769.574710	-769.559097	-769.614881

Table S15. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the products of the reactions between compounds **1**-**70** and **CH** (in au).

	E	ZPE	H	G
P-1+CH	-404.296327	-404.114157	-404.105220	-404.146858
P-2+CH	-425.371614	-425.179264	-425.169937	-425.212918
P-3+CH	-452.017035	-451.791741	-451.780306	-451.827933
P-4+CH	-516.558721	-516.372331	-516.362644	-516.406832
P-5+CH	-649.097083	-648.908317	-648.897765	-648.943521
P-6+CH	-416.143680	-415.893168	-415.880813	-415.930583
P-7+CH	-1256.788222	-1256.608359	-1256.597483	-1256.645820
P-8+CH	-884.962768	-884.780030	-884.769680	-884.814996
P-9+CH	-464.683881	-464.463463	-464.452870	-464.497975
P-10+CH	-464.684947	-464.464307	-464.453599	-464.499438
P-11+CH	-517.611857	-517.420859	-517.409896	-517.456618
P-12+CH	-911.603758	-911.388390	-911.375846	-911.426028
P-13+CH	-491.328851	-491.075493	-491.062753	-491.112733
P-14+CH	-491.330569	-491.077169	-491.064284	-491.115071
P-15+CH	-544.250075	-544.026407	-544.013159	-544.065352
P-16+CH	-496.523150	-496.343053	-496.332277	-496.378085
P-17+CH	-496.527182	-496.346762	-496.336014	-496.382207
P-18+CH	-496.531553	-496.350884	-496.340179	-496.386196
P-19+CH	-443.609805	-443.399428	-443.389094	-443.433696
P-20+CH	-443.607666	-443.397530	-443.387223	-443.431449
P-21+CH	-762.409224	-762.211647	-762.198890	-762.250647
P-22+CH	-455.456700	-455.177757	-455.164083	-455.216307
P-23+CH	-1296.101217	-1295.893237	-1295.880892	-1295.932397
P-24+CH	-721.055799	-720.866866	-720.854570	-720.906850
P-25+CH	-689.179718	-688.966006	-688.953378	-689.004782
P-26+CH	-588.750364	-588.572147	-588.559535	-588.609734
P-27+CH	-482.920267	-482.682233	-482.670453	-482.717737
P-28+CH	-482.916632	-482.678206	-482.666506	-482.713766
P-29+CH	-535.843321	-535.634930	-535.622831	-535.671347
P-30+CH	-535.839064	-535.630811	-535.618642	-535.667429
P-31+CH	-503.993459	-503.744809	-503.732869	-503.780930
P-32+CH	-609.829998	-609.641269	-609.628295	-609.679932
P-33+CH	-680.966280	-680.790662	-680.776123	-680.830469
P-34+CH	-628.060331	-627.854228	-627.840257	-627.892845
P-35+CH	-649.140426	-648.923606	-648.909414	-648.962811
P-36+CH	-543.299246	-543.022021	-543.008992	-543.058820
P-37+CH	-675.779636	-675.530381	-675.513934	-675.572371
P-38+CH	-575.152490	-574.916065	-574.902637	-574.953462
P-39+CH	-575.145112	-574.908783	-574.895296	-574.946770
P-40+CH	-522.225260	-521.958714	-521.945887	-521.994911
P-41+CH	-463.461388	-463.263063	-463.253780	-463.296193
P-42+CH	-502.776265	-502.550092	-502.539221	-502.584723
P-43+CH	-502.774796	-502.548727	-502.537963	-502.583325
P-44+CH	-555.700686	-555.504081	-555.492981	-555.539567
P-45+CH	-923.057475	-922.868607	-922.858065	-922.903524
P-46+CH	-595.015819	-594.791390	-594.778700	-594.828263
P-47+CH	-542.088071	-541.833878	-541.821626	-541.869729
P-48+CH	-502.802891	-502.574247	-502.564036	-502.608718
P-49+CH	-542.116122	-541.859696	-541.847971	-541.895479
P-50+CH	-542.113824	-541.857239	-541.845679	-541.892846
P-51+CH	-595.040016	-594.813225	-594.801142	-594.850089
P-52+CH	-962.396920	-962.177987	-962.166471	-962.214180
P-53+CH	-634.352195	-634.097412	-634.083943	-634.135212
P-54+CH	-581.423407	-581.138808	-581.125883	-581.175552
P-55+CH	-612.758290	-612.572071	-612.561661	-612.607177
P-56+CH	-538.725210	-538.519574	-538.509724	-538.553797
P-57+CH	-542.116847	-541.858981	-541.847681	-541.895084
P-58+CH	-581.427552	-581.141554	-581.128903	-581.178442
P-59+CH	-581.424859	-581.138888	-581.126190	-581.176302
P-60+CH	-634.353622	-634.097417	-634.084305	-634.135818
P-61+CH	-1001.712384	-1001.463956	-1001.451465	-1001.501045
P-62+CH	-673.662329	-673.377978	-673.363569	-673.416830
P-63+CH	-620.730945	-620.416732	-620.402880	-620.454490
P-64+CH	-691.323994	-691.078306	-691.066468	-691.115131
P-65+CH	-730.635950	-730.362116	-730.348907	-730.399750
P-66+CH	-730.629473	-730.355661	-730.342528	-730.393553
P-67+CH	-783.557087	-783.313281	-783.299621	-783.352117
P-68+CH	-1150.915822	-1150.679850	-1150.666746	-1150.717968
P-69+CH	-822.867737	-822.595957	-822.580907	-822.635575
P-70+CH	-769.937959	-769.635616	-769.621282	-769.673833

Table S16. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the transition structures of the reactions between compounds **1**-**70** and **BU** (in au).

	E	ZPE	H	G
TS-1+BU	-326.791120	-326.651430	-326.642400	-326.684022
TS-2+BU	-347.873275	-347.722883	-347.713656	-347.755623
TS-3+BU	-374.527566	-374.344346	-374.332886	-374.380276
TS-4+BU	-439.054059	-438.909967	-438.900360	-438.943585
TS-5+BU	-571.584541	-571.438437	-571.427880	-571.473497
TS-6+BU	-338.655618	-338.446127	-338.434070	-338.481869
TS-7+BU	-1179.301438	-1179.163168	-1179.152340	-1179.199205
TS-8+BU	-807.469571	-807.328422	-807.318080	-807.363203
TS-9+BU	-387.192154	-387.013776	-387.002899	-387.048707
TS-10+BU	-387.187290	-387.008548	-386.997886	-387.043055
TS-11+BU	-440.113209	-439.963960	-439.953042	-439.999470
TS-12+BU	-834.121575	-833.947728	-833.935167	-833.985416
TS-13+BU	-413.847102	-413.636128	-413.622880	-413.675103
TS-14+BU	-413.841795	-413.630282	-413.617368	-413.668013
TS-15+BU	-466.760532	-466.578519	-466.565430	-466.616791
TS-16+BU	-419.031884	-418.893577	-418.882574	-418.929288
TS-17+BU	-419.027712	-418.889163	-418.878474	-418.924468
TS-18+BU	-419.031092	-418.892560	-418.881860	-418.927808
TS-19+BU	-366.106184	-365.938142	-365.927707	-365.972392
TS-20+BU	-366.106117	-365.938386	-365.927769	-365.972809
TS-21+BU	-684.909451	-684.753799	-684.741224	-684.791881
TS-22+BU	-377.969980	-377.732020	-377.718565	-377.769339
TS-23+BU	-1218.615791	-1218.449413	-1218.437046	-1218.487309
TS-24+BU	-643.550688	-643.403842	-643.391683	-643.441630
TS-25+BU	-611.691375	-611.519439	-611.507117	-611.557050
TS-26+BU	-511.261797	-511.124926	-511.112275	-511.162890
TS-27+BU	-405.420996	-405.225048	-405.212986	-405.261006
TS-28+BU	-405.418875	-405.222758	-405.210759	-405.258747
TS-29+BU	-458.345609	-458.178868	-458.166686	-458.215605
TS-30+BU	-458.342549	-458.176060	-458.163840	-458.212789
TS-31+BU	-426.498627	-426.291697	-426.279685	-426.327505
TS-32+BU	-532.345777	-532.198224	-532.185297	-532.236621
TS-33+BU	-603.482582	-603.347713	-603.333270	-603.387986
TS-34+BU	-550.575569	-550.410732	-550.396631	-550.450076
TS-35+BU	-571.661586	-571.485788	-571.471586	-571.525057
TS-36+BU	-465.814185	-465.578806	-465.565547	-465.615606
TS-37+BU	-598.303644	-598.095313	-598.078926	-598.137248
TS-38+BU	-497.659418	-497.464736	-497.451078	-497.502801
TS-39+BU	-497.654326	-497.459669	-497.446026	-497.497804
TS-40+BU	-444.732120	-444.507870	-444.494619	-444.544843
TS-41+BU	-385.952863	-385.796387	-385.787067	-385.829417
TS-42+BU	-425.273618	-425.089303	-425.078197	-425.124456
TS-43+BU	-425.268565	-425.084163	-425.073286	-425.118951
TS-44+BU	-478.195014	-478.039828	-478.028732	-478.075417
TS-45+BU	-845.552405	-845.405072	-845.394480	-845.440292
TS-46+BU	-517.515477	-517.332283	-517.319507	-517.369562
TS-47+BU	-464.588846	-464.376493	-464.363902	-464.413076
TS-48+BU	-425.303167	-425.116266	-425.106162	-425.150343
TS-49+BU	-464.622065	-464.407285	-464.395472	-464.443242
TS-50+BU	-464.617788	-464.403023	-464.391413	-464.438593
TS-51+BU	-517.544610	-517.359095	-517.347172	-517.395652
TS-52+BU	-884.898095	-884.720616	-884.709158	-884.756880
TS-53+BU	-556.862319	-556.648815	-556.635302	-556.686872
TS-54+BU	-503.935683	-503.692818	-503.679655	-503.729847
TS-55+BU	-535.256640	-535.112294	-535.101966	-535.147144
TS-56+BU	-461.219916	-461.056421	-461.046698	-461.090207
TS-57+BU	-464.617701	-464.401183	-464.390079	-464.436469
TS-58+BU	-503.934487	-503.690084	-503.677332	-503.727027
TS-59+BU	-503.931236	-503.686731	-503.674177	-503.723407
TS-60+BU	-556.858179	-556.643061	-556.630116	-556.680946
TS-61+BU	-924.212754	-924.005482	-923.993134	-924.042544
TS-62+BU	-596.172101	-595.928906	-595.914522	-595.967869
TS-63+BU	-543.244930	-542.972210	-542.958256	-543.010019
TS-64+BU	-613.824363	-613.620374	-613.608684	-613.656668
TS-65+BU	-653.142109	-652.910280	-652.896916	-652.948204
TS-66+BU	-653.138117	-652.906140	-652.892950	-652.943790
TS-67+BU	-706.064331	-705.861879	-705.848295	-705.900711
TS-68+BU	-1073.418540	-1073.224282	-1073.211185	-1073.262644
TS-69+BU	-745.380045	-745.149480	-745.134434	-745.189424
TS-70+BU	-692.453577	-692.193537	-692.178866	-692.232448

Table S17. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the products of the reactions between compounds **1**-**70** and **BU** (in au).

	E	ZPE	H	G
P-1+BU	-326.887968	-326.742284	-326.734149	-326.773741
P-2+BU	-347.964150	-347.808243	-347.799819	-347.840306
P-3+BU	-374.607781	-374.419123	-374.408519	-374.454013
P-4+BU	-439.150094	-439.000015	-438.991076	-439.033661
P-5+BU	-571.689679	-571.537349	-571.527600	-571.571512
P-6+BU	-338.735381	-338.521428	-338.509793	-338.557907
P-7+BU	-1179.380031	-1179.236629	-1179.226525	-1179.273162
P-8+BU	-807.560083	-807.413507	-807.403995	-807.447102
P-9+BU	-387.277261	-387.093452	-387.083642	-387.126851
P-10+BU	-387.276723	-387.092685	-387.082805	-387.126405
P-11+BU	-440.198915	-440.044442	-440.034212	-440.079228
P-12+BU	-834.199844	-834.020769	-834.009017	-834.057196
P-13+BU	-413.921648	-413.705114	-413.693086	-413.741230
P-14+BU	-413.921800	-413.704926	-413.692909	-413.741427
P-15+BU	-466.840437	-466.653306	-466.640999	-466.690606
P-16+BU	-419.113607	-418.969880	-418.959966	-419.003716
P-17+BU	-419.120055	-418.975883	-418.966048	-419.009916
P-18+BU	-419.120497	-418.976393	-418.966495	-419.010570
P-19+BU	-366.202984	-366.029248	-366.019708	-366.062345
P-20+BU	-366.201529	-366.027995	-366.018486	-366.060755
P-21+BU	-685.000760	-684.839435	-684.827682	-684.876835
P-22+BU	-378.049708	-377.807578	-377.794554	-377.845582
P-23+BU	-1218.694237	-1218.522694	-1218.511195	-1218.560466
P-24+BU	-643.644625	-643.491957	-643.480501	-643.529471
P-25+BU	-611.775879	-611.598156	-611.586648	-611.634965
P-26+BU	-511.341315	-511.199484	-511.187727	-511.235963
P-27+BU	-405.514634	-405.312953	-405.302038	-405.347258
P-28+BU	-405.513823	-405.311924	-405.301065	-405.346100
P-29+BU	-458.435556	-458.263520	-458.252289	-458.298719
P-30+BU	-458.435108	-458.263199	-458.251921	-458.298522
P-31+BU	-426.588526	-426.376416	-426.365297	-426.411368
P-32+BU	-532.422288	-532.270056	-532.258003	-532.307155
P-33+BU	-603.558894	-603.419436	-603.405829	-603.458038
P-34+BU	-550.657190	-550.487504	-550.474375	-550.524983
P-35+BU	-571.736674	-571.556421	-571.543019	-571.594454
P-36+BU	-465.896749	-465.656458	-465.644085	-465.692047
P-37+BU	-598.375232	-598.162617	-598.146951	-598.203396
P-38+BU	-497.748427	-497.548484	-497.535841	-497.584872
P-39+BU	-497.745067	-497.545036	-497.532433	-497.581349
P-40+BU	-444.824298	-444.594519	-444.582365	-444.629773
P-41+BU	-386.048553	-385.886750	-385.878142	-385.919390
P-42+BU	-425.364914	-425.175439	-425.165225	-425.209799
P-43+BU	-425.364258	-425.174913	-425.164824	-425.209258
P-44+BU	-478.286960	-478.126916	-478.116532	-478.161908
P-45+BU	-845.644549	-845.492377	-845.482520	-845.527042
P-46+BU	-517.602855	-517.415090	-517.403111	-517.451566
P-47+BU	-464.677834	-464.460368	-464.448818	-464.496158
P-48+BU	-425.392059	-425.199867	-425.190530	-425.233260
P-49+BU	-464.706353	-464.486278	-464.475410	-464.520984
P-50+BU	-464.706927	-464.487054	-464.476300	-464.521702
P-51+BU	-517.629622	-517.439187	-517.428035	-517.474906
P-52+BU	-884.984491	-884.801964	-884.791386	-884.837088
P-53+BU	-556.941814	-556.723559	-556.710908	-556.760395
P-54+BU	-504.016636	-503.768402	-503.756269	-503.804118
P-55+BU	-535.342184	-535.192142	-535.182622	-535.226393
P-56+BU	-461.308890	-461.139563	-461.130513	-461.173203
P-57+BU	-464.709379	-464.487392	-464.477115	-464.521759
P-58+BU	-504.021015	-503.771059	-503.759379	-503.806619
P-59+BU	-504.022097	-503.772329	-503.760708	-503.807779
P-60+BU	-556.945321	-556.725149	-556.713047	-556.761766
P-61+BU	-924.299992	-924.087892	-924.076427	-924.123896
P-62+BU	-596.255802	-596.007887	-595.994320	-596.045654
P-63+BU	-543.329742	-543.051754	-543.038731	-543.088379
P-64+BU	-613.915026	-613.705466	-613.694579	-613.741017
P-65+BU	-653.219247	-652.981820	-652.969459	-653.018742
P-66+BU	-653.228024	-652.990696	-652.978381	-653.027345
P-67+BU	-706.149851	-705.942197	-705.929429	-705.980008
P-68+BU	-1073.499777	-1073.299911	-1073.287753	-1073.337233
P-69+BU	-745.454123	-745.218124	-745.204044	-745.257002
P-70+BU	-692.529802	-692.263931	-692.250347	-692.301655

Table S18. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the transition structures of the reactions between compounds **1**-**70** and **DMB** (in au).

	E	ZPE	H	G
TS-1+DMB	-405.426644	-405.230797	-405.218680	-405.267320
TS-2+DMB	-426.507727	-426.301220	-426.288916	-426.337943
TS-3+DMB	-453.163959	-452.924742	-452.910183	-452.964748
TS-4+DMB	-517.691090	-517.491134	-517.478355	-517.528715
TS-5+DMB	-650.219842	-650.017499	-650.003897	-650.056220
TS-6+DMB	-417.289129	-417.023372	-417.008345	-417.062623
TS-7+DMB	-1257.936608	-1257.742450	-1257.728439	-1257.782509
TS-8+DMB	-886.104704	-885.907372	-885.893971	-885.946069
TS-9+DMB	-465.826627	-465.592226	-465.578276	-465.630981
TS-10+DMB	-465.821614	-465.586947	-465.573131	-465.625491
TS-11+DMB	-518.748386	-518.543095	-518.529056	-518.582460
TS-12+DMB	-912.758342	-912.528422	-912.512776	-912.570143
TS-13+DMB	-492.483364	-492.216178	-492.199917	-492.258469
TS-14+DMB	-492.478238	-492.210827	-492.194739	-492.252815
TS-15+DMB	-545.397795	-545.159951	-545.143667	-545.202378
TS-16+DMB	-497.669507	-497.475166	-497.461079	-497.514927
TS-17+DMB	-497.664920	-497.470387	-497.456584	-497.509469
TS-18+DMB	-497.667651	-497.472941	-497.459222	-497.511698
TS-19+DMB	-444.741613	-444.517789	-444.504148	-444.556074
TS-20+DMB	-444.741483	-444.517895	-444.504098	-444.556421
TS-21+DMB	-763.544429	-763.332930	-763.317153	-763.375083
TS-22+DMB	-456.603365	-456.309617	-456.292993	-456.350845
TS-23+DMB	-1297.250969	-1297.028560	-1297.013089	-1297.070090
TS-24+DMB	-722.188452	-721.985659	-721.970379	-722.027220
TS-25+DMB	-690.328306	-690.100383	-690.084966	-690.141612
TS-26+DMB	-589.901317	-589.708693	-589.692811	-589.751081
TS-27+DMB	-484.055562	-483.803456	-483.788348	-483.843161
TS-28+DMB	-484.054370	-483.802382	-483.787172	-483.842489
TS-29+DMB	-536.981550	-536.758927	-536.743571	-536.799588
TS-30+DMB	-536.979679	-536.757390	-536.741927	-536.798317
TS-31+DMB	-505.132408	-504.869262	-504.854254	-504.908649
TS-32+DMB	-610.983764	-610.780277	-610.764138	-610.822879
TS-33+DMB	-682.122746	-681.932348	-681.914504	-681.977304
TS-34+DMB	-629.215152	-628.994394	-628.977103	-629.037724
TS-35+DMB	-650.299276	-650.067499	-650.050109	-650.110675
TS-36+DMB	-544.447903	-544.156450	-544.140046	-544.197152
TS-37+DMB	-676.942636	-676.678500	-676.658866	-676.724419
TS-38+DMB	-576.295044	-576.044346	-576.027513	-576.086266
TS-39+DMB	-576.291644	-576.040832	-576.024127	-576.082459
TS-40+DMB	-523.366668	-523.086753	-523.070160	-523.128464
TS-41+DMB	-464.586202	-464.373579	-464.361146	-464.410636
TS-42+DMB	-503.906969	-503.666606	-503.652381	-503.705710
TS-43+DMB	-503.901970	-503.661522	-503.647504	-503.700332
TS-44+DMB	-556.829538	-556.618502	-556.604177	-556.658276
TS-45+DMB	-924.186509	-923.983125	-923.969403	-924.022313
TS-46+DMB	-596.149613	-595.910586	-595.894514	-595.952152
TS-47+DMB	-543.222190	-542.953754	-542.938038	-542.994214
TS-48+DMB	-503.936238	-503.693311	-503.680091	-503.731214
TS-49+DMB	-543.255211	-542.984251	-542.969413	-543.023795
TS-50+DMB	-543.250790	-542.980119	-542.965299	-543.019648
TS-51+DMB	-596.178667	-595.937448	-595.922221	-595.978344
TS-52+DMB	-963.532025	-963.298348	-963.283845	-963.338278
TS-53+DMB	-635.496200	-635.226813	-635.210092	-635.268702
TS-54+DMB	-582.568717	-582.269931	-582.253598	-582.310860
TS-55+DMB	-613.892877	-613.692536	-613.679062	-613.731286
TS-56+DMB	-539.854485	-539.635054	-539.622196	-539.672776
TS-57+DMB	-543.250769	-542.978387	-542.964148	-543.017396
TS-58+DMB	-582.567886	-582.267425	-582.251599	-582.307918
TS-59+DMB	-582.564272	-582.264009	-582.248238	-582.304588
TS-60+DMB	-635.492418	-635.221422	-635.205304	-635.262997
TS-61+DMB	-1002.846794	-1002.583674	-1002.568199	-1002.624431
TS-62+DMB	-674.806186	-674.507308	-674.489650	-674.550271
TS-63+DMB	-621.878321	-621.549447	-621.532414	-621.590794
TS-64+DMB	-692.460244	-692.200112	-692.185371	-692.239909
TS-65+DMB	-731.778065	-731.490128	-731.473718	-731.531564
TS-66+DMB	-731.773896	-731.485773	-731.469537	-731.526913
TS-67+DMB	-784.701131	-784.442735	-784.425982	-784.485353
TS-68+DMB	-1152.055262	-1151.804496	-1151.788518	-1151.846030
TS-69+DMB	-824.016793	-823.730276	-823.712074	-823.773885
TS-70+DMB	-771.089778	-770.773433	-770.755801	-770.815605

Table S19. B3LYP/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the products of the reactions between compounds **1**-**70** and **DMB** (in au).

	E	ZPE	H	G
P-1+DMB	-405.523187	-405.321544	-405.310176	-405.357090
P-2+DMB	-426.599100	-426.387212	-426.375561	-426.423361
P-3+DMB	-453.242990	-452.998457	-452.984582	-453.037478
P-4+DMB	-517.785500	-517.579507	-517.567316	-517.617167
P-5+DMB	-650.324856	-650.116582	-650.103578	-650.154735
P-6+DMB	-417.370230	-417.100431	-417.085498	-417.141307
P-7+DMB	-1258.015175	-1257.815804	-1257.802436	-1257.856313
P-8+DMB	-886.195432	-885.992973	-885.980145	-886.030739
P-9+DMB	-465.912378	-465.672784	-465.659673	-465.710352
P-10+DMB	-465.911943	-465.672112	-465.658932	-465.709989
P-11+DMB	-518.834468	-518.623976	-518.610501	-518.662737
P-12+DMB	-912.835677	-912.600793	-912.585702	-912.641396
P-13+DMB	-492.557004	-492.284597	-492.269277	-492.324846
P-14+DMB	-492.553816	-492.280692	-492.265538	-492.320921
P-15+DMB	-545.476386	-545.233318	-545.217749	-545.274732
P-16+DMB	-497.749430	-497.549781	-497.536563	-497.587802
P-17+DMB	-497.755875	-497.555751	-497.542644	-497.593859
P-18+DMB	-497.756251	-497.556232	-497.543048	-497.594470
P-19+DMB	-444.838257	-444.608667	-444.595827	-444.645879
P-20+DMB	-444.836860	-444.607489	-444.594675	-444.644435
P-21+DMB	-763.636152	-763.419011	-763.403889	-763.460687
P-22+DMB	-456.684632	-456.386844	-456.370414	-456.429577
P-23+DMB	-1297.329435	-1297.102043	-1297.087232	-1297.143892
P-24+DMB	-722.280828	-722.072304	-722.057513	-722.113912
P-25+DMB	-690.411250	-690.177721	-690.162887	-690.218682
P-26+DMB	-589.977738	-589.779965	-589.764896	-589.820513
P-27+DMB	-484.150154	-483.892552	-483.878339	-483.930938
P-28+DMB	-484.149026	-483.891445	-483.877199	-483.929833
P-29+DMB	-537.071445	-536.843472	-536.828943	-536.882802
P-30+DMB	-537.070987	-536.843188	-536.828558	-536.882684
P-31+DMB	-505.223554	-504.955523	-504.941123	-504.994486
P-32+DMB	-611.058323	-610.850231	-610.834841	-610.891443
P-33+DMB	-682.195978	-682.000619	-681.983655	-682.043350
P-34+DMB	-629.293652	-629.068012	-629.051541	-629.109628
P-35+DMB	-650.372907	-650.136839	-650.120067	-650.179041
P-36+DMB	-544.531873	-544.235640	-544.219955	-544.275274
P-37+DMB	-677.012086	-676.743423	-676.724446	-676.788253
P-38+DMB	-576.384346	-576.128564	-576.112585	-576.169060
P-39+DMB	-576.380859	-576.124779	-576.108876	-576.165097
P-40+DMB	-523.459444	-523.173623	-523.158168	-523.212881
P-41+DMB	-464.684285	-464.466510	-464.454734	-464.502996
P-42+DMB	-504.000711	-503.755309	-503.741881	-503.793527
P-43+DMB	-504.000127	-503.754709	-503.741459	-503.792631
P-44+DMB	-556.923369	-556.707438	-556.693825	-556.746248
P-45+DMB	-924.280848	-924.072747	-924.059660	-924.111188
P-46+DMB	-596.239468	-595.995736	-595.980525	-596.035989
P-47+DMB	-543.313926	-543.040625	-543.025791	-543.080092
P-48+DMB	-504.026766	-503.778660	-503.766056	-503.816180
P-49+DMB	-543.341193	-543.065194	-543.051036	-543.103987
P-50+DMB	-543.341856	-543.066064	-543.052002	-543.104831
P-51+DMB	-596.264959	-596.018675	-596.004170	-596.058718
P-52+DMB	-963.619807	-963.381495	-963.367552	-963.420882
P-53+DMB	-635.577191	-635.302924	-635.286948	-635.343879
P-54+DMB	-582.651611	-582.347728	-582.332195	-582.387665
P-55+DMB	-613.979450	-613.773415	-613.760737	-613.811564
P-56+DMB	-539.945695	-539.720466	-539.708211	-539.758203
P-57+DMB	-543.344486	-543.066725	-543.053104	-543.105325
P-58+DMB	-582.656058	-582.350140	-582.335151	-582.389802
P-59+DMB	-582.657274	-582.351748	-582.336779	-582.391321
P-60+DMB	-635.580988	-635.304982	-635.289549	-635.345725
P-61+DMB	-1002.935464	-1002.667387	-1002.652626	-1002.707397
P-62+DMB	-674.891424	-674.587247	-674.570436	-674.628918
P-63+DMB	-621.965014	-621.630797	-621.614539	-621.671278
P-64+DMB	-692.550119	-692.284733	-692.270482	-692.324613
P-65+DMB	-731.857444	-731.563978	-731.548446	-731.604424
P-66+DMB	-731.863238	-731.569841	-731.554267	-731.610402
P-67+DMB	-784.785489	-784.521939	-784.505849	-784.563868
P-68+DMB	-1152.137274	-1151.881583	-1151.866183	-1151.922487
P-69+DMB	-824.089880	-823.798058	-823.780623	-823.841179
P-70+DMB	-771.165281	-770.843574	-770.826603	-770.885601

Table S20. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), zero-point corrected energies ($\Delta ZPE^{\ddagger}$), enthalpies ($\Delta H^{\ddagger}$) and Gibbs free energies ($\Delta G^{\ddagger}$) computed for the reactions between compounds **1**-**70** and **CP** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta ZPE^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$
TS-1+CP	16.4	18.4	17.6	31.0
TS-2+CP	16.3	18.4	17.5	31.1
TS-3+CP	10.3	12.4	11.6	24.9
TS-4+CP	12.1	14.1	13.3	27.1
TS-5+CP	17.5	19.3	18.5	32.6
TS-6+CP	15.6	18.0	16.9	31.8
TS-7+CP	12.6	14.7	13.9	27.7
TS-8+CP	16.1	18.0	17.3	31.1
TS-9+CP	19.8	21.7	20.9	34.8
TS-10+CP	20.0	22.0	21.1	35.1
TS-11+CP	14.9	16.8	16.0	29.9
TS-12+CP	8.8	10.7	10.1	23.4
TS-13+CP	13.3	15.3	14.6	28.1
TS-14+CP	16.3	18.4	17.6	31.4
TS-15+CP	10.7	12.8	12.0	25.7
TS-16+CP	9.3	11.2	10.6	24.0
TS-17+CP	15.3	17.1	16.4	30.2
TS-18+CP	14.6	16.6	15.7	29.6
TS-19+CP	21.5	23.4	22.6	36.4
TS-20+CP	20.5	22.3	21.6	35.3
TS-21+CP	14.5	16.4	15.6	29.9
TS-22+CP	20.3	22.7	21.6	36.9
TS-23+CP	18.1	20.1	19.3	33.6
TS-24+CP	5.6	7.7	6.9	21.6
TS-25+CP	12.1	14.0	13.2	27.8
TS-26+CP	10.2	12.0	11.4	25.2
TS-27+CP	24.8	26.5	25.8	39.9
TS-28+CP	24.5	26.3	25.5	39.8
TS-29+CP	19.1	20.9	20.2	34.4
TS-30+CP	20.5	22.3	21.5	35.7
TS-31+CP	24.9	26.9	26.0	40.8
TS-32+CP	9.9	11.7	11.1	24.9
TS-33+CP	10.5	12.1	11.5	25.8
TS-34+CP	16.8	18.6	17.9	32.3
TS-35+CP	16.8	18.8	18.0	32.8
TS-36+CP	27.0	29.0	27.9	43.4
TS-37+CP	15.1	17.2	16.5	31.0
TS-38+CP	24.2	26.1	25.2	40.0
TS-39+CP	24.5	26.3	25.4	40.5
TS-40+CP	28.5	30.3	29.3	44.6
TS-41+CP	17.0	18.7	17.9	31.6
TS-42+CP	20.9	22.6	21.8	35.8
TS-43+CP	22.7	24.5	23.6	37.9
TS-44+CP	15.1	16.7	16.0	30.0
TS-45+CP	17.3	18.9	18.2	32.0
TS-46+CP	20.2	21.8	21.1	35.7
TS-47+CP	26.3	27.9	27.1	41.6
TS-48+CP	21.4	23.3	22.5	36.6
TS-49+CP	25.7	27.6	26.7	41.4
TS-50+CP	26.8	28.8	27.9	42.8
TS-51+CP	20.2	22.1	21.3	35.7
TS-52+CP	22.8	24.7	23.9	38.3
TS-53+CP	25.7	27.6	26.8	41.9
TS-54+CP	30.2	32.3	31.2	47.4
TS-55+CP	12.2	14.0	13.3	27.1
TS-56+CP	19.6	21.6	20.8	34.7
TS-57+CP	23.2	25.1	24.4	38.5
TS-58+CP	28.9	30.7	29.9	44.2
TS-59+CP	28.8	30.6	29.8	44.4
TS-60+CP	22.2	23.9	23.2	37.5
TS-61+CP	25.8	27.6	27.0	41.2
TS-62+CP	29.0	30.8	30.0	44.8
TS-63+CP	33.2	35.1	34.2	49.5
TS-64+CP	17.4	19.1	18.5	32.4
TS-65+CP	22.7	24.5	23.8	38.1
TS-66+CP	23.3	25.2	24.4	39.0
TS-67+CP	16.0	17.7	17.1	31.4
TS-68+CP	19.4	21.1	20.5	34.6
TS-69+CP	22.6	24.4	23.7	38.5
TS-70+CP	27.4	29.3	28.3	44.2

Table S21. B3LYP/6-31G* reaction energies (ΔE_{rxn}), zero-point corrected energies (ΔZPE_{rxn}), enthalpies (ΔH_{rxn}) and Gibbs free energies (ΔG_{rxn}) computed for the reactions between compounds **1-70** and **CP** (in kcal/mol).

	ΔE_{rxn}	ΔZPE_{rxn}	ΔH_{rxn}	ΔG_{rxn}
P-1+CP	-22.1	-16.7	-18.2	-3.4
P-2+CP	-18.6	-13.5	-14.9	-0.4
P-3+CP	-18.9	-13.8	-15.1	-0.7
P-4+CP	-24.5	-19.3	-20.6	-6.3
P-5+CP	-24.9	-19.7	-21.0	-5.8
P-6+CP	-15.8	-11.1	-12.5	2.7
P-7+CP	-16.6	-11.8	-13.1	1.3
P-8+CP	-17.5	-12.8	-14.0	1.0
P-9+CP	-13.3	-8.5	-9.9	5.4
P-10+CP	-14.8	-10.0	-11.3	3.6
P-11+CP	-16.7	-12.0	-13.2	1.3
P-12+CP	-17.8	-13.1	-14.3	0.6
P-13+CP	-13.4	-8.5	-9.9	5.4
P-14+CP	-12.8	-7.9	-9.2	5.6
P-15+CP	-17.1	-12.2	-13.4	1.1
P-16+CP	-19.9	-15.1	-16.3	-1.3
P-17+CP	-19.4	-14.7	-15.9	-0.9
P-18+CP	-20.4	-15.4	-16.8	-1.8
P-19+CP	-17.0	-11.9	-13.4	1.8
P-20+CP	-17.4	-12.4	-13.8	1.6
P-21+CP	-20.8	-16.0	-17.2	-2.0
P-22+CP	-10.7	-6.1	-7.5	8.1
P-23+CP	-10.7	-6.0	-7.3	7.5
P-24+CP	-31.2	-26.0	-27.3	-12.0
P-25+CP	-16.4	-11.6	-12.7	2.4
P-26+CP	-17.2	-12.9	-14.0	1.2
P-27+CP	-12.4	-7.6	-9.0	6.8
P-28+CP	-12.2	-7.3	-8.8	7.3
P-29+CP	-14.4	-9.7	-11.1	4.6
P-30+CP	-14.0	-9.3	-10.6	5.0
P-31+CP	-9.0	-4.3	-5.8	9.9
P-32+CP	-14.5	-10.3	-11.3	3.5
P-33+CP	-13.4	-9.5	-10.5	5.0
P-34+CP	-9.7	-5.4	-6.7	9.3
P-35+CP	-6.3	-2.0	-3.3	12.6
P-36+CP	-4.7	0.0	-1.7	15.4
P-37+CP	-6.7	-2.3	-3.5	12.0
P-38+CP	-8.4	-3.9	-5.3	11.0
P-39+CP	-8.4	-3.7	-5.3	11.5
P-40+CP	-6.5	-1.7	-3.4	13.6
P-41+CP	-21.6	-17.0	-18.4	-3.4
P-42+CP	-16.9	-12.4	-13.8	1.9
P-43+CP	-15.0	-10.6	-12.0	3.6
P-44+CP	-20.7	-16.4	-17.6	-2.4
P-45+CP	-20.6	-16.3	-17.4	-2.2
P-46+CP	-14.7	-10.5	-11.8	4.2
P-47+CP	-10.2	-5.8	-7.3	9.1
P-48+CP	-12.8	-8.1	-9.3	5.8
P-49+CP	-8.1	-3.4	-4.8	11.2
P-50+CP	-6.3	-1.7	-3.1	12.7
P-51+CP	-10.8	-6.4	-7.6	7.8
P-52+CP	-12.3	-7.8	-9.0	6.3
P-53+CP	-4.3	0.1	-1.3	15.2
P-54+CP	-1.2	3.7	2.0	19.7
P-55+CP	-21.5	-16.7	-17.9	-3.0
P-56+CP	-17.1	-12.1	-13.3	1.5
P-57+CP	-12.6	-8.0	-9.2	5.8
P-58+CP	-7.6	-3.1	-4.4	11.2
P-59+CP	-5.5	-0.9	-2.2	13.1
P-60+CP	-10.6	-6.4	-7.5	7.6
P-61+CP	-13.8	-9.3	-10.4	5.0
P-62+CP	-3.8	0.4	-0.9	15.1
P-63+CP	-0.6	4.0	2.5	19.0
P-64+CP	-17.9	-13.3	-14.4	0.6
P-65+CP	-12.7	-8.1	-9.4	6.4
P-66+CP	-8.6	-3.9	-5.2	10.5
P-67+CP	-14.5	-10.2	-11.3	4.1
P-68+CP	-16.7	-12.3	-13.3	1.9
P-69+CP	-7.5	-3.2	-4.5	11.8
P-70+CP	-3.6	1.2	-0.4	16.9

Table S22. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), zero-point corrected energies ($\Delta ZPE^{\ddagger}$), enthalpies ($\Delta H^{\ddagger}$) and Gibbs free energies ($\Delta G^{\ddagger}$) computed for the reactions between compounds **1**-**70** and **CH** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta ZPE^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$
TS-1+CH	21.1	22.9	22.1	35.5
TS-2+CH	20.4	22.3	21.5	35.1
TS-3+CH	13.9	15.9	15.2	28.4
TS-4+CH	16.4	18.3	17.5	31.4
TS-5+CH	22.3	23.9	23.2	37.1
TS-6+CH	19.1	21.3	20.3	35.5
TS-7+CH	16.5	18.4	17.7	31.6
TS-8+CH	20.0	21.7	21.1	34.9
TS-9+CH	24.0	25.8	25.0	39.2
TS-10+CH	23.3	25.3	24.4	38.8
TS-11+CH	19.2	21.0	20.2	34.2
TS-12+CH	11.7	13.5	12.9	26.4
TS-13+CH	17.1	18.8	18.2	31.5
TS-14+CH	20.6	22.5	21.8	35.5
TS-15+CH	14.6	16.5	15.8	29.6
TS-16+CH	13.2	14.9	14.5	27.7
TS-17+CH	19.9	21.5	20.9	34.6
TS-18+CH	19.3	21.0	20.3	34.1
TS-19+CH	27.0	28.8	28.0	42.1
TS-20+CH	25.5	27.2	26.5	40.3
TS-21+CH	20.1	21.7	21.0	35.4
TS-22+CH	24.5	26.8	25.8	41.3
TS-23+CH	22.8	24.7	24.0	38.4
TS-24+CH	10.0	11.9	11.2	26.1
TS-25+CH	17.0	18.6	17.9	32.3
TS-26+CH	14.3	15.7	15.3	28.9
TS-27+CH	29.9	31.6	30.8	45.4
TS-28+CH	30.6	32.3	31.5	45.7
TS-29+CH	24.1	25.7	25.0	39.2
TS-30+CH	25.8	27.4	26.7	41.2
TS-31+CH	29.1	31.0	30.1	45.0
TS-32+CH	14.1	15.6	15.1	28.8
TS-33+CH	14.6	16.0	15.5	29.8
TS-34+CH	21.9	23.4	22.8	37.2
TS-35+CH	21.8	23.6	22.8	38.0
TS-36+CH	32.2	34.3	33.2	49.3
TS-37+CH	19.3	21.3	20.6	35.3
TS-38+CH	29.9	31.5	30.7	45.7
TS-39+CH	30.9	32.5	31.7	46.7
TS-40+CH	35.1	36.7	35.8	51.1
TS-41+CH	20.6	22.0	21.3	35.1
TS-42+CH	24.7	26.1	25.4	39.6
TS-43+CH	27.5	29.0	28.3	42.6
TS-44+CH	19.1	20.5	19.9	33.9
TS-45+CH	20.7	22.1	21.6	35.3
TS-46+CH	24.6	26.2	25.4	40.4
TS-47+CH	31.1	32.6	31.8	46.7
TS-48+CH	25.2	26.8	26.1	40.2
TS-49+CH	29.9	31.7	30.8	45.8
TS-50+CH	32.2	33.9	33.0	47.8
TS-51+CH	24.5	26.1	25.4	39.8
TS-52+CH	26.9	28.5	27.9	42.3
TS-53+CH	30.9	32.6	31.8	47.1
TS-54+CH	36.3	38.2	37.2	53.6
TS-55+CH	15.7	17.3	16.7	30.6
TS-56+CH	23.6	25.2	24.6	38.4
TS-57+CH	26.8	28.5	27.8	42.1
TS-58+CH	32.7	34.5	33.7	48.7
TS-59+CH	33.9	35.7	34.9	49.6
TS-60+CH	26.6	28.2	27.6	42.0
TS-61+CH	29.8	31.3	30.7	45.2
TS-62+CH	34.2	36.0	35.1	50.4
TS-63+CH	38.8	40.6	39.6	55.4
TS-64+CH	21.4	22.9	22.3	36.4
TS-65+CH	26.9	28.5	27.8	42.5
TS-66+CH	28.6	30.2	29.5	44.2
TS-67+CH	20.3	21.8	21.2	35.5
TS-68+CH	23.4	24.8	24.3	38.5
TS-69+CH	27.7	29.3	28.6	43.7
TS-70+CH	33.1	34.9	34.0	49.9

Table S23. B3LYP/6-31G* reaction energies (ΔE_{rxn}), zero-point corrected energies (ΔZPE_{rxn}), enthalpies (ΔH_{rxn}) and Gibbs free energies (ΔG_{rxn}) computed for the reactions between compounds **1-70** and **CH** (in kcal/mol).

	ΔE_{rxn}	ΔZPE_{rxn}	ΔH_{rxn}	ΔG_{rxn}
P-1+CH	-28.8	-23.5	-24.9	-10.1
P-2+CH	-25.5	-20.6	-21.9	-7.5
P-3+CH	-25.7	-20.6	-21.9	-7.4
P-4+CH	-32.6	-27.3	-28.6	-13.8
P-5+CH	-32.5	-27.3	-28.7	-13.2
P-6+CH	-22.3	-17.5	-18.9	-3.4
P-7+CH	-22.9	-18.2	-19.4	-4.9
P-8+CH	-24.2	-19.6	-20.7	-5.7
P-9+CH	-19.7	-15.0	-16.4	-1.0
P-10+CH	-21.3	-16.5	-17.8	-2.8
P-11+CH	-25.8	-21.1	-22.4	-7.3
P-12+CH	-24.3	-19.6	-20.7	-5.7
P-13+CH	-19.6	-14.7	-16.0	-0.6
P-14+CH	-19.0	-14.1	-15.4	-0.4
P-15+CH	-23.8	-18.9	-20.0	-5.4
P-16+CH	-26.1	-21.4	-22.6	-7.4
P-17+CH	-25.2	-20.5	-21.7	-6.7
P-18+CH	-26.9	-21.9	-23.2	-8.1
P-19+CH	-23.2	-18.1	-19.5	-4.1
P-20+CH	-23.4	-18.4	-19.7	-4.2
P-21+CH	-27.3	-22.6	-23.8	-8.7
P-22+CH	-16.6	-11.8	-13.3	2.9
P-23+CH	-16.5	-11.9	-13.1	1.8
P-24+CH	-39.3	-34.1	-35.3	-20.7
P-25+CH	-21.6	-17.0	-18.0	-3.1
P-26+CH	-22.6	-18.3	-19.4	-4.0
P-27+CH	-17.9	-13.1	-14.6	1.4
P-28+CH	-16.9	-11.9	-13.5	2.8
P-29+CH	-20.2	-15.6	-16.9	-1.1
P-30+CH	-19.1	-14.5	-15.8	-0.1
P-31+CH	-14.9	-10.2	-11.7	4.2
P-32+CH	-20.3	-16.1	-17.1	-2.2
P-33+CH	-18.2	-14.3	-15.4	0.3
P-34+CH	-13.9	-9.6	-10.9	5.3
P-35+CH	-11.1	-6.9	-8.2	8.1
P-36+CH	-9.1	-4.2	-6.0	11.5
P-37+CH	-11.5	-7.1	-8.3	7.6
P-38+CH	-13.1	-8.5	-10.0	6.7
P-39+CH	-11.8	-7.1	-8.7	8.0
P-40+CH	-10.5	-5.4	-7.2	10.3
P-41+CH	-32.2	-27.6	-28.9	-13.8
P-42+CH	-26.4	-22.1	-23.4	-7.5
P-43+CH	-24.4	-20.1	-21.5	-5.7
P-44+CH	-30.6	-26.4	-27.6	-12.1
P-45+CH	-31.1	-26.9	-28.1	-12.5
P-46+CH	-23.4	-19.4	-20.7	-4.3
P-47+CH	-18.2	-13.8	-15.3	1.5
P-48+CH	-21.7	-17.0	-18.3	-3.0
P-49+CH	-16.1	-11.5	-12.9	3.4
P-50+CH	-14.1	-9.4	-10.9	5.3
P-51+CH	-19.0	-14.7	-15.8	-0.2
P-52+CH	-21.4	-17.0	-18.2	-2.5
P-53+CH	-11.2	-6.8	-8.2	8.6
P-54+CH	-7.1	-2.2	-4.0	14.0
P-55+CH	-31.3	-26.5	-27.7	-12.6
P-56+CH	-26.4	-21.5	-22.6	-7.7
P-57+CH	-19.9	-15.5	-16.7	-1.7
P-58+CH	-13.9	-9.4	-10.7	5.2
P-59+CH	-11.4	-6.9	-8.2	7.3
P-60+CH	-17.2	-13.0	-14.1	1.2
P-61+CH	-21.1	-16.6	-17.8	-2.0
P-62+CH	-9.2	-4.8	-6.2	10.3
P-63+CH	-5.2	-0.5	-2.2	15.0
P-64+CH	-25.2	-20.7	-21.8	-6.7
P-65+CH	-19.0	-14.3	-15.6	0.4
P-66+CH	-14.6	-10.0	-11.3	4.6
P-67+CH	-21.2	-16.9	-18.0	-2.3
P-68+CH	-24.2	-19.8	-20.9	-5.3
P-69+CH	-13.0	-8.6	-9.9	6.7
P-70+CH	-8.4	-3.3	-5.0	13.0

Table S24. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), zero-point corrected energies ($\Delta ZPE^{\ddagger}$), enthalpies ($\Delta H^{\ddagger}$) and Gibbs free energies ($\Delta G^{\ddagger}$) computed for the reactions between compounds **1**-**70** and **BU** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta ZPE^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$
TS-1+BU	20.4	22.5	21.4	34.8
TS-2+BU	19.4	21.4	20.4	33.9
TS-3+BU	13.7	15.7	14.8	28.0
TS-4+BU	16.3	18.4	17.4	31.4
TS-5+BU	21.3	23.1	22.1	36.2
TS-6+BU	16.2	18.6	17.4	32.6
TS-7+BU	14.7	16.8	15.8	29.9
TS-8+BU	17.5	19.4	18.6	32.3
TS-9+BU	21.0	22.8	22.0	35.4
TS-10+BU	23.2	25.2	24.1	38.1
TS-11+BU	19.3	21.2	20.2	34.0
TS-12+BU	10.5	12.5	11.7	25.3
TS-13+BU	14.9	16.6	16.0	28.5
TS-14+BU	19.9	22.0	21.0	34.6
TS-15+BU	15.6	17.8	16.9	30.5
TS-16+BU	14.4	16.3	15.6	28.8
TS-17+BU	20.4	22.2	21.3	35.0
TS-18+BU	19.4	21.3	20.3	34.0
TS-19+BU	25.0	27.0	26.0	39.8
TS-20+BU	23.6	25.4	24.5	38.1
TS-21+BU	18.5	20.3	19.3	33.7
TS-22+BU	21.0	23.5	22.2	37.8
TS-23+BU	20.3	22.3	21.3	35.6
TS-24+BU	9.9	12.0	11.1	25.7
TS-25+BU	17.0	18.9	17.9	32.3
TS-26+BU	16.2	18.0	17.2	30.9
TS-27+BU	27.6	29.4	28.5	42.5
TS-28+BU	27.6	29.5	28.5	42.8
TS-29+BU	24.3	26.2	25.3	39.4
TS-30+BU	24.7	26.5	25.6	39.7
TS-31+BU	27.8	29.7	28.6	43.2
TS-32+BU	15.8	17.5	16.8	30.4
TS-33+BU	17.5	19.2	18.4	32.5
TS-34+BU	22.5	24.3	23.4	37.6
TS-35+BU	21.6	23.5	22.5	37.3
TS-36+BU	27.4	29.5	28.2	44.1
TS-37+BU	19.4	21.5	20.6	35.1
TS-38+BU	28.5	30.3	29.3	44.0
TS-39+BU	28.3	30.3	29.2	44.2
TS-40+BU	31.2	33.1	31.9	47.2
TS-41+BU	19.1	20.8	19.9	33.6
TS-42+BU	21.2	22.7	21.8	35.8
TS-43+BU	25.4	27.0	26.1	40.1
TS-44+BU	18.9	20.5	19.7	33.6
TS-45+BU	18.0	19.6	18.8	32.6
TS-46+BU	22.7	24.3	23.4	38.1
TS-47+BU	27.3	28.9	27.9	42.5
TS-48+BU	24.0	26.0	25.0	39.1
TS-49+BU	26.1	28.1	27.0	41.6
TS-50+BU	29.3	31.2	30.1	44.9
TS-51+BU	24.0	25.9	25.0	39.4
TS-52+BU	23.8	25.6	24.8	38.9
TS-53+BU	28.4	30.3	29.2	44.4
TS-54+BU	31.2	33.2	32.0	48.2
TS-55+BU	15.7	17.6	16.7	30.6
TS-56+BU	22.8	24.8	23.9	37.7
TS-57+BU	25.5	27.4	26.4	40.6
TS-58+BU	27.7	29.5	28.6	42.9
TS-59+BU	30.5	32.4	31.4	46.0
TS-60+BU	25.9	27.7	26.8	41.1
TS-61+BU	24.6	26.7	25.8	40.2
TS-62+BU	30.6	32.6	31.5	46.5
TS-63+BU	32.0	34.0	32.8	48.4
TS-64+BU	20.5	22.3	21.4	35.5
TS-65+BU	23.1	24.8	23.9	38.3
TS-66+BU	25.9	27.7	26.8	41.4
TS-67+BU	20.2	22.0	21.2	35.4
TS-68+BU	20.0	21.6	20.9	34.9
TS-69+BU	25.3	27.2	26.2	41.2
TS-70+BU	27.7	29.7	28.5	44.4

Table S25. B3LYP/6-31G* reaction energies (ΔE_{rxn}), zero-point corrected energies (ΔZPE_{rxn}), enthalpies (ΔH_{rxn}) and Gibbs free energies (ΔG_{rxn}) computed for the reactions between compounds **1**-**70** and **BU** (in kcal/mol).

	ΔE_{rxn}	ΔZPE_{rxn}	ΔH_{rxn}	ΔG_{rxn}
P-1+BU	-40.3	-34.6	-36.1	-21.5
P-2+BU	-37.7	-32.2	-33.7	-19.2
P-3+BU	-36.7	-31.2	-32.6	-18.3
P-4+BU	-44.0	-38.1	-39.5	-25.2
P-5+BU	-44.7	-38.9	-40.4	-25.3
P-6+BU	-33.9	-28.7	-30.2	-15.1
P-7+BU	-34.6	-29.3	-30.7	-16.5
P-8+BU	-39.3	-34.0	-35.3	-20.3
P-9+BU	-32.4	-27.2	-28.7	-13.6
P-10+BU	-32.9	-27.6	-29.2	-14.2
P-11+BU	-34.5	-29.3	-30.7	-16.0
P-12+BU	-38.7	-33.3	-34.6	-19.8
P-13+BU	-31.9	-26.6	-28.1	-13.0
P-14+BU	-30.3	-24.9	-26.4	-11.5
P-15+BU	-34.5	-29.2	-30.6	-15.8
P-16+BU	-36.9	-31.6	-33.0	-17.9
P-17+BU	-37.6	-32.2	-33.6	-18.6
P-18+BU	-36.7	-31.3	-32.8	-17.9
P-19+BU	-35.7	-30.2	-31.8	-16.6
P-20+BU	-36.3	-30.9	-32.4	-17.1
P-21+BU	-38.8	-33.5	-34.9	-19.6
P-22+BU	-29.1	-23.9	-25.5	-10.0
P-23+BU	-28.9	-23.7	-25.2	-10.3
P-24+BU	-49.1	-43.2	-44.7	-29.4
P-25+BU	-36.0	-30.5	-32.0	-16.6
P-26+BU	-33.7	-28.8	-30.1	-14.9
P-27+BU	-31.1	-25.8	-27.4	-11.6
P-28+BU	-32.0	-26.5	-28.2	-12.0
P-29+BU	-32.2	-26.9	-28.5	-12.8
P-30+BU	-33.4	-28.2	-29.7	-14.1
P-31+BU	-28.6	-23.4	-25.1	-9.4
P-32+BU	-32.2	-27.6	-28.8	-13.8
P-33+BU	-30.4	-25.8	-27.1	-11.5
P-34+BU	-28.7	-23.9	-25.4	-9.4
P-35+BU	-25.6	-20.8	-22.3	-6.3
P-36+BU	-24.4	-19.2	-21.1	-3.9
P-37+BU	-25.5	-20.7	-22.0	-6.4
P-38+BU	-27.4	-22.2	-23.9	-7.5
P-39+BU	-28.6	-23.3	-25.1	-8.2
P-40+BU	-26.7	-21.2	-23.1	-6.1
P-41+BU	-40.9	-35.9	-37.3	-22.8
P-42+BU	-36.1	-31.3	-32.8	-17.7
P-43+BU	-34.6	-29.9	-31.4	-16.5
P-44+BU	-38.8	-34.1	-35.4	-20.7
P-45+BU	-39.8	-35.2	-36.5	-21.8
P-46+BU	-32.1	-27.6	-29.1	-13.4
P-47+BU	-28.6	-23.8	-25.4	-9.6
P-48+BU	-31.7	-26.5	-28.0	-12.9
P-49+BU	-26.8	-21.5	-23.1	-7.2
P-50+BU	-26.6	-21.5	-23.1	-7.3
P-51+BU	-29.3	-24.3	-25.8	-10.3
P-52+BU	-30.5	-25.4	-26.8	-11.4
P-53+BU	-21.5	-16.6	-18.2	-1.8
P-54+BU	-19.6	-14.2	-16.1	1.6
P-55+BU	-38.0	-32.5	-33.9	-19.2
P-56+BU	-33.0	-27.4	-28.7	-14.3
P-57+BU	-32.1	-26.7	-28.2	-12.9
P-58+BU	-26.6	-21.3	-22.9	-7.0
P-59+BU	-26.5	-21.3	-22.9	-6.9
P-60+BU	-28.8	-23.8	-25.2	-9.6
P-61+BU	-30.1	-25.0	-26.5	-10.9
P-62+BU	-21.9	-17.0	-18.5	-2.3
P-63+BU	-21.3	-15.9	-17.7	-0.8
P-64+BU	-36.4	-31.1	-32.5	-17.4
P-65+BU	-25.3	-20.1	-21.6	-6.0
P-66+BU	-30.5	-25.3	-26.8	-11.1
P-67+BU	-33.4	-28.4	-29.7	-14.3
P-68+BU	-31.0	-25.8	-27.1	-11.9
P-69+BU	-21.2	-15.9	-17.5	-1.2
P-70+BU	-20.1	-14.4	-16.3	1.0

Table S26. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), zero-point corrected energies ($\Delta ZPE^{\ddagger}$), enthalpies ($\Delta H^{\ddagger}$) and Gibbs free energies ($\Delta G^{\ddagger}$) computed for the reactions between compounds **1**-**70** and **DMB** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta ZPE^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$
TS-1+DMB	19.9	21.2	20.6	33.6
TS-2+DMB	19.5	20.8	20.2	33.3
TS-3+DMB	12.6	13.8	13.4	26.0
TS-4+DMB	14.8	16.1	15.5	28.9
TS-5+DMB	20.9	22.1	21.5	35.3
TS-6+DMB	16.9	18.7	17.8	32.9
TS-7+DMB	14.4	15.6	15.1	28.6
TS-8+DMB	17.2	18.5	18.0	31.3
TS-9+DMB	21.1	22.1	21.7	34.8
TS-10+DMB	23.4	24.5	23.9	37.4
TS-11+DMB	18.9	20.1	19.6	32.9
TS-12+DMB	9.1	10.4	10.1	23.1
TS-13+DMB	13.9	15.0	14.7	27.1
TS-14+DMB	18.8	20.0	19.5	32.4
TS-15+DMB	14.0	15.2	14.8	27.8
TS-16+DMB	12.5	13.7	13.4	26.0
TS-17+DMB	18.8	19.8	19.4	32.7
TS-18+DMB	18.2	19.5	18.8	32.4
TS-19+DMB	24.5	25.6	25.0	38.3
TS-20+DMB	23.1	24.0	23.7	36.6
TS-21+DMB	18.2	19.2	18.7	32.5
TS-22+DMB	21.7	23.3	22.5	37.7
TS-23+DMB	20.0	21.2	20.7	34.6
TS-24+DMB	7.9	9.3	8.7	23.0
TS-25+DMB	15.5	16.6	16.1	30.2
TS-26+DMB	13.1	14.0	13.7	26.6
TS-27+DMB	27.7	28.7	28.2	42.0
TS-28+DMB	27.1	28.1	27.5	41.2
TS-29+DMB	23.5	24.5	24.1	37.7
TS-30+DMB	23.1	24.0	23.6	37.0
TS-31+DMB	28.3	29.6	28.9	43.3
TS-32+DMB	13.7	14.6	14.4	27.3
TS-33+DMB	14.0	14.7	14.5	27.4
TS-34+DMB	19.4	20.3	20.0	33.6
TS-35+DMB	19.6	20.8	20.3	34.5
TS-36+DMB	28.0	29.4	28.5	43.9
TS-37+DMB	16.7	17.9	17.5	31.4
TS-38+DMB	27.9	28.9	28.4	42.6
TS-39+DMB	26.6	27.9	27.2	42.1
TS-40+DMB	31.2	32.2	31.6	45.8
TS-41+DMB	19.9	21.0	20.4	33.7
TS-42+DMB	22.0	22.8	22.3	35.8
TS-43+DMB	26.2	27.0	26.5	40.1
TS-44+DMB	19.0	19.7	19.4	32.6
TS-45+DMB	18.3	19.2	18.8	32.2
TS-46+DMB	23.0	23.8	23.4	37.2
TS-47+DMB	28.1	28.9	28.4	42.6
TS-48+DMB	25.0	26.2	25.6	39.4
TS-49+DMB	27.1	28.3	27.7	42.1
TS-50+DMB	30.4	31.4	30.8	45.0
TS-51+DMB	24.4	25.3	24.9	38.5
TS-52+DMB	24.2	25.4	24.9	38.9
TS-53+DMB	28.8	29.9	29.3	44.0
TS-54+DMB	32.2	33.4	32.6	48.3
TS-55+DMB	14.7	15.8	15.4	28.7
TS-56+DMB	22.9	24.0	23.5	36.9
TS-57+DMB	26.4	27.5	27.0	40.8
TS-58+DMB	28.5	29.5	29.0	43.2
TS-59+DMB	31.5	32.5	32.0	46.1
TS-60+DMB	26.1	27.1	26.7	40.6
TS-61+DMB	25.0	26.2	25.7	39.8
TS-62+DMB	31.0	31.9	31.4	45.8
TS-63+DMB	32.7	34.1	33.3	48.7
TS-64+DMB	19.7	20.8	20.3	34.3
TS-65+DMB	22.2	23.3	22.8	37.0
TS-66+DMB	25.2	26.3	25.8	40.2
TS-67+DMB	18.9	19.8	19.5	33.3
TS-68+DMB	18.7	19.9	19.4	33.6
TS-69+DMB	23.9	25.0	24.5	39.2
TS-70+DMB	26.7	28.2	27.3	43.2

Table S27. B3LYP/6-31G* reaction energies (ΔE_{rxn}), zero-point corrected energies (ΔZPE_{rxn}), enthalpies (ΔH_{rxn}) and Gibbs free energies (ΔG_{rxn}) computed for the reactions between compounds **1**-**70** and **DMB** (in kcal/mol).

	ΔE_{rxn}	ΔZPE_{rxn}	ΔH_{rxn}	ΔG_{rxn}
P-1+DMB	-40.7	-35.7	-36.8	-22.8
P-2+DMB	-37.9	-33.2	-34.2	-20.3
P-3+DMB	-37.0	-32.4	-33.3	-19.6
P-4+DMB	-44.4	-39.4	-40.3	-26.6
P-5+DMB	-45.0	-40.1	-41.1	-26.5
P-6+DMB	-34.0	-29.7	-30.6	-16.4
P-7+DMB	-34.9	-30.5	-31.3	-17.7
P-8+DMB	-39.7	-35.3	-36.0	-21.8
P-9+DMB	-32.7	-28.4	-29.4	-15.0
P-10+DMB	-33.3	-28.9	-29.9	-15.6
P-11+DMB	-35.1	-30.6	-31.5	-17.4
P-12+DMB	-39.4	-35.0	-35.7	-21.6
P-13+DMB	-32.3	-28.0	-28.8	-14.5
P-14+DMB	-28.6	-23.9	-24.9	-10.4
P-15+DMB	-35.4	-30.8	-31.7	-17.6
P-16+DMB	-37.6	-33.2	-34.0	-19.7
P-17+DMB	-38.3	-33.8	-34.6	-20.3
P-18+DMB	-37.4	-32.8	-33.8	-19.6
P-19+DMB	-36.1	-31.4	-32.5	-18.0
P-20+DMB	-36.8	-32.2	-33.2	-18.6
P-21+DMB	-39.3	-34.8	-35.7	-21.3
P-22+DMB	-29.3	-25.1	-26.0	-11.7
P-23+DMB	-29.3	-25.0	-25.8	-11.7
P-24+DMB	-50.0	-45.1	-45.9	-31.4
P-25+DMB	-36.5	-31.9	-32.8	-18.1
P-26+DMB	-34.9	-30.7	-31.5	-17.0
P-27+DMB	-31.7	-27.2	-28.3	-13.1
P-28+DMB	-32.3	-27.8	-28.9	-13.6
P-29+DMB	-33.0	-28.5	-29.5	-14.5
P-30+DMB	-34.2	-29.8	-30.7	-15.9
P-31+DMB	-28.9	-24.5	-25.6	-10.5
P-32+DMB	-33.1	-29.3	-30.0	-15.7
P-33+DMB	-31.9	-28.2	-28.9	-14.0
P-34+DMB	-29.9	-25.8	-26.7	-11.5
P-35+DMB	-26.6	-22.7	-23.6	-8.4
P-36+DMB	-24.7	-20.3	-21.7	-5.1
P-37+DMB	-26.9	-22.8	-23.6	-8.7
P-38+DMB	-28.2	-23.9	-25.0	-9.4
P-39+DMB	-29.3	-24.8	-26.0	-9.8
P-40+DMB	-27.0	-22.3	-23.7	-7.2
P-41+DMB	-41.6	-37.4	-38.3	-24.3
P-42+DMB	-36.9	-32.9	-33.9	-19.3
P-43+DMB	-35.4	-31.4	-32.4	-17.8
P-44+DMB	-39.9	-36.1	-36.9	-22.6
P-45+DMB	-40.9	-37.1	-37.8	-23.6
P-46+DMB	-33.4	-29.7	-30.6	-15.4
P-47+DMB	-29.5	-25.6	-26.7	-11.3
P-48+DMB	-31.8	-27.4	-28.3	-13.9
P-49+DMB	-26.9	-22.5	-23.5	-8.2
P-50+DMB	-26.8	-22.5	-23.6	-8.5
P-51+DMB	-29.7	-25.7	-26.5	-11.9
P-52+DMB	-30.9	-26.8	-27.6	-13.0
P-53+DMB	-22.0	-17.8	-18.9	-3.2
P-54+DMB	-19.8	-15.4	-16.7	0.1
P-55+DMB	-39.6	-35.0	-35.9	-21.6
P-56+DMB	-34.3	-29.6	-30.4	-16.7
P-57+DMB	-32.4	-27.9	-28.8	-14.4
P-58+DMB	-26.9	-22.4	-23.4	-8.2
P-59+DMB	-26.8	-22.6	-23.6	-8.4
P-60+DMB	-29.5	-25.3	-26.2	-11.3
P-61+DMB	-30.6	-26.4	-27.2	-12.3
P-62+DMB	-22.5	-18.2	-19.2	-3.6
P-63+DMB	-21.7	-16.9	-18.2	-1.8
P-64+DMB	-36.7	-32.3	-33.1	-18.9
P-65+DMB	-27.6	-23.1	-24.1	-8.8
P-66+DMB	-30.9	-26.4	-27.4	-12.2
P-67+DMB	-34.1	-29.9	-30.6	-16.0
P-68+DMB	-32.8	-28.5	-29.3	-14.4
P-69+DMB	-21.9	-17.5	-18.5	-3.1
P-70+DMB	-20.6	-15.9	-17.1	-0.7

Table S28. CBS-QB3 energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for **CP** and the selected 35 dienophiles (in au).

	E	ZPE	H	G
CP	-193.708562	-193.712750	-193.707618	-193.739359
4	-282.702682	-282.707419	-282.701738	-282.735245
7	-1022.211461	-1022.217253	-1022.210516	-1022.247754
10	-230.822710	-230.828546	-230.821766	-230.857308
11	-283.712308	-283.718269	-283.711364	-283.747761
14	-257.372209	-257.380180	-257.371265	-257.411710
15	-310.252800	-310.260909	-310.251856	-310.293180
17	-262.649031	-262.654605	-262.648086	-262.683865
18	-262.650416	-262.656172	-262.649472	-262.685221
19	-209.765473	-209.771090	-209.764529	-209.799342
21	-528.343410	-528.351004	-528.342466	-528.384000
22	-221.493064	-221.502079	-221.492119	-221.535709
23	-1061.443129	-1061.450479	-1061.442185	-1061.483248
24	-486.978477	-486.985755	-486.977532	-487.019194
25	-455.127977	-455.135298	-455.127033	-455.168020
26	-354.756433	-354.763752	-354.755489	-354.795884
28	-248.993483	-249.000631	-248.992538	-249.031481
29	-301.883800	-301.890976	-301.882856	-301.922314
30	-301.881562	-301.888712	-301.880618	-301.920037
31	-270.053642	-270.060966	-270.052698	-270.092060
32	-375.820224	-375.827807	-375.819280	-375.860342
36	-309.280259	-309.289244	-309.279315	-309.323204
40	-288.224823	-288.233637	-288.223879	-288.267038
41	-229.609311	-229.613667	-229.608367	-229.640657
42	-268.842995	-268.849060	-268.842051	-268.878681
43	-268.842804	-268.848099	-268.841860	-268.876790
44	-321.728886	-321.734892	-321.727941	-321.764881
45	-688.771637	-688.777038	-688.770692	-688.806611
47	-308.077658	-308.085389	-308.076714	-308.117375
48	-268.877251	-268.882465	-268.876307	-268.911147
49	-308.110135	-308.117092	-308.109190	-308.148253
50	-308.110769	-308.117632	-308.109825	-308.148563
52	-728.037520	-728.043876	-728.036576	-728.074980
55	-378.781562	-378.786783	-378.780617	-378.815879
56	-304.807071	-304.811767	-304.806127	-304.839750
57	-308.104965	-308.111125	-308.104021	-308.141084

Table S29. CBS-QB3 energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the transition structures of the reactions between the selected 35 dienophiles and **CP** (in au).

	E	ZPE	H	G
TS-4+CP	-476.398238	-476.406744	-476.397293	-476.440385
TS-7+CP	-1215.908433	-1215.918170	-1215.907489	-1215.954465
TS-10+CP	-424.511678	-424.521244	-424.510734	-424.555672
TS-11+CP	-477.409238	-477.419053	-477.408294	-477.454433
TS-14+CP	-451.063784	-451.075594	-451.062840	-451.113040
TS-15+CP	-503.955496	-503.967556	-503.954552	-504.005832
TS-17+CP	-456.345245	-456.354803	-456.344301	-456.389808
TS-18+CP	-456.347421	-456.356962	-456.346477	-456.391895
TS-19+CP	-403.450695	-403.460075	-403.449751	-403.494262
TS-21+CP	-722.039120	-722.050615	-722.038176	-722.088619
TS-22+CP	-415.184179	-415.196739	-415.183235	-415.234572
TS-23+CP	-1255.136518	-1255.147790	-1255.135574	-1255.185684
TS-24+CP	-680.687873	-680.698917	-680.686929	-680.736562
TS-25+CP	-648.830219	-648.841431	-648.829275	-648.878714
TS-26+CP	-548.459086	-548.470548	-548.458142	-548.508162
TS-28+CP	-442.678001	-442.688994	-442.677057	-442.724883
TS-29+CP	-495.577896	-495.588981	-495.576952	-495.625443
TS-30+CP	-495.573401	-495.584537	-495.572457	-495.621044
TS-31+CP	-463.738573	-463.749423	-463.737628	-463.784925
TS-32+CP	-569.523751	-569.535512	-569.522807	-569.573579
TS-36+CP	-502.965648	-502.978018	-502.964704	-503.015082
TS-40+CP	-481.907749	-481.920042	-481.906805	-481.956967
TS-41+CP	-423.301150	-423.309342	-423.300206	-423.342391
TS-42+CP	-462.531473	-462.541425	-462.530528	-462.576593
TS-43+CP	-462.531422	-462.541118	-462.530478	-462.575631
TS-44+CP	-515.427902	-515.437897	-515.426957	-515.473414
TS-45+CP	-882.464364	-882.473815	-882.463420	-882.509056
TS-47+CP	-501.762539	-501.774062	-501.761595	-501.810693
TS-48+CP	-462.564802	-462.573837	-462.563858	-462.607909
TS-49+CP	-501.793955	-501.804656	-501.793011	-501.840503
TS-50+CP	-501.794476	-501.804942	-501.793532	-501.840206
TS-52+CP	-921.725582	-921.735833	-921.724638	-921.771709
TS-55+CP	-572.483212	-572.492480	-572.482268	-572.527292
TS-56+CP	-498.496278	-498.504897	-498.495333	-498.538653
TS-57+CP	-501.789729	-501.799805	-501.788785	-501.835145

Table S30. CBS-QB3 activation energies ($\Delta E^{\ddagger}$), zero-point corrected energies ($\Delta ZPE^{\ddagger}$), enthalpies ($\Delta H^{\ddagger}$) and Gibbs free energies ($\Delta G^{\ddagger}$) computed for the reactions between the selected 35 dienophiles and **CP** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta ZPE^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$
TS-4+CP	8.2	8.4	7.6	21.5
TS-7+CP	7.3	7.4	6.7	20.5
TS-10+CP	12.3	12.6	11.7	25.7
TS-11+CP	7.3	7.5	6.7	20.5
TS-14+CP	10.7	10.9	10.1	23.9
TS-15+CP	3.7	3.8	3.1	16.8
TS-17+CP	7.7	7.9	7.2	21.0
TS-18+CP	7.3	7.5	6.7	20.5
TS-19+CP	14.6	14.9	14.1	27.9
TS-21+CP	8.1	8.2	7.5	21.8
TS-22+CP	10.9	11.4	10.4	25.4
TS-23+CP	9.5	9.7	8.9	23.2
TS-24+CP	-0.5	-0.3	-1.1	13.8
TS-25+CP	4.0	4.2	3.4	18.0
TS-26+CP	3.7	3.7	3.1	17.0
TS-28+CP	15.1	15.3	14.5	28.8
TS-29+CP	9.1	9.3	8.5	22.7
TS-30+CP	10.5	10.6	9.9	24.1
TS-31+CP	14.8	15.2	14.2	29.2
TS-32+CP	3.2	3.2	2.6	16.4
TS-36+CP	14.5	15.0	13.9	29.8
TS-40+CP	16.1	16.5	15.5	31.0
TS-41+CP	10.5	10.7	9.9	23.6
TS-42+CP	12.6	12.8	12.0	26.0
TS-43+CP	12.5	12.4	11.9	25.4
TS-44+CP	6.0	6.1	5.4	19.3
TS-45+CP	9.9	10.0	9.3	23.2
TS-47+CP	14.9	15.1	14.3	28.9
TS-48+CP	13.2	13.4	12.6	26.7
TS-49+CP	15.5	15.8	14.9	29.6
TS-50+CP	15.6	16.0	15.0	29.9
TS-52+CP	12.9	13.0	12.3	26.8
TS-55+CP	4.3	4.4	3.7	17.5
TS-56+CP	12.1	12.3	11.6	25.4
TS-57+CP	14.9	15.1	14.3	28.4

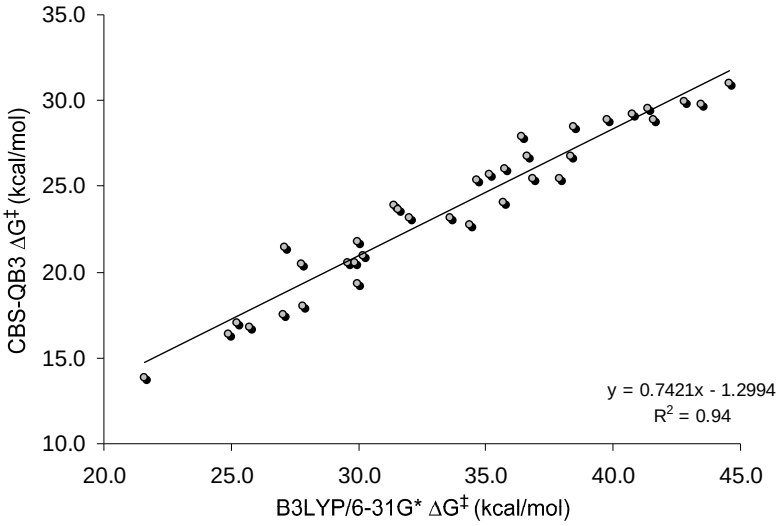


Figure S6. Plot of CBS-QB3 $\Delta G^{\ddagger}$ versus B3LYP/6-31G* $\Delta G^{\ddagger}$ correspondig to the reactions between the 35 selected dienophiles and **CP**.

Table S31. M06-2X/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for **CP** and the selected 35 dienophiles (in au).

	E	ZPE	H	G
CP	-194.004693	-193.910657	-193.905597	-193.937243
4	-282.962581	-282.906413	-282.900828	-282.934127
7	-1023.214772	-1023.164766	-1023.158101	-1023.195188
10	-231.117199	-231.026118	-231.019383	-231.054865
11	-284.030611	-283.969023	-283.962175	-283.998460
14	-257.740933	-257.616752	-257.607883	-257.648447
15	-310.646135	-310.551400	-310.542459	-310.583643
17	-262.961226	-262.910242	-262.903804	-262.939397
18	-262.962634	-262.911943	-262.905288	-262.940968
19	-210.053079	-209.972949	-209.966410	-210.001231
21	-528.754735	-528.686080	-528.677703	-528.718869
22	-221.879282	-221.729555	-221.719636	-221.763233
23	-1062.515689	-1062.437373	-1062.429063	-1062.470490
24	-487.373433	-487.313731	-487.305741	-487.346578
25	-455.545928	-455.461332	-455.453129	-455.493884
26	-355.160575	-355.110942	-355.102782	-355.142940
28	-249.349228	-249.240641	-249.232506	-249.271823
29	-302.264534	-302.185255	-302.177210	-302.216543
30	-302.261800	-302.182620	-302.174614	-302.213821
31	-270.414898	-270.295366	-270.287206	-270.326333
32	-376.230838	-376.170437	-376.161993	-376.202871
36	-309.710792	-309.562690	-309.552965	-309.595883
40	-288.648438	-288.511521	-288.501892	-288.544716
41	-229.888051	-229.818883	-229.813640	-229.845860
42	-269.189604	-269.092321	-269.085286	-269.122248
43	-269.191197	-269.093873	-269.087015	-269.123233
44	-322.100628	-322.032541	-322.025643	-322.062520
45	-689.458779	-689.398687	-689.392412	-689.428226
47	-308.492546	-308.367274	-308.359361	-308.398356
48	-269.225422	-269.125998	-269.119899	-269.154679
49	-308.526470	-308.399059	-308.391117	-308.430740
50	-308.526837	-308.399675	-308.391814	-308.431035
52	-728.794295	-728.704409	-728.697109	-728.735819
55	-379.143394	-379.086565	-379.080472	-379.115631
56	-305.137444	-305.061397	-305.055815	-305.089368
57	-308.522697	-308.393498	-308.386492	-308.423389

Table S32. M06-2X/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G) computed for the transition structures of the reactions between the selected 35 dienophiles and **CP** (in au).

	E	ZPE	H	G
TS-4+CP	-476.959270	-476.805856	-476.796698	-476.839088
TS-7+CP	-1217.211807	-1217.064422	-1217.054111	-1217.099939
TS-10+CP	-425.102716	-424.914481	-424.904270	-424.948509
TS-11+CP	-478.025201	-477.866692	-477.856199	-477.901733
TS-14+CP	-451.730810	-451.508953	-451.496706	-451.545689
TS-15+CP	-504.648387	-504.456446	-504.443855	-504.494190
TS-17+CP	-456.954796	-456.807196	-456.796923	-456.841865
TS-18+CP	-456.957371	-456.809670	-456.799408	-456.844300
TS-19+CP	-404.036180	-403.859059	-403.848958	-403.893069
TS-21+CP	-722.749610	-722.584291	-722.572161	-722.622100
TS-22+CP	-415.867869	-415.620525	-415.607480	-415.657405
TS-23+CP	-1256.506722	-1256.331280	-1256.319398	-1256.368545
TS-24+CP	-681.383887	-681.226746	-681.215191	-681.263644
TS-25+CP	-649.546839	-649.365346	-649.353444	-649.402287
TS-26+CP	-549.163304	-549.017122	-549.004990	-549.054233
TS-28+CP	-443.330038	-443.124582	-443.112934	-443.160063
TS-29+CP	-496.254889	-496.078741	-496.067015	-496.114804
TS-30+CP	-496.249461	-496.073398	-496.061641	-496.109461
TS-31+CP	-464.396314	-464.179872	-464.168299	-464.215192
TS-32+CP	-570.234231	-570.077239	-570.064853	-570.114751
TS-36+CP	-503.691039	-503.445874	-503.432810	-503.482884
TS-40+CP	-482.626208	-482.392437	-482.379537	-482.428981
TS-41+CP	-423.877135	-423.711338	-423.702453	-423.744120
TS-42+CP	-463.174482	-462.980320	-462.969724	-463.015062
TS-43+CP	-463.174028	-462.979901	-462.969524	-463.014195
TS-44+CP	-516.095693	-515.931097	-515.920421	-515.966331
TS-45+CP	-883.448451	-883.292082	-883.281988	-883.326793
TS-47+CP	-502.472014	-502.249882	-502.237672	-502.286239
TS-48+CP	-463.210253	-463.013998	-463.004339	-463.047621
TS-49+CP	-502.506736	-502.282568	-502.271155	-502.318285
TS-50+CP	-502.506149	-502.281722	-502.270535	-502.316797
TS-52+CP	-922.778552	-922.591869	-922.580957	-922.627376
TS-55+CP	-573.142729	-572.988972	-572.979105	-573.023273
TS-56+CP	-499.124659	-498.951488	-498.942252	-498.984810
TS-57+CP	-502.504814	-502.278894	-502.268146	-502.313950

Table S33. M06-2X/6-31G* activation energies ($\Delta E^{\ddagger}$), zero-point corrected energies ($\Delta ZPE^{\ddagger}$), enthalpies ($\Delta H^{\ddagger}$) and Gibbs free energies ($\Delta G^{\ddagger}$) computed for the reactions between the selected 35 dienophiles and **CP** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta ZPE^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$
TS-4+CP	5.0	7.0	6.1	20.3
TS-7+CP	4.8	6.9	6.0	20.4
TS-10+CP	12.0	14.0	13.0	27.4
TS-11+CP	6.3	8.2	7.3	21.3
TS-14+CP	9.3	11.6	10.5	25.1
TS-15+CP	1.5	3.5	2.6	16.8
TS-17+CP	7.0	8.6	7.8	21.8
TS-18+CP	6.2	8.1	7.2	21.3
TS-19+CP	13.5	15.4	14.5	28.5
TS-21+CP	6.2	7.8	7.0	21.3
TS-22+CP	10.1	12.4	11.1	27.0
TS-23+CP	8.6	10.5	9.6	24.6
TS-24+CP	-3.6	-1.5	-2.4	12.7
TS-25+CP	2.4	4.2	3.3	18.1
TS-26+CP	1.2	2.8	2.1	16.3
TS-28+CP	15.0	16.8	15.8	30.7
TS-29+CP	9.0	10.8	9.9	24.5
TS-30+CP	10.7	12.5	11.7	26.1
TS-31+CP	14.6	16.4	15.4	30.4
TS-32+CP	0.8	2.4	1.7	15.9
TS-36+CP	15.3	17.2	16.2	31.5
TS-40+CP	16.9	18.7	17.5	33.2
TS-41+CP	9.8	11.4	10.5	24.5
TS-42+CP	12.4	14.2	13.3	27.9
TS-43+CP	13.7	15.5	14.5	29.0
TS-44+CP	6.0	7.6	6.8	21.0
TS-45+CP	9.4	10.8	10.1	24.3
TS-47+CP	15.8	17.6	17.1	31.0
TS-48+CP	12.5	14.2	13.3	27.8
TS-49+CP	15.3	17.0	16.0	31.2
TS-50+CP	15.9	18.0	16.9	32.3
TS-52+CP	12.8	14.6	13.6	28.7
TS-55+CP	3.4	5.2	4.4	18.6
TS-56+CP	11.0	12.9	12.0	26.2
TS-57+CP	14.2	15.9	15.0	29.3

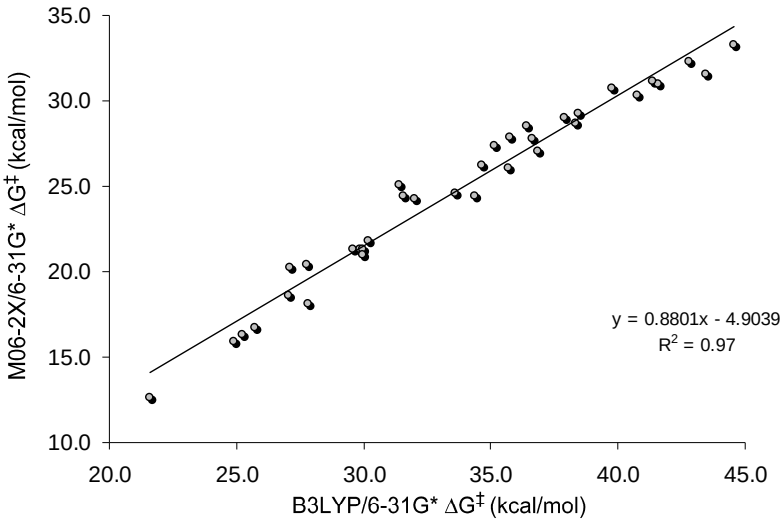


Figure S7. Plot of M06-2X/6-31G* $\Delta G^{\ddagger}$ versus B3LYP/6-31G* $\Delta G^{\ddagger}$ correspondig to the reactions between the 35 selected dienophiles and **CP**.

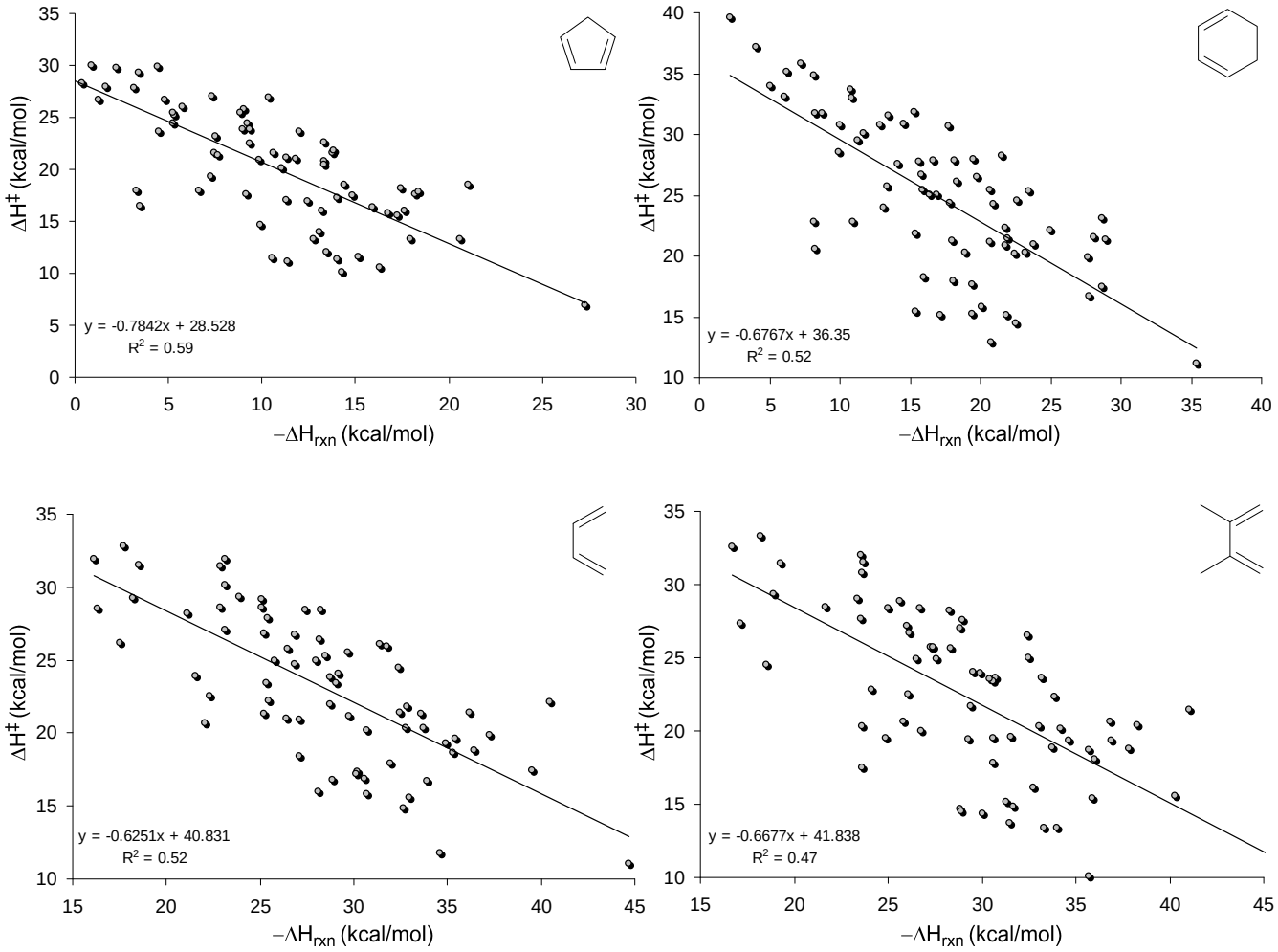


Figure S8. Plots of $\Delta H^{\ddagger}$ versus $-\Delta H_{rxn}$ correspondig to the reactions between **1-70** and the four dienes under study.

Table S34. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), diene distortion energy ($\Delta E_d^{\ddagger}{}_{\text{-diene}}$), dienophile distortion energy ($\Delta E_d^{\ddagger}{}_{\text{-C=C}}$), total distortion energy ($\Delta E_d^{\ddagger}$) and interaction energy ($\Delta E_i^{\ddagger}$) computed for the reactions of **1-70** and **CP** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta E_d^{\ddagger}{}_{\text{-diene}}$	$\Delta E_d^{\ddagger}{}_{\text{-C=C}}$	$\Delta E_d^{\ddagger}$	$\Delta E_i^{\ddagger}$
TS-1+CP	16.4	15.3	9.6	24.8	-8.4
TS-2+CP	16.3	16.1	9.2	25.3	-9.0
TS-3+CP	10.3	14.3	10.3	24.6	-14.3
TS-4+CP	12.1	13.4	9.9	23.3	-11.2
TS-5+CP	17.5	15.6	10.1	25.7	-8.2
TS-6+CP	15.6	16.8	7.7	24.5	-9.0
TS-7+CP	12.6	14.9	8.9	23.8	-11.2
TS-8+CP	16.1	16.1	11.9	28.0	-11.9
TS-9+CP	19.8	17.6	11.4	29.0	-9.2
TS-10+CP	20.0	17.4	11.6	29.0	-9.0
TS-11+CP	14.9	17.6	11.0	28.6	-13.7
TS-12+CP	8.8	13.4	12.1	25.5	-16.8
TS-13+CP	13.3	15.6	12.0	27.6	-14.3
TS-14+CP	16.2	16.3	14.7	31.0	-14.8
TS-15+CP	10.7	17.7	12.5	30.2	-19.6
TS-16+CP	9.3	12.1	10.6	22.7	-13.4
TS-17+CP	15.3	16.4	11.4	27.7	-12.5
TS-18+CP	14.6	16.3	12.0	28.3	-13.6
TS-19+CP	21.5	16.5	13.4	30.0	-8.4
TS-20+CP	20.5	16.1	12.1	28.3	-7.8
TS-21+CP	14.5	16.2	12.7	28.9	-14.3
TS-22+CP	20.3	18.6	11.1	29.7	-9.4
TS-23+CP	18.0	16.7	12.9	29.6	-11.6
TS-24+CP	5.6	13.6	11.0	24.6	-19.0
TS-25+CP	12.1	16.3	10.2	26.6	-14.5
TS-26+CP	10.2	14.8	13.8	28.6	-18.4
TS-27+CP	24.8	17.3	15.5	32.8	-8.0
TS-28+CP	24.5	17.3	15.0	32.3	-7.8
TS-29+CP	19.1	17.2	14.3	31.5	-12.4
TS-30+CP	20.5	17.5	15.0	32.5	-12.0
TS-31+CP	25.0	19.0	15.2	34.2	-9.2
TS-32+CP	9.9	16.2	12.3	28.5	-18.5
TS-33+CP	10.5	18.6	16.8	35.4	-24.9
TS-34+CP	16.8	17.0	18.0	35.0	-18.2
TS-35+CP	16.8	19.6	16.5	36.1	-19.3
TS-36+CP	27.1	20.0	17.0	37.1	-10.0
TS-37+CP	15.1	22.1	17.1	39.2	-24.0
TS-38+CP	24.2	18.7	17.7	36.4	-12.1
TS-39+CP	24.5	18.7	17.1	35.8	-11.3
TS-40+CP	28.5	18.8	18.0	36.8	-8.3
TS-41+CP	17.0	15.4	10.9	26.4	-9.4
TS-42+CP	20.9	16.8	13.8	30.6	-9.7
TS-43+CP	22.7	16.8	15.1	31.9	-9.2
TS-44+CP	15.1	16.1	12.0	28.1	-13.0
TS-45+CP	17.3	15.4	14.4	29.8	-12.5
TS-46+CP	20.2	17.5	15.4	32.9	-12.7
TS-47+CP	26.2	17.9	17.9	35.8	-9.6
TS-48+CP	21.4	17.8	12.3	30.1	-8.6
TS-49+CP	25.7	19.0	15.8	34.8	-9.2
TS-50+CP	26.8	19.5	16.4	36.0	-9.1
TS-51+CP	20.2	18.8	13.9	32.7	-12.5
TS-52+CP	22.8	18.1	16.3	34.4	-11.5
TS-53+CP	25.7	20.5	17.8	38.3	-12.5
TS-54+CP	30.2	20.6	19.3	39.9	-9.7
TS-55+CP	12.2	16.9	9.8	26.6	-14.5
TS-56+CP	19.7	16.8	11.8	28.6	-8.9
TS-57+CP	23.2	19.0	12.9	31.9	-8.8
TS-58+CP	28.9	21.0	17.6	38.6	-9.7
TS-59+CP	28.7	20.7	17.2	37.9	-9.2
TS-60+CP	22.2	19.8	15.0	34.8	-12.6
TS-61+CP	25.9	19.6	18.3	38.0	-12.1
TS-62+CP	29.0	21.7	19.7	41.3	-12.3
TS-63+CP	33.2	22.5	20.4	42.9	-9.7
TS-64+CP	17.4	16.5	11.2	27.7	-10.3
TS-65+CP	22.7	18.5	15.3	33.7	-11.0
TS-66+CP	23.3	19.1	15.5	34.6	-11.3
TS-67+CP	16.0	17.7	13.0	30.8	-14.8
TS-68+CP	19.4	16.8	15.9	32.7	-13.4
TS-69+CP	22.6	19.8	17.5	37.2	-14.6
TS-70+CP	27.4	20.5	18.3	38.8	-11.5

Table S35. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), diene distortion energy ($\Delta E_d^{\ddagger}{}_{\text{-diene}}$), dienophile distortion energy ($\Delta E_d^{\ddagger}{}_{\text{-C=C}}$), total distortion energy ($\Delta E_d^{\ddagger}$) and interaction energy ($\Delta E_i^{\ddagger}$) computed for the reactions of **1-70** and **CH** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta E_d^{\ddagger}{}_{\text{-diene}}$	$\Delta E_d^{\ddagger}{}_{\text{-C=C}}$	$\Delta E_d^{\ddagger}$	$\Delta E_i^{\ddagger}$
TS-1+CH	21.1	19.7	9.6	29.3	-8.2
TS-2+CH	20.5	20.1	9.0	29.2	-8.7
TS-3+CH	14.0	18.0	10.8	28.8	-14.8
TS-4+CH	16.4	17.6	10.0	27.6	-11.2
TS-5+CH	22.3	19.9	10.6	30.5	-8.2
TS-6+CH	19.1	20.4	7.4	27.8	-8.7
TS-7+CH	16.4	18.5	8.9	27.4	-11.0
TS-8+CH	20.1	19.8	12.2	32.0	-11.9
TS-9+CH	24.1	21.6	11.4	33.0	-8.9
TS-10+CH	23.4	20.3	14.1	34.4	-11.0
TS-11+CH	19.3	22.3	11.1	33.5	-14.2
TS-12+CH	11.7	15.8	13.1	29.0	-17.3
TS-13+CH	17.1	18.8	12.8	31.5	-14.4
TS-14+CH	20.7	20.5	16.6	37.1	-16.4
TS-15+CH	14.7	22.1	12.8	35.0	-20.3
TS-16+CH	13.3	15.2	12.2	27.5	-14.2
TS-17+CH	20.0	21.1	11.3	32.4	-12.4
TS-18+CH	19.3	20.9	12.3	33.2	-13.9
TS-19+CH	27.0	21.6	13.8	35.4	-8.4
TS-20+CH	25.6	20.8	12.5	33.3	-7.7
TS-21+CH	20.0	21.3	13.0	34.3	-14.3
TS-22+CH	24.6	22.8	11.9	34.7	-10.1
TS-23+CH	22.8	20.8	13.9	34.7	-11.9
TS-24+CH	10.0	18.3	11.0	29.3	-19.3
TS-25+CH	17.1	21.1	10.4	31.5	-14.4
TS-26+CH	14.3	18.7	14.8	33.5	-19.2
TS-27+CH	29.9	22.2	16.0	38.1	-8.2
TS-28+CH	30.6	22.8	16.4	39.1	-8.5
TS-29+CH	24.2	22.3	15.0	37.3	-13.2
TS-30+CH	25.9	22.6	15.2	37.8	-11.9
TS-31+CH	29.1	23.3	15.8	39.1	-10.0
TS-32+CH	14.1	20.4	13.4	33.8	-19.6
TS-33+CH	14.6	24.5	17.6	42.1	-27.5
TS-34+CH	21.8	22.1	19.7	41.8	-20.0
TS-35+CH	21.9	25.4	17.2	42.6	-20.7
TS-36+CH	32.3	25.9	18.1	44.0	-11.7
TS-37+CH	19.2	28.0	17.3	45.3	-26.1
TS-38+CH	29.8	24.6	18.6	43.2	-13.4
TS-39+CH	30.8	24.8	18.5	43.3	-12.5
TS-40+CH	35.0	25.0	19.4	44.4	-9.5
TS-41+CH	20.6	19.4	10.2	29.6	-9.0
TS-42+CH	24.7	21.0	13.5	34.5	-9.8
TS-43+CH	27.5	21.8	15.7	37.5	-10.0
TS-44+CH	19.1	20.6	11.8	32.4	-13.3
TS-45+CH	20.7	18.8	14.8	33.6	-12.8
TS-46+CH	24.7	22.8	15.6	38.3	-13.7
TS-47+CH	31.1	23.3	18.8	42.0	-10.9
TS-48+CH	25.2	22.1	11.4	33.6	-8.4
TS-49+CH	29.9	23.7	15.4	39.1	-9.2
TS-50+CH	32.2	25.0	16.3	41.3	-9.1
TS-51+CH	24.5	23.6	13.7	37.3	-12.8
TS-52+CH	26.9	22.1	16.6	38.6	-11.7
TS-53+CH	30.9	26.2	18.1	44.3	-13.4
TS-54+CH	36.3	26.8	20.1	46.9	-10.7
TS-55+CH	15.8	20.8	8.9	29.7	-13.9
TS-56+CH	23.7	21.0	11.0	32.0	-8.3
TS-57+CH	26.9	23.4	12.2	35.5	-8.7
TS-58+CH	32.9	25.3	17.3	42.7	-9.7
TS-59+CH	34.0	26.4	17.2	43.6	-9.6
TS-60+CH	26.7	25.1	15.2	40.3	-13.6
TS-61+CH	29.8	23.8	18.7	42.6	-12.8
TS-62+CH	34.3	28.0	20.2	48.2	-13.9
TS-63+CH	38.9	28.4	21.7	50.1	-11.2
TS-64+CH	21.4	21.0	10.6	31.6	-10.2
TS-65+CH	26.9	22.9	15.1	38.0	-11.1
TS-66+CH	28.6	24.7	15.3	40.0	-11.4
TS-67+CH	20.3	22.6	13.2	35.7	-15.5
TS-68+CH	23.4	20.9	16.8	37.7	-14.2
TS-69+CH	27.8	25.8	18.0	43.8	-16.0
TS-70+CH	33.2	27.0	19.6	46.6	-13.4

Table S36. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), diene distortion energy ($\Delta E_d^{\ddagger}{}_{\text{-diene}}$), dienophile distortion energy ($\Delta E_d^{\ddagger}{}_{\text{-C=C}}$), total distortion energy ($\Delta E_d^{\ddagger}$) and interaction energy ($\Delta E_i^{\ddagger}$) computed for the reactions of **1-70** and **BU** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta E_d^{\ddagger}{}_{\text{-diene}}$	$\Delta E_d^{\ddagger}{}_{\text{-C=C}}$	$\Delta E_d^{\ddagger}$	$\Delta E_i^{\ddagger}$
TS-1+BU	20.4	18.8	9.8	28.7	-8.2
TS-2+BU	19.4	18.5	9.3	27.8	-8.4
TS-3+BU	13.7	16.4	10.1	26.5	-12.9
TS-4+BU	16.3	17.3	9.8	27.1	-10.8
TS-5+BU	21.3	18.7	11.0	29.7	-8.4
TS-6+BU	16.2	17.7	6.8	24.5	-8.3
TS-7+BU	14.8	16.5	8.0	24.5	-9.8
TS-8+BU	17.5	17.1	10.8	27.9	-10.4
TS-9+BU	21.1	18.4	10.7	29.1	-8.0
TS-10+BU	23.2	20.1	11.4	31.5	-8.3
TS-11+BU	19.3	20.5	10.7	31.3	-12.0
TS-12+BU	10.4	14.4	10.1	24.5	-14.1
TS-13+BU	14.9	16.1	10.9	27.0	-12.1
TS-14+BU	19.9	18.3	14.8	33.1	-13.2
TS-15+BU	15.6	20.1	12.3	32.4	-16.7
TS-16+BU	14.4	15.4	11.0	26.5	-12.0
TS-17+BU	20.4	20.1	11.6	31.7	-11.4
TS-18+BU	19.4	19.9	11.5	31.4	-12.1
TS-19+BU	25.0	20.3	12.8	33.1	-8.1
TS-20+BU	23.6	18.9	12.0	30.9	-7.3
TS-21+BU	18.4	18.8	12.0	30.7	-12.3
TS-22+BU	21.0	19.5	10.3	29.9	-8.9
TS-23+BU	20.3	18.4	11.9	30.3	-10.1
TS-24+BU	9.8	16.2	9.6	25.8	-16.0
TS-25+BU	17.0	19.6	10.3	30.0	-13.0
TS-26+BU	16.2	18.3	13.5	31.8	-15.7
TS-27+BU	27.6	21.2	14.9	36.1	-8.5
TS-28+BU	27.6	20.3	14.6	35.0	-7.4
TS-29+BU	24.3	20.8	14.6	35.3	-11.1
TS-30+BU	24.7	20.9	14.3	35.2	-10.5
TS-31+BU	27.8	20.9	15.5	36.4	-8.5
TS-32+BU	15.8	19.5	12.2	31.7	-15.9
TS-33+BU	17.5	22.1	16.0	38.1	-20.6
TS-34+BU	22.5	20.3	17.3	37.7	-15.2
TS-35+BU	21.6	22.4	15.2	37.6	-16.0
TS-36+BU	27.6	21.2	15.9	37.2	-9.6
TS-37+BU	19.4	24.1	15.6	39.6	-20.2
TS-38+BU	28.5	21.9	17.2	39.1	-10.6
TS-39+BU	28.3	21.7	16.4	38.1	-9.8
TS-40+BU	31.2	22.2	17.7	39.9	-8.8
TS-41+BU	19.1	17.6	10.5	28.1	-9.1
TS-42+BU	21.2	18.8	12.4	31.3	-10.1
TS-43+BU	25.4	19.1	14.8	33.9	-8.5
TS-44+BU	18.9	18.8	11.7	30.5	-11.6
TS-45+BU	18.0	16.4	12.6	29.1	-11.1
TS-46+BU	22.7	20.0	14.5	34.5	-11.7
TS-47+BU	27.3	19.4	17.2	36.6	-9.3
TS-48+BU	24.0	21.3	11.7	33.0	-9.0
TS-49+BU	26.1	21.5	13.9	35.3	-9.2
TS-50+BU	29.4	22.8	15.6	38.4	-9.1
TS-51+BU	24.0	21.6	13.5	35.0	-11.0
TS-52+BU	23.8	19.8	14.5	34.2	-10.5
TS-53+BU	28.4	23.8	16.3	40.1	-11.7
TS-54+BU	31.2	22.1	17.8	39.9	-8.7
TS-55+BU	15.8	19.4	9.2	28.6	-12.9
TS-56+BU	22.9	19.8	11.3	31.0	-8.2
TS-57+BU	25.5	22.2	12.5	34.7	-9.3
TS-58+BU	27.7	21.5	15.1	36.6	-8.9
TS-59+BU	30.5	23.7	16.2	40.0	-9.4
TS-60+BU	25.9	23.8	14.5	38.3	-12.4
TS-61+BU	24.8	20.5	15.9	36.3	-11.5
TS-62+BU	30.7	25.3	17.5	42.9	-12.2
TS-63+BU	32.0	23.1	18.4	41.5	-9.5
TS-64+BU	20.5	19.3	10.8	30.1	-9.6
TS-65+BU	23.2	19.4	13.2	32.6	-9.4
TS-66+BU	25.9	21.3	14.4	35.7	-9.8
TS-67+BU	20.3	20.7	12.4	33.2	-12.9
TS-68+BU	19.9	19.0	13.4	32.5	-12.6
TS-69+BU	25.3	22.6	15.5	38.1	-12.7
TS-70+BU	27.6	22.6	16.4	39.0	-11.4

Table S37. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), diene distortion energy ($\Delta E_d^{\ddagger}{}_{-diene}$), dienophile distortion energy ($\Delta E_d^{\ddagger}{}_{-C=C}$), total distortion energy ($\Delta E_d^{\ddagger}$) and interaction energy ($\Delta E_i^{\ddagger}$) computed for the reactions of **1-70** and **DMB** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta E_d^{\ddagger}{}_{-diene}$	$\Delta E_d^{\ddagger}{}_{-C=C}$	$\Delta E_d^{\ddagger}$	$\Delta E_i^{\ddagger}$
TS-1+DMB	19.9	18.9	10.0	28.9	-9.0
TS-2+DMB	19.5	18.5	9.6	28.1	-8.6
TS-3+DMB	12.6	15.9	10.4	26.3	-13.7
TS-4+DMB	14.8	16.7	10.7	27.4	-12.5
TS-5+DMB	20.9	19.0	11.0	30.0	-9.1
TS-6+DMB	16.8	18.1	7.3	25.4	-8.6
TS-7+DMB	14.4	16.5	8.5	24.9	-10.5
TS-8+DMB	17.2	16.9	11.0	27.8	-10.6
TS-9+DMB	21.2	18.2	11.0	29.1	-8.0
TS-10+DMB	23.4	20.0	11.7	31.7	-8.3
TS-11+DMB	18.9	20.7	10.9	31.6	-12.7
TS-12+DMB	9.1	13.8	9.9	23.7	-14.6
TS-13+DMB	13.9	15.6	11.0	26.5	-12.7
TS-14+DMB	18.8	17.8	15.3	33.1	-14.3
TS-15+DMB	14.0	19.8	12.8	32.6	-18.6
TS-16+DMB	12.5	15.0	10.6	25.6	-13.1
TS-17+DMB	18.8	20.5	11.6	32.1	-13.3
TS-18+DMB	18.2	20.2	11.4	31.6	-13.4
TS-19+DMB	24.6	20.4	12.9	33.3	-8.7
TS-20+DMB	23.2	18.9	11.8	30.7	-7.6
TS-21+DMB	18.2	18.9	12.2	31.1	-12.9
TS-22+DMB	21.8	19.9	10.8	30.7	-8.9
TS-23+DMB	20.0	18.3	12.4	30.7	-10.7
TS-24+DMB	8.0	16.4	9.7	26.1	-18.2
TS-25+DMB	15.5	19.8	11.0	30.8	-15.3
TS-26+DMB	13.1	18.1	13.2	31.3	-18.2
TS-27+DMB	27.7	20.3	14.9	35.2	-7.5
TS-28+DMB	27.0	20.3	14.6	34.9	-7.9
TS-29+DMB	23.5	21.2	14.4	35.5	-12.0
TS-30+DMB	23.1	21.2	14.1	35.3	-12.2
TS-31+DMB	28.3	21.3	15.5	36.8	-8.5
TS-32+DMB	13.7	19.2	12.4	31.6	-17.9
TS-33+DMB	14.0	22.7	15.8	38.5	-24.5
TS-34+DMB	19.4	20.2	17.4	37.5	-18.2
TS-35+DMB	19.7	22.6	15.4	38.0	-18.3
TS-36+DMB	28.1	21.4	16.0	37.4	-9.4
TS-37+DMB	16.6	24.9	15.7	40.6	-24.0
TS-38+DMB	27.9	22.1	16.9	39.1	-11.1
TS-39+DMB	26.7	22.3	16.1	38.4	-11.7
TS-40+DMB	31.2	21.5	17.5	39.0	-7.8
TS-41+DMB	20.0	18.0	10.8	28.8	-8.8
TS-42+DMB	22.0	18.2	12.7	30.9	-8.9
TS-43+DMB	26.2	19.6	14.8	34.4	-8.2
TS-44+DMB	18.9	19.3	11.4	30.7	-11.8
TS-45+DMB	18.3	16.4	12.8	29.2	-10.9
TS-46+DMB	23.0	20.5	14.2	34.7	-11.7
TS-47+DMB	28.1	19.6	17.4	37.0	-9.0
TS-48+DMB	25.1	20.8	12.1	32.9	-7.8
TS-49+DMB	27.1	21.1	14.2	35.3	-8.1
TS-50+DMB	30.3	22.4	15.8	38.2	-7.9
TS-51+DMB	24.5	22.0	13.4	35.5	-10.9
TS-52+DMB	24.2	20.0	14.9	34.9	-10.7
TS-53+DMB	28.8	23.5	16.1	39.6	-10.8
TS-54+DMB	32.2	22.7	18.0	40.7	-8.5
TS-55+DMB	14.8	20.1	9.3	29.4	-14.6
TS-56+DMB	22.8	20.1	11.6	31.6	-8.8
TS-57+DMB	26.5	21.8	12.7	34.4	-8.0
TS-58+DMB	28.6	21.8	15.4	37.2	-8.6
TS-59+DMB	31.6	23.4	16.4	39.8	-8.2
TS-60+DMB	26.0	23.3	14.5	37.8	-11.8
TS-61+DMB	25.1	20.6	16.1	36.7	-11.6
TS-62+DMB	31.0	25.1	17.3	42.5	-11.5
TS-63+DMB	32.7	23.6	18.5	42.1	-9.4
TS-64+DMB	19.7	19.3	11.0	30.3	-10.6
TS-65+DMB	22.2	19.5	13.4	32.9	-10.7
TS-66+DMB	25.1	21.4	14.6	36.1	-11.0
TS-67+DMB	18.9	20.9	12.5	33.3	-14.5
TS-68+DMB	18.7	17.9	13.4	31.3	-12.6
TS-69+DMB	24.0	22.8	15.3	38.1	-14.1
TS-70+DMB	26.7	21.8	16.5	38.2	-11.6

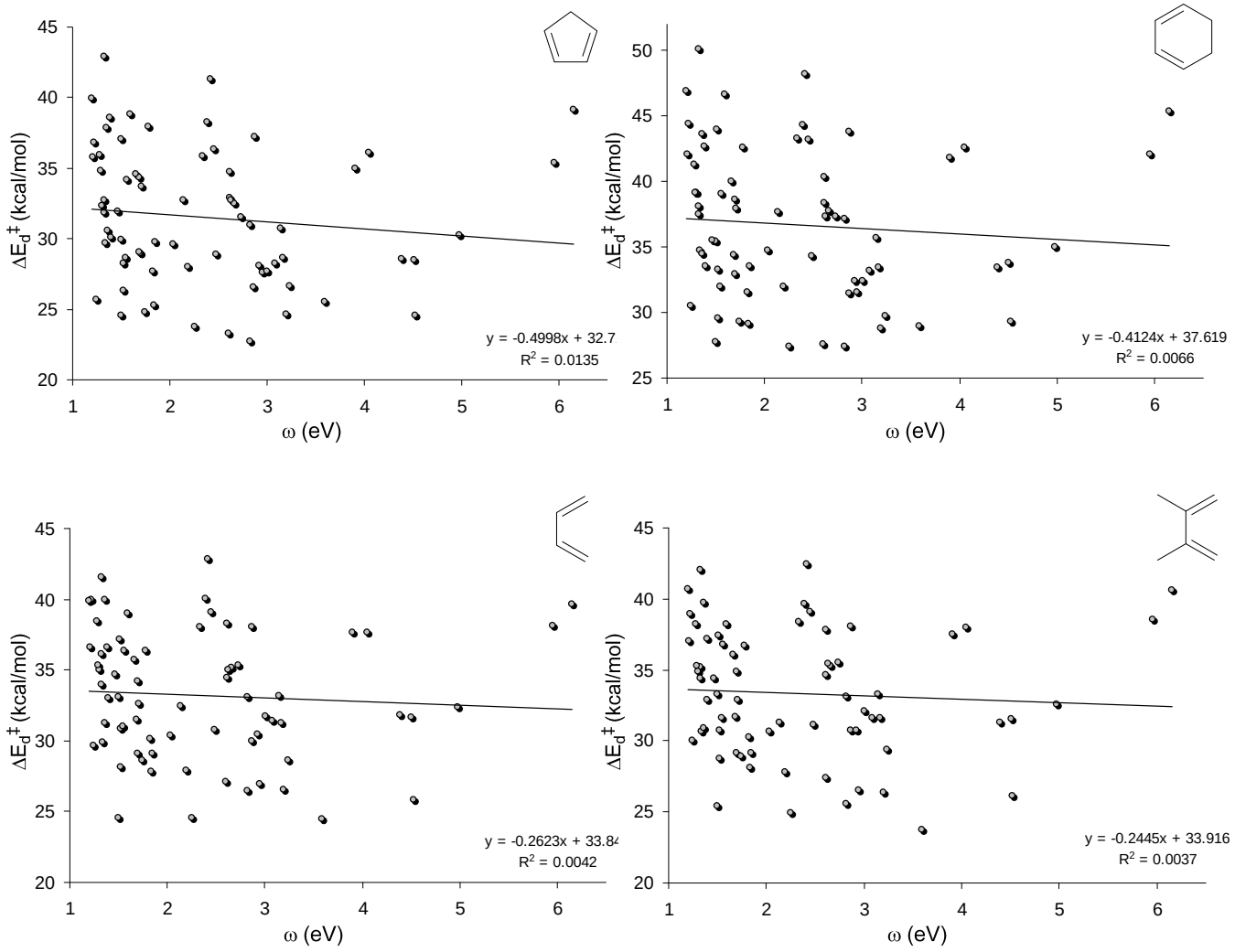


Figure S9. Plots of $\Delta E_d^{\ddagger}$ versus ω correspondig to the reactions between **1-70** and the four dienes under study.

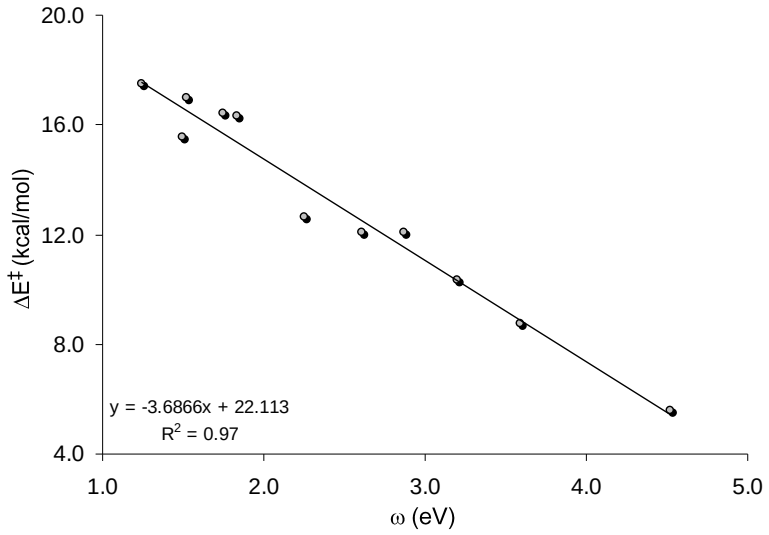


Figure S10. Plots of $\Delta E^{\ddagger}$ versus ω correspondig to the reactions between the similarly distorted TSs corresponding to the reactions of compounds **1-7**, **12**, **24-25** and **41** with **CP**.

Note that when the distortion energy is the same, a good linear correlation between the activation barrier and the electrophilicity is found.

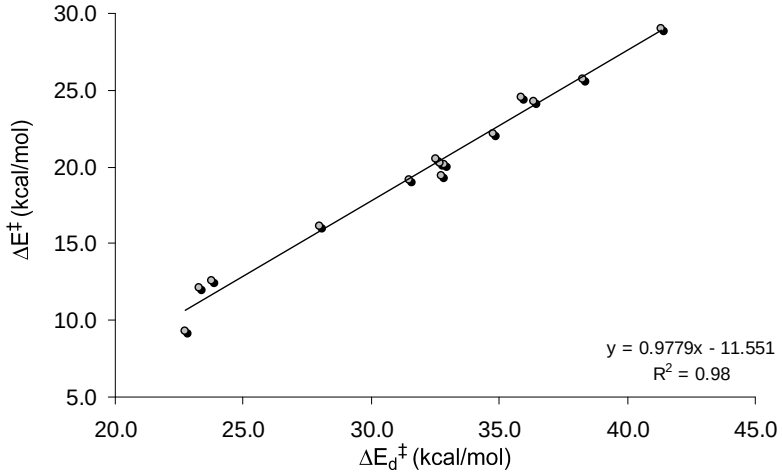


Figure S11. Plots of $\Delta E^{\ddagger}$ versus $\Delta E_d^{\ddagger}$ correspondig to the reactions between the similary electrophilic reagents **4**, **7-8**, **16**, **29-30**, **38-39**, **46**, **51**, **53**, **60**, **62** and **68** (2.1 eV < ω < 2.8 eV) with **CP**.

Note that when the dienophiles display similar ω indices, a good linear correlation between the activation barrier and the distortion energy is found.

Table S38. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), zero-point corrected energies ($\Delta ZPE^{\ddagger}$), enthalpies ($\Delta H^{\ddagger}$) and Gibbs free energies ($\Delta G^{\ddagger}$) computed for the reactions between ethylene (**ET**) and **CP**, **CH**, **BU** and **DMB** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta ZPE^{\ddagger}$	$\Delta H^{\ddagger}$	$\Delta G^{\ddagger}$
TS-ET+CP	19.9	22.3	21.1	34.4
TS-ET+CH	24.3	26.5	25.3	38.6
TS-ET+BU	22.4	24.8	23.4	36.8
TS-ET+DMB	23.4	25.1	24.1	36.9

Table S39. B3LYP/6-31G* activation energies ($\Delta E^{\ddagger}$), diene distortion energy ($\Delta E_d^{\ddagger}{}_{-diene}$), dienophile distortion energy ($\Delta E_d^{\ddagger}{}_{-C=C}$), total distortion energy ($\Delta E_d^{\ddagger}$) and interaction energy ($\Delta E_i^{\ddagger}$) computed for the reactions between ethylene (**ET**) and **CP**, **CH**, **BU** and **DMB** (in kcal/mol).

	$\Delta E^{\ddagger}$	$\Delta E_d^{\ddagger}{}_{-diene}$	$\Delta E_d^{\ddagger}{}_{-C=C}$	$\Delta E_d^{\ddagger}$	$\Delta E_i^{\ddagger}$
TS-ET+CP	19.9	16.4	7.5	23.9	-4.0
TS-ET+CH	24.3	20.8	7.5	28.3	-4.0
TS-ET+BU	22.4	19.6	7.9	27.5	-5.1
TS-ET+DMB	23.4	19.8	8.1	27.9	-4.5

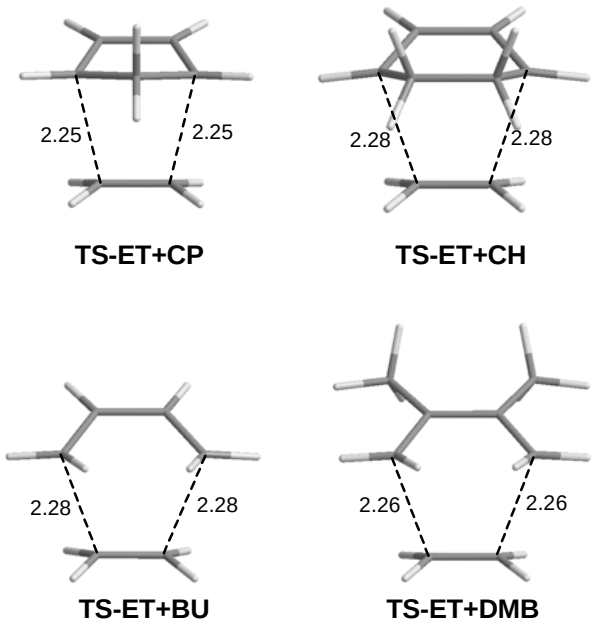


Figure S12. Optimized geometries for the transition structures found for the DA reactions between **ET** and **CP**, **CH**, **BU** and **DMB**.

Table S40. Results obtained by applying ANOVA of the selected most significant factors of the interaction energy ($\Delta E_i^{\ddagger}$)

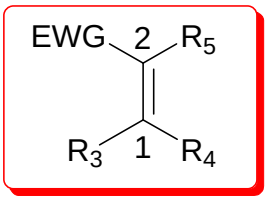
$$-\Delta E_i^{\ddagger} = a.\omega + b.\mathrm{NS} + c$$

Source	Sum of Squares	Mean Square	F value	Prob. > F	Significant
		cyclopentadiene			
ω	843.387368	843.387368	1106.07811	< 0.0001	Yes
NS	14.6690391	14.6690391	19.23802	< 0.0001	Yes
		1,3-cyclohexadiene			
ω	953.43047	953.43047	890.001771	< 0.0001	Yes
NS	58.9957605	58.9957605	55.07096	< 0.0001	Yes
		butadiene			
ω	460.583715	460.583715	743.540003	< 0.0001	Yes
NS	12.1924567	12.1924567	19.6828047	< 0.0001	Yes
		2,3-dimethyl-1,3-butadiene			
ω	852.120631	852.120631	1015.82913	< 0.0001	Yes
NS	6.72604758	6.72604758	8.01824861	0.0061	Yes

Table S41. Results obtained by applying ANOVA of the selected most significant factors of the diene distortion energy ($\Delta E_d^{\ddagger}{}_{-C=C}$) and coefficient values of Equation 4.

$$\Delta E_d^{\ddagger}{}_{-C=C} = a.\Delta d_{C1C2} + b.\Delta\phi + c.\tau + d.\chi_{C1} + e.\chi_{C2} + f.\Delta\phi^2 + g.\chi_{C2}^2 + h.\Delta\phi.\chi_{C1} + i.\Delta\phi.\chi_{C2} + j.\tau.\chi_{C2} + k$$

Source	Coefficient Value	Sum of Squares	Mean Square	F value	Prob. > F	Significant
Δd_{C1C2}	a = 109.4497	40.96231	40.96231	47.81965	< 0.0001	Yes
$\Delta\phi$	b = 5.270745	17.08504	17.08504	19.94518	< 0.0001	Yes
τ	c = 0.23307	32.15027	32.15027	37.53243	< 0.0001	Yes
χ_{C1}	d = -0.50563	8.971235	8.971235	10.47307	0.0014	Yes
χ_{C2}	e = -0.44627	38.47113	38.47113	44.91144	< 0.0001	Yes
$\Delta\phi^2$	f = -3.11435	43.29541	43.29541	50.54332	< 0.0001	Yes
χ_{C2}^2	g = 0.008037	32.4202	32.4202	37.84754	< 0.0001	Yes
$\Delta\phi.\chi_{C1}$	h = -0.43904	65.42868	65.42868	76.38184	< 0.0001	Yes
$\Delta\phi.\chi_{C2}$	I = -0.17773	27.64464	27.64464	32.27253	< 0.0001	Yes
$\tau.\chi_{C2}$	j = -0.00822	19.9772	19.9772	23.32151	< 0.0001	Yes
-	k = 11.71181	-	-	-	-	-



Bending angles:

$\phi_1 = \angle\ R_3\text{-}C_1\text{-}R_4$
$\phi_2 = \angle\ R_3\text{-}C_1\text{-}C_2$
$\phi_3 = \angle\ R_4\text{-}C_1\text{-}C_2$
$\phi_4 = \angle\ R_5\text{-}C_2\text{-}EWG$
$\phi_5 = \angle\ R_5\text{-}C_2\text{-}C_1$
$\phi_6 = \angle\ C_1\text{-}C_2\text{-}EWG$

Dihedral angles:

$\theta_1 = \angle\ R_3\text{-}C_1\text{-}C_2\text{-}EWG$
$\theta_2 = \angle\ R_4\text{-}C_1\text{-}C_2\text{-}R_5$
$\theta_3 = \angle\ R_4\text{-}C_1\text{-}C_2\text{-}EWG$
$\theta_4 = \angle\ R_3\text{-}C_1\text{-}C_2\text{-}R_5$

Out-of-plane deformations:

$\tau = (\theta_1+\theta_2)/2$
$\chi_{C1} = \theta_1 - \theta_3 + \pi(\text{mod } 2\pi)$
$= -\theta_2 + \theta_4 + \pi(\text{mod } 2\pi)$
$\chi_{C2} = \theta_2 - \theta_3 + \pi(\text{mod } 2\pi)$
$= -\theta_1 + \theta_4 + \pi(\text{mod } 2\pi)$

Figure S13. Definition of the bending angles, dihedral angles and out-of-plane deformations for the strained dienophiles.

Table S42. Δd_{C1C2}, $\Delta\phi$, $\theta_{1\text{-}4}$, τ, χ_{C1} and χ_{C1} values for the dienophile fragments derived from the transition structures of **CP**.

fragment from	Δd_{C1C2}	$\Delta\phi$	θ_1	θ_2	θ_3	θ_4	τ	χ_{C1}	χ_{C2}
TS-1+CP	0.063	-1.93	-7.0	9.8	-152.0	154.8	1.4	35.0	18.2
TS-2+CP	0.063	-1.85	-6.1	13.7	-150.6	158.2	3.8	35.5	15.8
TS-3+CP	0.066	-1.99	-15.0	18.0	-155.7	158.7	1.5	39.3	6.3
TS-4+CP	0.064	-1.87	-13.1	8.4	-157.4	152.7	-2.3	35.7	14.2
TS-5+CP	0.060	-1.94	5.0	2.7	-147.7	155.4	3.9	27.4	29.6
TS-6+CP	0.060	-1.39	-13.5	16.4	-159.9	162.8	1.4	33.6	3.7
TS-7+CP	0.062	-1.65	-13.4	17.7	-157.3	161.5	2.1	36.1	5.1
TS-8+CP	0.069	-2.48	-12.5	13.0	-151.3	151.8	0.3	41.2	15.7
TS-9+CP	0.069	-2.32	-11.2	9.7	-152.0	150.5	-0.8	39.1	18.3
TS-10+CP	0.065	-2.22	-0.6	17.7	-142.9	160.0	8.5	37.7	19.4
TS-11+CP	0.068	-2.09	6.7	4.9	-145.0	156.5	5.8	28.3	30.2
TS-12+CP	0.070	-2.44	-22.3	16.4	-159.1	153.3	-2.9	43.2	4.5
TS-13+CP	0.071	-2.32	-19.8	13.8	-157.7	151.7	-3.0	42.0	8.5
TS-14+CP	0.070	-2.37	-10.2	22.3	-148.2	160.3	6.1	42.0	9.5
TS-15+CP	0.072	-2.23	-7.6	15.2	-148.5	156.2	3.8	39.1	16.3
TS-16+CP	0.069	-2.25	-17.7	14.6	-156.8	153.7	-1.6	40.9	8.6
TS-17+CP	0.067	-2.16	0.0	0.0	-150.1	150.1	0.0	29.9	29.9
TS-18+CP	0.068	-2.25	5.2	3.0	-145.7	154.0	4.1	29.1	31.3
TS-19+CP	0.067	-2.36	-0.5	13.8	-143.4	156.7	6.7	37.1	22.8
TS-20+CP	0.068	-2.37	-11.6	3.1	-154.3	145.8	-4.2	37.3	22.6
TS-21+CP	0.066	-2.42	-1.5	19.2	-141.2	158.9	8.8	40.3	19.6
TS-22+CP	0.064	-1.72	-9.8	21.3	-153.0	164.5	5.8	36.9	5.7
TS-23+CP	0.066	-2.03	-9.3	22.6	-149.9	163.2	6.6	39.5	7.5
TS-24+CP	0.064	-2.15	-0.4	-1.6	148.8	-150.8	-1.0	30.8	29.6
TS-25+CP	0.070	-1.78	17.2	-5.5	159.3	-147.6	5.8	37.9	15.2
TS-26+CP	0.075	-2.60	-18.3	9.0	-155.6	146.3	-4.6	42.7	15.4
TS-27+CP	0.072	-2.66	-15.7	-2.1	-156.9	139.1	-8.9	38.8	25.2
TS-28+CP	0.073	-2.67	-4.9	7.6	-146.3	149.0	1.3	38.6	26.1
TS-29+CP	0.072	-2.55	-0.3	3.7	-146.2	149.7	1.7	34.1	30.0
TS-30+CP	0.072	-2.63	-7.2	-6.0	-153.7	140.5	-6.6	33.5	32.3
TS-31+CP	0.068	-2.43	-3.6	13.1	-144.7	154.1	4.7	39.0	22.3
TS-32+CP	0.077	-2.46	-6.6	18.9	-145.0	157.3	6.1	41.6	16.1
TS-33+CP	0.085	-2.77	0.0	0.0	-146.6	146.6	0.0	33.4	33.4
TS-34+CP	0.082	-2.91	11.7	-14.5	147.2	-150.0	-1.4	44.6	18.3
TS-35+CP	0.086	-2.72	-10.6	9.8	-149.0	148.3	-0.4	41.6	21.2
TS-36+CP	0.077	-2.76	-15.0	6.4	-152.2	143.6	-4.3	42.8	21.4
TS-37+CP	0.086	-2.64	-4.8	-1.1	-150.4	144.5	-3.0	34.4	30.7
TS-38+CP	0.078	-2.91	-6.7	-3.2	-150.5	140.6	-5.0	36.1	32.7
TS-39+CP	0.077	-2.92	0.0	0.0	-145.1	145.1	0.0	34.9	34.9
TS-40+CP	0.077	-2.98	-9.3	3.0	-148.7	142.4	-3.2	40.6	28.3
TS-41+CP	0.063	-2.84	0.1	17.8	-141.6	159.4	8.9	38.4	20.7
TS-42+CP	0.070	-3.52	-1.7	12.4	-140.8	151.5	5.3	40.9	26.8
TS-43+CP	0.067	-3.46	1.1	19.5	-136.7	157.3	10.3	42.2	23.8
TS-44+CP	0.068	-3.28	1.9	3.3	-144.3	149.5	2.6	33.8	32.4
TS-45+CP	0.067	-3.97	-0.8	20.4	-136.0	155.6	9.8	44.9	23.6
TS-46+CP	0.074	-3.93	0.2	0.7	-143.0	143.8	0.4	36.8	36.4
TS-47+CP	0.073	-4.11	-0.7	13.3	-137.0	149.6	6.3	43.8	29.7
TS-48+CP	0.067	-2.51	-6.5	11.0	-148.6	153.1	2.2	37.9	20.4
TS-49+CP	0.073	-3.05	-10.4	4.4	-150.2	144.2	-3.0	40.2	25.4
TS-50+CP	0.070	-2.98	-3.4	14.1	-142.4	153.1	5.3	41.0	23.5
TS-51+CP	0.071	-2.90	-0.2	0.8	-146.8	147.4	0.3	33.3	32.4
TS-52+CP	0.073	-3.36	-9.1	8.5	-146.7	146.1	-0.3	42.4	24.8
TS-53+CP	0.077	-3.36	-4.5	-3.3	-148.3	140.4	-3.9	36.3	35.0
TS-54+CP	0.075	-3.46	-7.8	7.1	-144.9	144.2	-0.3	42.9	28.0
TS-55+CP	0.063	-2.08	0.0	0.0	-151.7	151.7	0.0	28.3	28.3
TS-56+CP	0.064	-2.55	-7.0	8.7	-149.6	151.2	0.8	37.4	21.7
TS-57+CP	0.068	-2.38	-4.0	10.9	-146.3	153.3	3.5	37.6	22.8
TS-58+CP	0.074	-2.94	-12.0	4.0	-150.5	142.4	-4.0	41.5	25.6
TS-59+CP	0.071	-2.81	1.0	14.8	-138.8	154.6	7.9	40.3	26.4
TS-60+CP	0.073	-2.71	4.1	1.8	-143.5	149.4	2.9	32.4	34.7
TS-61+CP	0.074	-3.13	-11.8	6.3	-148.7	143.2	-2.8	43.1	25.0
TS-62+CP	0.079	-2.98	-4.3	-5.4	-149.4	139.8	-4.8	34.8	35.9
TS-63+CP	0.079	-3.10	-8.2	6.4	-145.6	143.7	-0.9	42.7	28.0
TS-64+CP	0.067	-2.34	-4.3	14.0	-146.2	155.9	4.8	38.1	19.8
TS-65+CP	0.073	-2.96	-9.8	7.1	-148.3	145.6	-1.4	41.6	24.6
TS-66+CP	0.072	-2.71	-0.5	15.8	-140.6	155.9	7.6	39.9	23.6
TS-67+CP	0.072	-2.71	3.5	3.4	-143.5	150.4	3.4	33.0	33.1
TS-68+CP	0.073	-3.14	-9.8	11.0	-146.2	147.5	0.6	43.5	22.8
TS-69+CP	0.078	-3.11	-3.3	-2.7	-147.4	141.4	-3.0	35.9	35.3
TS-70+CP	0.080	-3.11	-7.1	8.4	-144.8	146.1	0.6	42.3	26.8

Table S43. Δd_{C1C2}, $\Delta\phi$, $\theta_{1\text{-}4}$, τ, χ_{C1} and χ_{C1} values for the dienophile fragments derived from the transition structures of **CH**.

fragment from	Δd_{C1C2}	$\Delta\phi$	θ_1	θ_2	θ_3	θ_4	τ	χ_{C1}	χ_{C2}
TS-1+CH	0.060	-1.98	-5.8	9.9	-150.8	155.0	2.1	34.9	19.2
TS-2+CH	0.059	-1.85	-4.2	15.4	-148.9	160.0	5.6	35.3	15.7
TS-3+CH	0.064	-2.03	-14.4	21.3	-154.5	161.5	3.5	39.8	4.1
TS-4+CH	0.062	-1.92	-13.0	6.7	-157.5	151.2	-3.1	35.5	15.8
TS-5+CH	0.058	-2.06	4.3	1.7	-147.8	153.9	3.0	27.8	30.5
TS-6+CH	0.056	-1.36	-11.5	18.6	-158.3	165.4	3.5	33.3	3.1
TS-7+CH	0.059	-1.65	-11.6	19.7	-155.5	163.6	4.1	36.1	4.8
TS-8+CH	0.068	-2.65	-12.7	16.6	-149.6	153.5	2.0	43.1	13.8
TS-9+CH	0.066	-2.39	-10.4	10.9	-150.8	151.3	0.3	39.6	18.3
TS-10+CH	0.068	-2.40	-14.9	17.7	-153.1	155.8	1.4	41.9	9.2
TS-11+CH	0.065	-2.15	8.1	5.7	-143.5	157.3	6.9	28.4	30.8
TS-12+CH	0.069	-2.53	-25.2	19.8	-161.2	155.8	-2.7	44.0	-0.9
TS-13+CH	0.070	-2.40	-20.7	15.0	-157.8	152.2	-2.8	42.8	7.1
TS-14+CH	0.070	-2.53	-9.4	28.4	-145.5	164.5	9.5	43.9	6.1
TS-15+CH	0.069	-2.26	-5.9	18.3	-146.3	158.7	6.2	39.6	15.4
TS-16+CH	0.074	-2.62	-20.1	18.6	-155.9	154.3	-0.8	44.3	5.5
TS-17+CH	0.064	-2.20	0.0	0.0	-150.0	150.0	0.0	30.0	30.0
TS-18+CH	0.066	-2.35	-6.4	-1.4	145.4	-153.2	-3.9	28.1	33.2
TS-19+CH	0.065	-2.52	0.9	13.2	-141.8	155.9	7.1	37.4	25.0
TS-20+CH	0.067	-2.54	-10.5	5.2	-151.9	146.5	-2.7	38.7	23.0
TS-21+CH	0.064	-2.64	-1.8	17.4	-140.7	156.3	7.8	41.1	21.9
TS-22+CH	0.061	-1.80	-7.0	26.9	-149.0	168.9	10.0	38.0	4.2
TS-23+CH	0.064	-2.14	-5.8	28.1	-145.2	167.5	11.1	40.6	6.7
TS-24+CH	0.062	-2.16	-1.9	1.9	-149.8	149.9	0.0	32.0	28.3
TS-25+CH	0.068	-1.87	15.0	-5.5	157.2	-147.6	4.8	37.9	17.4
TS-26+CH	0.077	-2.84	-20.1	12.9	-154.8	147.5	-3.6	45.4	12.3
TS-27+CH	0.071	-2.83	-13.1	1.2	-153.2	141.3	-5.9	39.9	25.7
TS-28+CH	0.073	-2.99	-2.4	10.7	-141.7	150.0	4.2	40.7	27.6
TS-29+CH	0.071	-2.71	-0.3	-5.9	144.1	-150.3	-3.1	35.7	30.0
TS-30+CH	0.069	-2.77	-7.2	-3.8	-151.9	140.9	-5.5	35.3	31.9
TS-31+CH	0.070	-2.51	-8.5	14.7	-147.1	153.3	3.1	41.4	18.1
TS-32+CH	0.079	-2.70	-8.5	20.5	-144.6	156.7	6.0	43.9	14.8
TS-33+CH	0.086	-2.92	0.0	0.0	-145.8	145.8	0.0	34.2	34.2
TS-34+CH	0.086	-3.19	-13.0	17.8	-145.7	150.6	2.4	47.3	16.4
TS-35+CH	0.086	-2.88	-9.5	9.7	-147.4	147.6	0.1	42.0	22.9
TS-36+CH	0.075	-2.97	-9.3	13.2	-144.9	148.8	1.9	44.4	21.9
TS-37+CH	0.083	-2.75	-4.4	1.3	-148.4	145.2	-1.6	36.0	30.3
TS-38+CH	0.077	-3.13	1.1	4.2	147.0	-141.8	2.6	34.1	37.1
TS-39+CH	0.077	-3.21	0.0	0.0	-143.5	143.5	0.0	36.5	36.5
TS-40+CH	0.076	-3.28	-4.3	7.8	-142.1	145.7	1.8	42.2	30.1
TS-41+CH	0.058	-2.71	1.2	18.0	-141.6	160.8	9.6	37.2	20.4
TS-42+CH	0.066	-3.62	-0.8	15.0	-139.3	153.5	7.1	41.5	25.7
TS-43+CH	0.065	-3.58	3.3	23.6	-133.0	160.0	13.5	43.6	23.4
TS-44+CH	0.065	-3.22	3.3	6.0	-142.7	152.0	4.6	34.0	31.3
TS-45+CH	0.066	-4.12	-1.0	24.1	-134.7	157.7	11.5	46.3	21.2
TS-46+CH	0.072	-4.12	1.2	5.7	-139.7	146.7	3.5	39.1	34.5
TS-47+CH	0.071	-4.38	0.8	18.8	-133.0	152.6	9.8	46.3	28.2
TS-48+CH	0.061	-2.41	-5.0	11.0	-148.2	154.3	3.0	36.7	20.7
TS-49+CH	0.068	-3.14	-9.4	6.4	-148.5	145.6	-1.5	40.9	25.0
TS-50+CH	0.065	-3.09	-2.1	13.4	-141.3	152.6	5.7	40.8	25.3
TS-51+CH	0.067	-2.93	1.3	1.7	-145.5	148.5	1.5	33.2	32.8
TS-52+CH	0.071	-3.50	-10.2	11.6	-146.0	147.4	0.7	44.3	22.4
TS-53+CH	0.075	-3.54	-3.7	0.9	-145.1	142.3	-1.4	38.6	34.0
TS-54+CH	0.072	-3.72	-6.1	12.1	-140.7	146.7	3.0	45.4	27.2
TS-55+CH	0.058	-1.92	0.0	0.0	-152.8	152.8	0.0	27.2	27.2
TS-56+CH	0.059	-2.49	-4.7	9.3	-148.3	152.8	2.3	36.5	22.5
TS-57+CH	0.063	-2.32	-2.1	12.5	-145.0	155.5	5.2	37.0	22.5
TS-58+CH	0.071	-2.99	-11.7	6.0	-149.4	143.7	-2.8	42.3	24.6
TS-59+CH	0.067	-2.96	3.2	14.9	-136.6	154.7	9.0	40.2	28.5
TS-60+CH	0.071	-2.86	6.2	3.7	-140.7	150.7	5.0	33.1	35.6
TS-61+CH	0.074	-3.33	-13.5	11.1	-147.5	145.1	-1.2	46.0	21.4
TS-62+CH	0.079	-3.23	-3.4	1.2	-144.4	142.2	-1.1	38.9	34.4
TS-63+CH	0.077	-3.39	-6.0	13.5	-139.9	147.4	3.7	46.1	26.6
TS-64+CH	0.063	-2.27	-2.8	14.7	-145.5	157.4	6.0	37.3	19.8
TS-65+CH	0.071	-3.00	-9.4	9.5	-147.1	147.2	0.0	42.3	23.4
TS-66+CH	0.069	-2.80	0.9	14.8	-139.7	155.4	7.8	39.5	25.5
TS-67+CH	0.070	-2.78	4.8	3.6	-142.4	150.8	4.2	32.8	34.0
TS-68+CH	0.076	-3.41	-11.8	16.7	-144.9	149.8	2.4	46.9	18.3
TS-69+CH	0.078	-3.31	-2.6	2.5	-143.5	143.4	0.0	39.0	34.0
TS-70+CH	0.081	-3.38	-5.5	14.3	-140.2	149.0	4.4	45.3	25.5

Table S44. Δd_{C1C2}, $\Delta\phi$, $\theta_{1\text{-}4}$, τ, χ_{C1} and χ_{C1} values for the dienophile fragments derived from the transition structures of **BU**.

fragment from	Δd_{C1C2}	$\Delta\phi$	θ_1	θ_2	θ_3	θ_4	τ	χ_{C1}	χ_{C2}
TS-1+BU	0.060	-2.03	-5.2	9.4	-150.3	154.5	2.1	34.9	20.3
TS-2+BU	0.058	-1.92	-2.1	16.0	-146.7	160.6	6.9	35.4	17.3
TS-3+BU	0.060	-1.89	-10.3	21.5	-152.0	163.3	5.6	38.3	6.4
TS-4+BU	0.060	-1.96	-11.0	4.6	-156.4	150.1	-3.2	34.5	18.9
TS-5+BU	0.058	-2.13	4.8	1.4	-147.4	153.6	3.1	27.8	31.3
TS-6+BU	0.052	-1.24	-11.5	18.7	-159.6	166.8	3.6	31.9	1.7
TS-7+BU	0.055	-1.49	-10.6	19.6	-156.2	165.2	4.5	34.4	4.2
TS-8+BU	0.060	-2.23	-4.0	25.7	-143.7	165.4	10.8	40.3	10.6
TS-9+BU	0.060	-2.04	-4.1	19.5	-146.3	161.7	7.7	37.8	14.2
TS-10+BU	0.060	-2.28	0.7	15.3	-142.7	158.8	8.0	36.6	21.9
TS-11+BU	0.063	-2.17	4.7	4.4	-145.8	154.9	4.6	29.5	29.8
TS-12+BU	0.057	-1.94	-12.2	26.5	-153.3	167.7	7.2	38.9	0.1
TS-13+BU	0.059	-1.86	-11.5	22.2	-153.4	164.1	5.3	38.1	4.4
TS-14+BU	0.064	-2.29	-7.1	24.8	-145.9	163.7	8.9	41.1	9.3
TS-15+BU	0.065	-2.23	-4.9	16.4	-146.4	157.9	5.8	38.5	17.2
TS-16+BU	0.067	-2.33	-11.1	21.1	-149.8	159.8	5.0	41.3	9.1
TS-17+BU	0.064	-2.28	0.0	0.0	-149.4	149.4	0.0	30.6	30.6
TS-18+BU	0.064	-2.27	2.1	-3.2	-150.6	149.5	-0.6	27.3	32.7
TS-19+BU	0.063	-2.34	-3.0	7.6	-147.7	152.3	2.3	35.3	24.7
TS-20+BU	0.064	-2.35	-5.3	10.6	-147.9	153.2	2.7	37.4	21.4
TS-21+BU	0.061	-2.37	-2.4	12.8	-144.7	155.2	5.2	37.6	22.4
TS-22+BU	0.057	-1.59	-9.7	22.5	-154.2	167.0	6.4	35.5	3.3
TS-23+BU	0.059	-1.89	-8.5	22.7	-150.5	164.8	7.1	38.0	6.8
TS-24+BU	0.059	-2.03	8.2	5.0	157.5	-144.4	6.6	30.7	27.5
TS-25+BU	0.067	-1.97	14.8	-5.3	156.4	-146.9	4.8	38.4	18.3
TS-26+BU	0.071	-2.63	-9.8	17.5	-147.2	154.9	3.9	42.7	15.3
TS-27+BU	0.067	-2.51	-3.8	10.2	-146.1	152.5	3.2	37.7	23.7
TS-28+BU	0.068	-2.63	-3.3	9.3	-145.2	151.3	3.0	38.0	25.5
TS-29+BU	0.069	-2.66	-2.5	2.6	-147.5	147.6	0.1	35.0	29.9
TS-30+BU	0.067	-2.60	-2.0	1.7	-147.8	147.5	-0.2	34.2	30.5
TS-31+BU	0.063	-2.47	2.0	15.7	-140.1	157.8	8.8	37.8	24.2
TS-32+BU	0.072	-2.53	-10.2	13.6	-148.8	152.2	1.7	41.4	17.6
TS-33+BU	0.077	-2.71	0.0	0.0	-147.1	147.1	0.0	32.9	32.9
TS-34+BU	0.077	-2.84	-6.9	16.4	-144.0	153.5	4.8	42.9	19.6
TS-35+BU	0.078	-2.61	-4.5	9.7	-146.1	151.3	2.6	38.5	24.2
TS-36+BU	0.068	-2.43	-1.3	21.9	-140.5	161.1	10.3	40.8	17.6
TS-37+BU	0.075	-2.48	-0.4	10.7	-143.9	154.3	5.2	36.5	25.4
TS-38+BU	0.072	-2.82	2.0	2.8	-144.0	148.8	2.4	34.0	33.1
TS-39+BU	0.072	-2.86	0.0	0.0	-145.9	145.9	0.0	34.1	34.1
TS-40+BU	0.072	-2.85	-0.2	13.2	-140.4	153.4	6.5	39.8	26.4
TS-41+BU	0.057	-2.77	3.1	20.9	-139.2	163.1	12.0	37.8	20.0
TS-42+BU	0.061	-3.18	2.3	24.2	-136.5	163.0	13.2	41.2	19.2
TS-43+BU	0.062	-3.46	4.0	20.5	-135.0	159.5	12.2	41.0	24.5
TS-44+BU	0.062	-3.22	3.8	7.2	-142.0	153.1	5.5	34.2	30.7
TS-45+BU	0.058	-3.50	2.0	29.8	-133.9	165.7	15.9	44.1	16.2
TS-46+BU	0.067	-3.74	3.5	13.6	-137.0	154.2	8.6	39.5	29.4
TS-47+BU	0.065	-3.88	3.6	25.1	-131.9	160.6	14.3	44.5	22.9
TS-48+BU	0.061	-2.50	-3.4	12.3	-146.4	155.2	4.4	37.1	21.4
TS-49+BU	0.065	-2.82	-4.8	17.0	-144.0	156.1	6.1	40.8	19.1
TS-50+BU	0.064	-2.96	-2.6	11.1	-143.5	152.0	4.3	39.0	25.4
TS-51+BU	0.065	-2.91	-0.1	-0.1	-147.4	147.2	-0.1	32.7	32.7
TS-52+BU	0.065	-3.15	-4.3	21.5	-140.8	158.1	8.6	43.4	17.6
TS-53+BU	0.070	-3.22	-1.0	7.2	-142.8	149.0	3.1	38.2	30.0
TS-54+BU	0.068	-3.25	-4.0	16.3	-140.9	153.2	6.1	43.1	22.8
TS-55+BU	0.057	-2.03	0.0	0.1	-152.1	152.2	0.0	27.9	27.8
TS-56+BU	0.059	-2.59	-3.6	9.9	-146.8	153.1	3.2	36.9	23.3
TS-57+BU	0.064	-2.41	0.1	14.7	-142.3	157.2	7.4	37.5	22.9
TS-58+BU	0.068	-2.65	-4.5	17.7	-143.0	156.2	6.6	41.5	19.3
TS-59+BU	0.066	-2.85	3.2	14.0	-137.9	155.1	8.6	38.9	28.1
TS-60+BU	0.069	-2.81	4.5	1.9	-142.9	149.4	3.2	32.5	35.2
TS-61+BU	0.070	-2.96	-4.9	23.6	-140.1	158.9	9.4	44.7	16.3
TS-62+BU	0.075	-2.96	1.2	11.0	-139.5	151.8	6.1	39.3	29.5
TS-63+BU	0.074	-2.94	-1.1	22.1	-137.0	158.0	10.5	44.1	20.9
TS-64+BU	0.063	-2.33	-0.7	16.4	-143.2	159.0	7.9	37.5	20.4
TS-65+BU	0.067	-2.59	-3.9	19.0	-143.0	158.0	7.5	40.9	18.1
TS-66+BU	0.066	-2.63	1.9	14.3	-140.4	156.7	8.1	37.6	25.2
TS-67+BU	0.067	-2.68	4.6	4.0	-143.1	151.7	4.3	32.3	32.9
TS-68+BU	0.068	-2.87	-4.6	24.8	-140.6	160.8	10.1	44.0	14.6
TS-69+BU	0.073	-2.94	1.7	10.5	-140.0	152.2	6.1	38.3	29.5
TS-70+BU	0.074	-2.84	-1.5	20.8	-139.0	158.3	9.6	42.5	20.1

Table S45. Δd_{C1C2}, $\Delta\phi$, $\theta_{1\text{-}4}$, τ, χ_{C1} and χ_{C1} values for the dienophile fragments derived from the transition structures of **DMB**.

fragment from	Δd_{C1C2}	$\Delta\phi$	θ_1	θ_2	θ_3	θ_4	τ	χ_{C1}	χ_{C2}
TS-1+DMB	0.062	-2.08	-8.9	10.1	-152.2	153.5	0.6	36.6	17.6
TS-2+DMB	0.060	-1.97	-4.3	17.0	-147.5	160.3	6.4	36.8	15.4
TS-3+DMB	0.061	-1.94	-12.9	22.8	-153.8	163.7	4.9	39.1	3.5
TS-4+DMB	0.063	-2.05	-15.5	8.6	-158.0	151.1	-3.4	37.5	13.3
TS-5+DMB	0.059	-2.12	2.2	1.0	-148.9	152.1	1.6	28.9	30.2
TS-6+DMB	0.054	-1.32	-13.0	19.6	-160.1	166.7	3.3	32.9	0.3
TS-7+DMB	0.056	-1.57	-12.5	20.4	-157.1	165.0	3.9	35.4	2.5
TS-8+DMB	0.061	-2.28	-6.0	26.2	-145.0	165.1	10.1	41.1	8.9
TS-9+DMB	0.062	-2.10	-6.5	20.3	-147.5	161.3	6.9	39.0	12.2
TS-10+DMB	0.062	-2.31	-0.7	17.1	-142.9	159.2	8.2	37.9	20.0
TS-11+DMB	0.064	-2.16	6.1	3.9	-145.4	155.5	5.0	28.5	30.7
TS-12+DMB	0.056	-1.90	-14.3	25.7	-155.8	167.2	5.7	38.5	-1.5
TS-13+DMB	0.060	-1.86	-14.0	21.8	-155.6	163.3	3.9	38.4	2.7
TS-14+DMB	0.066	-2.31	-10.6	25.5	-148.8	163.6	7.4	41.9	5.7
TS-15+DMB	0.067	-2.27	-8.8	18.9	-148.4	158.5	5.1	40.4	12.7
TS-16+DMB	0.067	-2.30	-16.6	19.1	-155.0	157.5	1.3	41.5	5.9
TS-17+DMB	0.065	-2.24	0.0	0.0	-149.8	149.8	0.0	30.2	30.2
TS-18+DMB	0.064	-2.22	-3.4	1.2	-151.4	149.2	-1.1	32.0	27.4
TS-19+DMB	0.064	-2.32	-6.1	8.4	-149.5	151.7	1.1	36.6	22.2
TS-20+DMB	0.065	-2.35	-8.6	10.3	-150.2	151.9	0.9	38.4	19.5
TS-21+DMB	0.062	-2.40	-4.2	13.9	-145.4	155.0	4.8	38.9	20.7
TS-22+DMB	0.057	-1.64	-10.7	23.5	-154.5	167.3	6.4	36.2	2.1
TS-23+DMB	0.060	-1.93	-9.8	24.1	-151.2	165.4	7.1	38.7	4.7
TS-24+DMB	0.060	-1.97	8.2	5.5	158.2	-144.5	6.9	30.0	27.3
TS-25+DMB	0.069	-2.00	18.5	-7.8	158.0	-147.3	5.3	40.4	14.2
TS-26+DMB	0.072	-2.58	-13.6	18.4	-150.2	155.0	2.4	43.4	11.4
TS-27+DMB	0.068	-2.55	-7.4	9.4	-148.4	150.4	1.0	39.0	22.2
TS-28+DMB	0.069	-2.61	-6.8	9.1	-147.7	150.0	1.2	39.1	23.2
TS-29+DMB	0.070	-2.61	-4.3	0.6	-149.7	146.0	-1.9	34.6	29.7
TS-30+DMB	0.068	-2.53	-2.6	1.5	-148.7	147.5	-0.6	34.0	29.9
TS-31+DMB	0.064	-2.48	-0.8	15.2	-142.0	156.4	7.2	38.8	22.8
TS-32+DMB	0.075	-2.56	-10.9	19.3	-147.7	156.1	4.2	43.2	13.0
TS-33+DMB	0.079	-2.64	0.0	0.0	-147.6	147.6	0.0	32.4	32.4
TS-34+DMB	0.079	-2.82	-11.8	18.1	-147.4	153.7	3.2	44.4	14.6
TS-35+DMB	0.080	-2.61	-5.3	15.0	-144.8	154.5	4.9	40.5	20.2
TS-36+DMB	0.069	-2.45	-3.7	22.2	-142.0	160.5	9.3	41.7	15.8
TS-37+DMB	0.076	-2.41	-2.0	13.1	-144.4	155.5	5.6	37.6	22.5
TS-38+DMB	0.073	-2.80	0.0	-1.0	-147.0	146.0	-0.5	33.0	34.0
TS-39+DMB	0.074	-2.78	0.0	0.0	-146.4	146.4	0.0	33.6	33.6
TS-40+DMB	0.073	-2.86	-5.2	10.5	-144.4	149.7	2.7	40.8	25.1
TS-41+DMB	0.059	-2.81	2.0	22.4	-139.1	163.5	12.2	38.9	18.5
TS-42+DMB	0.062	-3.20	1.4	27.0	-136.2	164.6	14.2	42.4	16.8
TS-43+DMB	0.063	-3.43	2.4	20.4	-136.2	159.1	11.4	41.4	23.3
TS-44+DMB	0.063	-3.18	2.0	3.6	-144.8	150.5	2.8	33.2	31.6
TS-45+DMB	0.059	-3.46	1.3	32.8	-133.9	167.9	17.0	44.8	13.4
TS-46+DMB	0.067	-3.65	2.6	13.7	-137.9	154.2	8.2	39.5	28.4
TS-47+DMB	0.066	-3.85	2.7	26.9	-132.1	161.7	14.8	45.2	21.0
TS-48+DMB	0.063	-2.55	-4.3	14.2	-145.9	155.9	5.0	38.3	19.9
TS-49+DMB	0.066	-2.85	-5.8	18.5	-144.0	156.7	6.4	41.8	17.5
TS-50+DMB	0.065	-2.94	-2.9	12.6	-143.3	152.9	4.8	39.7	24.2
TS-51+DMB	0.066	-2.90	-0.3	-1.4	-148.2	146.5	-0.8	32.1	33.2
TS-52+DMB	0.067	-3.20	-5.5	24.1	-140.8	159.4	9.3	44.7	15.1
TS-53+DMB	0.070	-3.17	-1.9	6.6	-143.7	148.5	2.4	38.2	29.7
TS-54+DMB	0.069	-3.26	-4.8	17.7	-141.0	153.8	6.4	43.9	21.3
TS-55+DMB	0.059	-1.97	0.0	0.0	-152.5	152.5	0.0	27.5	27.5
TS-56+DMB	0.061	-2.57	-5.5	11.3	-147.6	153.5	2.9	37.9	21.1
TS-57+DMB	0.065	-2.40	0.5	16.2	-141.6	158.3	8.4	37.9	22.2
TS-58+DMB	0.069	-2.67	-5.6	19.5	-143.1	157.1	7.0	42.4	17.3
TS-59+DMB	0.067	-2.83	3.4	15.1	-137.4	156.0	9.3	39.2	27.5
TS-60+DMB	0.070	-2.81	6.1	1.6	-142.3	150.0	3.8	31.5	36.1
TS-61+DMB	0.071	-2.97	-6.1	25.0	-140.8	159.6	9.4	45.4	14.3
TS-62+DMB	0.075	-2.90	1.4	11.0	-139.7	152.1	6.2	38.9	29.2
TS-63+DMB	0.074	-2.92	-1.4	22.8	-137.1	158.5	10.7	44.3	20.1
TS-64+DMB	0.064	-2.31	-1.0	18.2	-143.0	160.2	8.6	38.1	18.8
TS-65+DMB	0.068	-2.57	-5.0	20.1	-143.6	158.6	7.5	41.4	16.4
TS-66+DMB	0.067	-2.60	1.9	16.3	-139.9	158.1	9.1	38.2	23.8
TS-67+DMB	0.068	-2.65	5.8	3.9	-142.7	152.3	4.8	31.5	33.4
TS-68+DMB	0.068	-2.79	-6.6	25.0	-142.6	161.0	9.2	44.0	12.4
TS-69+DMB	0.073	-2.88	1.4	10.7	-140.4	152.5	6.0	38.1	28.9
TS-70+DMB	0.075	-2.80	-2.1	21.3	-139.5	158.7	9.6	42.6	19.2

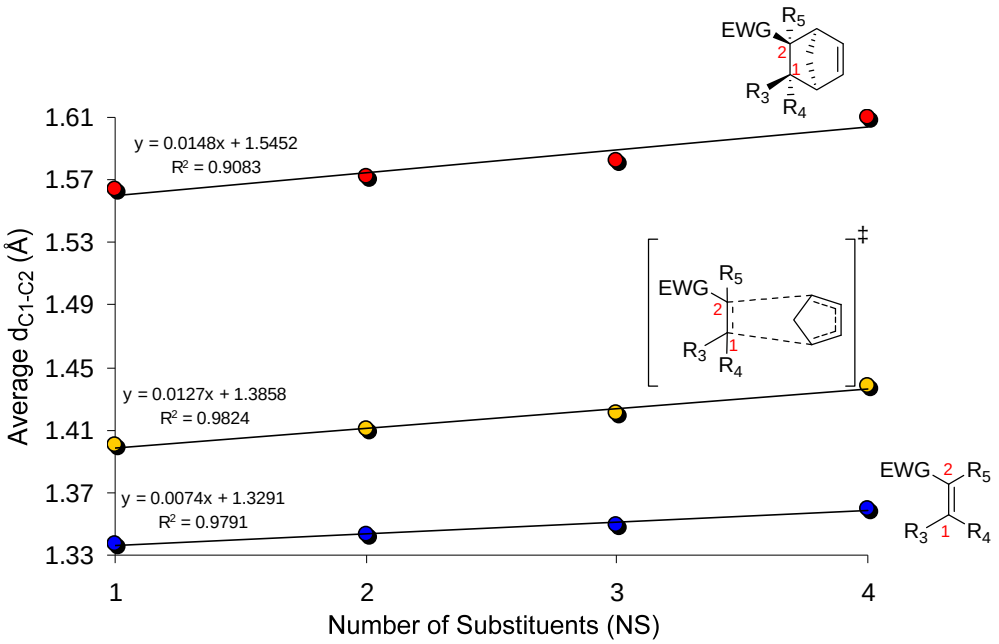


Figure S14. Plots of the averaged C1-C2 distance (d_{C1C2}) versus the number of substituents of the dienophile (NS) for the dienophile reagents (in blue), the transition structures (in yellow) and the Diels-Alder products (in red), corresponding for the reactions between **1-70** and **CP**.

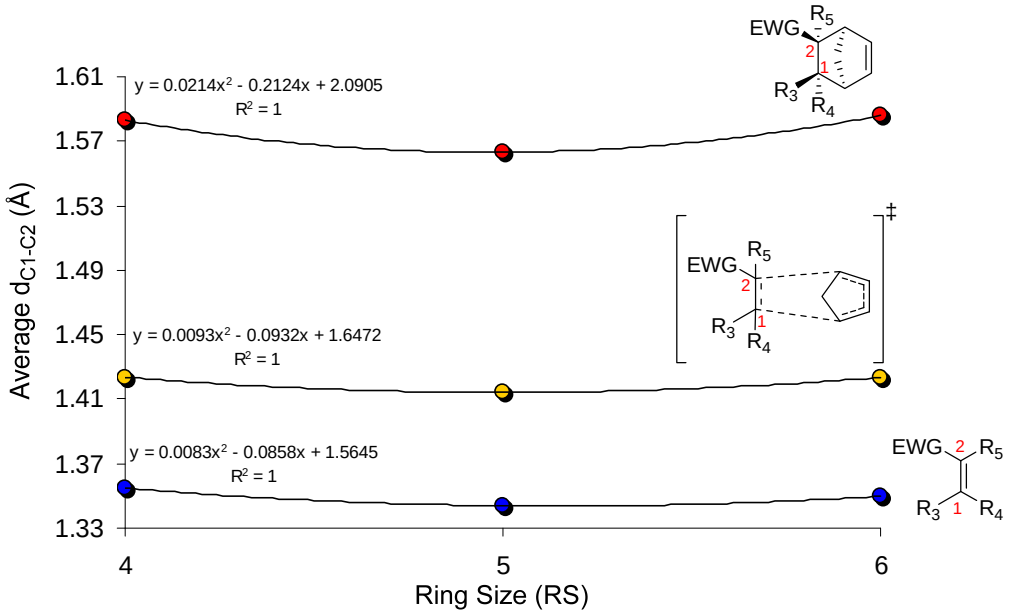


Figure S15. Plots of the averaged C1-C2 distance (d_{C1C2}) versus the ring size of the dienophile (RS) for the dienophile reagents (in blue), the transition structures (in yellow) and the Diels-Alder products (in red), corresponding for the reactions between **41-70** and **CP**.

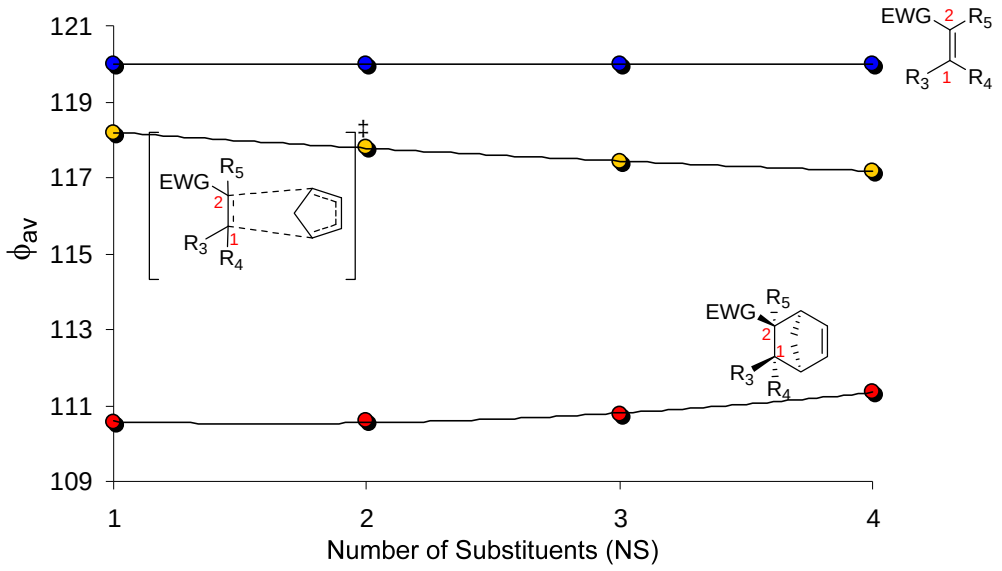


Figure S16. Plots of the average bending angles (ϕ_{av}) versus the number of substituents of the dienophile (NS) for the dienophile reagents (in blue), the transition structures (in yellow) and the Diels-Alder products (in red), corresponding for the reactions between **1-70** and **CP**.

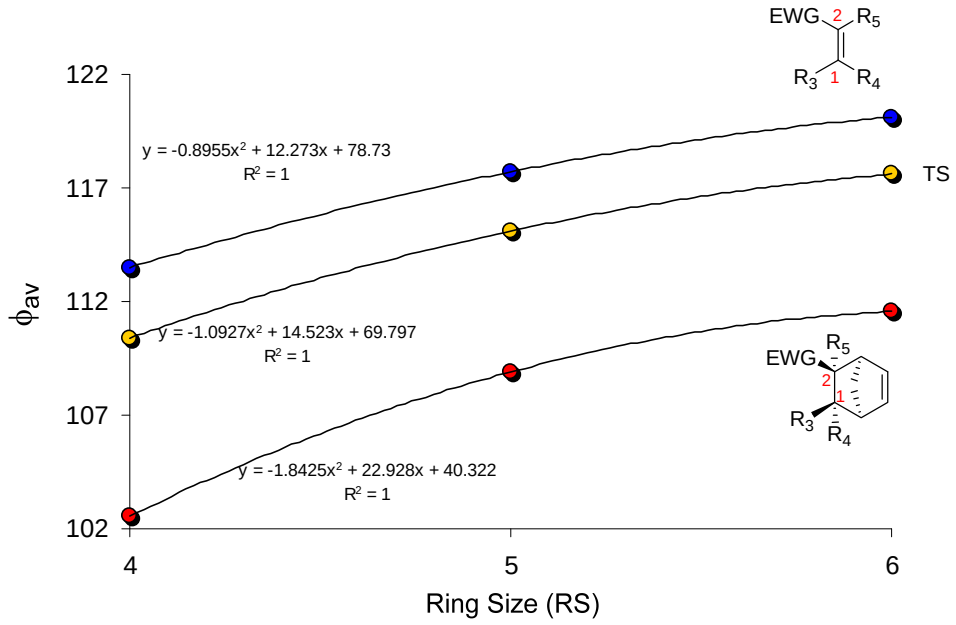


Figure S17. Plots of the average bending angles (ϕ_{av}) versus the ring size of the dienophile (RS) for the dienophile reagents (in blue), the transition structures (in yellow) and the Diels-Alder products (in red), corresponding for the reactions between **41-70** and **CP**.

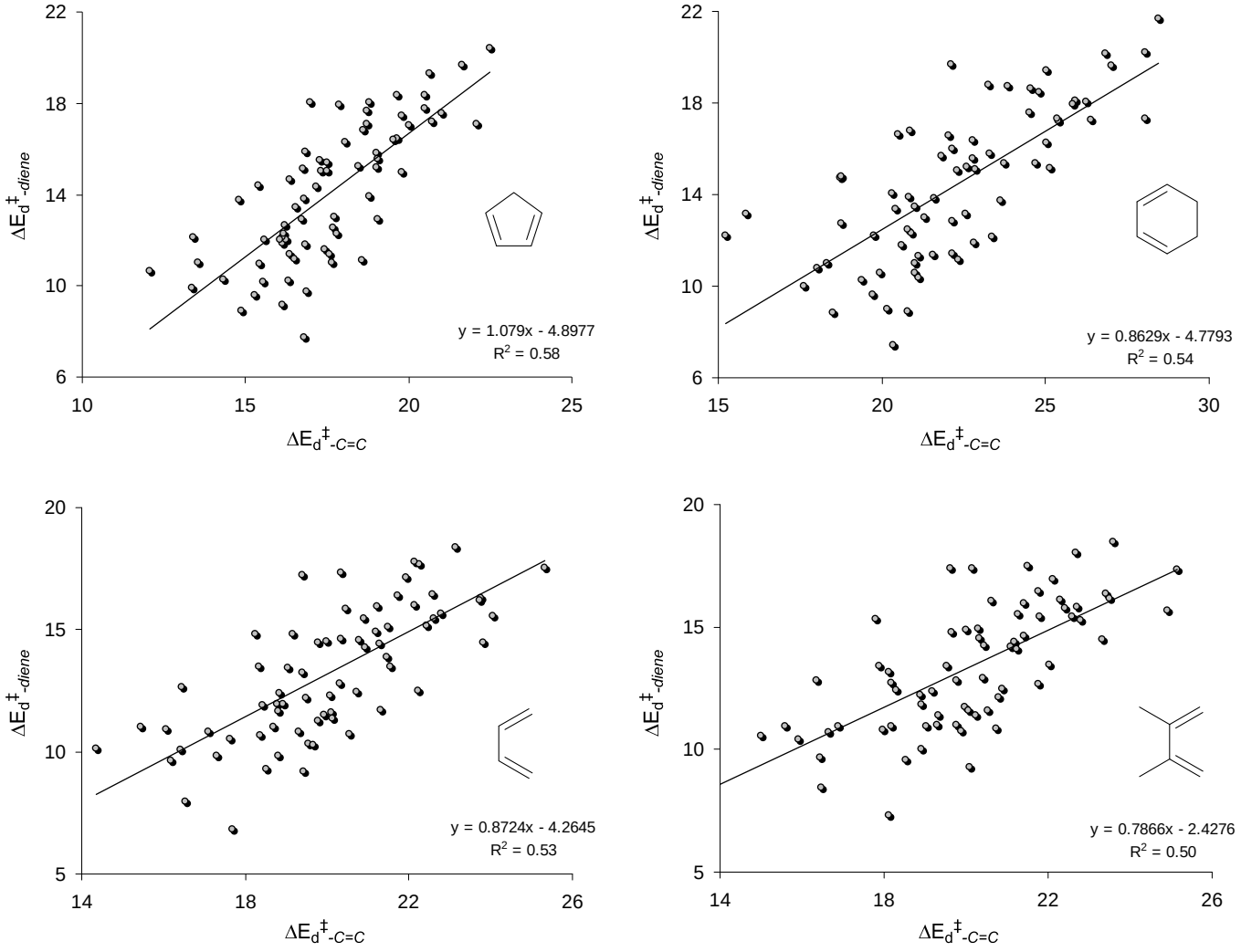
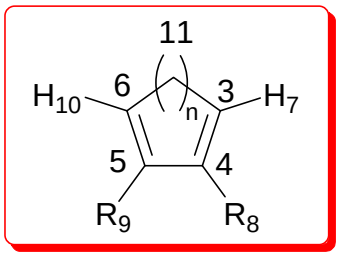


Figure S18. Plots of $\Delta E_d^{\ddagger}$-*diene* versus $\Delta E_d^{\ddagger}$-*C=C* correspondig to the reactions between **1-70** and the four dienes under study.

Table S46. Results obtained by applying ANOVA of the selected most significant factors of the diene distortion energy ($\Delta E_d^{\ddagger}{}_{-C=C}$) and coefficient values of Equation 5.

$$\Delta E_d^{\ddagger}{}_{-diene} = a.\Delta d_{C3C6} + b.\chi_{C6} + c.\chi_{C3} + d.\chi_{C6}{}^2 + e.\chi_{C3}{}^2 + f$$

Source	Coefficient Value	Sum of Squares	Mean Square	F value	Prob. > F	Significant
			cyclopentadiene			
Δd_{C3C6}	*a* = -217.685	45.88610	45.88610	260.94924	< 0.0001	Yes
χ_{C6}	*b* = -0.285	0.27930	0.27930	1.58833	0.2121	No
χ_{C3}	*c* = -0.105	0.33095	0.33095	1.88206	0.1749	No
$\chi_{C6}{}^2$	*d* = 0.012	1.96658	1.96658	11.18372	0.0014	Yes
$\chi_{C3}{}^2$	*e* = 0.011	4.77900	4.77900	27.17766	< 0.0001	yes
-	*f* = 0.79	-	-	-	-	-
			1,3-cyclohexadiene			
Δd_{C3C6}	*a* = -138.328	100.23622	100.23622	289.32730	< 0.0001	yes
χ_{C6}	*b* = -0.629	2.50709	2.50709	7.23661	0.0091	Yes
χ_{C3}	*c* = -0.449	8.24540	8.24540	23.79997	< 0.0001	Yes
$\chi_{C6}{}^2$	*d* = 0.015	6.93259	6.93259	20.01062	< 0.0001	Yes
$\chi_{C3}{}^2$	*e* = 0.016	20.99933	20.99933	60.61361	< 0.0001	yes
-	*f* = 10.945	-	-	-	-	-
			butadiene			
Δd_{C3C6}	*a* = -54.766	36.69622	36.69622	114.57877	< 0.0001	Yes
χ_{C6}	*b* = 0.00923	0.05793	0.05793	0.18089	0.6720	No
χ_{C3}	*c* = -0.138	0.32853	0.32853	1.02578	0.3150	No
$\chi_{C6}{}^2$	*d* = 0.0063	72.43945	72.43945	226.18200	< 0.0001	Yes
$\chi_{C3}{}^2$	*e* = 0.013	5.01638	5.01638	15.66294	0.0002	yes
-	*f* = -0.211	-	-	-	-	-
			2,3-dimethyl-1,3-butadiene			
Δd_{C3C6}	*a* = -61.212	32.92785	32.92785	166.17339	< 0.0001	yes
χ_{C6}	*b* = -0.14	0.18140	0.18140	0.91546	0.3423	No
χ_{C3}	*c* = -0.075	0.29812	0.29812	1.50451	0.2245	Yes
$\chi_{C6}{}^2$	*d* = 0.008	2.67525	2.67525	13.50090	0.0005	Yes
$\chi_{C3}{}^2$	*e* = 0.01	7.58077	7.58077	38.25707	< 0.0001	yes
-	*f* = 1.182	-	-	-	-	-



Dihedral angles:

$\theta_1 = \angle\ R_9\text{-}C_5\text{-}C_6\text{-}H_{10}$
$\theta_2 = \angle\ C_4\text{-}C_5\text{-}C_6\text{-}R_{11}$
$\theta_3 = \angle\ C_4\text{-}C_5\text{-}C_6\text{-}H_{10}$
$\theta_4 = \angle\ R_9\text{-}C_5\text{-}C_6\text{-}R_{11}$
$\theta_5 = \angle\ R_5\text{-}C_4\text{-}C_3\text{-}R_{11}$
$\theta_6 = \angle\ H_7\text{-}C_3\text{-}C_4\text{-}R_8$
$\theta_7 = \angle\ R_{11}\text{-}C_3\text{-}C_4\text{-}R_8$
$\theta_8 = \angle\ H_7\text{-}C_3\text{-}C_4\text{-}C_5$

Out-of-plane deformations:

$\tau_{56} = (\theta_1+\theta_2)/2$
$\tau_{34} = (\theta_5+\theta_6)/2$
$\chi_{C6} = \theta_2 - \theta_3 + \pi(\text{mod } 2\pi)$
$\chi_{C5} = \theta_1 - \theta_3 + \pi(\text{mod } 2\pi)$
$\chi_{C4} = \theta_5 - \theta_7 + \pi(\text{mod } 2\pi)$
$\chi_{C3} = \theta_6 - \theta_7 + \pi(\text{mod } 2\pi)$

Figure S19. Definition of the dihedral angles and out-of-plane deformations for the strained dienes.

Table S47. $\theta_{1\text{-}8}$ values for the diene fragments derived from the transition structures of **CP**.

fragment from	θ_1	θ_2	θ_3	θ_4	θ_5	θ_5	θ_7	θ_8
TS-1+CP	21.1	-19.9	-167.4	168.6	15.1	-9.1	-171.3	177.3
TS-2+CP	21.2	-20.5	-167.4	168.1	15.6	-7.9	-170.2	177.9
TS-3+CP	23.7	-20.0	-164.2	167.9	12.4	-3.2	-172.0	-178.8
TS-4+CP	22.0	-18.5	-165.8	169.3	13.9	-6.3	-172.6	-179.8
TS-5+CP	16.8	-18.8	-171.1	169.2	17.6	-13.5	-170.2	174.3
TS-6+CP	22.2	-20.3	-166.1	168.0	16.3	-10.5	-169.5	175.3
TS-7+CP	23.5	-19.5	-164.4	168.4	14.3	-6.4	-171.2	179.0
TS-8+CP	24.3	-20.9	-165.3	168.6	13.9	-4.4	-170.9	-179.6
TS-9+CP	23.6	-21.6	-166.2	168.2	15.6	-7.1	-169.9	178.4
TS-10+CP	21.2	-20.9	-167.5	167.7	16.6	-8.8	-169.9	177.6
TS-11+CP	13.8	-18.7	-173.2	168.3	19.0	-14.1	-168.0	172.9
TS-12+CP	26.2	-19.2	-161.9	168.9	10.2	-0.9	-173.3	-177.5
TS-13+CP	25.9	-20.7	-163.0	168.1	12.6	-3.0	-171.9	-178.5
TS-14+CP	23.9	-21.2	-164.1	166.8	13.4	-3.4	-171.2	-178.9
TS-15+CP	19.8	-20.5	-167.8	167.0	16.1	-6.9	-169.4	178.6
TS-16+CP	24.9	-18.4	-162.8	169.3	9.9	-2.0	-174.3	-177.7
TS-17+CP	14.9	-18.2	-173.1	169.7	18.2	-14.9	-169.7	173.1
TS-18+CP	13.3	-17.8	-173.6	169.1	18.3	-15.2	-169.6	172.7
TS-19+CP	20.8	-20.3	-167.6	168.2	16.2	-10.3	-171.0	177.0
TS-20+CP	22.5	-20.6	-166.9	168.8	15.2	-8.7	-171.2	177.8
TS-21+CP	18.1	-19.7	-169.8	168.1	16.4	-8.8	-169.4	176.9
TS-22+CP	22.7	-21.0	-165.7	167.5	17.3	-11.4	-169.0	174.9
TS-23+CP	24.4	-20.3	-163.7	167.8	15.4	-7.2	-170.7	178.9
TS-24+CP	12.9	-17.0	-174.6	170.6	16.1	-11.5	-170.5	175.2
TS-25+CP	-20.1	19.7	168.1	-168.5	-16.2	8.6	170.4	-178.1
TS-26+CP	23.5	-19.5	-165.2	169.2	12.8	-3.7	-172.4	-178.5
TS-27+CP	21.7	-21.2	-167.4	167.9	16.1	-9.4	-170.6	177.3
TS-28+CP	22.1	-20.7	-167.1	168.5	16.4	-10.2	-170.9	177.1
TS-29+CP	-16.5	19.0	171.5	-169.0	-18.3	12.2	168.4	-174.5
TS-30+CP	16.3	-19.0	-172.4	169.6	18.6	-14.4	-169.5	173.7
TS-31+CP	20.1	-21.8	-168.3	166.6	17.6	-9.8	-168.9	176.7
TS-32+CP	-22.7	20.4	164.8	-167.2	-13.5	3.9	171.6	178.8
TS-33+CP	13.6	-18.7	-173.9	168.9	18.7	-13.6	-168.9	173.9
TS-34+CP	-24.5	20.6	164.5	-168.4	-14.1	4.4	171.8	178.5
TS-35+CP	-23.2	21.9	164.3	-165.6	-15.7	5.5	170.3	179.5
TS-36+CP	22.9	-22.8	-166.4	166.6	16.9	-8.4	-168.9	177.4
TS-37+CP	-17.7	21.5	169.4	-165.7	-19.0	11.0	168.1	-176.1
TS-38+CP	-16.4	19.5	171.7	-168.6	-19.3	13.5	168.0	-173.8
TS-39+CP	15.9	-19.4	-172.8	169.4	19.4	-15.9	-169.4	172.8
TS-40+CP	21.5	-21.7	-167.5	167.4	17.1	-10.8	-170.2	176.5
TS-41+CP	19.4	-20.8	-167.9	166.5	14.8	-8.8	-170.6	176.5
TS-42+CP	20.8	-22.2	-167.3	165.8	14.7	-8.1	-170.3	176.9
TS-43+CP	19.3	-21.1	-168.0	166.2	16.0	-10.2	-170.2	176.1
TS-44+CP	-15.6	18.1	171.3	-168.8	-18.2	11.8	167.8	-174.2
TS-45+CP	22.0	-21.8	-165.6	165.8	12.7	-4.0	-171.4	-179.9
TS-46+CP	-14.9	18.3	171.7	-168.4	-19.6	13.2	167.1	-173.5
TS-47+CP	20.6	-22.3	-167.5	165.8	15.9	-9.4	-170.0	176.5
TS-48+CP	20.9	-21.4	-167.0	166.5	16.7	-9.2	-169.5	177.1
TS-49+CP	22.4	-22.4	-166.2	166.2	16.7	-8.3	-169.3	177.6
TS-50+CP	20.6	-21.9	-167.3	166.0	18.1	-10.3	-168.9	176.7
TS-51+CP	-15.7	20.1	172.0	-167.6	-19.0	13.0	167.2	-173.2
TS-52+CP	23.3	-21.9	-165.0	166.4	15.6	-5.2	-169.9	-179.8
TS-53+CP	-14.9	20.4	172.6	-167.1	-20.3	14.8	166.7	-172.2
TS-54+CP	22.3	-22.7	-166.3	165.9	18.0	-9.5	-168.7	177.2
TS-55+CP	-14.3	18.6	173.2	-168.9	-18.6	14.3	168.9	-173.2
TS-56+CP	19.3	-20.3	-168.4	167.4	16.8	-10.8	-170.3	176.3
TS-57+CP	20.4	-22.2	-167.5	165.8	17.5	-9.3	-169.2	177.4
TS-58+CP	21.7	-23.6	-166.8	164.9	17.7	-8.3	-168.6	178.0
TS-59+CP	19.9	-22.6	-168.1	165.4	18.8	-10.4	-168.6	177.0
TS-60+CP	-16.1	20.8	172.1	-167.4	-19.4	12.4	166.9	-173.9
TS-61+CP	22.4	-23.0	-165.7	165.1	16.3	-5.4	-169.4	-179.7
TS-62+CP	-16.4	21.2	171.6	-166.8	-20.7	12.9	166.1	-173.8
TS-63+CP	20.9	-23.9	-167.5	164.4	18.9	-10.1	-168.1	176.9
TS-64+CP	21.5	-20.8	-167.0	167.7	15.9	-8.3	-170.7	178.3
TS-65+CP	23.4	-22.3	-166.0	167.1	16.2	-7.6	-170.1	178.8
TS-66+CP	21.7	-21.8	-166.9	166.9	17.7	-9.7	-170.0	178.0
TS-67+CP	-15.9	19.7	172.5	-168.7	-18.3	13.2	168.8	-174.0
TS-68+CP	24.3	-21.4	-164.5	167.3	14.4	-4.1	-171.2	-178.5
TS-69+CP	-15.8	20.4	172.5	-167.9	-19.7	14.7	168.2	-173.2
TS-70+CP	23.4	-22.8	-165.9	166.5	17.7	-9.0	-169.5	178.3

Table S48. Δd_{C3C6}, τ_{56}, τ_{34}, χ_{C3}, χ_{C4}, χ_{C5} and χ_{C6} values for the diene fragments derived from the transition structures of **CP**.

fragment from	Δd_{C3C6}	τ_{56}	τ_{34}	χ_{C3}	χ_{C4}	χ_{C5}	χ_{C6}
TS-1+CP	-0.043	0.6	3.0	17.8	6.4	8.5	32.5
TS-2+CP	-0.044	0.4	3.9	17.7	5.8	8.6	33.1
TS-3+CP	-0.034	1.8	4.6	11.2	4.4	8.0	35.8
TS-4+CP	-0.037	1.8	3.8	13.7	6.5	7.8	32.8
TS-5+CP	-0.047	1.0	2.1	23.3	7.8	8.0	27.7
TS-6+CP	-0.039	0.9	2.9	21.0	5.8	8.3	34.2
TS-7+CP	-0.035	2.0	3.9	15.2	5.5	7.9	35.1
TS-8+CP	-0.043	1.7	4.8	13.5	4.8	9.5	35.7
TS-9+CP	-0.046	1.0	4.3	17.2	5.6	9.8	35.4
TS-10+CP	-0.049	0.1	3.9	19.0	6.5	8.6	33.5
TS-11+CP	-0.051	2.5	2.4	26.1	7.0	6.9	25.5
TS-12+CP	-0.029	3.5	4.6	7.7	3.5	8.2	37.3
TS-13+CP	-0.035	2.6	4.8	11.1	4.5	8.9	37.8
TS-14+CP	-0.040	1.4	5.0	12.3	4.6	8.0	37.1
TS-15+CP	-0.049	0.4	4.6	17.5	5.5	7.6	32.8
TS-16+CP	-0.030	3.2	4.0	7.7	4.2	7.7	35.5
TS-17+CP	-0.051	1.7	1.7	25.2	7.9	7.9	25.2
TS-18+CP	-0.051	2.3	1.5	25.6	7.9	6.9	24.3
TS-19+CP	-0.048	0.3	3.0	19.3	7.3	8.5	32.6
TS-20+CP	-0.046	1.0	3.3	17.4	6.5	9.4	33.6
TS-21+CP	-0.048	0.8	3.8	19.4	5.7	7.9	30.0
TS-22+CP	-0.044	0.9	3.0	22.4	6.4	8.4	35.2
TS-23+CP	-0.040	2.1	4.1	16.5	6.1	8.1	36.6
TS-24+CP	-0.048	2.0	2.3	21.0	6.6	7.5	22.3
TS-25+CP	-0.045	0.2	3.8	18.1	6.7	8.2	31.6
TS-26+CP	-0.043	2.0	4.5	11.3	5.2	8.7	34.3
TS-27+CP	-0.051	0.2	3.3	18.8	6.7	9.1	33.8
TS-28+CP	-0.050	0.7	3.1	19.3	7.3	9.2	33.6
TS-29+CP	-0.054	1.2	3.0	23.8	6.7	8.0	27.5
TS-30+CP	-0.055	1.4	2.1	24.9	8.0	8.7	26.6
TS-31+CP	-0.053	0.9	3.9	20.9	6.5	8.4	33.5
TS-32+CP	-0.041	1.2	4.8	12.3	5.1	7.5	35.6
TS-33+CP	-0.060	2.5	2.5	24.8	7.5	7.5	24.8
TS-34+CP	-0.047	2.0	4.8	12.6	5.9	9.0	36.1
TS-35+CP	-0.049	0.7	5.1	15.2	6.0	7.4	37.6
TS-36+CP	-0.052	0.1	4.3	19.6	5.8	9.3	36.4
TS-37+CP	-0.061	1.9	4.0	22.9	7.2	7.2	32.1
TS-38+CP	-0.058	1.6	2.9	25.5	7.3	8.1	27.8
TS-39+CP	-0.058	1.7	1.7	26.6	8.7	8.8	26.6
TS-40+CP	-0.054	0.1	3.2	20.6	7.3	9.1	34.2
TS-41+CP	-0.042	0.7	3.0	18.2	5.4	7.3	32.9
TS-42+CP	-0.045	0.7	3.3	17.8	5.0	8.0	34.9
TS-43+CP	-0.047	0.9	2.9	19.9	6.3	7.3	33.1
TS-44+CP	-0.047	1.3	3.2	24.0	5.9	6.9	26.7
TS-45+CP	-0.040	0.1	4.4	12.6	4.1	7.6	36.2
TS-46+CP	-0.051	1.7	3.2	26.1	6.8	6.6	26.5
TS-47+CP	-0.049	0.9	3.3	19.4	5.9	8.1	34.8
TS-48+CP	-0.047	0.3	3.8	19.6	6.2	7.9	34.4
TS-49+CP	-0.049	0.0	4.2	19.0	5.9	8.6	36.2
TS-50+CP	-0.052	0.6	3.9	21.4	7.0	7.9	34.6
TS-51+CP	-0.053	2.2	3.0	25.8	6.2	7.7	28.2
TS-52+CP	-0.047	0.7	5.2	15.3	5.4	8.4	36.9
TS-53+CP	-0.058	2.8	2.7	28.1	7.0	7.5	27.8
TS-54+CP	-0.054	0.2	4.3	20.8	6.7	8.6	36.4
TS-55+CP	-0.050	2.1	2.1	25.4	7.5	7.5	25.4
TS-56+CP	-0.048	0.5	3.0	20.5	7.1	7.7	32.0
TS-57+CP	-0.050	0.9	4.1	20.1	6.7	8.0	34.6
TS-58+CP	-0.054	0.9	4.7	19.7	6.3	8.5	36.9
TS-59+CP	-0.055	1.3	4.2	21.8	7.4	8.0	34.5
TS-60+CP	-0.056	2.3	3.5	25.5	6.3	8.2	28.7
TS-61+CP	-0.051	0.3	5.5	16.0	5.7	8.1	37.3
TS-62+CP	-0.061	2.4	3.9	26.8	6.8	8.0	29.6
TS-63+CP	-0.058	1.5	4.4	22.0	7.0	8.3	36.4
TS-64+CP	-0.046	0.3	3.8	17.6	6.6	8.5	33.7
TS-65+CP	-0.049	0.5	4.3	17.4	6.4	9.4	36.2
TS-66+CP	-0.051	0.0	4.0	19.7	7.7	8.6	34.9
TS-67+CP	-0.053	1.9	2.6	24.4	7.1	8.4	27.2
TS-68+CP	-0.045	1.4	5.2	12.9	5.6	8.8	37.0
TS-69+CP	-0.059	2.3	2.5	26.5	7.9	8.3	27.9
TS-70+CP	-0.053	0.3	4.4	19.5	7.2	9.3	36.9

Table S49. $\theta_{1\text{-}8}$ values for the diene fragments derived from the transition structures of **CH**.

fragment from	θ_1	θ_2	θ_3	θ_4	θ_5	θ_5	θ_7	θ_8
TS-1+CH	11.1	-37.8	175.5	157.8	30.4	-2.0	-163.0	-168.6
TS-2+CH	11.4	-37.9	175.3	158.2	30.9	-0.3	-161.5	-168.0
TS-3+CH	15.2	-36.7	-179.9	158.4	24.6	2.4	-165.3	-167.7
TS-4+CH	12.3	-36.1	178.0	158.3	27.8	-0.6	-166.1	-166.7
TS-5+CH	7.7	-36.0	172.6	159.1	34.0	-5.1	-161.0	-170.0
TS-6+CH	12.1	-36.9	177.0	158.3	31.0	-4.2	-160.1	-173.0
TS-7+CH	14.0	-36.0	179.2	158.8	27.8	-1.3	-163.3	-170.2
TS-8+CH	15.7	-39.0	179.4	157.3	25.2	2.0	-164.2	-168.5
TS-9+CH	13.4	-40.0	176.5	156.9	29.9	0.4	-161.5	-168.3
TS-10+CH	15.7	-37.6	-177.6	155.6	28.4	-1.2	-165.4	-167.4
TS-11+CH	-4.3	36.6	-170.4	-157.4	-35.7	4.6	158.0	170.9
TS-12+CH	18.7	-34.7	-174.7	158.6	16.8	3.6	-170.5	-169.0
TS-13+CH	17.1	-37.9	-178.1	157.4	23.1	2.6	-166.3	-168.0
TS-14+CH	16.7	-38.4	-178.5	156.8	26.2	3.0	-164.1	-166.7
TS-15+CH	10.0	-38.2	175.6	156.2	31.6	1.3	-160.0	-167.1
TS-16+CH	19.0	-34.5	-174.2	158.7	15.9	2.1	-171.7	-170.3
TS-17+CH	5.6	-35.4	170.8	159.4	35.4	-5.6	-159.4	-170.8
TS-18+CH	7.0	-36.0	171.5	159.4	34.0	-3.6	-158.8	-170.8
TS-19+CH	10.3	-38.4	175.3	156.6	33.1	-2.8	-161.7	-168.0
TS-20+CH	12.9	-39.3	176.2	157.4	29.8	-1.0	-162.6	-168.6
TS-21+CH	7.8	-37.7	173.3	156.7	33.3	-1.5	-160.5	-167.7
TS-22+CH	12.9	-38.3	177.8	156.8	32.8	-4.9	-158.6	-173.5
TS-23+CH	14.9	-37.4	-179.9	157.4	29.7	-1.6	-161.9	-170.0
TS-24+CH	-4.9	33.9	-169.8	-161.2	-32.3	2.9	160.8	169.8
TS-25+CH	-9.8	37.3	-175.0	-157.5	-32.4	1.8	161.3	168.1
TS-26+CH	16.3	-37.1	-178.5	157.7	22.7	2.5	-166.7	-168.1
TS-27+CH	12.2	-40.1	175.5	156.6	31.3	-0.8	-160.8	-168.7
TS-28+CH	12.2	-39.9	175.9	156.4	32.7	-1.8	-160.9	-168.2
TS-29+CH	7.1	-37.4	172.2	157.5	34.8	-2.9	-158.1	-170.0
TS-30+CH	7.4	-37.6	171.2	158.6	35.3	-4.2	-158.6	-170.3
TS-31+CH	12.2	-39.8	177.8	154.6	32.8	-2.7	-161.4	-168.6
TS-32+CH	-14.4	38.7	179.7	-155.4	-24.9	-2.5	165.2	167.4
TS-33+CH	3.6	-36.7	170.1	156.8	36.7	-3.6	-156.8	-170.1
TS-34+CH	16.1	-39.6	-178.8	155.2	26.6	2.8	-164.6	-166.0
TS-35+CH	-12.0	41.3	-178.9	-151.8	-31.3	-1.9	161.0	165.7
TS-36+CH	12.9	-42.7	176.4	153.7	33.2	0.6	-158.0	-168.3
TS-37+CH	3.7	-38.8	169.6	155.3	39.0	-3.8	-152.9	-171.9
TS-38+CH	5.8	-38.0	171.9	155.9	37.5	-4.1	-156.8	-169.7
TS-39+CH	6.0	-38.1	170.7	157.2	38.1	-6.0	-157.2	-170.7
TS-40+CH	11.0	-41.5	174.7	154.8	34.6	-1.6	-158.5	-168.5
TS-41+CH	9.2	-37.3	174.2	157.8	31.0	-1.6	-160.9	-169.7
TS-42+CH	11.1	-40.3	175.1	155.7	29.6	-0.3	-161.0	-169.8
TS-43+CH	9.2	-38.5	174.3	156.5	33.9	-1.7	-159.2	-168.7
TS-44+CH	-5.7	36.1	-172.2	-157.4	-34.0	2.9	159.1	169.8
TS-45+CH	13.7	-39.1	179.3	155.2	23.4	1.6	-164.8	-170.2
TS-46+CH	4.7	-37.7	170.1	157.0	35.8	-3.7	-156.4	-171.5
TS-47+CH	11.2	-41.2	175.3	154.7	32.4	-0.4	-159.3	-168.7
TS-48+CH	9.8	-38.9	174.6	156.3	4.4	2.2	169.3	-162.6
TS-49+CH	11.9	-41.3	175.8	154.8	32.5	0.5	-158.9	-168.0
TS-50+CH	8.9	-40.5	174.5	153.9	36.6	-1.5	-158.2	-166.6
TS-51+CH	-5.3	38.9	-170.6	-155.8	-35.6	2.8	157.1	170.1
TS-52+CH	14.3	-40.8	179.0	154.5	27.8	2.4	-161.7	-168.0
TS-53+CH	5.2	-39.3	170.9	155.0	38.7	-2.7	-154.2	-169.7
TS-54+CH	11.9	-42.7	176.2	153.0	35.4	0.9	-156.8	-166.9
TS-55+CH	4.5	-35.3	170.0	159.2	35.3	-4.5	-159.2	-170.0
TS-56+CH	8.7	-37.6	173.5	157.6	33.5	-2.1	-160.2	-168.4
TS-57+CH	10.1	-39.9	174.4	155.8	34.6	-0.3	-158.7	-167.0
TS-58+CH	11.8	-42.9	175.5	153.4	33.3	0.9	-158.5	-167.4
TS-59+CH	8.3	-41.4	173.8	153.2	37.7	-1.4	-157.2	-166.5
TS-60+CH	-5.4	39.8	-170.4	-155.3	-36.9	2.7	155.9	169.8
TS-61+CH	14.3	-42.5	178.8	153.0	28.8	3.0	-161.0	-167.2
TS-62+CH	4.8	-40.6	170.3	153.8	39.7	-3.0	-153.5	-169.8
TS-63+CH	12.2	-44.2	176.3	151.7	35.9	1.2	-156.5	-166.5
TS-64+CH	11.4	-38.5	175.1	157.7	32.1	-0.8	-161.6	-167.1
TS-65+CH	13.9	-41.2	176.9	155.8	30.8	0.3	-161.4	-167.4
TS-66+CH	10.4	-40.6	175.1	154.8	36.0	-1.7	-159.7	-166.0
TS-67+CH	-6.4	38.1	-170.6	-157.6	-34.9	3.8	158.7	170.2
TS-68+CH	17.3	-40.2	-177.7	154.8	23.8	2.2	-165.5	-168.6
TS-69+CH	6.6	-39.3	171.0	156.2	38.3	-3.7	-155.9	-169.5
TS-70+CH	14.6	-43.5	178.0	153.1	34.1	0.7	-159.1	-166.1

Table S50. Δd_{C3C6}, τ_{56}, τ_{34}, χ_{C3}, χ_{C4}, χ_{C5} and χ_{C6} values for the diene fragments derived from the transition structures of **CH**.

fragment from	Δd_{C3C6}	τ_{56}	τ_{34}	χ_{C3}	χ_{C4}	χ_{C5}	χ_{C6}
TS-1+CH	-0.114	13.4	14.2	19.0	13.4	15.6	33.3
TS-2+CH	-0.113	13.3	15.3	18.9	12.4	16.1	33.2
TS-3+CH	-0.084	10.7	13.5	12.3	9.9	15.1	36.8
TS-4+CH	-0.104	11.9	13.6	14.5	13.9	14.3	34.1
TS-5+CH	-0.122	14.2	14.5	24.1	15.0	15.1	28.6
TS-6+CH	-0.101	12.4	13.4	24.1	11.2	15.1	33.8
TS-7+CH	-0.092	11.0	13.3	18.0	11.2	14.8	35.2
TS-8+CH	-0.095	11.7	13.6	13.7	9.5	16.3	38.4
TS-9+CH	-0.113	13.3	15.1	18.2	11.4	17.0	36.5
TS-10+CH	-0.105	11.0	13.6	15.8	13.8	13.3	40.0
TS-11+CH	-0.127	16.1	15.5	26.5	13.7	13.9	27.0
TS-12+CH	-0.051	8.0	10.2	5.8	7.4	13.4	40.1
TS-13+CH	-0.078	10.4	12.9	11.1	9.4	15.2	39.8
TS-14+CH	-0.091	10.8	14.6	12.9	10.3	15.2	39.9
TS-15+CH	-0.118	14.1	16.5	18.7	11.6	14.4	33.8
TS-16+CH	-0.057	7.7	9.0	6.2	7.6	13.2	40.3
TS-17+CH	-0.126	14.9	14.9	26.2	14.8	14.8	26.2
TS-18+CH	-0.123	14.5	15.2	24.8	12.8	15.4	27.6
TS-19+CH	-0.127	14.1	15.2	21.1	14.9	15.0	33.6
TS-20+CH	-0.116	13.2	14.4	18.3	12.4	16.7	35.5
TS-21+CH	-0.122	15.0	15.9	21.0	13.8	14.5	31.1
TS-22+CH	-0.110	12.7	13.9	26.3	11.4	15.1	36.1
TS-23+CH	-0.100	11.2	14.1	19.7	11.6	14.8	37.6
TS-24+CH	-0.111	14.5	14.7	22.1	13.1	15.1	23.7
TS-25+CH	-0.118	13.8	15.3	20.5	13.7	14.8	32.3
TS-26+CH	-0.086	10.4	12.6	10.8	9.4	14.8	38.6
TS-27+CH	-0.124	14.0	15.3	20.0	12.1	16.7	35.7
TS-28+CH	-0.127	13.8	15.5	20.9	13.6	16.3	35.7
TS-29+CH	-0.130	15.1	15.9	24.8	12.9	14.9	29.6
TS-30+CH	-0.133	15.1	15.6	25.6	13.9	16.2	28.8
TS-31+CH	-0.126	13.8	15.0	21.4	14.2	14.4	37.6
TS-32+CH	-0.095	12.2	13.7	12.3	10.1	14.0	39.0
TS-33+CH	-0.138	16.5	16.5	26.8	13.5	13.5	26.8
TS-34+CH	-0.104	11.8	14.7	12.6	11.2	14.9	40.9
TS-35+CH	-0.124	14.7	16.6	17.1	12.4	13.1	40.2
TS-36+CH	-0.130	14.9	16.9	21.5	11.2	16.5	39.1
TS-37+CH	-0.146	17.5	17.6	30.9	11.9	14.1	28.4
TS-38+CH	-0.141	16.1	16.7	27.2	14.3	13.9	30.0
TS-39+CH	-0.142	16.1	16.0	28.7	15.3	15.3	28.7
TS-40+CH	-0.137	15.2	16.5	23.1	13.1	16.3	36.2
TS-41+CH	-0.111	14.0	14.7	20.7	11.9	15.0	31.4
TS-42+CH	-0.113	14.6	14.6	19.4	10.6	16.0	35.4
TS-43+CH	-0.123	14.6	16.1	22.6	13.1	14.9	32.7
TS-44+CH	-0.119	15.2	15.6	23.8	13.1	13.5	28.3
TS-45+CH	-0.088	12.7	12.5	13.6	8.3	14.4	38.5
TS-46+CH	-0.129	16.5	16.1	27.3	12.3	14.6	27.7
TS-47+CH	-0.124	15.0	16.0	21.1	11.7	15.9	36.5
TS-48+CH	-0.123	14.6	3.3	13.0	15.1	15.2	33.5
TS-49+CH	-0.124	14.7	16.5	20.6	11.5	16.1	37.1
TS-50+CH	-0.137	15.8	17.6	23.2	14.9	14.4	35.0
TS-51+CH	-0.131	16.8	16.4	25.8	12.7	14.7	29.5
TS-52+CH	-0.103	13.3	15.1	15.8	9.5	15.3	39.9
TS-53+CH	-0.142	17.0	18.0	28.4	12.9	14.3	30.2
TS-54+CH	-0.134	15.4	18.2	22.4	12.2	15.7	39.0
TS-55+CH	-0.122	15.4	15.4	25.3	14.5	14.5	25.3
TS-56+CH	-0.122	14.5	15.7	21.9	13.7	15.2	31.1
TS-57+CH	-0.128	14.9	17.1	21.6	13.3	15.7	34.3
TS-58+CH	-0.129	15.5	17.1	20.6	11.8	16.3	38.4
TS-59+CH	-0.141	16.5	18.1	24.2	14.9	14.5	35.1
TS-60+CH	-0.137	17.2	17.1	26.7	12.9	15.1	30.2
TS-61+CH	-0.109	14.1	15.9	16.0	9.8	15.5	41.3
TS-62+CH	-0.149	17.9	18.3	29.6	13.2	14.4	30.9
TS-63+CH	-0.138	16.0	18.5	22.3	12.4	15.9	40.5
TS-64+CH	-0.119	13.6	15.7	19.2	13.7	16.2	33.6
TS-65+CH	-0.119	13.7	15.6	18.3	12.2	17.0	38.1
TS-66+CH	-0.136	15.1	17.1	22.0	15.7	15.4	35.6
TS-67+CH	-0.129	15.9	15.6	25.1	13.6	15.8	28.7
TS-68+CH	-0.088	11.4	13.0	12.3	9.2	15.0	42.5
TS-69+CH	-0.144	16.4	17.3	27.8	14.2	15.6	30.4
TS-70+CH	-0.130	14.4	17.4	20.2	13.2	16.6	41.5

Table S51. $\theta_{1\text{-}8}$ values for the diene fragments derived from the transition structures of **BU**.

fragment from	θ_1	θ_2	θ_3	θ_4	θ_5	θ_5	θ_7	θ_8
TS-1+BU	10.2	-36.4	175.8	158.0	26.2	-2.5	-165.7	-170.5
TS-2+BU	10.8	-36.5	176.0	158.3	25.5	-0.8	-165.6	-169.6
TS-3+BU	13.3	-35.5	179.6	158.2	19.2	1.6	-170.0	-169.2
TS-4+BU	10.6	-34.9	177.0	158.7	24.0	-1.8	-168.3	-169.6
TS-5+BU	7.2	-33.4	173.3	160.5	30.2	-5.5	-163.2	-172.0
TS-6+BU	10.7	-35.1	177.3	158.3	24.8	-5.2	-165.6	-174.8
TS-7+BU	12.1	-34.5	179.0	158.6	21.8	-2.6	-168.4	-172.4
TS-8+BU	12.9	-36.8	179.0	157.1	19.7	1.0	-168.9	-170.4
TS-9+BU	12.1	-37.6	177.3	157.2	23.1	0.0	-166.8	-170.1
TS-10+BU	9.9	-37.1	175.3	157.5	28.6	-1.4	-163.7	-169.2
TS-11+BU	-5.0	33.4	-172.0	-159.6	-33.2	4.5	159.8	171.5
TS-12+BU	13.3	-33.2	-178.6	158.8	15.2	2.0	-172.1	-170.7
TS-13+BU	13.4	-35.5	-179.9	157.8	18.3	1.7	-170.3	-169.8
TS-14+BU	14.1	-37.0	-179.8	156.9	21.2	1.9	-168.6	-168.2
TS-15+BU	9.0	-36.9	175.5	156.7	27.1	-0.2	-164.0	-169.1
TS-16+BU	15.1	-34.0	-177.4	158.5	15.7	1.3	-172.2	-170.9
TS-17+BU	5.7	-32.8	171.9	161.0	32.8	-5.7	-161.0	-171.9
TS-18+BU	-7.4	33.2	-173.1	-161.0	-32.3	3.6	160.2	171.1
TS-19+BU	9.1	-37.0	175.0	157.1	29.0	-3.5	-164.2	-170.4
TS-20+BU	11.6	-37.4	176.7	157.5	24.6	-1.2	-166.4	-170.2
TS-21+BU	6.9	-34.5	173.5	159.0	28.4	-2.3	-163.5	-170.4
TS-22+BU	11.1	-36.6	177.6	156.8	26.9	-5.7	-164.2	-174.6
TS-23+BU	12.6	-36.1	179.4	157.0	23.8	-2.8	-167.2	-171.8
TS-24+BU	5.3	-28.7	172.1	164.5	28.6	-3.1	-163.1	-171.4
TS-25+BU	-9.5	35.3	-175.8	-158.4	-27.4	2.7	164.8	170.6
TS-26+BU	13.6	-35.9	179.5	158.3	22.0	1.5	-167.7	-168.8
TS-27+BU	11.7	-37.8	176.6	157.4	27.2	-0.7	-163.8	-169.6
TS-28+BU	10.8	-37.8	176.3	156.8	27.3	-2.3	-164.8	-170.1
TS-29+BU	-7.0	34.7	-173.1	-159.1	-31.6	4.0	160.9	171.6
TS-30+BU	7.2	-34.8	172.5	159.9	32.2	-4.2	-160.9	-171.1
TS-31+BU	10.1	-36.8	175.5	157.8	30.0	-1.3	-161.9	-169.4
TS-32+BU	-11.8	37.1	-178.7	-156.0	-23.1	-0.8	167.1	169.1
TS-33+BU	4.3	-33.8	171.1	159.4	33.8	-4.3	-159.4	-171.1
TS-34+BU	13.0	-37.1	178.8	157.1	25.3	1.1	-165.8	-167.8
TS-35+BU	-10.4	38.4	-177.7	-154.3	-28.3	0.3	163.7	168.3
TS-36+BU	12.5	-39.3	177.5	155.7	27.0	0.2	-163.2	-169.6
TS-37+BU	5.8	-36.7	171.8	157.3	34.1	-3.5	-157.5	-171.9
TS-38+BU	5.5	-34.0	171.9	159.7	34.5	-5.0	-158.3	-172.2
TS-39+BU	6.0	-34.1	171.9	160.0	34.1	-6.0	-160.0	-171.9
TS-40+BU	11.5	-37.8	176.7	157.1	29.0	-1.1	-162.6	-169.5
TS-41+BU	9.7	-35.2	175.5	159.0	26.2	-0.9	-164.7	-169.9
TS-42+BU	11.1	-37.5	176.7	156.9	23.9	0.1	-166.1	-169.9
TS-43+BU	9.3	-35.1	175.3	158.9	29.6	-1.6	-162.7	-169.3
TS-44+BU	-4.6	33.2	-171.9	-159.5	-30.6	4.4	161.9	171.9
TS-45+BU	12.0	-36.6	178.7	156.7	19.5	1.2	-169.2	-170.1
TS-46+BU	6.1	-34.5	172.5	159.2	31.9	-2.5	-160.0	-170.6
TS-47+BU	11.3	-37.7	176.9	156.8	26.7	0.0	-164.3	-169.0
TS-48+BU	9.9	-37.4	175.6	157.0	29.4	-1.0	-162.9	-168.8
TS-49+BU	11.9	-39.5	177.4	155.0	26.1	0.5	-164.3	-169.1
TS-50+BU	9.0	-37.5	175.2	156.4	32.1	-1.7	-161.4	-168.3
TS-51+BU	-5.2	36.1	-171.3	-157.9	-32.6	4.1	159.8	171.7
TS-52+BU	12.7	-39.4	178.8	154.5	23.1	1.5	-166.4	-169.0
TS-53+BU	6.4	-36.6	172.8	156.9	34.4	-2.7	-158.2	-170.1
TS-54+BU	11.8	-39.8	177.6	154.4	28.6	0.2	-162.9	-168.3
TS-55+BU	4.4	-32.6	170.7	161.1	32.5	-4.4	-161.2	-170.7
TS-56+BU	9.1	-35.7	174.7	158.8	30.2	-1.8	-162.7	-168.9
TS-57+BU	11.0	-38.3	176.2	156.5	30.0	-0.4	-162.4	-168.0
TS-58+BU	12.6	-40.7	178.1	153.8	26.6	0.5	-164.2	-168.7
TS-59+BU	9.5	-38.4	175.2	155.9	33.1	-1.4	-160.5	-167.8
TS-60+BU	-5.2	37.2	-171.1	-157.0	-33.9	4.4	158.9	171.6
TS-61+BU	13.7	-40.4	-179.8	153.1	22.9	1.5	-166.6	-168.9
TS-62+BU	7.5	-38.2	173.7	155.7	35.4	-2.3	-157.4	-169.5
TS-63+BU	13.1	-41.2	178.7	153.2	29.0	0.7	-162.4	-167.9
TS-64+BU	11.7	-36.3	176.8	158.6	27.3	-0.8	-165.2	-168.3
TS-65+BU	13.4	-38.4	178.6	156.4	24.1	0.1	-166.8	-169.0
TS-66+BU	10.9	-36.9	176.2	157.9	30.9	-1.6	-163.0	-167.7
TS-67+BU	-5.5	35.0	-171.0	-159.4	-31.9	5.3	161.4	172.1
TS-68+BU	14.5	-37.8	-179.0	155.6	19.8	1.0	-169.7	-169.5
TS-69+BU	8.1	-36.3	173.6	158.2	33.8	-3.3	-159.7	-169.8
TS-70+BU	14.3	-39.7	179.4	155.1	26.9	0.3	-164.9	-167.9

Table S52. Δd_{C3C6}, τ_{56}, τ_{34}, χ_{C3}, χ_{C4}, χ_{C5} and χ_{C6} values for the diene fragments derived from the transition structures of **BU**.

fragment from	Δd_{C3C6}	τ_{56}	τ_{34}	χ_{C3}	χ_{C4}	χ_{C5}	χ_{C6}
TS-1+BU	-0.209	-13.1	11.9	16.8	-12.0	14.4	-32.2
TS-2+BU	-0.197	-12.8	12.4	15.2	-11.2	14.8	-32.5
TS-3+BU	-0.154	-11.1	10.4	8.4	-9.2	13.7	-35.1
TS-4+BU	-0.200	-12.1	11.1	13.5	-12.3	13.6	-31.8
TS-5+BU	-0.218	-13.1	12.4	22.3	-13.5	13.9	-26.7
TS-6+BU	-0.167	-12.2	9.8	19.6	-10.4	13.4	-32.3
TS-7+BU	-0.163	-11.2	9.6	14.2	-10.2	13.1	-33.4
TS-8+BU	-0.164	-12.0	10.4	10.1	-8.7	13.9	-35.9
TS-9+BU	-0.187	-12.8	11.5	13.3	-9.9	14.8	-35.0
TS-10+BU	-0.217	-13.6	13.6	17.8	-12.3	14.6	-32.4
TS-11+BU	-0.222	14.2	-14.3	24.7	-13.0	13.1	-25.4
TS-12+BU	-0.121	-9.9	8.6	5.9	-7.3	-12.0	34.6
TS-13+BU	-0.141	-11.0	10.0	8.0	-8.5	-13.3	35.6
TS-14+BU	-0.171	-11.4	11.6	9.5	-9.8	-13.9	37.2
TS-15+BU	-0.205	-13.9	13.4	16.2	-11.1	13.6	-32.3
TS-16+BU	-0.152	-9.5	8.5	6.6	-7.8	-12.5	36.6
TS-17+BU	-0.228	-13.6	13.6	24.7	-13.8	13.8	-24.7
TS-18+BU	-0.220	12.9	-14.3	23.3	-12.5	14.2	-26.3
TS-19+BU	-0.226	-13.9	12.7	19.4	-13.1	14.1	-32.0
TS-20+BU	-0.208	-12.9	11.7	14.8	-11.0	14.9	-34.1
TS-21+BU	-0.212	-13.8	13.1	18.8	-12.0	13.4	-27.9
TS-22+BU	-0.183	-12.8	10.6	21.5	-11.1	13.5	-34.2
TS-23+BU	-0.181	-11.8	10.5	15.6	-11.0	13.1	-35.5
TS-24+BU	-0.200	-11.7	12.7	20.0	-11.7	13.2	-20.7
TS-25+BU	-0.221	12.9	-12.3	18.0	-12.2	13.7	-31.1
TS-26+BU	-0.189	-11.1	11.7	10.8	-9.7	14.1	-35.3
TS-27+BU	-0.222	-13.0	13.3	16.8	-11.0	15.2	-34.4
TS-28+BU	-0.227	-13.5	12.5	17.4	-12.2	14.6	-34.0
TS-29+BU	-0.227	13.9	-13.8	23.1	-12.5	13.8	-27.8
TS-30+BU	-0.237	-13.8	14.0	23.3	-13.1	14.7	-27.3
TS-31+BU	-0.228	-13.3	14.4	19.4	-12.0	14.6	-32.3
TS-32+BU	-0.200	12.7	-11.9	12.1	-10.1	13.1	-35.7
TS-33+BU	-0.241	-14.7	14.7	24.9	-13.2	13.2	-24.9
TS-34+BU	-0.212	-12.1	13.2	13.1	-11.1	14.2	-35.9
TS-35+BU	-0.231	14.0	-14.0	16.6	-12.0	12.7	-36.1
TS-36+BU	-0.214	-13.4	13.6	16.6	-10.2	15.0	-36.8
TS-37+BU	-0.243	-15.5	15.3	26.1	-11.6	14.0	-28.5
TS-38+BU	-0.249	-14.2	14.7	26.7	-12.8	13.6	-25.9
TS-39+BU	-0.249	-14.0	14.0	26.0	-14.1	14.1	-26.0
TS-40+BU	-0.239	-13.1	13.9	18.5	-11.6	14.9	-34.5
TS-41+BU	-0.190	-12.7	12.7	16.2	-10.9	14.2	-30.7
TS-42+BU	-0.183	-13.2	12.0	13.8	-10.0	14.4	-34.2
TS-43+BU	-0.212	-12.9	14.0	18.9	-12.3	14.0	-30.4
TS-44+BU	-0.209	14.3	-13.1	22.4	-12.5	12.7	-25.1
TS-45+BU	-0.162	-12.3	10.3	9.6	-8.7	13.3	-35.2
TS-46+BU	-0.217	-14.2	14.7	22.5	-11.9	13.6	-27.0
TS-47+BU	-0.204	-13.2	13.4	15.7	-10.9	14.5	-34.5
TS-48+BU	-0.215	-13.7	14.2	18.1	-12.3	14.4	-32.9
TS-49+BU	-0.204	-13.8	13.3	15.2	-10.4	14.5	-36.9
TS-50+BU	-0.235	-14.2	15.2	20.4	-13.4	13.9	-32.6
TS-51+BU	-0.233	15.4	-14.2	24.3	-12.4	14.0	-27.4
TS-52+BU	-0.188	-13.4	12.3	12.1	-9.5	13.9	-38.2
TS-53+BU	-0.241	-15.1	15.8	24.5	-12.6	13.6	-29.5
TS-54+BU	-0.226	-14.0	14.4	16.9	-11.5	14.2	-37.4
TS-55+BU	-0.213	-14.1	14.1	23.2	-13.7	13.7	-23.3
TS-56+BU	-0.215	-13.3	14.2	19.0	-12.9	14.4	-30.4
TS-57+BU	-0.218	-13.6	14.8	18.0	-12.4	14.7	-34.5
TS-58+BU	-0.201	-14.0	13.6	15.3	-10.8	14.5	-38.8
TS-59+BU	-0.238	-14.5	15.8	20.9	-13.5	14.3	-33.6
TS-60+BU	-0.243	16.0	-14.7	25.5	-12.8	14.2	-28.3
TS-61+BU	-0.176	-13.3	12.2	11.9	-9.6	-13.5	40.6
TS-62+BU	-0.249	-15.3	16.5	24.9	-12.8	13.9	-31.8
TS-63+BU	-0.218	-14.0	14.8	16.9	-11.4	14.4	-39.9
TS-64+BU	-0.212	-12.3	13.2	15.6	-12.5	14.9	-33.1
TS-65+BU	-0.196	-12.5	12.1	13.1	-10.9	14.8	-37.0
TS-66+BU	-0.234	-13.0	14.6	18.7	-13.9	14.8	-33.1
TS-67+BU	-0.233	14.8	-13.3	23.9	-13.3	14.5	-26.0
TS-68+BU	-0.167	-11.7	10.4	9.2	-9.5	-13.5	38.8
TS-69+BU	-0.246	-14.1	15.2	23.6	-13.5	14.5	-29.9
TS-70+BU	-0.215	-12.7	13.6	14.8	-11.8	14.9	-39.2

Table S53. $\theta_{1\text{-}8}$ values for the diene fragments derived from the transition structures of **DMB**.

fragment from	θ_1	θ_2	θ_3	θ_4	θ_5	θ_5	θ_7	θ_8
TS-1+DMB	10.7	-35.9	178.5	156.2	23.8	-2.2	-166.3	-172.2
TS-2+DMB	11.0	-35.9	178.6	156.6	23.3	0.3	-165.2	-171.2
TS-3+DMB	13.7	-33.7	-177.3	157.3	16.0	2.6	-170.3	-171.2
TS-4+DMB	11.7	-33.7	-178.5	156.6	18.9	0.0	-169.5	-171.6
TS-5+DMB	7.8	-33.0	175.5	159.3	29.2	-4.4	-161.8	-173.4
TS-6+DMB	10.5	-34.3	180.0	156.3	23.7	-3.4	-163.3	-176.4
TS-7+DMB	12.2	-33.2	-178.0	157.0	19.6	-0.9	-167.5	-173.9
TS-8+DMB	13.0	-35.5	-178.4	155.9	17.4	1.7	-168.8	-172.1
TS-9+DMB	12.5	-36.6	-179.9	155.9	20.8	0.9	-166.5	-171.9
TS-10+DMB	10.4	-36.5	178.0	155.9	26.3	0.0	-163.0	-170.7
TS-11+DMB	-3.4	32.3	-173.3	-157.8	-32.7	4.4	158.0	173.7
TS-12+DMB	13.1	-30.8	-176.3	158.6	12.8	2.4	-172.3	-172.4
TS-13+DMB	13.5	-33.6	-177.3	157.3	15.6	2.3	-170.5	-171.6
TS-14+DMB	15.1	-35.3	-176.5	156.3	18.1	3.1	-168.9	-170.0
TS-15+DMB	10.1	-36.4	178.8	155.0	23.7	1.5	-164.3	-170.4
TS-16+DMB	15.4	-32.1	-174.9	158.2	12.6	0.5	-174.0	-172.9
TS-17+DMB	5.8	-31.9	173.8	160.0	31.9	-5.8	-160.0	-173.8
TS-18+DMB	-6.8	32.4	-174.7	-159.7	-31.2	3.2	158.7	173.2
TS-19+DMB	9.3	-36.6	177.7	155.1	26.8	-2.8	-164.2	-171.9
TS-20+DMB	11.7	-36.7	179.0	156.0	22.5	-1.3	-166.9	-171.9
TS-21+DMB	7.2	-34.3	175.9	157.0	26.6	-1.0	-162.7	-171.7
TS-22+DMB	10.7	-35.6	-179.7	154.8	25.8	-3.7	-161.6	-176.2
TS-23+DMB	12.5	-34.8	-177.5	155.3	21.9	-0.4	-165.2	-173.3
TS-24+DMB	4.3	-28.0	173.6	162.7	27.4	-2.4	-161.6	-173.4
TS-25+DMB	-9.3	35.4	-178.6	-155.3	-24.6	1.2	164.7	171.9
TS-26+DMB	14.2	-35.0	-177.9	157.0	18.3	1.6	-168.9	-171.2
TS-27+DMB	10.2	-37.4	178.8	154.1	25.3	0.1	-163.1	-171.5
TS-28+DMB	11.1	-37.2	178.8	155.2	25.2	-2.1	-165.2	-171.7
TS-29+DMB	-6.7	34.1	-174.9	-157.8	-30.9	2.8	158.6	173.3
TS-30+DMB	6.9	-34.1	174.3	158.5	31.2	-4.2	-160.0	-173.0
TS-31+DMB	8.8	-36.6	177.8	154.4	28.6	0.2	-160.2	-171.0
TS-32+DMB	-12.0	36.3	178.2	-153.9	-19.6	-1.1	168.5	170.9
TS-33+DMB	4.2	-33.1	173.0	158.1	33.1	-4.2	-158.1	-173.0
TS-34+DMB	14.4	-36.5	-177.6	155.4	20.8	1.5	-167.6	-170.1
TS-35+DMB	-10.6	38.3	179.0	-151.2	-25.3	-0.8	164.2	169.7
TS-36+DMB	10.4	-39.0	179.7	151.8	25.3	1.6	-161.8	-171.3
TS-37+DMB	5.4	-37.5	173.8	154.1	32.5	-2.0	-156.2	-173.4
TS-38+DMB	-5.0	33.8	-174.3	-156.9	-33.2	3.6	157.0	173.5
TS-39+DMB	5.8	-33.4	173.7	158.7	33.4	-5.8	-158.7	-173.7
TS-40+DMB	9.9	-37.5	178.8	153.6	27.4	-0.8	-162.0	-171.4
TS-41+DMB	6.8	-35.3	177.7	153.8	23.8	0.6	-163.5	-172.1
TS-42+DMB	8.3	-37.2	179.4	151.7	21.0	1.8	-165.1	-172.1
TS-43+DMB	6.6	-35.4	177.3	153.9	27.7	-0.5	-161.3	-171.5
TS-44+DMB	-4.5	32.8	-174.4	-157.3	-29.8	1.7	158.6	173.3
TS-45+DMB	9.4	-35.6	-178.5	152.3	16.4	2.5	-168.7	-172.4
TS-46+DMB	3.1	-34.2	174.3	154.6	30.7	-1.0	-157.6	-172.7
TS-47+DMB	8.2	-37.4	179.2	151.6	24.3	1.7	-162.8	-171.2
TS-48+DMB	8.0	-37.3	178.0	152.8	27.6	1.4	-160.4	-170.6
TS-49+DMB	9.4	-39.5	179.7	150.2	24.6	2.5	-162.1	-170.8
TS-50+DMB	6.7	-37.4	177.3	152.1	30.9	0.7	-158.3	-170.2
TS-51+DMB	-3.5	35.9	-173.4	-154.2	-31.8	1.9	156.8	173.3
TS-52+DMB	10.6	-39.0	-178.4	149.9	20.8	3.2	-165.1	-170.8
TS-53+DMB	4.0	-36.1	174.6	153.2	34.1	-0.3	-154.3	-171.8
TS-54+DMB	9.3	-39.5	-180.0	149.8	27.4	2.7	-159.9	-170.0
TS-55+DMB	3.8	-31.9	172.8	159.1	31.9	-3.8	-159.1	-172.8
TS-56+DMB	8.0	-35.6	176.8	155.5	28.2	-1.3	-162.3	-170.9
TS-57+DMB	8.0	-38.1	178.1	151.8	28.8	1.5	-159.7	-170.0
TS-58+DMB	9.9	-40.4	-179.4	148.9	24.6	2.7	-162.1	-170.6
TS-59+DMB	6.1	-38.1	177.0	151.0	32.2	0.6	-157.4	-169.8
TS-60+DMB	-4.4	37.0	-173.7	-153.7	-32.8	1.2	155.5	172.9
TS-61+DMB	11.7	-39.6	-177.1	149.1	20.6	3.2	-165.3	-170.9
TS-62+DMB	4.3	-37.8	175.2	151.3	35.2	-0.2	-153.5	-171.5
TS-63+DMB	10.1	-40.7	-179.3	148.7	28.0	2.8	-159.5	-169.8
TS-64+DMB	10.2	-35.9	178.7	155.5	25.3	0.0	-164.3	-170.3
TS-65+DMB	11.7	-37.9	-179.4	153.2	22.2	0.9	-166.0	-170.9
TS-66+DMB	9.2	-36.8	178.0	154.3	29.1	-0.7	-161.7	-169.8
TS-67+DMB	-5.4	34.5	-173.6	-157.3	-30.6	3.5	159.6	173.4
TS-68+DMB	13.1	-36.4	-176.7	153.4	17.6	1.5	-169.6	-171.3
TS-69+DMB	6.1	-35.7	175.1	155.3	32.9	-2.5	-157.7	-171.8
TS-70+DMB	12.2	-39.1	-178.9	152.0	25.4	1.1	-163.7	-169.9

Table S54. Δd_{C3C6}, τ_{56}, τ_{34}, χ_{C3}, χ_{C4}, χ_{C5} and χ_{C6} values for the diene fragments derived from the transition structures of **DMB**.

fragment from	Δd_{C3C6}	τ_{56}	τ_{34}	χ_{C3}	χ_{C4}	χ_{C5}	χ_{C6}
TS-1+DMB	-0.194	12.6	10.8	16.0	10.0	12.1	34.4
TS-2+DMB	-0.184	12.4	11.8	14.5	8.5	12.4	34.5
TS-3+DMB	-0.143	10.0	9.3	7.1	6.3	11.0	36.4
TS-4+DMB	-0.174	11.0	9.4	10.5	8.5	10.3	35.2
TS-5+DMB	-0.203	12.6	12.4	22.6	10.9	12.2	28.5
TS-6+DMB	-0.161	11.9	10.1	20.1	7.0	10.5	34.2
TS-7+DMB	-0.154	10.5	9.3	13.4	7.1	10.2	35.2
TS-8+DMB	-0.157	11.2	9.6	9.5	6.2	11.4	37.0
TS-9+DMB	-0.172	12.0	10.8	12.6	7.3	12.4	36.6
TS-10+DMB	-0.199	13.0	13.1	17.0	9.4	12.3	34.5
TS-11+DMB	-0.208	14.5	14.1	26.4	10.7	10.1	25.6
TS-12+DMB	-0.124	8.8	7.6	5.3	5.1	9.4	34.5
TS-13+DMB	-0.137	10.0	9.0	7.2	6.1	10.8	36.3
TS-14+DMB	-0.156	10.1	10.6	8.0	7.0	11.6	38.8
TS-15+DMB	-0.188	13.1	12.6	14.1	8.0	11.4	35.1
TS-16+DMB	-0.144	8.4	6.5	5.5	6.6	10.3	37.2
TS-17+DMB	-0.215	13.1	13.1	25.7	12.0	12.0	25.7
TS-18+DMB	-0.207	12.8	14.0	24.4	10.0	12.1	27.1
TS-19+DMB	-0.208	13.6	12.0	18.7	10.9	11.7	34.3
TS-20+DMB	-0.193	12.5	10.6	14.4	9.4	12.7	35.7
TS-21+DMB	-0.197	13.6	12.8	18.3	9.3	11.2	30.2
TS-22+DMB	-0.174	12.5	11.1	22.0	7.4	10.4	35.9
TS-23+DMB	-0.167	11.1	10.7	15.2	7.1	10.0	37.2
TS-24+DMB	-0.189	11.8	12.5	20.8	9.0	10.7	21.5
TS-25+DMB	-0.199	13.1	11.7	16.5	9.3	10.7	34.1
TS-26+DMB	-0.172	10.4	10.0	9.5	7.2	12.0	37.1
TS-27+DMB	-0.203	13.6	12.7	16.8	8.4	11.4	36.1
TS-28+DMB	-0.207	13.0	11.6	16.9	10.4	12.3	36.0
TS-29+DMB	-0.219	13.7	14.0	24.2	9.5	11.8	29.0
TS-30+DMB	-0.221	13.6	13.5	24.1	11.2	12.6	28.4
TS-31+DMB	-0.212	13.9	14.4	19.6	8.8	11.0	34.4
TS-32+DMB	-0.180	12.1	10.3	10.5	8.0	10.2	38.1
TS-33+DMB	-0.229	14.4	14.4	26.0	11.2	11.2	26.0
TS-34+DMB	-0.190	11.1	11.2	10.9	8.4	12.0	39.0
TS-35+DMB	-0.209	13.9	13.0	15.0	9.4	9.6	39.3
TS-36+DMB	-0.196	14.3	13.5	16.6	7.2	10.8	38.7
TS-37+DMB	-0.228	16.0	15.2	25.8	8.6	11.6	31.3
TS-38+DMB	-0.230	14.4	14.8	26.7	10.1	10.7	28.1
TS-39+DMB	-0.233	13.8	13.8	27.1	12.1	12.1	27.1
TS-40+DMB	-0.218	13.8	13.3	18.8	9.4	11.1	36.3
TS-41+DMB	-0.177	14.2	12.2	15.9	7.3	9.1	33.1
TS-42+DMB	-0.169	14.5	11.4	13.1	6.1	8.9	36.6
TS-43+DMB	-0.198	14.4	13.6	19.2	9.0	9.3	32.7
TS-44+DMB	-0.197	14.2	14.0	23.1	8.4	10.1	27.1
TS-45+DMB	-0.151	13.1	9.4	8.8	5.1	7.9	37.0
TS-46+DMB	-0.204	15.5	14.9	23.4	8.3	8.8	28.5
TS-47+DMB	-0.189	14.6	13.0	15.5	7.1	9.0	36.6
TS-48+DMB	-0.197	14.6	14.5	18.1	8.0	10.0	35.3
TS-49+DMB	-0.186	15.1	13.6	15.4	6.7	9.7	39.1
TS-50+DMB	-0.216	15.3	15.8	21.1	9.2	9.4	34.7
TS-51+DMB	-0.215	16.2	15.0	25.0	8.6	10.2	29.3
TS-52+DMB	-0.171	14.2	12.0	11.6	5.9	8.9	40.7
TS-53+DMB	-0.223	16.1	16.9	25.9	8.4	9.3	30.8
TS-54+DMB	-0.207	15.1	15.0	17.4	7.3	9.3	39.5
TS-55+DMB	-0.205	14.1	14.1	24.7	11.0	11.0	24.7
TS-56+DMB	-0.201	13.8	13.4	19.0	10.4	11.2	32.5
TS-57+DMB	-0.199	15.1	15.1	18.8	8.6	9.8	36.2
TS-58+DMB	-0.182	15.3	13.6	15.3	6.7	9.3	41.0
TS-59+DMB	-0.219	16.0	16.4	22.1	9.6	9.1	35.2
TS-60+DMB	-0.224	16.3	15.8	25.6	8.3	10.7	30.7
TS-61+DMB	-0.166	14.0	11.9	11.5	5.9	8.8	42.5
TS-62+DMB	-0.230	16.8	17.5	26.7	8.7	9.1	33.0
TS-63+DMB	-0.201	15.3	15.4	17.7	7.5	9.4	41.4
TS-64+DMB	-0.192	12.9	12.7	15.6	9.6	11.4	34.6
TS-65+DMB	-0.181	13.1	11.6	13.1	8.2	11.1	38.5
TS-66+DMB	-0.213	13.8	14.2	19.0	10.9	11.1	34.8
TS-67+DMB	-0.215	14.6	13.5	24.0	10.2	11.7	28.1
TS-68+DMB	-0.158	11.6	9.5	8.9	7.1	9.8	39.7
TS-69+DMB	-0.226	14.8	15.2	24.8	10.7	10.9	30.8
TS-70+DMB	-0.200	13.4	13.2	15.2	9.0	11.1	40.2

Table S55. Results obtained by applying ANOVA of the selected most significant factors of the distortion energy ($\Delta E_d^{\ddagger}$).

$$\Delta E_d^{\ddagger} \sim a.\mathrm{NS} + b.\mathrm{RS} + c.\omega + d.\Delta d + e.\ \Delta d^2 + f$$

Source	Sum of Squares	Mean Square	F value	Prob. > F	Significant
cyclopentadiene, acyclic dienophile					
NS	541.307418	541.307418	255.302404	< 0.0001	Yes
Δd	19.2813963	19.2813963	9.09388393	0.0047	Yes
Δd^2	34.9674761	34.9674761	16.4920716	0.0003	Yes
1,3-cyclohexadiene, acyclic dienophile					
NS	828.348766	828.348766	300.933046	< 0.0001	Yes
Δd	12.6220048	12.6220048	4.585482	0.0391	Yes
Δd^2	33.3766019	33.3766019	12.1254753	0.0013	Yes
butadiene, acyclic dienophile					
NS	500.172332	500.172332	204.606593	< 0.0001	Yes
Δd	8.91571247	8.91571247	3.64717006	0.0642	No
Δd^2	30.4772341	30.4772341	12.467389	0.0012	Yes
2,3-dimethyl-1,3-butadiene, acyclic dienophile					
NS	468.346637	468.346637	190.507623	< 0.0001	Yes
Δd	16.6827613	16.6827613	6.78598489	0.0133	Yes
Δd^2	46.1834736	46.1834736	18.7858801	0.0001	Yes
cyclopentadiene, cyclic dienophile					
NS	313.489542	313.489542	144.497017	< 0.0001	Yes
RS	124.344859	124.344859	57.3143878	< 0.0001	Yes
ω	65.0953644	65.0953644	30.0044649	< 0.0001	Yes
Δd	8.38609293	8.38609293	3.86540937	0.0605	No
1,3-cyclohexadiene, cyclic dienophile					
NS	595.317282	595.317282	273.628315	< 0.0001	Yes
RS	165.305079	165.305079	75.9799046	< 0.0001	Yes
ω	89.0675208	89.0675208	40.9384984	< 0.0001	Yes
Δd	14.0664356	14.0664356	6.46541802	0.0176	Yes
butadiene, cyclic dienophile					
NS	249.82791	249.82791	112.175589	< 0.0001	Yes
RS	112.217068	112.217068	50.3867469	< 0.0001	Yes
ω	71.3928979	71.3928979	32.0562277	< 0.0001	Yes
Δd	55.6381374	55.6381374	24.98216	< 0.0001	Yes
2,3-dimethyl-1,3-butadiene, cyclic dienophile					
NS	226.888912	226.888912	98.8200493	< 0.0001	Yes
RS	91.606532	91.606532	39.8986531	< 0.0001	Yes
ω	74.1711259	74.1711259	32.3047709	< 0.0001	Yes
Δd	58.2771873	58.2771873	25.3822651	< 0.0001	Yes

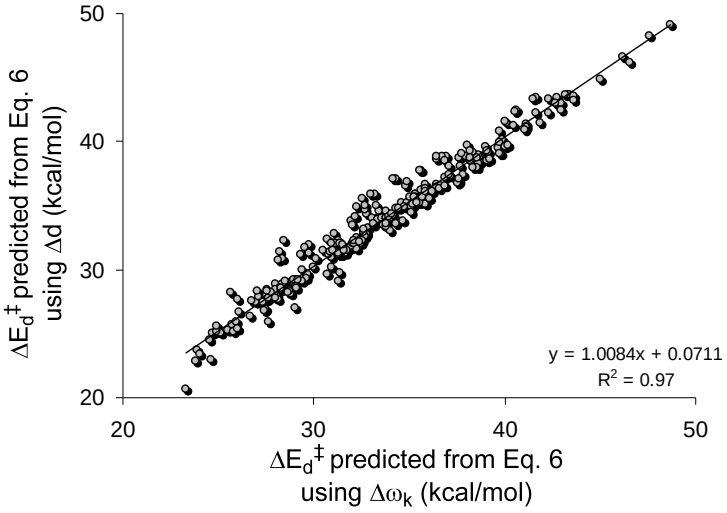


Figure S20. Plot of $\Delta E_d^{\ddagger}$ predicted from Eq. 6 (using Δd) versus $\Delta E_d^{\ddagger}$ predicted from Eq. 6 (using $\Delta\omega_k$) for the 280 reactions under study.

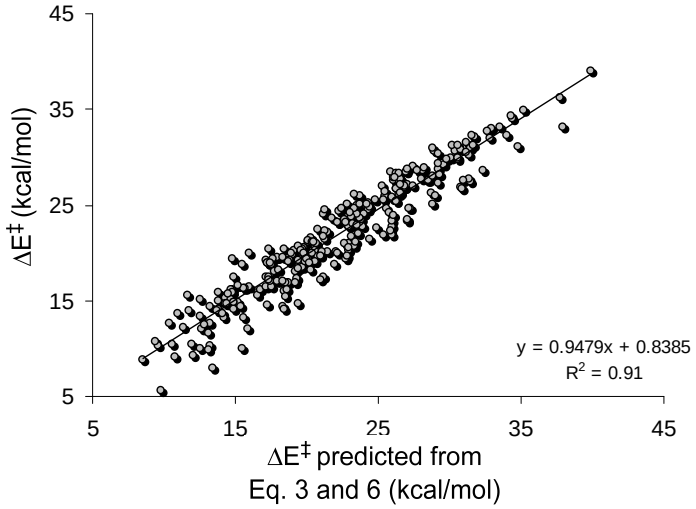


Figure S21. Plot of B3LYP/6-31G* activatio barriers ($\Delta E^{\ddagger}$) versus the barrier heights predicted from Eq. 3 and 6 for the 280 reactions under study.

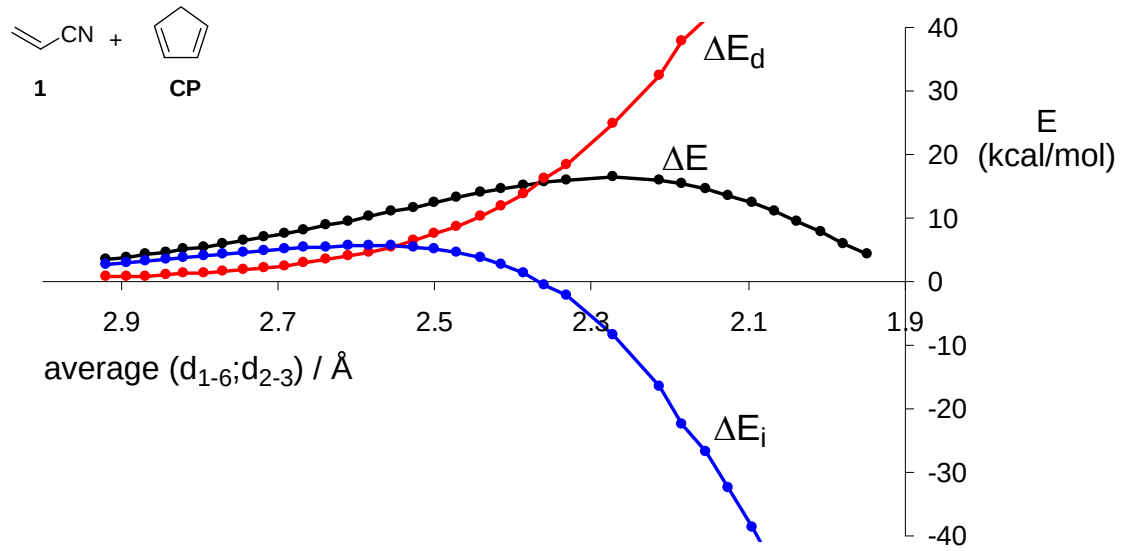


Figure S22. Distortion/interaction analysis of the Diels-Alder reaction between **1** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

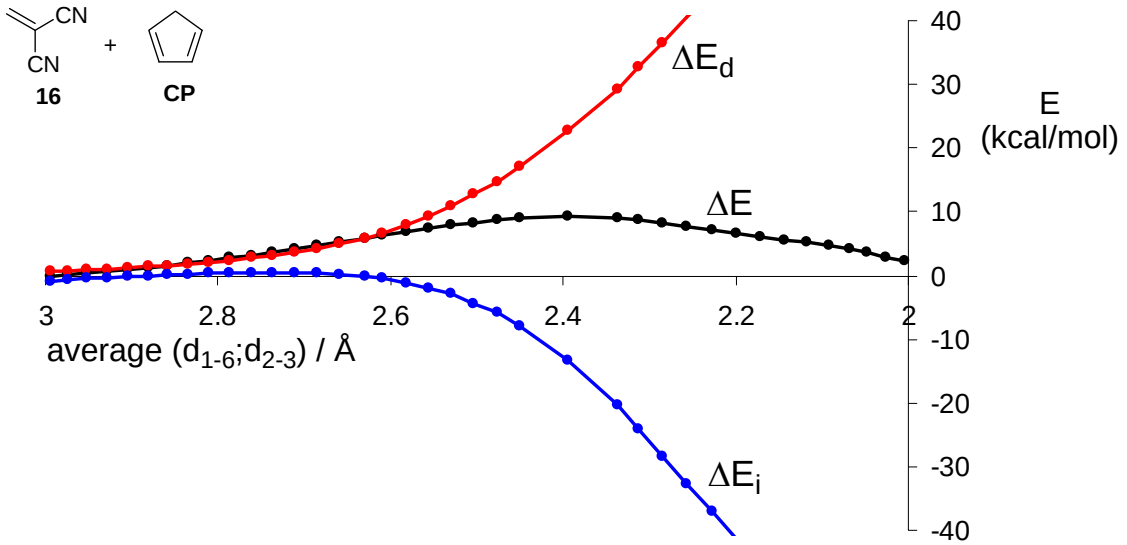


Figure S23. Distortion/interaction analysis of the Diels-Alder reaction between **16** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

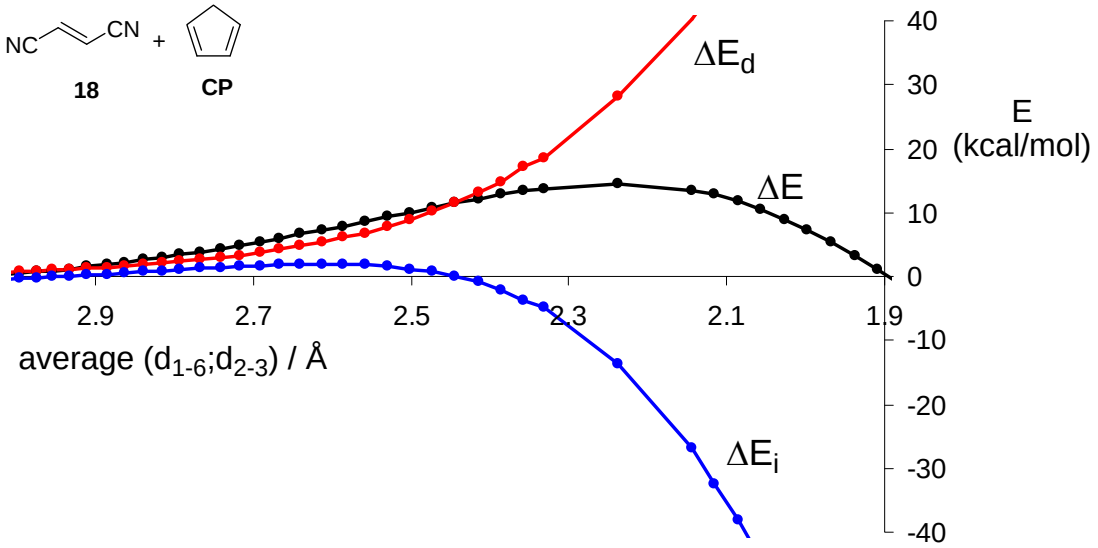


Figure S24. Distortion/interaction analysis of the Diels-Alder reaction between **18** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

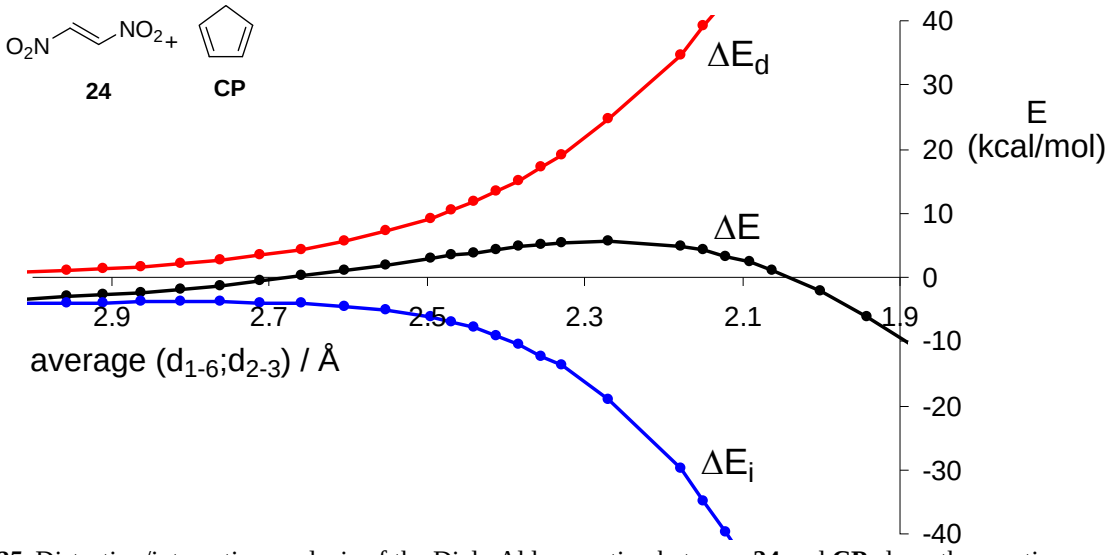


Figure S25. Distortion/interaction analysis of the Diels-Alder reaction between **24** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

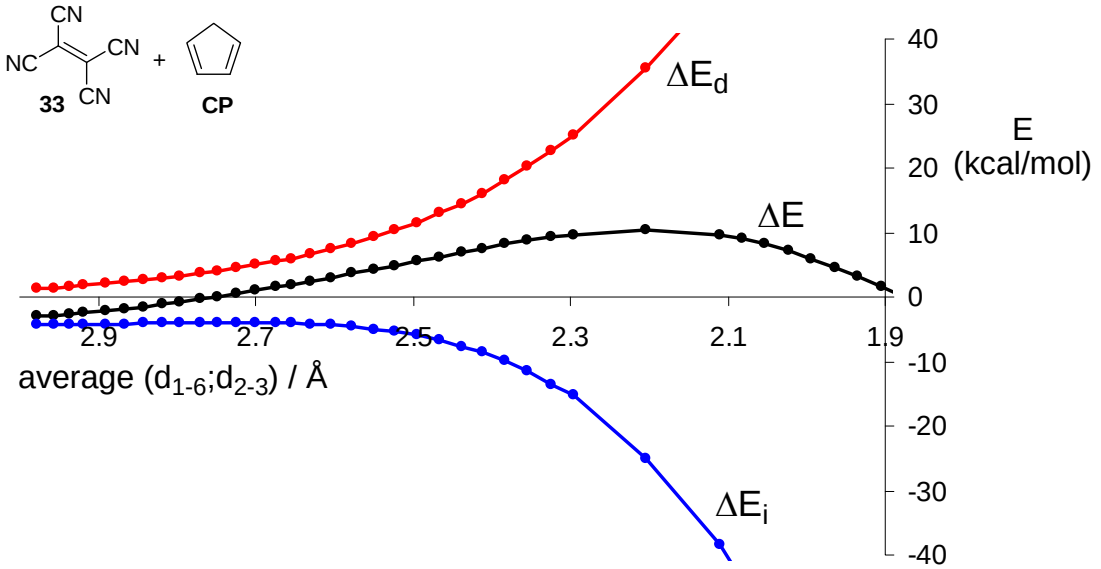


Figure S26. Distortion/interaction analysis of the Diels-Alder reaction between **33** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

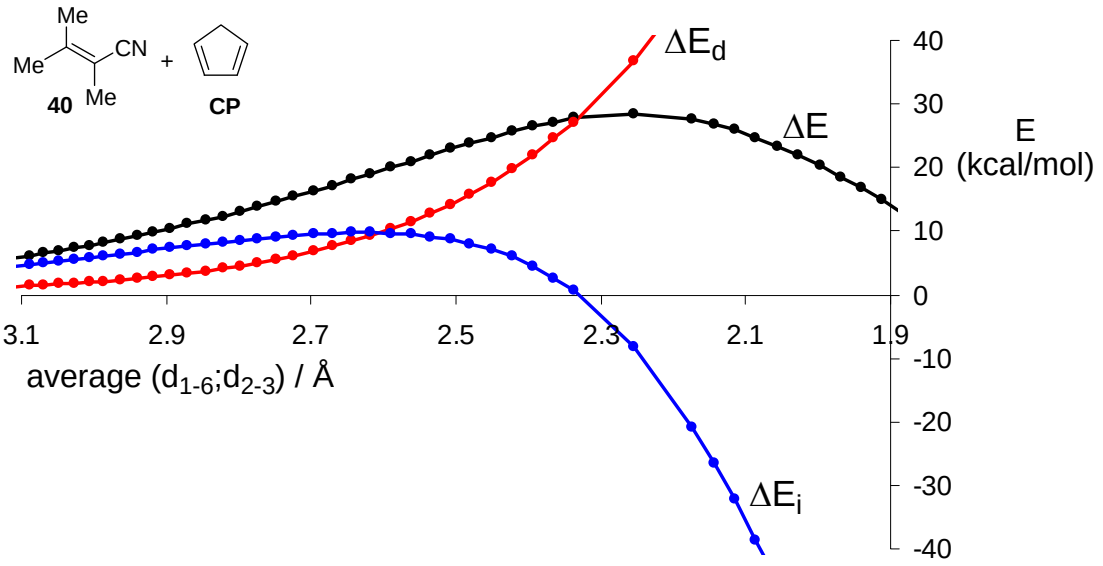


Figure S27. Distortion/interaction analysis of the Diels-Alder reaction between **40** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

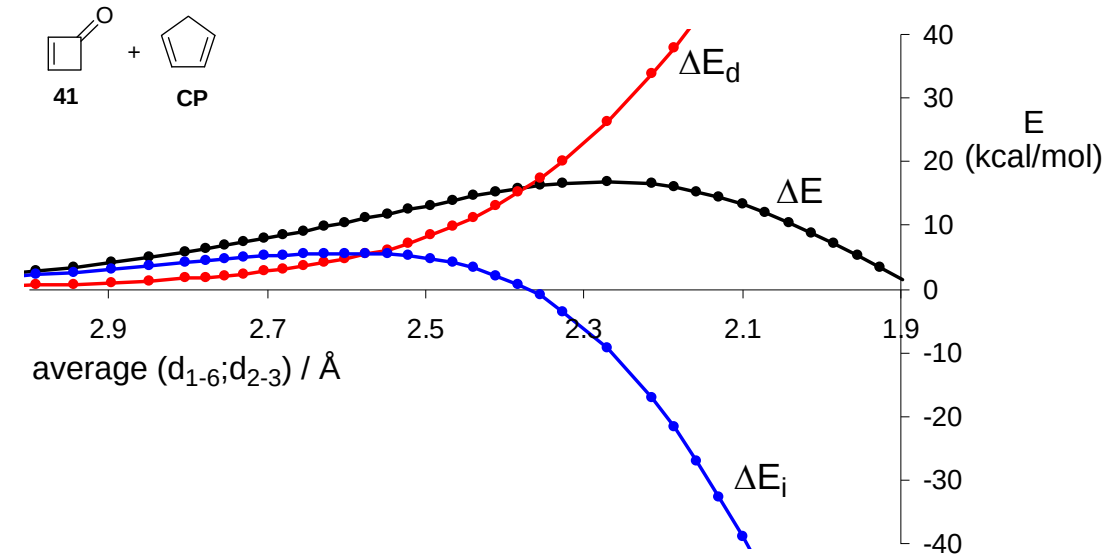


Figure S28. Distortion/interaction analysis of the Diels-Alder reaction between **41** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

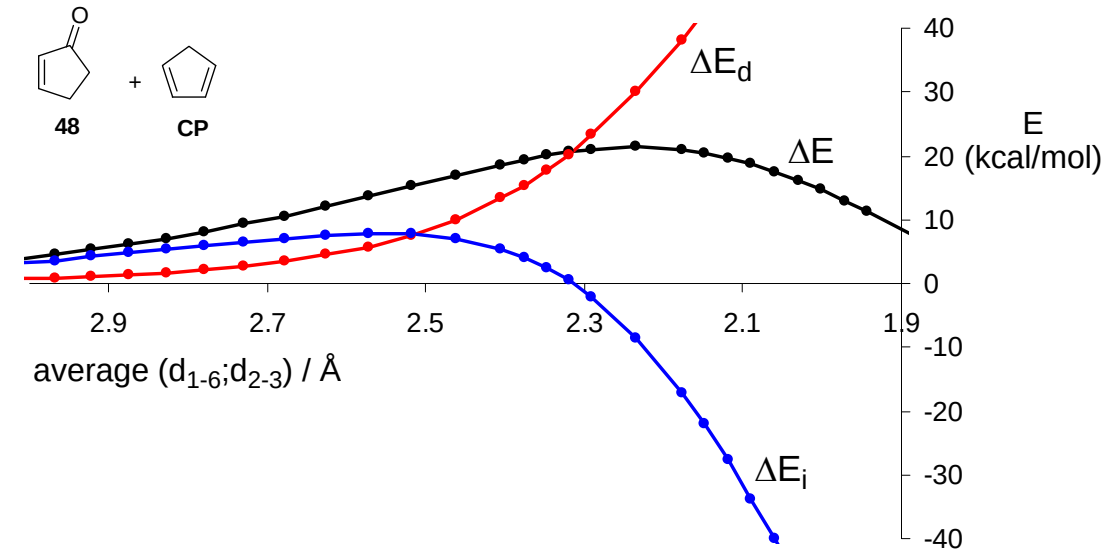


Figure S29. Distortion/interaction analysis of the Diels-Alder reaction between **48** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

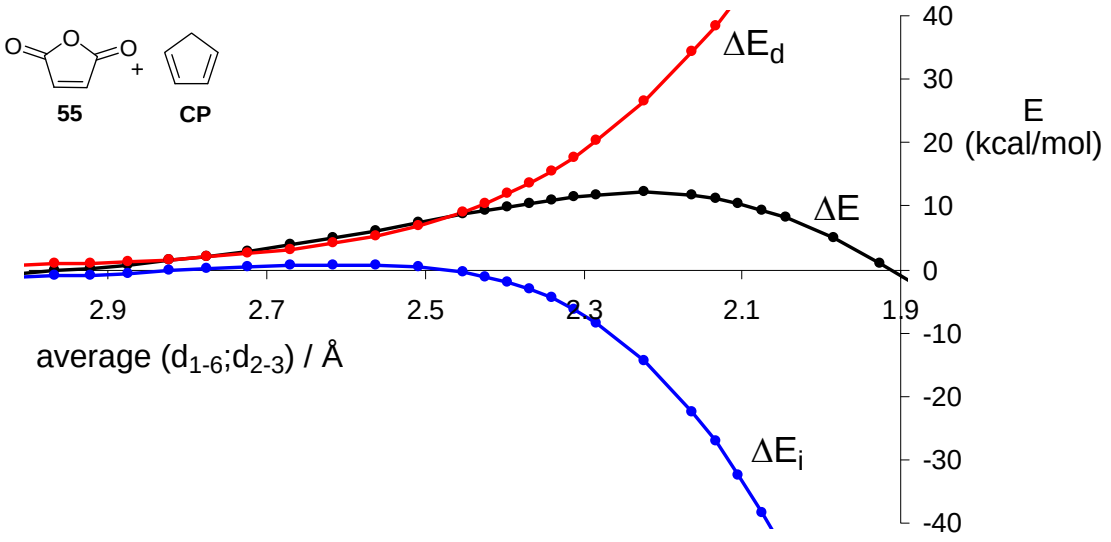


Figure S30. Distortion/interaction analysis of the Diels-Alder reaction between **55** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

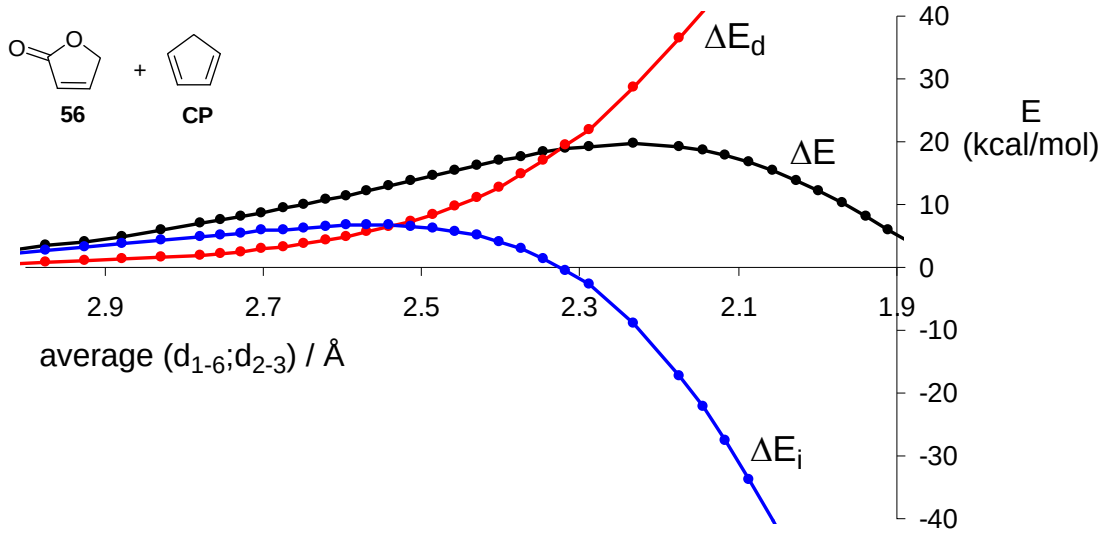


Figure S31. Distortion/interaction analysis of the Diels-Alder reaction between **56** and **CP** along the reaction coordinate projected onto the average forming C-C distances.

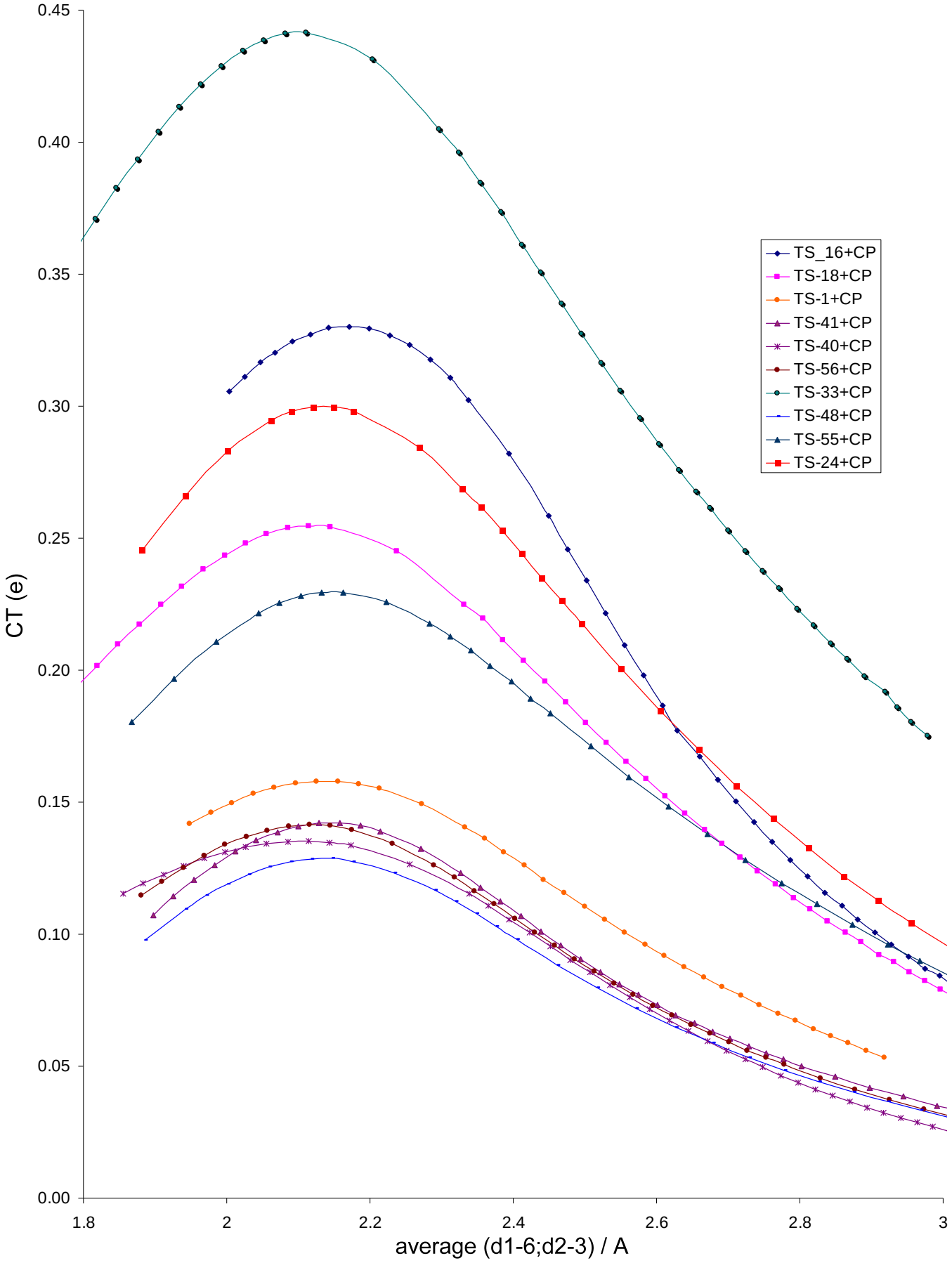


Figure S32. Plot of charge transfer (CT) versus the average bond forming C-C distances for the reactions of compounds **1**, **16**, **18**, **24**, **33**, **40**, **41**, **48**, **55** and **56** with **CP**.

Cartesian coordinates of B3LYP/6-31G* optimized geometries of all reagents, TSs and products under study.

CP

B3LYP/6-31G(d) Geometry

C 0	-1.184605	-0.603316	0.000074
C 0	-1.105864	0.901505	0.000022
C 0	0.377042	1.169229	0.000034
C 0	1.037102	-0.007176	0.000086
C 0	0.065590	-1.109886	0.000110
H 0	-2.114404	-1.160817	0.000075
H 0	-1.604263	1.340615	0.878249
H 0	-1.604245	1.340549	-0.878249
H 0	0.812943	2.161863	0.000013
H 0	2.114404	-0.140017	0.000109
H 0	0.333117	-2.161863	0.000152

CH

B3LYP/6-31G(d) Geometry

C 0	-1.173192	-0.726224	-0.103992
C 0	-0.026655	-1.425057	-0.064415
C 0	1.282375	-0.731771	0.239498
C 0	1.282377	0.731769	-0.239498
C 0	-0.026651	1.425058	0.064415
C 0	-1.173191	0.726227	0.103992
H 0	-2.123966	-1.227269	-0.271916
H 0	-0.028853	-2.506312	-0.184428
H 0	2.123963	-1.272145	-0.209644
H 0	1.448797	-0.763119	1.330072
H 0	1.448800	0.763116	-1.330072
H 0	2.123966	1.272139	0.209644
H 0	-0.028847	2.506312	0.184427
H 0	-2.123964	1.227274	0.271917

BU

B3LYP/6-31G(d) Geometry

C 0	-0.564669	-1.705847	0.000001
C 0	-0.564669	-0.364047	0.000001
C 0	0.564670	0.364047	0.000001
C 0	0.564670	1.705847	-0.000001
H 0	-1.512018	-2.269991	0.000003
H 0	0.367439	-2.294642	0.000001
H 0	-1.542843	0.148021	0.000003
H 0	1.542843	-0.148023	0.000001
H 0	1.512018	2.269993	0.000001
H 0	-0.367438	2.294642	-0.000003

DMB

B3LYP/6-31G(d) Geometry

C 0	1.027818	-1.532254	-0.000134
C 0	0.705685	-0.227103	-0.000010
C 0	-0.705751	0.227041	-0.000044
C 0	-1.028011	1.532155	-0.000125
C 0	1.798510	0.818872	0.000030
C 0	-1.798500	-0.819005	0.000036
H 0	2.065828	-1.853209	-0.000121
H 0	0.284552	-2.322315	-0.000215
H 0	-2.066054	1.852999	-0.000151
H 0	-0.284851	2.322315	-0.000194
H 0	1.732916	1.468391	-0.881712
H 0	1.732774	1.468434	0.881753
H 0	2.786372	0.349666	0.000081
H 0	-2.786372	-0.349832	0.000172
H 0	-1.732891	-1.468491	-0.881753
H 0	-1.732669	-1.468592	0.881734

1

B3LYP/6-31G(d) Geometry

C 0	0.220841	0.431947	-0.000000
C 0	1.243285	-0.432065	-0.000000
C 0	-1.148679	0.016572	-0.000000
N 0	-2.268674	-0.298602	-0.000000
H 0	0.390568	1.506122	0.000000
H 0	2.268674	-0.076304	0.000000
H 0	1.086086	-1.506122	-0.000000

2

B3LYP/6-31G(d) Geometry

C 0	1.317646	0.177940	-0.000331
C 0	0.115889	-0.410297	-0.000064
C 0	-1.123937	0.388921	-0.000018
O 0	-2.243257	-0.084648	-0.000363
H 0	2.243257	-0.389930	-0.000132
H 0	1.412193	1.262508	-0.000558
H 0	-0.003681	-1.491307	0.000259
H 0	-0.964542	1.491307	0.000558

3

B3LYP/6-31G(d) Geometry

C 0	2.227963	0.334110	-0.000358
C 0	1.101348	-0.395906	-0.000272
C 0	-0.193710	0.253513	-0.000296
O 0	-1.248949	-0.397752	-0.000195
B 0	-2.700969	0.285635	-0.000219
H 0	3.210101	-0.128059	-0.000345
H 0	2.199189	1.421385	-0.000445
H 0	1.110788	-1.482471	-0.000182
H 0	-0.248279	1.350519	-0.000369
H 0	-3.209820	-0.148963	1.007256
H 0	-3.210101	-0.149654	-1.007256
H 0	-2.495382	1.482471	-0.000663

4

B3LYP/6-31G(d) Geometry

C 0	-0.098764	-0.415828	-0.000882
C 0	-1.230799	0.276592	0.000836
N 0	1.200044	0.263022	-0.000143
O 0	2.186278	-0.474634	0.001030
O 0	1.228526	1.492120	-0.000443
H 0	0.008569	-1.492120	-0.002430
H 0	-2.186278	-0.236805	0.000577
H 0	-1.218390	1.360921	0.002430

5

B3LYP/6-31G(d) Geometry

C 0	0.014503	-0.447510	-0.000343
C 0	-1.118552	0.247837	-0.000314
C 0	1.369854	0.186668	-0.000320
F 0	2.082840	-0.194147	-1.086218
F 0	2.082391	-0.193124	1.086218
F 0	1.317882	1.533916	-0.000977
H 0	0.033396	-1.533916	-0.000329
H 0	-2.082840	-0.250719	-0.000331
H 0	-1.120494	1.333193	-0.000287

6

B3LYP/6-31G(d) Geometry

C	0	1.924949	-0.250698	-0.029604
C	0	0.741807	-0.886639	-0.048530
B	0	-0.651418	-0.176326	-0.048725
C	0	-1.948975	-1.081898	-0.038902
C	0	-0.808460	1.395758	-0.038850
H	0	2.878794	-0.777246	-0.033822
H	0	1.990846	0.835381	-0.009837
H	0	0.775875	-1.979914	-0.068902
H	0	-2.070714	-1.494225	0.977062
H	0	-1.858840	-1.956525	-0.697316
H	0	-2.878794	-0.554780	-0.281035
H	0	-1.292806	1.708734	-0.977062
H	0	0.111464	1.979914	0.068613
H	0	-1.503341	1.705120	0.755334

7

B3LYP/6-31G(d) Geometry

C	0	-1.678937	-0.578327	-0.000123
C	0	-0.367844	-0.872593	0.000070
B	0	0.752845	0.184175	0.000015
Cl	0	2.445435	-0.330512	-0.000069
Cl	0	0.416321	1.922528	-0.000004
H	0	-2.445435	-1.350530	-0.000028
H	0	-2.032641	0.449920	-0.000349
H	0	-0.074715	-1.922528	0.000349

8

B3LYP/6-31G(d) Geometry

C	0	-0.743368	0.904563	-0.000039
C	0	-0.241089	-0.335134	0.000001
C	0	1.228201	-0.564699	0.000008
O	0	1.769740	-1.645474	-0.000058
Cl	0	-1.252427	-1.756097	-0.000014
H	0	-1.808934	1.104342	-0.000113
H	0	-0.067815	1.756097	-0.000036
H	0	1.808934	0.383244	0.000113

9

B3LYP/6-31G(d) Geometry

C	0	-0.160928	0.005279	-0.000198
C	0	-1.188319	-0.857031	-0.000257
C	0	1.211939	-0.555784	-0.000352
O	0	2.223526	0.119192	-0.000258
C	0	-0.288495	1.503362	0.000005
H	0	-2.223526	-0.526916	-0.000161
H	0	-1.019790	-1.931982	-0.000411
H	0	1.264294	-1.667335	-0.000462
H	0	0.210339	1.931763	0.876803
H	0	0.210136	1.931982	-0.876803
H	0	-1.336171	1.816512	0.000162

10

B3LYP/6-31G(d) Geometry

C	0	-0.367643	0.482957	-0.000127
C	0	0.538440	-0.507823	-0.000082
C	0	-1.818880	0.204357	-0.000191
O	0	-2.314681	-0.908935	-0.000062
C	0	2.022464	-0.333942	-0.000070
H	0	-0.062189	1.528554	-0.000112
H	0	0.155416	-1.528554	-0.000115
H	0	-2.469205	1.106223	0.000373
H	0	2.469205	-0.819257	-0.878503
H	0	2.315126	0.720599	-0.000179
H	0	2.469150	-0.819056	0.878503

11

B3LYP/6-31G(d) Geometry

C	0	-0.576500	-0.401357	-0.000004
C	0	0.503567	0.401724	0.000104
C	0	-1.936641	0.174458	-0.000099
O	0	-2.946811	-0.498206	-0.000196
C	0	1.845460	-0.080845	0.000149
N	0	2.946811	-0.456747	0.000196
H	0	-0.493581	-1.484607	-0.000052
H	0	0.384608	1.484607	0.000144
H	0	-1.977472	1.285793	0.000121

12

B3LYP/6-31G(d) Geometry

C	0	-1.929749	0.859496	-0.000446
C	0	-1.150967	-0.233834	-0.000417
C	0	0.300863	-0.088670	-0.000348
O	0	1.075641	-1.048273	-0.000373
Cl	0	-1.800101	-1.847569	-0.000427
H	0	-3.011937	0.797242	-0.000466
H	0	-1.478433	1.847569	-0.000427
H	0	0.705342	0.931735	-0.000394
B	0	2.681780	-0.877838	-0.000475
H	0	3.011937	-1.457276	-1.007808
H	0	3.011899	-1.455630	1.007808
H	0	2.870395	0.321072	-0.001456

13

B3LYP/6-31G(d) Geometry

C	0	2.076074	-0.948331	-0.000277
C	0	1.157284	0.035788	-0.000271
C	0	-0.239957	-0.376253	-0.000322
O	0	-1.164404	0.450596	-0.000335
C	0	1.468809	1.508016	-0.000293
H	0	3.141455	-0.737377	-0.000230
H	0	1.786149	-1.996052	-0.000347
H	0	-0.488742	-1.445509	-0.000362
H	0	2.547934	1.681153	-0.000071
H	0	1.032398	1.996052	0.878131
H	0	1.032797	1.995854	-0.879020
B	0	-2.718297	0.035882	-0.000260
H	0	-3.141455	0.553080	-1.008198
H	0	-3.141164	0.552316	1.008198
H	0	-2.727117	-1.178521	-0.000713

14

B3LYP/6-31G(d) Geometry

C	0	1.737668	0.388940	-0.000084
C	0	0.634792	-0.386431	-0.000094
C	0	-0.677518	0.210941	-0.000111
O	0	-1.713577	-0.474431	-0.000109
B	0	-3.183116	0.168144	-0.000082
C	0	3.145082	-0.105693	-0.000094
H	0	1.605801	1.472246	-0.000098
H	0	0.691484	-1.472246	-0.000089
H	0	-0.772344	1.305467	-0.000126
H	0	-3.683634	-0.275415	1.008074

H 0 -3.683765 -0.275634 -1.008074
H 0 -3.011040 1.371473 -0.000222
H 0 3.198402 -1.197803 -0.000200
H 0 3.683762 0.273201 0.878730
H 0 3.683765 0.273377 -0.878836

15

B3LYP/6-31G(d) Geometry
C 0 1.463277 0.410620 -0.000291
C 0 0.390098 -0.410591 -0.000179
C 0 -0.947105 0.143828 0.000091
O 0 -1.943882 -0.594211 -0.000268
B 0 -3.442457 -0.043725 -0.000333
C 0 2.805929 -0.062153 -0.000252
N 0 3.910369 -0.429368 -0.000241
H 0 1.335738 1.491871 -0.000253
H 0 0.490127 -1.491871 -0.000165
H 0 -1.089465 1.232315 -0.000372
H 0 -3.909916 -0.532503 1.003230
H 0 -3.910369 -0.533363 -1.003230
H 0 -3.348165 1.165268 -0.000776

16

B3LYP/6-31G(d) Geometry
C 0 0.000000 1.076165 0.000001
C 0 0.000000 -0.270489 0.000000
C 0 -1.225646 -1.024562 0.000000
C 0 1.225646 -1.024562 0.000000
N 0 -2.216346 -1.631602 0.000000
N 0 2.216346 -1.631602 -0.000002
H 0 0.931606 1.631602 0.000001
H 0 -0.931606 1.631602 0.000002

17

B3LYP/6-31G(d) Geometry
C 0 0.674101 0.582569 0.000001
C 0 -0.674153 0.582574 -0.000001
C 0 1.479665 -0.593689 0.000002
C 0 -1.479691 -0.593695 -0.000002
N 0 -2.171080 -1.529363 -0.000003
N 0 2.171080 -1.529339 0.000003
H 0 1.207034 1.529363 0.000002
H 0 -1.207081 1.529363 -0.000002

18

B3LYP/6-31G(d) Geometry
C 0 -0.006832 -0.673929 0.000000
C 0 0.006832 0.673929 0.000000
C 0 -1.221649 -1.420569 0.000001
N 0 -2.200462 -2.049553 0.000002
C 0 1.221649 1.420569 -0.000001
N 0 2.200462 2.049553 -0.000002
H 0 0.918804 -1.243808 -0.000001
H 0 -0.918804 1.243808 0.000001

19

B3LYP/6-31G(d) Geometry
C 0 0.776801 -0.443001 -0.000008
C 0 -0.238876 0.435386 -0.000132
C 0 2.223719 -0.063140 -0.000313
C 0 -1.610361 0.034830 -0.000201
N 0 -2.733479 -0.271194 -0.000301
H 0 0.546869 -1.507513 -0.000175
H 0 -0.052469 1.507513 -0.000264
H 0 2.733479 -0.476447 0.879947
H 0 2.732926 -0.478336 -0.879947
H 0 2.360538 1.022525 -0.001375

20

B3LYP/6-31G(d) Geometry
C 0 -0.928811 1.106794 -0.000882
C 0 -0.369432 -0.112096 -0.000937
C 0 1.065274 -0.231080 -0.000840
C 0 -1.145468 -1.408625 -0.000888
N 0 2.220871 -0.366068 -0.000914
H 0 -2.008918 1.220880 -0.000969
H 0 -0.330887 2.012105 -0.000789
H 0 -0.898989 -2.012105 -0.882149
H 0 -0.901344 -2.010474 0.882149
H 0 -2.220871 -1.210999 -0.002495

21

B3LYP/6-31G(d) Geometry
C 0 -0.396227 0.366576 -0.000296
C 0 0.698066 -0.399583 -0.000467
C 0 -1.746825 -0.236336 -0.000243
O 0 -2.770824 0.414936 -0.000471
C 0 2.096089 0.140752 -0.000390
F 0 2.770281 -0.291046 1.087633
F 0 2.129679 1.485975 -0.001049
F 0 2.770824 -0.292129 -1.087633
H 0 -0.339360 1.451354 -0.000230
H 0 0.637050 -1.485975 -0.000576
H 0 -1.767411 -1.348194 -0.000426

22

B3LYP/6-31G(d) Geometry
C 0 1.359708 0.184694 -0.033546
C 0 0.278572 -0.618918 -0.063596
B 0 -1.197763 -0.127595 -0.058292
C 0 -2.354142 -1.210102 -0.041952
C 0 -1.597714 1.403950 -0.046200
C 0 2.791800 -0.258488 -0.041277
H 0 1.210618 1.265322 -0.000873
H 0 0.478450 -1.695326 -0.096395
H 0 -2.499983 -1.529777 1.004103
H 0 -2.105995 -2.122944 -0.598780
H 0 -3.325897 -0.839111 -0.389027
H 0 -2.083760 1.647658 -1.004103
H 0 -0.784231 2.122944 0.099146
H 0 -2.363279 1.598069 0.718633
H 0 3.325897 0.158935 -0.906270
H 0 2.880614 -1.349102 -0.073277
H 0 3.319401 0.107075 0.850728

23

B3LYP/6-31G(d) Geometry
C 0 -0.983465 0.160587 -0.000368
C 0 0.127003 -0.605044 -0.000380
B 0 1.555314 -0.051216 -0.000349
C 0 -2.391142 -0.344614 -0.000320
Cl 0 2.934835 -1.164098 -0.000328
Cl 0 1.908132 1.688760 -0.000336
H 0 -0.869649 1.245223 -0.000351
H 0 0.000021 -1.688760 -0.000413
H 0 -2.934416 0.028809 0.878510

H 0 -2.436792 -1.437746 -0.000814
H 0 -2.934835 0.029673 -0.878510

24

B3LYP/6-31G(d) Geometry
C 0 -0.495139 0.441844 -0.000922
C 0 0.495149 -0.441842 0.001119
N 0 -1.884072 -0.019242 -0.000382
N 0 1.884080 0.019255 0.000001
O 0 -2.732292 0.869348 -0.001796
O 0 -2.098789 -1.229074 0.001285
O 0 2.732292 -0.869337 -0.002902
O 0 2.098781 1.229087 0.001933
H 0 -0.379425 1.516538 -0.002840
H 0 0.379447 -1.516538 0.002902

25

B3LYP/6-31G(d) Geometry
C 0 0.399057 -0.765386 0.000576
C 0 -0.947071 -0.753640 0.000435
C 0 1.321262 0.387851 0.000317
C 0 -1.988301 0.341541 0.000064
O 0 -3.154705 0.004595 -0.000181
O 0 -1.624711 1.622650 0.000049
O 0 1.027534 1.577845 0.000638
O 0 2.603093 -0.015404 -0.000461
H 0 0.902290 -1.727817 0.000682
H 0 -1.441346 -1.721098 0.000510
H 0 -0.640093 1.727817 0.000460
H 0 3.154705 0.790191 -0.000682

26

B3LYP/6-31G(d) Geometry
C 0 -0.480377 -1.212755 0.000003
C 0 0.517353 -0.290491 0.000002
C 0 -1.860736 -0.877683 0.000002
C 0 0.270411 1.121846 -0.000001
C 0 1.888977 -0.710118 0.000000
N 0 0.087326 2.269541 -0.000003
N 0 -3.000688 -0.643175 0.000002
N 0 3.000688 -1.049467 -0.000002
H 0 -0.228890 -2.269541 0.000003

27

B3LYP/6-31G(d) Geometry
C 0 1.791899 0.413694 -0.000191
C 0 0.638145 -0.540013 -0.000315
C 0 -0.670590 -0.223767 -0.000301
C 0 -1.080456 1.154307 -0.000162
C 0 -1.786301 -1.244985 -0.000201
N 0 -1.447160 2.259232 -0.000283
H 0 2.427157 0.248330 0.879993
H 0 1.465531 1.457121 0.000029
H 0 2.427189 0.248654 -0.880415
H 0 0.887874 -1.600896 -0.000408
H 0 -2.426620 -1.129412 0.882184
H 0 -2.427189 -1.129343 -0.882184
H 0 -1.376678 -2.259232 -0.000361

28

B3LYP/6-31G(d) Geometry
C 0 0.241792 0.009764 -0.000347
C 0 -0.757603 -0.895048 -0.000295
C 0 1.594028 -0.481741 -0.000369
C 0 -2.231210 -0.629821 -0.000407
N 0 2.700350 -0.843797 -0.000410
C 0 0.109014 1.516240 -0.000368
H 0 -0.474772 -1.946507 -0.000279
H 0 -2.700223 -1.090783 -0.879867
H 0 -2.700350 -1.090566 0.879068
H 0 -2.482344 0.433154 -0.000589
H 0 0.597676 1.946465 0.881612
H 0 -0.935617 1.832887 -0.001115
H 0 0.598958 1.946507 -0.881612

29

B3LYP/6-31G(d) Geometry
C 0 0.469050 -0.907124 -0.000604
C 0 -0.512988 0.023907 -0.000625
C 0 1.853976 -0.571270 -0.000565
C 0 -1.874333 -0.431404 -0.000623
C 0 -0.300297 1.515074 -0.000594
N 0 -2.989788 -0.761897 -0.000531
N 0 2.989788 -0.316018 -0.000568
H 0 0.227369 -1.965952 -0.000580
H 0 -0.770317 1.965952 -0.882085
H 0 -0.768352 1.965757 0.882085
H 0 0.764155 1.759011 -0.001639

30

B3LYP/6-31G(d) Geometry
C 0 0.801020 -0.384214 -0.000137
C 0 -0.395813 -1.013254 -0.000109
C 0 2.114584 -1.124073 -0.000276
C 0 0.878817 1.048664 -0.000215
C 0 -1.657557 -0.351646 -0.000207
N 0 -2.707482 0.150294 -0.000288
N 0 1.005082 2.204939 -0.000184
H 0 -0.425440 -2.099800 -0.000003
H 0 2.707482 -0.854797 -0.881957
H 0 2.707186 -0.855977 0.881957
H 0 1.952612 -2.204939 -0.001064

31

B3LYP/6-31G(d) Geometry
C 0 -0.362735 -0.553473 0.000126
C 0 0.900007 -0.073088 0.000135
C 0 -1.599918 0.234478 -0.000206
O 0 -2.711076 -0.269777 0.000330
C 0 2.074216 -1.017634 0.000128
C 0 1.273592 1.387762 0.000211
H 0 -0.526163 -1.629669 0.000380
H 0 -1.494211 1.339279 -0.000197
H 0 2.708715 -0.847080 -0.880553
H 0 2.711076 -0.844503 0.878571
H 0 1.760369 -2.064889 0.002007
H 0 1.892552 1.617503 -0.877491
H 0 0.418445 2.064889 -0.002061
H 0 1.888500 1.618358 0.880553

32

B3LYP/6-31G(d) Geometry
C 0 -0.536679 -1.073087 0.000108
C 0 0.658565 -0.432366 0.000288
C 0 -1.842743 -0.373299 -0.000424
O 0 -2.889624 -0.987707 0.000324
C 0 1.892731 -1.164852 0.000424

C 0 0.773902 1.001286 0.000135
N 0 2.889624 -1.762764 -0.000142
N 0 0.882467 2.158587 0.000112
H 0 -0.568494 -2.158587 0.000254
H 0 -1.810079 0.732926 0.000231

33

B3LYP/6-31G(d) Geometry
C 0 0.686052 0.000003 0.000000
C 0 -0.686052 -0.000003 0.000000
C 0 1.433147 1.219348 -0.000001
C 0 1.433158 -1.219336 0.000000
N 0 2.059033 2.199271 -0.000002
C 0 -1.433147 -1.219348 0.000000
C 0 -1.433158 1.219336 -0.000001
N 0 -2.059033 -2.199271 0.000002
N 0 2.059051 -2.199254 0.000002
N 0 -2.059051 2.199254 -0.000002

34

B3LYP/6-31G(d) Geometry
C 0 0.516511 0.115579 -0.000830
C 0 -0.525299 -0.767591 -0.000865
C 0 1.875666 -0.341349 -0.000834
C 0 0.323670 1.536065 -0.000792
C 0 -1.866649 -0.268915 -0.000857
C 0 -0.366852 -2.262722 -0.000769
N 0 -2.978494 0.073569 -0.000845
N 0 2.978494 -0.710112 -0.000855
N 0 0.188849 2.690715 -0.000772
H 0 -0.856914 -2.690294 0.881728
H 0 -0.859266 -2.690715 -0.881728
H 0 0.685066 -2.553618 -0.002036

35

B3LYP/6-31G(d) Geometry
C 0 0.516753 -0.445887 -0.000894
C 0 -0.765809 0.018857 -0.000806
C 0 1.648414 0.531400 -0.000882
O 0 2.805416 0.165447 -0.000974
C 0 0.881556 -1.895180 -0.000808
C 0 -1.892711 -0.870296 -0.000459
C 0 -1.092556 1.419702 -0.000551
N 0 -2.805416 -1.590932 0.000019
N 0 -1.381600 2.545997 -0.000404
H 0 1.377126 1.603136 -0.000753
H 0 1.500689 -2.119339 0.875531
H 0 0.005792 -2.545997 -0.002100
H 0 1.503107 -2.118832 -0.875531

36

B3LYP/6-31G(d) Geometry
C 0 -0.393535 0.285839 -0.000197
C 0 0.915210 -0.080029 -0.000190
C 0 -1.480635 -0.717674 -0.000189
O 0 -2.669204 -0.438012 -0.000075
C 0 2.023670 0.943673 -0.000112
C 0 -0.856992 1.729162 -0.000159
C 0 1.440444 -1.497164 -0.000128
H 0 -1.179110 -1.781667 -0.000293
H 0 2.669204 0.806068 0.878526
H 0 2.669064 0.806337 -0.878892
H 0 1.663839 1.973114 0.000068
H 0 -1.948530 1.751844 -0.000392
H 0 -0.504946 2.272696 0.884307
H 0 -0.504507 2.272912 -0.884307
H 0 2.080296 -1.657175 -0.878527
H 0 2.080048 -1.657174 0.878460
H 0 0.675609 -2.272912 -0.000227

37

B3LYP/6-31G(d) Geometry
C 0 1.581562 0.030693 -0.000358
C 0 0.398592 -0.662081 -0.000373
C 0 -0.849508 0.097751 -0.000386
O 0 -1.934385 -0.504987 -0.000405
B 0 -3.352829 0.212719 -0.000302
C 0 2.845626 -0.644170 -0.000342
C 0 1.651008 1.464208 -0.000361
N 0 1.723044 2.624917 -0.000362
N 0 3.873633 -1.188332 -0.000328
C 0 0.310405 -2.157533 -0.000368
H 0 -0.844132 1.192919 -0.000385
H 0 -3.873107 -0.232474 0.999186
H 0 -3.873633 -0.233207 -0.999186
H 0 -3.129383 1.401478 -0.000799
H 0 1.296100 -2.624917 -0.000374
H 0 -0.250026 -2.498883 -0.878053
H 0 -0.250016 -2.498876 0.877327

38

B3LYP/6-31G(d) Geometry
C 0 0.506350 -0.452764 -0.000653
C 0 -0.506473 0.452680 -0.000762
C 0 1.861303 0.018659 -0.000927
C 0 0.337242 -1.952363 -0.000423
C 0 -1.861381 -0.018909 -0.000734
C 0 -0.337738 1.952260 -0.000424
N 0 -2.975188 -0.357001 -0.001051
N 0 2.975188 0.356508 -0.000957
H 0 0.817778 -2.390058 0.882134
H 0 -0.718519 -2.231047 -0.000940
H 0 0.818791 -2.390597 -0.882157
H 0 -0.819282 2.390597 -0.882135
H 0 -0.818510 2.389651 0.882157
H 0 0.717989 2.231085 -0.000782

39

B3LYP/6-31G(d) Geometry
C 0 -0.679613 0.035056 -0.000001
C 0 0.679638 0.035056 -0.000013
C 0 -1.570865 1.253567 -0.000027
C 0 -1.389138 -1.213570 -0.000005
C 0 1.389163 -1.213570 -0.000012
C 0 1.570890 1.253567 0.000007
N 0 2.028466 -2.185693 -0.000025
N 0 -2.028442 -2.185693 0.000006
H 0 -2.222850 1.243252 -0.881188
H 0 -2.222797 1.243348 0.881174
H 0 -1.005396 2.185692 -0.000090
H 0 2.222850 1.243273 0.881188
H 0 2.222849 1.243325 -0.881174
H 0 1.005423 2.185693 0.000031

40

B3LYP/6-31G(d) Geometry

C	0	0.757140	-0.375101	-0.000331
C	0	-0.416532	0.302329	-0.000334
C	0	2.107758	0.291688	-0.000380
C	0	-1.654512	-0.429899	-0.000346
C	0	-0.610240	1.805109	-0.000294
N	0	-2.684918	-0.972817	-0.000373
C	0	0.818427	-1.881731	-0.000300
H	0	2.684918	-0.026464	0.878262
H	0	2.684423	-0.025542	-0.879676
H	0	2.067677	1.381542	0.000253
H	0	-1.182637	2.119069	-0.881234
H	0	-1.181657	2.119203	0.881234
H	0	0.336172	2.347370	-0.000913
H	0	1.369903	-2.240161	-0.879937
H	0	1.369016	-2.240155	0.879914
H	0	-0.169132	-2.347370	-0.000749

41

B3LYP/6-31G(d) Geometry

C	0	-1.080328	0.099471	-0.000422
C	0	-0.122249	-0.851121	0.000161
C	0	-0.140993	1.300360	-0.000213
C	0	0.960269	0.180698	-0.000219
O	0	2.164262	0.187044	-0.000251
H	0	-2.164262	0.044278	-0.000098
H	0	-0.131331	-1.936159	-0.001151
H	0	-0.158176	1.935606	0.893359
H	0	-0.158052	1.936159	-0.893359

42

B3LYP/6-31G(d) Geometry

C	0	0.357429	-1.023383	-0.000414
C	0	-0.267620	0.176573	-0.000260
C	0	1.787160	-0.491820	-0.000111
C	0	1.050782	0.889841	-0.000149
O	0	1.411983	2.040596	-0.000376
C	0	-1.676696	0.661009	-0.000190
H	0	-0.023239	-2.040596	-0.000756
H	0	2.390065	-0.697884	-0.892929
H	0	2.389684	-0.698035	0.892929
H	0	-1.872103	1.286030	0.879808
H	0	-2.390065	-0.169198	0.000081
H	0	-1.872255	1.285748	-0.880336

43

B3LYP/6-31G(d) Geometry

C	0	-0.673819	0.130086	0.000022
C	0	0.264788	-0.847845	-0.000106
C	0	0.319412	1.295548	-0.000028
C	0	1.375298	0.138272	-0.000008
O	0	2.581231	0.105223	0.000318
C	0	-2.159639	0.144287	0.000257
H	0	0.216696	-1.932603	0.000043
H	0	0.322386	1.932527	0.893373
H	0	0.322175	1.932603	-0.893373
H	0	-2.538988	0.682165	0.879493
H	0	-2.581231	-0.865237	0.000336
H	0	-2.539254	0.682131	-0.878879

44

B3LYP/6-31G(d) Geometry

C	0	0.331489	0.142729	-0.000189
C	0	-0.588808	-0.853628	-0.000256
C	0	-0.668806	1.305886	-0.000146
C	0	-1.711847	0.136740	-0.000188
O	0	-2.912396	0.084361	-0.000171
C	0	1.748332	0.142883	-0.000323
N	0	2.912396	0.171392	-0.000094
H	0	-0.520282	-1.935855	0.000282
H	0	-0.671111	1.935855	-0.895744
H	0	-0.670912	1.935429	0.895744

45

B3LYP/6-31G(d) Geometry

C	0	0.187078	-1.061336	-0.000103
C	0	-0.501709	0.098284	-0.000088
C	0	1.564736	-0.404586	-0.000041
C	0	0.744815	0.931737	-0.000096
O	0	1.016690	2.099774	-0.000078
Cl	0	-2.177046	0.500168	-0.000062
H	0	-0.121305	-2.099774	-0.000109
H	0	2.177046	-0.561387	-0.895420
H	0	2.176940	-0.561345	0.895420

46

B3LYP/6-31G(d) Geometry

C	0	0.330440	-0.508921	0.000078
C	0	-0.643960	0.441947	0.000090
C	0	1.743655	-0.415281	0.000057
C	0	-0.597900	-1.728609	0.000021
C	0	-1.703417	-0.623688	0.000053
C	0	-0.685900	1.926485	0.000018
O	0	-2.906828	-0.633823	0.000035
N	0	2.906828	-0.350865	0.000029
H	0	-0.566317	-2.359065	0.895123
H	0	-0.566279	-2.359005	-0.895123
H	0	-1.228174	2.293638	-0.879904
H	0	-1.227254	2.293504	0.880554
H	0	0.318731	2.359065	-0.000513

47

B3LYP/6-31G(d) Geometry

C	0	-0.682289	-0.519978	-0.000067
C	0	0.280828	0.439351	-0.000097
C	0	0.274099	-1.713871	-0.000036
C	0	1.358285	-0.588187	-0.000107
O	0	2.566438	-0.581488	-0.000108
C	0	-2.168927	-0.491632	-0.000126
C	0	0.304172	1.930232	-0.000067
H	0	0.260716	-2.352289	-0.892915
H	0	0.260745	-2.352165	0.892915
H	0	-2.566438	-1.016495	-0.879379
H	0	-2.562517	0.529826	-0.000654
H	0	-2.566371	-1.015476	0.879779
H	0	-0.706574	2.352289	-0.000678
H	0	0.835566	2.312774	-0.880173
H	0	0.834401	2.312724	0.880759

48

B3LYP/6-31G(d) Geometry

C	0	0.029089	1.022968	-0.000727
C	0	-1.266966	0.677733	-0.001529
C	0	0.883784	-0.188844	-0.002108
O	0	2.099053	-0.230088	-0.002127

C 0	-0.060214	-1.405460	-0.000261
C 0	-1.486351	-0.817741	-0.002374
H 0	0.440257	2.026293	0.000224
H 0	-2.099053	1.377284	-0.001364
H 0	0.147908	-2.021892	0.880796
H 0	0.149478	-2.026293	-0.877767
H 0	-2.072755	-1.126105	0.873456
H 0	-2.069411	-1.125127	-0.880796

49

B3LYP/6-31G(d) Geometry

C 0	0.507946	-0.217595	-0.000012
C 0	-0.491212	-1.117085	-0.000019
C 0	-0.072904	1.152586	-0.000015
O 0	0.555736	2.195555	-0.000027
C 0	-1.602275	1.017123	-0.000010
C 0	-1.870717	-0.501883	-0.000024
C 0	1.987893	-0.435129	-0.000017
H 0	-0.348378	-2.195555	-0.000029
H 0	-2.012382	1.526252	-0.878875
H 0	-2.012370	1.526226	0.878875
H 0	-2.446442	-0.827264	-0.876908
H 0	-2.446458	-0.827283	0.876843
H 0	2.244136	-1.498862	-0.000147
H 0	2.446445	0.036526	0.877309
H 0	2.446458	0.036747	-0.877215

50

B3LYP/6-31G(d) Geometry

C 0	-0.295999	-0.873861	-0.000914
C 0	0.744026	-0.018992	-0.000911
C 0	-1.582060	-0.149479	-0.000769
O 0	-2.700522	-0.630044	-0.000759
C 0	2.198734	-0.366283	-0.000564
C 0	-1.252807	1.354645	-0.000500
C 0	0.286201	1.428731	-0.001056
H 0	-0.238456	-1.957256	-0.000983
H 0	2.362220	-1.447672	-0.001337
H 0	2.699575	0.059532	0.879528
H 0	2.700522	0.060835	-0.879528
H 0	-1.705712	1.824369	0.879112
H 0	-1.706595	1.825065	-0.879285
H 0	0.685551	1.957256	0.875380
H 0	0.684748	1.956668	-0.878215

51

B3LYP/6-31G(d) Geometry

C 0	0.547204	-0.926886	-0.000102
C 0	-0.397519	0.034343	-0.000442
C 0	1.898178	-0.309501	-0.000457
O 0	2.958665	-0.899834	-0.000749
C 0	-1.805063	-0.195367	-0.000487
C 0	1.703687	1.215553	-0.000353
C 0	0.179777	1.443387	-0.000498
N 0	-2.958665	-0.349484	-0.000602
H 0	0.383450	-1.997755	0.000446
H 0	2.197983	1.641045	-0.879745
H 0	2.197355	1.640388	0.879745
H 0	-0.170335	1.997755	-0.878966
H 0	-0.170347	1.997612	0.878121

52

B3LYP/6-31G(d) Geometry

C 0	0.531373	-0.134335	-0.001327
C 0	-0.238853	-1.232022	-0.001657
C 0	-0.290997	1.109869	-0.001437
O 0	0.111630	2.251889	-0.002245
C 0	-1.754495	0.648441	-0.000263
C 0	-1.709866	-0.895836	-0.002013
Cl 0	2.261343	-0.071868	-0.001157
H 0	0.132335	-2.251889	-0.001837
H 0	-2.261343	1.062256	-0.878246
H 0	-2.258514	1.059756	0.880572
H 0	-2.206256	-1.328174	-0.880572
H 0	-2.207522	-1.330455	0.874677

53

B3LYP/6-31G(d) Geometry

C 0	-0.544823	0.512649	-0.000574
C 0	0.391589	-0.464164	-0.000756
C 0	-1.894693	-0.124133	-0.000607
O 0	-2.951383	0.476017	-0.000640
C 0	1.798865	-0.237021	-0.000834
C 0	-1.708090	-1.645293	-0.000377
C 0	-0.184417	-1.872617	-0.000661
C 0	-0.376484	1.994124	-0.000483
N 0	2.951383	-0.070953	-0.000335
H 0	-2.203364	-2.071107	-0.879318
H 0	-2.202719	-2.070368	0.879318
H 0	0.162247	-2.429361	-0.879136
H 0	0.162405	-2.429115	0.877951
H 0	-0.869050	2.429245	-0.878107
H 0	0.676101	2.288284	0.000598
H 0	-0.870850	2.429361	0.876071

54

B3LYP/6-31G(d) Geometry

C 0	0.313624	0.432501	-0.000261
C 0	-0.745546	-0.407010	-0.000351
C 0	1.573096	-0.350314	-0.000234
O 0	2.701595	0.110648	-0.000327
C 0	-2.199920	-0.054218	-0.000219
C 0	1.210455	-1.840272	-0.000128
C 0	-0.328107	-1.866912	-0.000401
C 0	0.363963	1.928734	-0.000279
H 0	-2.372896	1.025076	-0.000381
H 0	-2.701180	-0.480913	0.879481
H 0	-2.701595	-0.481331	-0.879481
H 0	1.650481	-2.323198	0.879077
H 0	1.650867	-2.323456	-0.878997
H 0	-0.741209	-2.385029	0.876201
H 0	-0.740850	-2.384835	-0.877290
H 0	0.911938	2.292438	0.877200
H 0	-0.629826	2.385029	-0.001498
H 0	0.914110	2.292243	-0.876468

55

B3LYP/6-31G(d) Geometry

C 0	0.667837	0.699048	0.000011
C 0	-0.667835	0.699048	0.000009
C 0	-1.131998	-0.718114	0.000003
C 0	1.132001	-0.718113	-0.000003
O 0	0.000001	-1.530918	-0.000308
O 0	-2.245530	-1.159453	0.000306

O 0	2.245530	-1.159454	0.000308
H 0	1.360262	1.530919	0.000098
H 0	-1.360258	1.530919	0.000094

56

B3LYP/6-31G(d) Geometry

C 0	-1.245993	-1.256638	-0.000008
O 0	0.129629	-1.644061	0.000003
C 0	0.931210	-0.519436	-0.000107
C 0	0.034749	0.665063	0.000017
C 0	-1.231841	0.245329	-0.000052
O 0	2.133364	-0.580492	-0.000007
H 0	-1.735935	-1.676880	0.888044
H 0	-1.735923	-1.676926	-0.888044
H 0	0.417451	1.676926	0.000085
H 0	-2.133364	0.847990	-0.000075

57

B3LYP/6-31G(d) Geometry

C 0	0.769740	1.231121	0.061837
C 0	-0.571668	1.194630	-0.014792
C 0	1.628166	-0.001284	0.168380
C 0	0.884894	-1.258647	-0.305918
C 0	-0.519626	-1.338325	0.308025
C 0	-1.334371	-0.072632	0.054720
O 0	-2.552313	-0.093308	-0.044232
H 0	1.279893	2.194001	0.050441
H 0	-1.165163	2.100347	-0.110644
H 0	1.949176	-0.120600	1.216465
H 0	2.552313	0.141066	-0.406493
H 0	0.797199	-1.225635	-1.399960
H 0	1.461508	-2.158113	-0.061192
H 0	-0.442170	-1.460148	1.399960
H 0	-1.089791	-2.194001	-0.066494

58

B3LYP/6-31G(d) Geometry

C 0	0.142426	-1.363112	-0.148025
C 0	-0.869517	-0.475291	-0.080586
C 0	1.601699	-0.997457	-0.203485
C 0	1.856585	0.424236	0.312835
C 0	0.867800	1.411360	-0.317249
C 0	-0.582687	0.987240	-0.113518
O 0	-1.483144	1.810392	-0.024711
C 0	-2.319223	-0.871500	0.006555
H 0	-0.096000	-2.427194	-0.167528
H 0	1.955673	-1.090905	-1.243883
H 0	2.185743	-1.728184	0.371021
H 0	1.731798	0.434997	1.403812
H 0	2.889251	0.729491	0.107698
H 0	1.040541	1.466540	-1.403812
H 0	0.982304	2.427194	0.073383
H 0	-2.434136	-1.959823	0.008454
H 0	-2.889251	-0.456934	-0.832780
H 0	-2.778229	-0.467557	0.916044

59

B3LYP/6-31G(d) Geometry

C 0	-0.838000	-0.591369	0.064230
C 0	0.240934	-1.397619	-0.011999
C 0	-0.689664	0.909378	0.190378
C 0	0.673948	1.413200	-0.300311
C 0	1.815707	0.588103	0.304580
C 0	1.631237	-0.907235	0.063380
O 0	2.584571	-1.668920	-0.025352
C 0	-2.240927	-1.131156	0.044882
H 0	0.131469	-2.475276	-0.113427
H 0	-0.837317	1.187048	1.247191
H 0	-1.501613	1.405057	-0.358472
H 0	0.710249	1.331649	-1.394796
H 0	0.795305	2.475276	-0.057660
H 0	1.848764	0.740908	1.394796
H 0	2.795254	0.880345	-0.086055
H 0	-2.259648	-2.224066	0.007166
H 0	-2.795254	-0.743530	-0.820884
H 0	-2.794053	-0.806364	0.937135

60

B3LYP/6-31G(d) Geometry

C 0	-0.634557	-0.361747	0.066288
C 0	0.285528	-1.349126	-0.008404
C 0	-0.264297	1.105018	0.183273
C 0	1.166752	1.363216	-0.306523
C 0	2.157659	0.365919	0.309302
C 0	1.743163	-1.078367	0.063830
O 0	2.549326	-1.989101	-0.036147
C 0	-2.032114	-0.682830	0.048112
N 0	-3.174233	-0.906391	0.037226
H 0	-0.004823	-2.390853	-0.107613
H 0	-0.373472	1.407957	1.235745
H 0	-0.984436	1.708414	-0.380566
H 0	1.191276	1.271366	-1.400113
H 0	1.461339	2.390853	-0.067856
H 0	2.203836	0.509703	1.400113
H 0	3.174233	0.500175	-0.071821

61

B3LYP/6-31G(d) Geometry

C 0	0.304128	-1.276330	0.166627
C 0	1.073636	-0.176588	0.104977
C 0	-1.199946	-1.225476	0.204664
C 0	-1.744888	0.109906	-0.316639
C 0	-0.999810	1.288125	0.320410
C 0	0.512051	1.208490	0.124183
O 0	1.208318	2.200578	0.033653
Cl 0	2.819852	-0.301094	0.026191
H 0	0.780413	-2.253707	0.193814
H 0	-1.533070	-1.395115	1.241662
H 0	-1.604070	-2.064121	-0.376170
H 0	-1.617231	0.147054	-1.406236
H 0	-2.819852	0.186902	-0.118855
H 0	-1.182213	1.302652	1.406236
H 0	-1.332855	2.253707	-0.071310

62

B3LYP/6-31G(d) Geometry

C 0	-0.635322	-0.243818	-0.105080
C 0	0.188580	0.835519	-0.056427
C 0	-0.152890	-1.682820	-0.177463
C 0	1.286050	-1.826207	0.326507
C 0	2.191663	-0.780137	-0.329842
C 0	1.672135	0.634216	-0.123685
O 0	2.424148	1.593420	-0.050534
C 0	-2.059150	-0.069798	-0.102579
C 0	-0.276411	2.259669	0.042493

N 0	-3.219826	0.023269	-0.104292
H 0	-0.228933	-2.026537	-1.220530
H 0	-0.832841	-2.319945	0.399182
H 0	1.302031	-1.692604	1.416046
H 0	1.655482	-2.837387	0.123821
H 0	2.237791	-0.956603	-1.416046
H 0	3.219826	-0.819619	0.041819
H 0	-1.364945	2.333697	0.087086
H 0	0.087610	2.837387	-0.814548
H 0	0.152797	2.733622	0.932096

63

B3LYP/6-31G(d) Geometry

C 0	-0.957780	-0.242460	-0.120392
C 0	-0.103442	0.809163	-0.059000
C 0	-0.483294	-1.679107	-0.185891
C 0	0.947197	-1.865291	0.323617
C 0	1.870974	-0.836180	-0.328049
C 0	1.370762	0.589305	-0.128432
O 0	2.162726	1.521583	-0.068817
C 0	-2.454875	-0.077654	-0.136159
C 0	-0.550855	2.251253	0.044356
H 0	-0.557745	-2.025890	-1.230335
H 0	-1.179227	-2.312852	0.380709
H 0	0.962718	-1.730416	1.413371
H 0	1.296663	-2.885009	0.123787
H 0	1.921746	-1.016979	-1.413371
H 0	2.896416	-0.888236	0.050038
H 0	-2.772342	0.957585	-0.273470
H 0	-2.892583	-0.447461	0.802312
H 0	-2.896416	-0.682124	-0.940045
H 0	-1.260255	2.403576	0.865006
H 0	-1.036013	2.594052	-0.878646
H 0	0.321167	2.885009	0.215803

64

B3LYP/6-31G(d) Geometry

C 0	0.965632	0.961426	-0.060977
C 0	-0.325963	1.283970	0.117837
C 0	-1.288168	0.226636	0.605534
O 0	-0.616121	-0.666082	1.510866
C 0	0.249988	-1.354864	0.638939
C 0	1.406612	-0.425939	0.222420
C 0	-1.642662	-0.768013	-0.527705
O 0	-0.514955	-1.646574	-0.539407
O 0	2.552082	-0.819658	0.099947
H 0	1.716119	1.669841	-0.400160
H 0	-0.710052	2.275610	-0.111501
H 0	-2.157231	0.642988	1.117725
H 0	0.606852	-2.275610	1.104286
H 0	-1.752150	-0.301460	-1.510866
H 0	-2.552082	-1.327431	-0.277256

65

B3LYP/6-31G(d) Geometry

C 0	1.041848	-0.349696	-0.267647
C 0	0.065534	-1.264419	-0.421693
C 0	-1.352332	-0.826067	-0.694000
O 0	-1.353473	0.369173	-1.496394
C 0	-0.856687	1.315538	-0.581655
C 0	0.649720	1.086325	-0.368850
C 0	-2.027705	-0.278304	0.587504
O 0	-1.514228	1.054050	0.667416
O 0	1.436437	2.008959	-0.246672
C 0	2.487792	-0.658975	-0.008601
H 0	0.266875	-2.329630	-0.320492
H 0	-1.939755	-1.585792	-1.212687
H 0	-1.072384	2.329630	-0.923505
H 0	-1.764541	-0.826872	1.496394
H 0	-3.117901	-0.253562	0.470027
H 0	3.117901	-0.264611	-0.814199
H 0	2.656691	-1.736779	0.073302
H 0	2.826804	-0.173559	0.913634

66

B3LYP/6-31G(d) Geometry

C 0	0.255665	1.565237	0.044585
C 0	-0.761384	0.707938	0.261462
C 0	-0.405560	-0.711991	0.666338
O 0	0.771579	-0.721828	1.487478
C 0	1.770300	-0.384590	0.551636
C 0	1.652678	1.109609	0.197846
C 0	0.106450	-1.526056	-0.547849
O 0	1.480535	-1.142154	-0.631409
O 0	2.630021	1.817378	0.026226
C 0	-2.210814	1.050397	0.085977
H 0	0.095928	2.602409	-0.239759
H 0	-1.210215	-1.203346	1.218053
H 0	2.758197	-0.641562	0.938061
H 0	-0.400503	-1.285644	-1.487478
H 0	0.030384	-2.602409	-0.351842
H 0	-2.342548	2.079373	-0.259683
H 0	-2.758197	0.927223	1.030434
H 0	-2.689963	0.381504	-0.642498

67

B3LYP/6-31G(d) Geometry

C 0	0.277784	1.582781	0.066101
C 0	-0.563476	0.552070	0.303008
C 0	0.025037	-0.802173	0.686674
O 0	1.206259	-0.598295	1.467445
C 0	2.110458	-0.099605	0.504888
C 0	1.742237	1.359016	0.182975
C 0	0.628070	-1.508368	-0.549052
O 0	1.899254	-0.865568	-0.685106
O 0	2.568555	2.231617	-0.000424
C 0	-1.979656	0.662732	0.161156
N 0	-3.137713	0.706965	0.051903
H 0	-0.067588	2.576630	-0.201006
H 0	-0.674768	-1.411748	1.258941
H 0	3.137713	-0.200727	0.858911
H 0	0.050201	-1.374782	-1.467445
H 0	0.766117	-2.576630	-0.346655

68

B3LYP/6-31G(d) Geometry

C 0	1.176148	-0.162286	-0.348799
C 0	0.365865	-1.221934	-0.501856
C 0	-1.110287	-0.981382	-0.718831
O 0	-1.307873	0.218284	-1.484119
C 0	-0.930810	1.206463	-0.558099
C 0	0.604569	1.218615	-0.398948
C 0	-1.809699	-0.571560	0.600360
O 0	-1.489737	0.819102	0.701758
O 0	1.244757	2.240458	-0.282217
Cl 0	2.895135	-0.312445	-0.109532

H 0 0.737532 -2.240458 -0.438515
H 0 -1.594145 -1.807524 -1.242004
H 0 -1.306083 2.184271 -0.865121
H 0 -1.437545 -1.096745 1.484119
H 0 -2.895135 -0.701822 0.516837

69

B3LYP/6-31G(d) Geometry
C 0 0.086023 0.953633 -0.265660
C 0 0.624540 -0.282193 -0.429093
C 0 -0.284336 -1.476530 -0.700380
O 0 -1.403074 -1.056597 -1.488943
C 0 -2.127913 -0.281076 -0.562125
C 0 -1.405380 1.057757 -0.357309
C 0 -1.009474 -1.926889 0.587689
O 0 -2.083973 -0.985777 0.683324
O 0 -1.997694 2.113129 -0.232567
C 0 0.848534 2.215859 -0.009077
C 0 2.024524 -0.534785 -0.309167
N 0 3.157654 -0.786352 -0.214110
H 0 0.235204 -2.277390 -1.227388
H 0 -3.157654 -0.146378 -0.897500
H 0 -0.393064 -1.872469 1.488943
H 0 -1.408184 -2.940903 0.468541
H 0 1.923995 2.037254 0.057680
H 0 0.500393 2.682484 0.919423
H 0 0.654440 2.940903 -0.807819

70

B3LYP/6-31G(d) Geometry
C 0 0.818893 0.458831 -0.268690
C 0 0.372819 -0.811143 -0.414844
C 0 -1.101989 -1.039303 -0.691428
O 0 -1.641367 0.015372 -1.502018
C 0 -1.630752 1.087482 -0.590658
C 0 -0.183952 1.556464 -0.372173
C 0 -1.950256 -0.853368 0.590735
O 0 -2.122638 0.564417 0.651310
O 0 0.087341 2.740460 -0.255552
C 0 1.226347 -2.039883 -0.285036
C 0 2.251031 0.856519 -0.007964
H 0 -1.283320 -1.987460 -1.203099
H 0 -2.271815 1.897596 -0.942591
H 0 -1.456175 -1.204345 1.502018
H 0 -2.926039 -1.343252 0.487215
H 0 2.246236 -1.808881 0.028814
H 0 1.274820 -2.580062 -1.241108
H 0 0.797077 -2.740460 0.444951
H 0 2.926039 0.488130 -0.788916
H 0 2.611998 0.468012 0.952067
H 0 2.320847 1.946128 0.021118

TS-1+CP

B3LYP/6-31G(d) Geometry
C 0 -1.766708 -0.619522 0.468826
C 0 -1.697483 0.883239 0.267410
C 0 -0.260552 1.135755 0.631032
C 0 0.143860 0.122713 1.491831
C 0 -0.789568 -0.927274 1.433007
H 0 -2.697828 -1.171655 0.375175
H 0 -2.339642 1.357926 1.028552
H 0 -2.016604 1.252559 -0.709546
H 0 0.242850 2.086827 0.499512
H 0 1.082773 0.096493 2.033117
H 0 -0.688225 -1.882288 1.937877
C 0 -0.797936 -1.057146 -1.309704
C 0 0.215980 -0.100045 -1.457760
C 0 1.580166 -0.420578 -1.211790
N 0 2.697828 -0.689617 -1.012355
H 0 -1.692538 -0.943513 -1.915529
H 0 -0.519466 -2.086827 -1.113898
H 0 0.039223 0.802851 -2.033117

TS-2+CP

B3LYP/6-31G(d) Geometry
C 0 -1.373958 -0.642538 0.831775
C 0 -1.354097 0.873725 0.896396
C 0 0.127942 1.116989 0.980648
C 0 0.706834 -0.011694 1.553472
C 0 -0.215716 -1.070826 1.508051
H 0 -2.302143 -1.207159 0.840194
H 0 -1.808198 1.176379 1.855562
H 0 -1.882794 1.397543 0.098319
H 0 0.592785 2.093092 0.904542
H 0 1.736483 -0.088782 1.885693
H 0 -0.010070 -2.093092 1.808720
C 0 -0.775074 -0.731695 -1.150030
C 0 0.079616 0.358432 -1.357690
C 0 1.527188 0.199511 -1.461492
O 0 2.302143 1.042956 -1.885693
H 0 -1.786782 -0.681980 -1.544316
H 0 -0.349659 -1.731754 -1.165187
H 0 -0.312474 1.312652 -1.699049
H 0 1.901508 -0.794621 -1.118937

TS-3+CP

B3LYP/6-31G(d) Geometry
C 0 -3.004202 0.242332 -0.125773
C 0 -2.691833 -0.219026 1.289668
C 0 -1.572773 -1.183496 1.029774
C 0 -1.669925 -1.626506 -0.279370
C 0 -2.589436 -0.811504 -0.967967
H 0 -3.884601 0.839751 -0.346830
H 0 -3.562095 -0.792428 1.652173
H 0 -2.487486 0.563129 2.022119
H 0 -0.929747 -1.602434 1.794910
H 0 -1.076652 -2.419955 -0.719936
H 0 -2.832308 -0.897760 -2.022119
C 0 -1.515639 1.573183 -0.329602
C 0 -0.422794 1.143723 0.447095
C 0 0.673760 0.434858 -0.111645
O 0 1.713378 0.161227 0.535674
B 0 2.881990 -0.725372 -0.076962
H 0 -2.088183 2.419955 0.041382
H 0 -1.405436 1.575729 -1.410312
H 0 -0.336545 1.432223 1.490392
H 0 0.619549 0.109563 -1.159348
H 0 2.891897 -1.719851 0.621188
H 0 2.569358 -0.944522 -1.235490
H 0 3.884601 -0.058257 0.048995

TS-4+CP

B3LYP/6-31G(d) Geometry
C 0 0.664121 -1.540860 0.169793
C 0 1.243835 -0.538388 0.975360
C 0 1.660914 0.528850 0.160034
C 0 0.767382 -1.165883 -1.156412

C 0	1.742557	-0.026827	-1.252985
H 0	0.126397	-2.404306	0.543331
H 0	1.241065	-0.534207	2.059642
H 0	2.330136	1.308838	0.512650
H 0	0.406957	-1.735171	-2.005521
H 0	2.754204	-0.439514	-1.401909
H 0	1.558680	0.686207	-2.059642
C 0	-0.911910	0.749053	-0.894574
C 0	-0.079131	1.564750	-0.135730
N 0	-1.907698	-0.039913	-0.245704
O 0	-1.861560	-0.139998	0.993757
O 0	-2.754204	-0.598970	-0.956494
H 0	-1.040758	0.794801	-1.965527
H 0	0.386308	2.404306	-0.644278
H 0	-0.354577	1.737566	0.897356

TS-5+CP

B3LYP/6-31G(d) Geometry

C 0	1.051799	-1.508201	0.223285
C 0	1.747635	-0.541963	0.971016
C 0	2.073170	0.532921	0.137422
C 0	0.943486	-1.067875	-1.095622
C 0	1.968766	0.022541	-1.282676
H 0	0.561405	-2.383690	0.633510
H 0	1.884220	-0.564744	2.047271
H 0	2.728723	1.349153	0.424721
H 0	0.531784	-1.652647	-1.910305
H 0	2.928925	-0.450569	-1.548923
H 0	1.742851	0.768641	-2.047271
C 0	0.104987	1.506003	-0.045564
C 0	-0.621277	0.605030	-0.814224
C 0	-1.769148	-0.149936	-0.230420
F 0	-1.589174	-0.433679	1.080793
F 0	-2.008483	-1.323862	-0.868574
F 0	-2.928925	0.557585	-0.319185
H 0	0.535188	2.383690	-0.516463
H 0	-0.108440	1.607107	1.011935
H 0	-0.718943	0.755582	-1.884976

TS-6+CP

B3LYP/6-31G(d) Geometry

C 0	-1.263298	0.258113	-1.612131
C 0	-2.141574	0.985418	-0.793285
C 0	-2.507071	0.191457	0.312237
C 0	-1.101274	-1.021106	-1.083711
C 0	-2.223238	-1.240557	-0.100612
H 0	-0.719890	0.661247	-2.459763
H 0	-2.382602	2.036583	-0.914301
H 0	-3.338446	0.445263	0.964048
H 0	-0.536409	-1.823766	-1.543432
H 0	-3.099111	-1.606383	-0.664528
H 0	-2.028745	-1.945603	0.707925
C 0	-0.875119	0.376316	1.578599
C 0	0.119076	-0.450520	1.033176
B 0	1.269146	-0.028632	0.103957
C 0	2.349438	-1.101789	-0.360020
C 0	1.502676	1.490204	-0.308822
H 0	-1.421241	0.040671	2.459763
H 0	-0.752452	1.454909	1.534266
H 0	0.090455	-1.492588	1.359911
H 0	2.135611	-2.131099	-0.045776
H 0	3.338446	-0.835441	0.044139
H 0	2.477893	-1.101734	-1.452288
H 0	2.248082	1.919146	0.380850
H 0	0.615739	2.131099	-0.243433
H 0	1.929998	1.600467	-1.314228

TS-7+CP

B3LYP/6-31G(d) Geometry

C 0	-0.900031	0.164371	-1.612524
C 0	-1.726558	0.933423	-0.773034
C 0	-2.113970	0.158111	0.338732
C 0	-0.812036	-1.122341	-1.102906
C 0	-1.894542	-1.288286	-0.072826
H 0	-0.347064	0.544574	-2.463672
H 0	-1.919009	1.994505	-0.891049
H 0	-2.938521	0.447655	0.984481
H 0	-0.257367	-1.942639	-1.543066
H 0	-2.806902	-1.630736	-0.590710
H 0	-1.688716	-1.994505	0.732306
C 0	-0.523453	0.316702	1.592877
C 0	0.492283	-0.514384	1.088164
B 0	1.659887	-0.063705	0.248902
Cl 0	2.938521	-1.210114	-0.252108
Cl 0	1.879905	1.646652	-0.234919
H 0	-1.082047	-0.022853	2.463672
H 0	-0.374431	1.391891	1.565559
H 0	0.476950	-1.559332	1.393557

TS-8+CP

B3LYP/6-31G(d) Geometry

C 0	-1.440139	-1.032199	0.500077
C 0	-0.905549	-1.305478	-0.895370
C 0	-0.563207	0.087083	-1.332120
C 0	-1.359016	0.972822	-0.615861
C 0	-1.948393	0.288254	0.460207
H 0	-1.914129	-1.812741	1.089729
H 0	-1.745666	-1.665976	-1.513103
H 0	-0.101586	-2.037239	-0.974571
H 0	0.023336	0.326193	-2.211324
H 0	-1.443962	2.037239	-0.806242
H 0	-2.560249	0.743906	1.232136
C 0	0.326033	-0.785531	1.413962
C 0	1.261568	-0.277844	0.494262
C 0	1.614102	1.137903	0.414223
O 0	2.560249	1.623728	-0.178405
Cl 0	2.354948	-1.394203	-0.325638
H 0	0.460322	-1.812642	1.741119
H 0	0.022361	-0.114307	2.211324
H 0	0.901880	1.773074	0.987770

TS-9+CP

B3LYP/6-31G(d) Geometry

C 0	-2.131364	-0.739089	-0.579969
C 0	-1.423628	-1.387810	0.443782
C 0	-0.849797	-0.429990	1.275089
C 0	-1.934932	0.655965	-0.459374
C 0	-1.521020	0.882811	0.983910
H 0	-2.605160	-1.231655	-1.422929
H 0	-1.267043	-2.458567	0.518885
H 0	-0.264594	-0.635569	2.164014
H 0	-2.550172	1.374825	-0.994457
H 0	-0.933751	1.778958	1.182782
H 0	-2.439894	0.944584	1.592132
C 0	0.869704	0.507920	-0.328658

C 0	-0.098705	0.914755	-1.269714
C 0	1.482838	-0.815540	-0.455117
O 0	2.502834	-1.168978	0.120970
C 0	1.598543	1.493137	0.555728
H 0	-0.227689	0.311900	-2.164014
H 0	-0.195674	1.982619	-1.457894
H 0	0.955454	-1.507902	-1.149875
H 0	1.740251	1.112181	1.572055
H 0	2.605160	1.673243	0.155020
H 0	1.085048	2.458567	0.605602

TS-10+CP

B3LYP/6-31G(d) Geometry

C 0	-1.568627	-1.534057	-0.953761
C 0	-0.567296	-2.270016	-0.303072
C 0	-0.370846	-1.733423	0.970417
C 0	-1.974997	-0.473332	-0.120321
C 0	-1.563742	-0.872361	1.283859
H 0	-1.870913	-1.666710	-1.987701
H 0	0.034341	-3.051715	-0.754113
H 0	0.315963	-2.120387	1.714454
H 0	-2.868113	0.114362	-0.313346
H 0	-1.393830	-0.056185	1.987701
H 0	-2.356804	-1.515948	1.701861
C 0	0.646655	0.362221	0.360159
C 0	-0.427452	0.910941	-0.366261
C 0	1.786821	-0.274415	-0.291974
O 0	2.868113	-0.494749	0.232299
C 0	-1.097224	2.186977	0.111284
H 0	0.813834	0.667098	1.391401
H 0	-0.346758	0.838664	-1.449982
H 0	1.604201	-0.557713	-1.355733
H 0	-0.454434	3.051715	-0.098804
H 0	-2.055441	2.362509	-0.389333
H 0	-1.274934	2.171168	1.192540

TS-11+CP

B3LYP/6-31G(d) Geometry

C 0	-0.223227	1.663066	-0.863880
C 0	-1.389308	1.436595	-0.124611
C 0	-1.050343	0.768599	1.068223
C 0	0.873229	1.149066	-0.153907
C 0	0.428239	0.991654	1.279493
H 0	-0.186317	2.059085	-1.873308
H 0	-2.400328	1.629910	-0.466556
H 0	-1.749936	0.570336	1.873308
H 0	1.910825	1.279073	-0.441471
H 0	0.958698	0.239249	1.865168
H 0	0.555063	1.962788	1.786243
C 0	-0.616455	-1.257286	0.340714
C 0	0.515193	-1.033526	-0.477270
C 0	-1.930449	-1.530043	-0.270907
O 0	-2.861208	-2.059085	0.304577
C 0	1.804926	-1.490476	-0.062906
N 0	2.861208	-1.837660	0.285533
H 0	-0.477205	-1.680600	1.331490
H 0	0.374585	-0.988598	-1.553871
H 0	-2.023644	-1.197536	-1.330487

TS-12+CP

B3LYP/6-31G(d) Geometry

C 0	2.911476	0.491676	0.338620
C 0	2.480856	0.719216	-1.103139
C 0	1.634427	-0.488382	-1.349770
C 0	1.967612	-1.467899	-0.431693
C 0	2.809376	-0.904989	0.548629
H 0	3.717332	1.070971	0.781890
H 0	3.382312	0.645930	-1.735130
H 0	2.009564	1.676413	-1.329162
H 0	0.968844	-0.609981	-2.196541
H 0	1.592901	-2.485263	-0.433070
H 0	3.200706	-1.433087	1.412291
C 0	1.342933	1.185339	1.318593
C 0	0.179688	1.099825	0.523358
C 0	-0.678337	-0.031340	0.535660
O 0	-1.759037	-0.116539	-0.090673
B 0	-2.598966	-1.472606	-0.112640
Cl 0	-0.303452	2.485263	-0.441450
H 0	1.725326	2.184738	1.507081
H 0	1.370692	0.548075	2.196541
H 0	-0.364998	-0.879519	1.156118
H 0	-2.538489	-1.832821	-1.271137
H 0	-2.034590	-2.227111	0.662965
H 0	-3.717332	-1.157795	0.223386

TS-13+CP

B3LYP/6-31G(d) Geometry

C 0	-2.955031	0.030120	-0.340067
C 0	-2.586350	0.189209	1.128184
C 0	-1.547126	-0.880950	1.273679
C 0	-1.760328	-1.835404	0.291089
C 0	-2.670454	-1.322891	-0.650697
H 0	-3.822567	0.534564	-0.758027
H 0	-3.467430	-0.104198	1.724361
H 0	-2.294466	1.187485	1.453140
H 0	-0.877117	-0.981066	2.119670
H 0	-1.247834	-2.788296	0.220332
H 0	-2.982476	-1.830309	-1.557781
C 0	-1.452872	0.997907	-1.178912
C 0	-0.323318	0.967391	-0.323225
C 0	0.648363	-0.060641	-0.487444
O 0	1.737281	-0.070989	0.142702
B 0	2.761400	-1.281423	0.032323
C 0	-0.011567	2.090979	0.636918
H 0	-1.953985	1.958926	-1.282177
H 0	-1.391199	0.459646	-2.119670
H 0	0.460821	-0.870744	-1.201874
H 0	2.765627	-1.768715	1.146021
H 0	2.313362	-2.027997	-0.822709
H 0	3.822567	-0.775880	-0.259111
H 0	-0.850313	2.788296	0.727307
H 0	0.854567	2.660811	0.275520
H 0	0.257667	1.724986	1.632977

TS-14+CP

B3LYP/6-31G(d) Geometry

C 0	-2.875180	-0.786491	-0.128781
C 0	-2.456735	-1.164957	1.284107
C 0	-1.137151	-1.822625	1.010531
C 0	-1.150279	-2.300344	-0.294627
C 0	-2.240589	-1.730668	-0.971178
H 0	-3.877483	-0.424041	-0.341171
H 0	-3.158020	-1.936111	1.646121
H 0	-2.446122	-0.360731	2.020866
H 0	-0.401394	-2.070159	1.766849
H 0	-0.391719	-2.936036	-0.737460

H 0	-2.471731	-1.880965	-2.020866
C 0	-1.760737	0.858265	-0.345167
C 0	-0.592169	0.650805	0.431011
C 0	0.632288	0.202499	-0.126624
O 0	1.711041	0.177177	0.516454
B 0	3.040603	-0.443111	-0.095718
C 0	-2.727127	1.953183	0.079932
H 0	-1.610750	0.817524	-1.422751
H 0	-0.562391	0.980197	1.466749
H 0	0.650703	-0.137979	-1.170456
H 0	3.269653	-1.404555	0.611651
H 0	2.776306	-0.739884	-1.249508
H 0	3.877483	0.425310	0.012801
H 0	-2.279237	2.936036	-0.110170
H 0	-2.954375	1.897803	1.150241
H 0	-3.669580	1.906315	-0.474533

TS-15+CP

B3LYP/6-31G(d) Geometry

C 0	2.631074	0.881848	-0.181660
C 0	2.230993	1.006495	1.276308
C 0	0.770199	1.318922	1.119956
C 0	0.599415	1.941892	-0.123491
C 0	1.740126	1.715867	-0.899365
H 0	3.660699	0.720034	-0.485361
H 0	2.729362	1.900583	1.686062
H 0	2.484573	0.163210	1.920205
H 0	0.054651	1.344731	1.933949
H 0	-0.308280	2.432512	-0.457259
H 0	1.865620	2.017471	-1.933949
C 0	1.769034	-0.975375	-0.429633
C 0	0.617509	-0.978491	0.406272
C 0	-0.692859	-0.790837	-0.133756
O 0	-1.728360	-0.982608	0.536306
B 0	-3.186767	-0.647912	-0.032686
C 0	2.886242	-1.797321	-0.044457
N 0	3.806619	-2.432512	0.275746
H 0	1.605720	-0.951766	-1.504195
H 0	0.678623	-1.379205	1.412648
H 0	-0.801076	-0.447559	-1.171515
H 0	-3.579719	0.230552	0.705996
H 0	-3.014520	-0.290206	-1.184066
H 0	-3.806619	-1.678133	0.089700

TS-16+CP

B3LYP/6-31G(d) Geometry

C 0	-1.721765	-0.611388	0.885040
C 0	-1.682950	0.900046	0.713611
C 0	-0.312256	1.215311	1.223620
C 0	0.129001	0.173279	2.012116
C 0	-0.763117	-0.913325	1.874812
H 0	-2.651914	-1.167874	0.802564
H 0	-2.425157	1.335355	1.404018
H 0	-1.906281	1.287526	-0.282382
H 0	0.180334	2.171590	1.091908
H 0	1.047911	0.158868	2.586344
H 0	-0.647152	-1.878770	2.356366
C 0	-0.817385	-1.141947	-0.802408
C 0	0.263583	-0.270201	-1.080163
C 0	1.586266	-0.625936	-0.687380
C 0	0.084331	0.875635	-1.907602
N 0	2.651914	-0.957240	-0.348484
N 0	-0.102571	1.806141	-2.586344
H 0	-1.696691	-1.036043	-1.432201
H 0	-0.570753	-2.171590	-0.566361

TS-17+CP

B3LYP/6-31G(d) Geometry

C 0	-1.617263	-0.161950	0.758969
C 0	-1.618811	1.347770	0.760925
C 0	-0.131738	1.608274	0.760589
C 0	0.475695	0.503977	1.375910
C 0	-0.424852	-0.569152	1.374942
H 0	-2.520286	-0.762008	0.719974
H 0	-2.029680	1.691678	1.724299
H 0	-2.193900	1.831097	-0.031935
H 0	0.302527	2.601773	0.722992
H 0	1.516329	0.449463	1.674283
H 0	-0.190819	-1.584848	1.672449
C 0	-0.946423	-0.138126	-1.368316
C 0	-0.036923	0.945641	-1.367401
C 0	-0.514167	-1.490764	-1.543583
C 0	1.370355	0.754883	-1.541626
N 0	2.520286	0.631962	-1.674200
N 0	-0.193421	-2.601773	-1.677014
H 0	-1.953027	0.058612	-1.724299
H 0	-0.405056	1.903207	-1.722680

TS-18+CP

B3LYP/6-31G(d) Geometry

C 0	-1.844975	-0.595948	1.005841
C 0	-1.730807	0.878240	0.704881
C 0	-0.266878	1.091977	0.997738
C 0	0.104819	0.123993	1.945490
C 0	-0.850669	-0.900266	1.945908
H 0	-2.758840	-1.162391	0.863874
H 0	-2.315089	1.427222	1.461533
H 0	-2.086055	1.194260	-0.277559
H 0	0.236176	2.045178	0.873091
H 0	1.045889	0.105704	2.483140
H 0	-0.769878	-1.832591	2.494461
C 0	-0.690834	-1.040173	-0.878614
C 0	0.272519	-0.002856	-0.857886
C 0	-1.797663	-0.961055	-1.779026
C 0	1.643866	-0.319037	-0.598226
N 0	2.758840	-0.572065	-0.377881
N 0	-2.714337	-0.887300	-2.494461
H 0	-0.383153	-2.045178	-0.612417
H 0	0.116518	0.859287	-1.499489

TS-19+CP

B3LYP/6-31G(d) Geometry

C 0	-1.329059	-0.673944	1.339866
C 0	-1.361504	0.837305	1.462432
C 0	0.109495	1.122187	1.579853
C 0	0.714845	-0.006871	2.128299
C 0	-0.169177	-1.091308	2.019688
H 0	-2.236103	-1.270655	1.302156
H 0	-1.846493	1.091860	2.420142
H 0	-1.891014	1.375822	0.674564
H 0	0.539120	2.117626	1.566678
H 0	1.743693	-0.066678	2.464360
H 0	0.065899	-2.117626	2.282300
C 0	-0.703214	-0.660136	-0.665493

C 0	0.220519	0.403647	-0.725207
C 0	-2.027880	-0.546801	-1.395650
C 0	1.621621	0.162090	-0.783020
N 0	2.768660	-0.045334	-0.834859
H 0	-0.277177	-1.659682	-0.674747
H 0	-0.103714	1.372660	-1.095688
H 0	-1.883648	-0.752514	-2.464360
H 0	-2.454102	0.459174	-1.314637
H 0	-2.768660	-1.261797	-1.022445

TS-20+CP

B3LYP/6-31G(d) Geometry

C 0	-1.552271	-0.882915	1.444900
C 0	-1.608667	0.629450	1.556345
C 0	-0.143064	0.943369	1.653805
C 0	0.494692	-0.170466	2.186125
C 0	-0.371561	-1.273981	2.110109
H 0	-2.452653	-1.491746	1.442939
H 0	-2.087139	0.880967	2.518299
H 0	-2.161572	1.149050	0.772205
H 0	0.270607	1.944577	1.610508
H 0	1.530693	-0.209211	2.502934
H 0	-0.108556	-2.294196	2.369203
C 0	-0.995363	-0.908675	-0.523498
C 0	-0.084181	0.145054	-0.738180
C 0	1.311750	-0.161386	-0.749961
C 0	-0.486845	1.433296	-1.434469
N 0	2.452653	-0.404640	-0.777661
H 0	-1.997795	-0.781905	-0.927329
H 0	-0.633177	-1.929627	-0.564424
H 0	-1.550224	1.642618	-1.281726
H 0	-0.323525	1.355075	-2.518299
H 0	0.089236	2.294196	-1.081225

TS-21+CP

B3LYP/6-31G(d) Geometry

C 0	0.929854	-1.909330	-0.955226
C 0	1.993807	-1.244285	-0.328608
C 0	1.587140	-0.840775	0.946102
C 0	-0.188789	-1.890978	-0.102350
C 0	0.345662	-1.616253	1.287617
H 0	0.926536	-2.257745	-1.982872
H 0	2.941615	-0.994357	-0.792920
H 0	2.218974	-0.345767	1.674801
H 0	-1.086517	-2.471652	-0.280778
H 0	-0.347091	-1.145374	1.982872
H 0	0.655690	-2.581920	1.722161
C 0	0.085494	0.902764	0.337360
C 0	-0.829233	0.135616	-0.396870
C 0	1.125257	1.699078	-0.321312
O 0	1.770707	2.581920	0.216181
C 0	-2.261680	0.064140	0.051119
F 0	-2.384252	-0.119470	1.387779
F 0	-2.923928	1.205920	-0.249674
F 0	-2.941615	-0.939295	-0.555618
H 0	-0.137484	1.179902	1.363676
H 0	-0.761599	0.167391	-1.481290
H 0	1.294415	1.437848	-1.391867

TS-22+CP

B3LYP/6-31G(d) Geometry

C 0	0.523593	-2.299423	0.256486
C 0	1.622219	-1.800986	0.968042
C 0	2.302753	-0.857357	0.167872
C 0	0.514049	-1.730894	-1.020480
C 0	1.891946	-1.166597	-1.258956
H 0	-0.254147	-2.934098	0.666819
H 0	1.828993	-1.995975	2.015494
H 0	3.302461	-0.506815	0.409943
H 0	-0.175629	-1.990429	-1.815409
H 0	2.535034	-1.985487	-1.626254
H 0	1.962139	-0.344229	-1.971214
C 0	1.176023	0.872270	0.367637
C 0	0.053605	0.629236	-0.452437
B 0	-1.317166	0.082002	-0.031976
C 0	-2.488793	-0.029039	-1.105886
C 0	-1.672414	-0.240863	1.486216
C 0	2.195083	1.932098	-0.019430
H 0	1.013596	0.805769	1.441947
H 0	0.167080	0.957127	-1.490250
H 0	-2.187687	0.199084	-2.136160
H 0	-3.302461	0.664727	-0.843101
H 0	-2.951506	-1.026689	-1.102285
H 0	-2.184931	0.639787	1.907093
H 0	-0.812046	-0.438507	2.136160
H 0	-2.378757	-1.074754	1.593704
H 0	1.787151	2.934098	0.167978
H 0	2.447141	1.879637	-1.085171
H 0	3.123642	1.847066	0.556076

TS-23+CP

B3LYP/6-31G(d) Geometry

C 0	0.421216	-2.296702	0.119081
C 0	1.419582	-1.714372	0.914393
C 0	2.030182	-0.657868	0.201462
C 0	0.426469	-1.682685	-1.128985
C 0	1.717774	-0.924789	-1.261651
H 0	-0.302952	-3.028295	0.458141
H 0	1.595678	-1.944044	1.960025
H 0	2.985482	-0.240976	0.508940
H 0	-0.222577	-1.932791	-1.960025
H 0	2.483274	-1.619497	-1.648052
H 0	1.700528	-0.055941	-1.920263
C 0	0.784095	0.916911	0.473664
C 0	-0.319573	0.664641	-0.375961
B 0	-1.634271	0.056678	0.027843
Cl 0	-2.985482	-0.087283	-1.139441
Cl 0	-1.968387	-0.480544	1.705217
C 0	1.712247	2.081631	0.163339
H 0	0.597406	0.786748	1.537613
H 0	-0.249148	1.052797	-1.392466
H 0	1.205507	3.028295	0.388786
H 0	1.993075	2.106059	-0.895932
H 0	2.629297	2.050528	0.761236

TS-24+CP

B3LYP/6-31G(d) Geometry

C 0	0.620814	1.493275	-0.979894
C 0	1.670068	1.224537	-0.085371
C 0	1.129145	0.804976	1.135217
C 0	-0.597935	1.259583	-0.336052
C 0	-0.324332	1.204727	1.145895
H 0	0.741231	1.729639	-2.031213
H 0	2.722634	1.216239	-0.343199
H 0	1.708898	0.611505	2.031213
H 0	-1.574816	1.457525	-0.764257

H 0	-0.398311	2.229036	1.546504
H 0	-0.995379	0.573348	1.729930
C 0	0.512320	-1.270636	0.514409
C 0	-0.508168	-1.022414	-0.397388
N 0	1.793217	-1.715813	-0.003033
N 0	-1.882602	-1.249244	0.012311
O 0	2.567933	-2.229036	0.805761
O 0	2.037506	-1.530776	-1.199823
O 0	-2.135272	-1.362243	1.218587
O 0	-2.722634	-1.301039	-0.887107
H 0	0.318124	-1.619723	1.517513
H 0	-0.369386	-1.125418	-1.461523

TS-25+CP

B3LYP/6-31G(d) Geometry

C 0	0.623396	0.672544	1.203852
C 0	-0.779191	0.676807	1.216287
C 0	-1.241604	0.981891	-0.062234
C 0	1.074474	0.924779	-0.111154
C 0	-0.093121	1.570555	-0.834224
H 0	1.257321	0.380104	2.033069
H 0	-1.396415	0.376302	2.055141
H 0	-2.282710	1.084610	-0.346663
H 0	2.109069	1.156461	-0.343820
H 0	-0.058206	2.654147	-0.632550
H 0	-0.122438	1.436874	-1.916846
C 0	-0.536495	-1.109133	-1.125181
C 0	0.859281	-0.890481	-1.030131
C 0	-1.357638	-1.929631	-0.256872
C 0	1.924595	-1.665869	-0.277329
O 0	3.075564	-1.594699	-0.658929
O 0	1.594172	-2.352582	0.817875
O 0	-1.035329	-2.444698	0.819045
O 0	-2.617300	-2.090253	-0.729169
H 0	-1.020557	-0.833331	-2.055141
H 0	1.306022	-0.548510	-1.959699
H 0	0.607294	-2.386645	0.943149
H 0	-3.075564	-2.654147	-0.079063

TS-26+CP

B3LYP/6-31G(d) Geometry

C 0	-1.574641	-0.358581	0.983497
C 0	-1.659637	1.152746	1.110984
C 0	-0.212792	1.493792	1.289553
C 0	0.452083	0.378066	1.780846
C 0	-0.387344	-0.740025	1.658494
H 0	-2.460673	-0.987647	0.982528
H 0	-2.193461	1.381653	2.048117
H 0	-2.172448	1.686992	0.309076
H 0	0.187818	2.499076	1.229855
H 0	1.481737	0.355215	2.117554
H 0	-0.112517	-1.760633	1.899631
C 0	-1.030470	-0.407964	-0.943033
C 0	-0.088241	0.646639	-1.178740
C 0	-0.619500	-1.778353	-1.128771
C 0	1.315354	0.395008	-1.213165
C 0	-0.554590	1.887331	-1.704633
N 0	2.460673	0.182063	-1.228693
N 0	-0.324472	-2.895282	-1.254613
N 0	-0.970810	2.895282	-2.117554
H 0	-2.026853	-0.217460	-1.337078

TS-27+CP

B3LYP/6-31G(d) Geometry

C 0	-1.567335	-0.525290	1.400792
C 0	-1.626586	0.984815	1.515436
C 0	-0.159159	1.295327	1.612713
C 0	0.469690	0.184329	2.167873
C 0	-0.398293	-0.916337	2.087099
H 0	-2.466870	-1.135776	1.383641
H 0	-2.103647	1.237350	2.477847
H 0	-2.179473	1.505061	0.732188
H 0	0.256082	2.296292	1.574906
H 0	1.501431	0.146912	2.498757
H 0	-0.143567	-1.934168	2.362004
C 0	-0.981446	-0.552335	-0.578076
C 0	-0.086599	0.535899	-0.737433
C 0	-0.535226	-1.985372	-0.792602
C 0	1.318787	0.272085	-0.771085
C 0	-0.513458	1.828377	-1.415617
N 0	2.466870	0.068134	-0.815960
H 0	-1.985263	-0.346346	-0.951232
H 0	0.439269	-2.174458	-0.334193
H 0	-0.437203	-2.195194	-1.866081
H 0	-1.257806	-2.696886	-0.378363
H 0	-1.583140	2.009900	-1.273514
H 0	-0.335845	1.773533	-2.498757
H 0	0.037563	2.696886	-1.040999

TS-28+CP

B3LYP/6-31G(d) Geometry

C 0	-1.337888	-0.890020	1.387495
C 0	-1.411895	0.618676	1.518182
C 0	0.050219	0.943766	1.626063
C 0	0.687676	-0.167851	2.174504
C 0	-0.164773	-1.276226	2.070255
H 0	-2.230533	-1.509413	1.360585
H 0	-1.898679	0.856113	2.479491
H 0	-1.966136	1.144487	0.739252
H 0	0.452287	1.950706	1.607794
H 0	1.718613	-0.199179	2.507816
H 0	0.102499	-2.296435	2.325493
C 0	-0.743749	-0.874417	-0.601541
C 0	0.166793	0.210270	-0.717103
C 0	-2.076444	-0.850833	-1.326910
C 0	1.560620	-0.107343	-0.688052
C 0	-0.182507	1.513663	-1.415358
N 0	2.698910	-0.364366	-0.680735
H 0	-0.285609	-1.858608	-0.585188
H 0	-1.920787	-0.914911	-2.412525
H 0	-2.648889	0.062509	-1.136624
H 0	-2.698910	-1.702478	-1.034491
H 0	-1.175577	1.876409	-1.134842
H 0	-0.181364	1.387768	-2.507816
H 0	0.542974	2.296435	-1.176595

TS-29+CP

B3LYP/6-31G(d) Geometry

C 0	-1.315636	-0.266014	1.175831
C 0	-1.295208	1.240589	1.132876
C 0	0.196602	1.477137	1.131375
C 0	0.779395	0.382946	1.799446
C 0	-0.139484	-0.673755	1.817789
H 0	-2.226844	-0.851226	1.117022
H 0	-1.701964	1.620184	2.084583

H 0	-1.864870	1.702156	0.324597
H 0	0.642631	2.465881	1.093539
H 0	1.814113	0.325105	2.117609
H 0	0.069769	-1.679144	2.166704
C 0	-0.536147	-0.308227	-0.990180
C 0	0.329711	0.821971	-0.928134
C 0	-1.833012	-0.091271	-1.563704
C 0	0.022319	-1.713310	-1.133602
C 0	1.743799	0.646875	-1.082043
N 0	2.894320	0.511247	-1.198372
N 0	-2.894320	0.070362	-2.017679
H 0	-0.040652	1.765072	-1.319334
H 0	0.893321	-1.845616	-0.486771
H 0	0.345057	-1.894075	-2.166704
H 0	-0.727817	-2.465881	-0.876446

TS-30+CP

B3LYP/6-31G(d) Geometry

C 0	-1.599086	-0.385626	1.499019
C 0	-1.634842	1.123061	1.507749
C 0	-0.155378	1.413476	1.480457
C 0	0.483373	0.327124	2.096373
C 0	-0.391657	-0.764488	2.112860
H 0	-2.490840	-1.003862	1.483225
H 0	-2.035055	1.453740	2.480386
H 0	-2.238546	1.594575	0.730953
H 0	0.259485	2.414239	1.423171
H 0	1.528490	0.297092	2.381973
H 0	-0.131354	-1.774389	2.407887
C 0	-0.978305	-0.379826	-0.601853
C 0	-0.068474	0.712045	-0.682965
C 0	-0.551456	-1.739335	-0.744660
C 0	1.340901	0.438736	-0.758712
C 0	-0.492993	1.987657	-1.400368
N 0	2.490840	0.271195	-0.829330
N 0	-0.237138	-2.854800	-0.854346
H 0	-1.981065	-0.197214	-0.980855
H 0	-1.556878	2.189606	-1.246527
H 0	-0.327819	1.886101	-2.480386
H 0	0.079734	2.854800	-1.059493

TS-31+CP

B3LYP/6-31G(d) Geometry

C 0	1.598960	-1.429304	1.072137
C 0	0.499294	-2.220616	0.714640
C 0	0.201191	-1.989112	-0.632941
C 0	1.971588	-0.635012	-0.031075
C 0	1.413738	-1.343771	-1.249463
H 0	2.001166	-1.334971	2.075343
H 0	-0.093954	-2.822824	1.394360
H 0	-0.570229	-2.500720	-1.197619
H 0	2.903493	-0.077032	-0.063079
H 0	1.232638	-0.727705	-2.130680
H 0	2.120708	-2.140419	-1.538421
C 0	-0.640913	0.197131	-0.521781
C 0	0.490677	0.891738	-0.021432
C 0	-1.820636	-0.196308	0.247879
O 0	-2.903493	-0.468426	-0.251624
C 0	0.515455	1.370385	1.424667
C 0	1.149958	1.884616	-0.972347
H 0	-0.835221	0.244034	-1.591681
H 0	-1.689315	-0.247681	1.350237
H 0	0.169459	0.612573	2.130680
H 0	1.529745	1.664337	1.718167
H 0	-0.127890	2.253670	1.542469
H 0	0.577826	2.822824	-0.986288
H 0	2.169876	2.134632	-0.658389
H 0	1.187684	1.513272	-2.001247

TS-32+CP

B3LYP/6-31G(d) Geometry

C 0	0.079161	1.203948	0.946049
C 0	1.321339	0.942091	0.351057
C 0	1.122391	0.600890	-1.015867
C 0	-0.907848	1.143745	-0.031065
C 0	-0.249388	1.153492	-1.375492
H 0	-0.092157	1.341140	2.007243
H 0	2.268085	0.878323	0.876665
H 0	1.944779	0.596662	-1.726416
H 0	-1.970560	1.284222	0.128226
H 0	-0.793336	0.640061	-2.170058
H 0	-0.113153	2.200857	-1.692737
C 0	0.608769	-1.292510	-1.011364
C 0	-0.652940	-1.422960	-0.345288
C 0	1.841768	-1.910879	-0.424642
O 0	2.807419	-2.200857	-1.096803
C 0	-1.847900	-1.545901	-1.114574
C 0	-0.721168	-1.771884	1.037926
N 0	-2.807419	-1.621813	-1.772954
N 0	-0.743176	-2.049253	2.170058
H 0	0.572737	-1.409730	-2.092440
H 0	1.826794	-2.065596	0.673125

TS-33+CP

B3LYP/6-31G(d) Geometry

C 0	-1.846239	0.146860	0.971562
C 0	-1.733121	1.619758	0.673053
C 0	-0.270131	1.824359	0.971647
C 0	0.093891	0.858434	1.937102
C 0	-0.859572	-0.156388	1.937024
H 0	-2.755929	-0.425770	0.826659
H 0	-2.319162	2.170321	1.426166
H 0	-2.079172	1.944939	-0.309327
H 0	0.244702	2.767994	0.826937
H 0	1.027614	0.846659	2.487002
H 0	-0.789707	-1.087607	2.486858
C 0	-0.715082	-0.335802	-0.857343
C 0	0.282254	0.725832	-0.857160
C 0	-1.817474	-0.246888	-1.778534
C 0	-0.291774	-1.680353	-0.563805
C 0	1.650572	0.387138	-0.563560
N 0	-2.737026	-0.174871	-2.487002
C 0	0.124898	1.820630	-1.778281
N 0	0.026624	-2.767994	-0.304469
N 0	2.755929	0.137173	-0.304152
N 0	-0.004216	2.733987	-2.486653

TS-34+CP

B3LYP/6-31G(d) Geometry

C 0	-1.338342	-0.445056	1.605995
C 0	-1.299650	1.040234	1.427599
C 0	0.196328	1.254396	1.266357
C 0	0.811722	0.180481	1.966949
C 0	-0.109637	-0.862912	2.111281
H 0	-2.241856	-1.041889	1.557953
H 0	-1.607838	1.518133	2.372149

H 0	-1.945745	1.434467	0.642747
H 0	0.634607	2.248674	1.259742
H 0	1.867562	0.122127	2.205474
H 0	0.121397	-1.862170	2.460617
C 0	-0.535512	-0.423126	-0.817962
C 0	0.342370	0.717598	-0.657273
C 0	-1.841111	-0.238386	-1.361620
C 0	-0.024669	-1.755753	-0.818208
C 0	1.763012	0.439945	-0.764631
C 0	-0.031426	2.015087	-1.383797
N 0	2.912164	0.286143	-0.844066
N 0	-2.912164	-0.057762	-1.786444
N 0	0.393791	-2.843206	-0.808017
H 0	-1.080443	2.272660	-1.225240
H 0	0.123089	1.887985	-2.460617
H 0	0.596485	2.843206	-1.046355

TS-35+CP

B3LYP/6-31G(d) Geometry

C 0	-0.706363	2.198819	0.101397
C 0	0.619853	1.969319	-0.268506
C 0	0.655893	0.979557	-1.299010
C 0	-1.537901	1.450460	-0.735616
C 0	-0.734348	1.011301	-1.919312
H 0	-1.031049	2.775594	0.959283
H 0	1.491660	2.375733	0.232833
H 0	1.547127	0.833778	-1.903840
H 0	-2.620136	1.416411	-0.686971
H 0	-1.078994	0.101184	-2.409344
H 0	-0.743303	1.816213	-2.672684
C 0	0.477491	-0.764825	-0.397343
C 0	-0.852504	-0.762237	0.180883
C 0	1.630024	-0.617874	0.567571
O 0	2.743869	-1.033015	0.334189
C 0	-1.898355	-1.511486	-0.439932
C 0	-1.063574	-0.421761	1.554421
C 0	0.768415	-1.764364	-1.509417
N 0	-2.743869	-2.105798	-0.979803
N 0	-1.220458	-0.132337	2.672684
H 0	1.402386	-0.074694	1.505468
H 0	1.747762	-1.567977	-1.949771
H 0	0.797284	-2.775594	-1.088603
H 0	0.006094	-1.755201	-2.290292

TS-36+CP

B3LYP/6-31G(d) Geometry

C 0	2.022892	-1.052482	0.704955
C 0	1.151569	-2.090361	0.355043
C 0	0.556648	-1.785056	-0.873214
C 0	1.922177	-0.024402	-0.264579
C 0	1.385424	-0.705151	-1.508717
H 0	2.559482	-0.976086	1.644586
H 0	0.899856	-2.941009	0.979463
H 0	-0.132875	-2.425325	-1.411906
H 0	2.652363	0.778964	-0.326332
H 0	0.877003	-0.067302	-2.230313
H 0	2.232335	-1.180505	-2.033144
C 0	-0.864529	0.108966	-0.191124
C 0	0.196401	0.978805	0.231587
C 0	-1.554272	-0.785132	0.752361
O 0	-2.652363	-1.290562	0.552299
C 0	-1.653901	0.373341	-1.456546
C 0	0.402490	1.246069	1.723457
C 0	0.392245	2.263595	-0.572597
H 0	-1.019941	-1.003233	1.697342
H 0	-2.307317	-0.475208	-1.669072
H 0	-2.303055	1.252005	-1.326379
H 0	-1.031372	0.573352	-2.332809
H 0	0.398709	0.341703	2.332809
H 0	1.357953	1.756519	1.891923
H 0	-0.391890	1.904659	2.101488
H 0	-0.459137	2.941009	-0.417497
H 0	1.292612	2.794198	-0.244376
H 0	0.476569	2.092707	-1.648964

TS-37+CP

B3LYP/6-31G(d) Geometry

C 0	-2.677142	1.309052	-0.453787
C 0	-2.152419	1.139463	-1.851709
C 0	-0.667183	1.244693	-1.571715
C 0	-0.551772	2.115975	-0.447276
C 0	-1.761005	2.130934	0.236718
H 0	-3.718881	1.179762	-0.181785
H 0	-2.445308	2.019922	-2.446192
H 0	-2.496211	0.254606	-2.386428
H 0	0.087038	1.195340	-2.351277
H 0	0.369643	2.583939	-0.117248
H 0	-1.935837	2.590492	1.202233
C 0	-1.784261	-0.716364	0.055934
C 0	-0.577050	-0.671873	-0.757919
C 0	0.693554	-0.444827	-0.059091
O 0	1.776221	-0.713183	-0.597154
C 0	-2.882680	-1.526193	-0.392513
C 0	-1.700957	-0.565935	1.483709
C 0	-0.477934	-1.562658	-1.986024
N 0	-1.623901	-0.419083	2.635692
N 0	-3.784418	-2.150767	-0.782481
H 0	0.697369	0.007648	0.939286
H 0	-1.408408	-1.585788	-2.555366
H 0	-0.258967	-2.590492	-1.673690
H 0	0.337660	-1.239578	-2.635692
B 0	3.206264	-0.330095	0.066189
H 0	3.673881	0.428573	-0.753091
H 0	2.929404	0.177802	1.133175
H 0	3.784418	-1.386973	0.127690

TS-38+CP

B3LYP/6-31G(d) Geometry

C 0	-1.258539	-0.539607	1.478272
C 0	-1.275398	0.966867	1.464675
C 0	0.209568	1.235196	1.439684
C 0	0.822653	0.151163	2.098831
C 0	-0.069277	-0.925399	2.118900
H 0	-2.158442	-1.143780	1.432313
H 0	-1.671929	1.319590	2.431007
H 0	-1.874328	1.429342	0.679990
H 0	0.634768	2.232986	1.400835
H 0	1.861052	0.115297	2.407936
H 0	0.166203	-1.928813	2.456288
C 0	-0.535295	-0.553825	-0.659912
C 0	0.342874	0.583512	-0.656740
C 0	-1.835683	-0.367146	-1.239859
C 0	0.015401	-1.966461	-0.795058
C 0	1.754598	0.302291	-0.714623
C 0	-0.032912	1.877110	-1.375489
N 0	2.901170	0.107184	-0.771330

N 0	-2.901170	-0.238704	-1.694549
H 0	0.891917	-2.099206	-0.156957
H 0	0.324975	-2.161206	-1.829720
H 0	-0.737627	-2.710474	-0.520794
H 0	-1.082494	2.133227	-1.216948
H 0	0.116036	1.763078	-2.456288
H 0	0.589805	2.710474	-1.038951

TS-39+CP

B3LYP/6-31G(d) Geometry

C 0	-1.391272	-0.400933	1.457614
C 0	-1.395468	1.106368	1.490456
C 0	0.089620	1.364258	1.458924
C 0	0.701698	0.258377	2.076908
C 0	-0.196277	-0.811957	2.076192
H 0	-2.294953	-1.000797	1.423237
H 0	-1.784529	1.432024	2.469319
H 0	-1.991369	1.606876	0.726921
H 0	0.523351	2.358446	1.425428
H 0	1.745413	0.201742	2.363269
H 0	0.040714	-1.830168	2.361904
C 0	-0.745735	-0.375176	-0.677061
C 0	0.177558	0.725287	-0.676638
C 0	-2.094454	-0.254678	-1.379607
C 0	-0.210155	-1.710264	-0.734084
C 0	1.585419	0.429940	-0.733018
C 0	-0.175201	2.032967	-1.378510
N 0	2.734658	0.252147	-0.789374
N 0	0.164673	-2.811080	-0.790962
H 0	-1.960074	-0.246898	-2.469319
H 0	-2.624005	0.661028	-1.105888
H 0	-2.734658	-1.105561	-1.132525
H 0	-1.169021	2.395289	-1.104810
H 0	-0.159300	1.899906	-2.468300
H 0	0.551507	2.811080	-1.130827

TS-40+CP

B3LYP/6-31G(d) Geometry

C 0	-1.308136	-0.500976	1.385138
C 0	-1.351537	1.007580	1.516321
C 0	0.120232	1.300025	1.590731
C 0	0.737841	0.180647	2.153018
C 0	-0.141277	-0.906637	2.070215
H 0	-2.212974	-1.103276	1.367243
H 0	-1.810388	1.257190	2.488171
H 0	-1.910699	1.545624	0.750823
H 0	0.544001	2.298086	1.563867
H 0	1.770506	0.131534	2.479122
H 0	0.101010	-1.927973	2.343427
C 0	-0.720222	-0.517152	-0.625759
C 0	0.184637	0.589150	-0.716667
C 0	-2.078790	-0.377906	-1.302367
C 0	-0.154395	-1.924250	-0.771181
C 0	1.589662	0.314316	-0.735710
C 0	-0.181736	1.901513	-1.395990
N 0	2.738287	0.111465	-0.770962
H 0	-1.959391	-0.413318	-2.394787
H 0	-2.595509	0.555384	-1.064259
H 0	-2.738287	-1.206574	-1.023277
H 0	0.794526	-2.044513	-0.245012
H 0	0.028988	-2.145975	-1.831993
H 0	-0.860269	-2.673278	-0.394795
H 0	-1.157747	2.278304	-1.078788
H 0	-0.222844	1.779772	-2.488171
H 0	0.562875	2.673278	-1.181571

TS-41+CP

B3LYP/6-31G(d) Geometry

C 0	1.229632	0.230347	1.211117
C 0	0.905384	-1.099365	0.876928
C 0	0.996927	-1.252798	-0.501070
C 0	1.442343	0.960716	0.030652
C 0	1.747864	-0.065298	-1.045203
H 0	1.192712	0.648895	2.211221
H 0	0.550623	-1.853334	1.571035
H 0	0.855295	-2.182920	-1.039257
H 0	1.887661	1.951433	0.024312
H 0	1.507026	0.226550	-2.069309
H 0	2.827277	-0.291122	-1.008552
C 0	-0.936474	0.050812	-1.216862
C 0	-0.521903	1.276211	-0.648822
C 0	-1.955840	-0.161120	-0.169942
C 0	-1.540587	1.180921	0.501591
O 0	-2.827277	-0.972391	0.052432
H 0	-0.836574	-0.372282	-2.211221
H 0	-0.230421	2.182920	-1.168899
H 0	-1.129584	1.108993	1.516093
H 0	-2.345757	1.925163	0.491477

TS-42+CP

B3LYP/6-31G(d) Geometry

C 0	-1.621806	-1.463350	0.163737
C 0	-1.165087	-0.937967	1.388211
C 0	-0.918516	0.420362	1.233264
C 0	-1.559749	-0.451808	-0.815501
C 0	-1.573057	0.857862	-0.049851
H 0	-1.846854	-2.507792	-0.022992
H 0	-0.955592	-1.516617	2.281358
H 0	-0.603476	1.095679	2.020486
H 0	-2.043181	-0.550650	-1.783655
H 0	-1.125380	1.713374	-0.556321
H 0	-2.622578	1.119550	0.168666
C 0	1.117239	0.361211	-0.237241
C 0	0.454376	-0.368294	-1.263300
C 0	1.793446	-0.859000	0.255858
C 0	1.133269	-1.693767	-0.870811
O 0	2.622578	-1.098254	1.108614
C 0	1.557522	1.784812	-0.064818
H 0	0.276517	-0.032216	-2.281358
H 0	0.474421	-2.513941	-0.558055
H 0	1.870884	-2.077172	-1.586340
H 0	0.787205	2.513941	-0.335571
H 0	2.431453	1.991777	-0.699100
H 0	1.862614	1.971180	0.970280

TS-43+CP

B3LYP/6-31G(d) Geometry

C 0	1.190070	-0.779098	1.148084
C 0	0.900875	-1.871286	0.310943
C 0	0.959646	-1.447173	-1.015203
C 0	1.359834	0.371540	0.359382
C 0	1.684518	-0.126364	-1.035996
H 0	1.158631	-0.798467	2.232382
H 0	0.576867	-2.851509	0.642863
H 0	0.839748	-2.089330	-1.880374
H 0	1.772948	1.296353	0.751247

H 0	1.430995	0.545854	-1.858050
H 0	2.768551	-0.324843	-1.090702
C 0	-0.977372	-0.077133	-1.148929
C 0	-0.642160	0.887062	-0.158558
C 0	-1.955127	-0.741990	-0.269217
C 0	-1.616482	0.260784	0.865651
O 0	-2.768551	-1.633747	-0.381384
C 0	-0.444641	2.371816	-0.340169
H 0	-0.899367	-0.059728	-2.232382
H 0	-1.175053	-0.159766	1.777207
H 0	-2.474174	0.888936	1.139854
H 0	-1.404622	2.846392	-0.587145
H 0	0.251462	2.596262	-1.156185
H 0	-0.069193	2.851509	0.570189

TS-44+CP

B3LYP/6-31G(d) Geometry

C 0	0.748086	1.422696	1.126076
C 0	1.792425	1.401356	0.188583
C 0	1.247215	1.234113	-1.095605
C 0	-0.469908	1.269675	0.455914
C 0	-0.218509	1.594383	-0.995718
H 0	0.874497	1.448012	2.203115
H 0	2.850983	1.391792	0.423695
H 0	1.823421	1.319210	-2.010813
H 0	-1.446947	1.338852	0.920307
H 0	-0.887840	1.117070	-1.713880
H 0	-0.312500	2.685068	-1.128534
C 0	0.688053	-0.874293	-1.123700
C 0	-0.294961	-0.954406	-0.096638
C 0	1.679848	-1.592210	-0.268403
C 0	0.653512	-1.657093	0.895192
O 0	2.797584	-2.018226	-0.420944
C 0	-1.697318	-1.135372	-0.218761
N 0	-2.850983	-1.279670	-0.311593
H 0	0.573152	-0.886097	-2.203115
H 0	0.908388	-1.100175	1.804179
H 0	0.381220	-2.685068	1.160124

TS-45+CP

B3LYP/6-31G(d) Geometry

C 0	1.847687	0.522934	0.023392
C 0	1.342586	0.329846	1.327671
C 0	0.626322	-0.853758	1.360523
C 0	1.330614	-0.482974	-0.820486
C 0	0.922570	-1.619738	0.103223
H 0	2.427245	1.380103	-0.302040
H 0	1.439501	1.031414	2.149048
H 0	0.118714	-1.267329	2.223862
H 0	1.751111	-0.677240	-1.803624
H 0	0.127047	-2.275252	-0.251711
H 0	1.811165	-2.248787	0.281630
C 0	-1.417153	-0.172574	-0.164464
C 0	-0.537298	0.187352	-1.214451
C 0	-1.632228	1.209476	0.292246
C 0	-0.691926	1.679600	-0.854311
O 0	-2.320028	1.773012	1.109742
Cl 0	-2.427245	-1.581606	0.060929
H 0	-0.560267	-0.210578	-2.223862
H 0	0.221391	2.205811	-0.551956
H 0	-1.235876	2.275252	-1.595855

TS-46+CP

B3LYP/6-31G(d) Geometry

C 0	-1.845888	1.562305	-0.328584
C 0	-0.778245	1.858573	-1.187859
C 0	0.425945	1.564231	-0.530937
C 0	-1.332232	1.093529	0.892386
C 0	0.115685	1.524486	0.944723
H 0	-2.896120	1.578714	-0.598485
H 0	-0.873097	2.152210	-2.227683
H 0	1.411597	1.790504	-0.922360
H 0	-1.938031	0.916052	1.774580
H 0	0.152770	2.554019	1.338095
H 0	0.787460	0.918644	1.554262
C 0	0.338870	-0.679925	-0.568910
C 0	-0.651440	-0.974876	0.427507
C 0	1.743004	-0.875177	-0.472172
C 0	-0.568901	-1.102842	-1.741206
C 0	-1.607262	-1.414519	-0.636474
C 0	-0.540202	-1.538137	1.817022
O 0	-2.708458	-1.910045	-0.633138
N 0	2.896120	-1.029158	-0.388302
H 0	-0.251189	-2.006329	-2.274562
H 0	-0.831351	-0.323693	-2.466233
H 0	-1.529424	-1.603328	2.280632
H 0	0.113062	-0.947520	2.466233
H 0	-0.126284	-2.554019	1.776924

TS-47+CP

B3LYP/6-31G(d) Geometry

C 0	-1.587893	-0.739062	-1.207602
C 0	-1.177919	-1.753670	-0.325350
C 0	-0.877333	-1.182070	0.908975
C 0	-1.456316	0.506701	-0.561261
C 0	-1.477166	0.198679	0.922851
H 0	-1.827975	-0.882007	-2.255788
H 0	-1.021356	-2.793614	-0.590471
H 0	-0.586480	-1.730617	1.797781
H 0	-1.892988	1.417599	-0.961349
H 0	-0.994081	0.930313	1.571446
H 0	-2.528582	0.118005	1.248188
C 0	1.175530	0.039711	0.395628
C 0	0.605544	0.872619	-0.620920
C 0	1.780414	-0.859504	-0.607336
C 0	1.209912	0.008865	-1.751901
O 0	2.528582	-1.814717	-0.565359
C 0	1.659638	0.292998	1.793768
C 0	0.583974	2.382675	-0.633241
H 0	0.508992	-0.472919	-2.445001
H 0	2.006365	0.496890	-2.329703
H 0	0.905965	0.748350	2.445001
H 0	2.524720	0.972273	1.784339
H 0	1.990567	-0.644161	2.253352
H 0	1.610064	2.772545	-0.696056
H 0	0.133745	2.793614	0.277778
H 0	0.031418	2.778718	-1.492022

TS-48+CP

B3LYP/6-31G(d) Geometry

C 0	1.349328	0.499437	1.094900
C 0	1.029649	-0.866983	1.155974
C 0	1.140756	-1.413427	-0.120744
C 0	1.598267	0.852292	-0.247946
C 0	1.942008	-0.447433	-0.954014

H 0	1.279192	1.196168	1.923704
H 0	0.651702	-1.387286	2.029568
H 0	0.997072	-2.459039	-0.367661
H 0	2.062045	1.795820	-0.523973
H 0	1.757141	-0.473122	-2.029568
H 0	3.013267	-0.654176	-0.790846
C 0	-0.731239	-0.352031	-1.184458
C 0	-0.282055	0.979184	-1.096354
C 0	-1.826275	-0.594624	-0.230951
O 0	-2.523770	-1.592397	-0.138483
C 0	-1.960098	0.673806	0.628678
C 0	-1.198665	1.762520	-0.151302
H 0	-0.579564	-1.014643	-2.027951
H 0	0.109994	1.491992	-1.971467
H 0	-1.494972	0.479993	1.604210
H 0	-3.013267	0.904431	0.812775
H 0	-0.656117	2.459039	0.496847
H 0	-1.896716	2.363143	-0.749745

TS-49+CP

B3LYP/6-31G(d) Geometry

C 0	-1.437986	-1.196730	0.461218
C 0	-1.020281	-0.274512	1.433764
C 0	-0.914310	0.984171	0.847809
C 0	-1.516882	-0.535752	-0.788433
C 0	-1.671502	0.935734	-0.451726
H 0	-1.535351	-2.266541	0.612939
H 0	-0.726292	-0.519390	2.448969
H 0	-0.646480	1.897526	1.366481
H 0	-2.024837	-0.981087	-1.640688
H 0	-1.359312	1.639906	-1.222915
H 0	-2.736585	1.130000	-0.239189
C 0	1.041703	0.590728	-0.622795
C 0	0.401509	-0.381092	-1.430789
C 0	1.940885	-0.089007	0.335469
O 0	2.724789	0.452325	1.101795
C 0	1.316744	2.032910	-0.958837
C 0	1.768757	-1.601810	0.154286
C 0	1.056072	-1.747964	-1.202648
H 0	0.112043	-0.124663	-2.448969
H 0	1.619800	2.578497	-0.060314
H 0	0.465561	2.544588	-1.417581
H 0	2.153001	2.103187	-1.669584
H 0	1.150109	-1.987753	0.974870
H 0	2.736585	-2.108140	0.213018
H 0	0.342283	-2.578497	-1.228772
H 0	1.789566	-1.930355	-1.999685

TS-50+CP

B3LYP/6-31G(d) Geometry

C 0	1.273906	-0.966789	1.185508
C 0	0.760833	-2.044685	0.451038
C 0	0.911700	-1.770108	-0.911227
C 0	1.705066	0.035937	0.290264
C 0	1.940649	-0.677261	-1.029062
H 0	1.219807	-0.862301	2.264259
H 0	0.224434	-2.892341	0.863776
H 0	0.649695	-2.449971	-1.714081
H 0	2.318843	0.873964	0.609796
H 0	1.884929	-0.063275	-1.928829
H 0	2.943131	-1.136721	-0.998723
C 0	-0.635564	-0.035890	-1.188998
C 0	-0.069780	0.957703	-0.353804
C 0	-1.828476	-0.637430	-0.571931
O 0	-2.630863	-1.396073	-1.092656
C 0	0.528562	2.234933	-0.914769
C 0	-1.906685	-0.105888	0.868146
C 0	-0.969762	1.115052	0.885026
H 0	-0.500168	-0.084050	-2.264259
H 0	-0.274535	2.892341	-1.275191
H 0	1.201250	2.048660	-1.758037
H 0	1.084855	2.792083	-0.152148
H 0	-1.561772	-0.893435	1.550028
H 0	-2.943131	0.120452	1.135256
H 0	-0.399003	1.213593	1.814666
H 0	-1.550869	2.041702	0.774320

TS-51+CP

B3LYP/6-31G(d) Geometry

C 0	-0.330094	1.660386	1.131317
C 0	0.638714	2.043365	0.196878
C 0	0.181951	1.706472	-1.093641
C 0	-1.419797	1.093289	0.451866
C 0	-1.318267	1.549294	-0.983292
H 0	-0.211016	1.695552	2.209137
H 0	1.632117	2.411069	0.430195
H 0	0.686618	2.008359	-2.005508
H 0	-2.355431	0.805835	0.919050
H 0	-1.798949	0.907661	-1.723254
H 0	-1.773109	2.550580	-1.061000
C 0	0.400276	-0.426103	-1.144265
C 0	-0.514831	-0.889789	-0.164285
C 0	1.791010	-0.645206	-0.661717
O 0	2.809035	-0.520927	-1.314014
C 0	-1.774630	-1.462758	-0.520636
C 0	1.710662	-1.067588	0.811692
C 0	0.240181	-1.460167	1.050711
N 0	-2.809035	-1.925784	-0.793693
H 0	0.200273	-0.465192	-2.209137
H 0	2.014886	-0.216477	1.433002
H 0	2.419940	-1.876880	1.006819
H 0	-0.155799	-1.088477	1.999935
H 0	0.123831	-2.550580	1.061878

TS-52+CP

B3LYP/6-31G(d) Geometry

C 0	1.965366	0.185509	0.189509
C 0	1.367500	-0.237340	1.388518
C 0	0.699353	-1.434145	1.159609
C 0	1.591298	-0.704979	-0.848531
C 0	1.189640	-1.991188	-0.145857
H 0	2.500824	1.119064	0.052138
H 0	1.348789	0.325371	2.315794
H 0	0.140394	-2.000125	1.895281
H 0	2.117935	-0.718887	-1.800039
H 0	0.492545	-2.639194	-0.676906
H 0	2.105691	-2.574101	0.048737
C 0	-1.143537	-0.584093	-0.351567
C 0	-0.261594	-0.150917	-1.367796
C 0	-1.641347	0.538334	0.465440
O 0	-2.500824	0.512645	1.326564
Cl 0	-2.079533	-2.066717	-0.433548
C 0	-0.888660	1.782301	-0.030320
C 0	-0.312824	1.380801	-1.402974
H 0	-0.247362	-0.682833	-2.315794
H 0	-0.092630	2.025720	0.684229

H 0	-1.567258	2.639194	-0.065079
H 0	0.659612	1.837864	-1.613466
H 0	-0.996977	1.688520	-2.204177

TS-53+CP

B3LYP/6-31G(d) Geometry

C 0	0.173152	1.969784	-1.023421
C 0	-0.811656	2.048338	-0.035038
C 0	-0.340555	1.406749	1.128318
C 0	1.284619	1.279369	-0.499804
C 0	1.164335	1.362632	1.001743
H 0	0.053533	2.277560	-2.056815
H 0	-1.820947	2.420176	-0.175940
H 0	-0.863003	1.425349	2.078946
H 0	2.236444	1.180816	-1.011441
H 0	1.686050	0.588238	1.563747
H 0	1.563257	2.336585	1.329905
C 0	-0.439300	-0.726092	0.605961
C 0	0.525807	-0.790520	-0.447512
C 0	-1.800116	-0.796048	-0.012557
O 0	-2.847000	-0.909805	0.597285
C 0	-0.278988	-1.325768	1.984028
C 0	1.801716	-1.402252	-0.231838
C 0	-1.651841	-0.743476	-1.535140
C 0	-0.162605	-1.020021	-1.806935
N 0	2.847000	-1.889769	-0.063951
H 0	-1.147475	-1.073788	2.598531
H 0	-0.233580	-2.420176	1.912699
H 0	0.631233	-0.998854	2.492621
H 0	-1.956301	0.249633	-1.885692
H 0	-2.326800	-1.468430	-1.999027
H 0	-0.011636	-2.063006	-2.111143
H 0	0.255824	-0.392156	-2.598531

TS-54+CP

B3LYP/6-31G(d) Geometry

C 0	-1.442157	-1.185772	-1.130528
C 0	-0.873074	-2.071484	-0.206434
C 0	-0.789030	-1.434746	1.034108
C 0	-1.659304	0.061051	-0.493489
C 0	-1.727223	-0.260089	0.987640
H 0	-1.555130	-1.375434	-2.192873
H 0	-0.457058	-3.045926	-0.439583
H 0	-0.428900	-1.894148	1.947740
H 0	-2.285240	0.830356	-0.939358
H 0	-1.509840	0.561093	1.670173
H 0	-2.745086	-0.617346	1.218912
C 0	0.905598	0.222521	0.579552
C 0	0.187511	0.967709	-0.403334
C 0	1.884683	-0.667680	-0.084294
O 0	2.745086	-1.337442	0.468556
C 0	1.193567	0.641377	1.997952
C 0	1.682602	-0.556064	-1.598522
C 0	0.833709	0.712686	-1.776780
C 0	-0.246075	2.398212	-0.136747
H 0	1.749808	-0.153559	2.503276
H 0	0.300384	0.876821	2.584769
H 0	1.827249	1.540828	2.011946
H 0	1.159998	-1.451305	-1.957411
H 0	2.650539	-0.523165	-2.107552
H 0	0.097601	0.636689	-2.584769
H 0	1.480582	1.568490	-2.018331
H 0	0.637120	3.045926	-0.043478
H 0	-0.823383	2.501160	0.787503
H 0	-0.852593	2.792282	-0.960087

TS-55+CP

B3LYP/6-31G(d) Geometry

C 0	0.512738	-0.700656	1.186171
C 0	0.512776	0.700621	1.186209
C 0	0.826397	1.156229	-0.103402
C 0	0.826301	-1.156213	-0.103479
C 0	1.477490	0.000009	-0.827283
H 0	0.192651	-1.328437	2.010139
H 0	0.192722	1.328377	2.010210
H 0	0.997001	2.196944	-0.356531
H 0	0.996899	-2.196924	-0.356634
H 0	2.551917	-0.000046	-0.580099
H 0	1.386755	0.000051	-1.915225
C 0	-1.063219	0.699392	-1.181527
C 0	-1.063181	-0.699373	-1.181506
C 0	-2.071203	-1.142244	-0.192529
C 0	-2.071220	1.142255	-0.192543
O 0	-2.551917	-0.000003	0.459650
O 0	-2.467599	-2.241653	0.084757
O 0	-2.467640	2.241653	0.084749
H 0	-0.805852	1.345640	-2.010207
H 0	-0.805856	-1.345611	-2.010210

TS-56+CP

B3LYP/6-31G(d) Geometry

C 0	0.646845	-0.980947	1.073966
C 0	0.984646	0.376307	1.194988
C 0	1.314989	0.882429	-0.075766
C 0	0.808937	-1.368781	-0.255201
C 0	1.660614	-0.323294	-0.928185
H 0	0.211539	-1.591805	1.856809
H 0	0.875537	0.966800	2.098436
H 0	1.784564	1.851209	-0.223657
H 0	0.674633	-2.377306	-0.629388
H 0	2.720847	-0.573581	-0.757060
H 0	1.516028	-0.208127	-2.004523
C 0	-0.578477	1.100265	-0.990973
C 0	-1.006896	-0.214656	-1.197816
C 0	-2.072910	-0.528037	-0.229414
O 0	-2.720847	-1.535218	-0.074651
C 0	-1.526446	1.696172	0.034215
O 0	-2.242394	0.580181	0.581474
H 0	-0.196094	1.729309	-1.788412
H 0	-0.897787	-0.802256	-2.098436
H 0	-2.245171	2.377306	-0.443152
H 0	-1.042300	2.226161	0.858470

TS-57+CP

B3LYP/6-31G(d) Geometry

C 0	-1.257629	0.719751	1.314177
C 0	-1.573117	-0.604857	0.974577
C 0	-1.835587	-0.672395	-0.410222
C 0	-1.384379	1.517876	0.176847
C 0	-2.208463	0.741819	-0.818208
H 0	-0.865712	1.049679	2.270506
H 0	-1.490571	-1.459217	1.638203
H 0	-2.291566	-1.543411	-0.874301
H 0	-1.241919	2.591942	0.147795
H 0	-3.274823	0.895810	-0.581704
H 0	-2.059775	0.995461	-1.869194

C 0	0.042778	-0.582847	-1.301584
C 0	0.444808	0.757556	-1.114783
C 0	1.610950	1.143899	-0.301952
O 0	1.986537	2.308724	-0.221135
C 0	0.890251	-1.704058	-0.715527
C 0	2.420257	0.020930	0.349863
C 0	1.638359	-1.282225	0.556403
H 0	-0.395253	-0.821258	-2.270506
H 0	0.155174	1.518743	-1.832332
H 0	1.623492	-2.006769	-1.479946
H 0	0.276245	-2.591942	-0.518953
H 0	2.843599	0.399814	1.286308
H 0	3.274823	-0.157883	-0.321093
H 0	2.318840	-2.083356	0.870497
H 0	0.920181	-1.149032	1.372256

TS-58+CP

B3LYP/6-31G(d) Geometry

C 0	1.230922	-0.360077	-1.462747
C 0	1.597277	-1.368162	-0.560200
C 0	1.830178	-0.781116	0.707981
C 0	1.313574	0.873665	-0.816240
C 0	2.163479	0.669695	0.409205
H 0	0.840583	-0.519204	-2.462523
H 0	1.561580	-2.433814	-0.759175
H 0	2.326258	-1.325695	1.508351
H 0	1.118377	1.835459	-1.276321
H 0	3.223648	0.718151	0.107061
H 0	2.021915	1.377005	1.224360
C 0	-0.023872	-0.410353	1.470369
C 0	-0.526397	0.719796	0.768829
C 0	-1.625438	0.579820	-0.215066
O 0	-2.091446	1.554414	-0.798737
C 0	-0.784560	-1.731553	1.426176
C 0	-2.301293	-0.783982	-0.377737
C 0	-1.479947	-1.992015	0.083947
C 0	-0.411804	2.117033	1.353446
H 0	0.372458	-0.186131	2.462523
H 0	-1.544069	-1.702287	2.223425
H 0	-0.118261	-2.567702	1.674715
H 0	-2.627465	-0.883260	-1.418886
H 0	-3.223648	-0.710280	0.219191
H 0	-2.126520	-2.874696	0.167600
H 0	-0.731004	-2.233449	-0.675083
H 0	0.343354	2.167752	2.143728
H 0	-1.371422	2.407857	1.802429
H 0	-0.189671	2.874696	0.596879

TS-59+CP

B3LYP/6-31G(d) Geometry

C 0	0.946639	-1.734449	0.924315
C 0	1.480797	-0.515280	1.360631
C 0	1.945900	0.208944	0.242354
C 0	1.118304	-1.826443	-0.461791
C 0	2.190262	-0.835080	-0.831901
H 0	0.378880	-2.430241	1.533027
H 0	1.418794	-0.130040	2.373155
H 0	2.568776	1.094343	0.340296
H 0	0.842688	-2.682848	-1.066631
H 0	3.173445	-1.297353	-0.640591
H 0	2.184789	-0.484996	-1.864097
C 0	0.177192	0.955239	-0.674127
C 0	-0.358459	-0.232955	-1.236544
C 0	-1.643649	-0.830751	-0.830340
O 0	-2.129116	-1.783305	-1.431414
C 0	-0.623900	1.639578	0.435898
C 0	-2.415811	-0.152858	0.301213
C 0	-1.545592	0.703390	1.227840
C 0	0.834431	1.957155	-1.616405
H 0	-0.077325	-0.507918	-2.250280
H 0	-1.241682	2.417179	-0.043271
H 0	0.049879	2.176739	1.115941
H 0	-2.970509	-0.922069	0.849220
H 0	-3.173445	0.476945	-0.190467
H 0	-2.181538	1.296259	1.897076
H 0	-0.946831	0.051458	1.870518
H 0	1.459176	1.473590	-2.373155
H 0	1.452556	2.682848	-1.074908
H 0	0.060374	2.526618	-2.149614

TS-60+CP

B3LYP/6-31G(d) Geometry

C 0	0.381069	-2.112273	0.380942
C 0	1.219583	-1.405777	1.248767
C 0	2.165154	-0.696720	0.491470
C 0	0.773789	-1.841912	-0.948127
C 0	2.202231	-1.349593	-0.868086
H 0	-0.510954	-2.658856	0.667852
H 0	1.091363	-1.328411	2.323302
H 0	2.997099	-0.138078	0.906691
H 0	0.366110	-2.361533	-1.808880
H 0	2.863781	-2.229523	-0.809599
H 0	2.552440	-0.723590	-1.689566
C 0	0.820914	0.938953	-0.390593
C 0	0.076273	0.120805	-1.289028
C 0	-1.404270	-0.028303	-1.165729
O 0	-2.041706	-0.652117	-1.999823
C 0	0.127753	1.620525	0.793334
C 0	-2.093058	0.691445	-0.011535
C 0	-1.182810	0.932826	1.198956
C 0	1.932036	1.672896	-0.925891
N 0	2.840341	2.275969	-1.338854
H 0	0.404595	0.071191	-2.323302
H 0	-0.089700	2.658856	0.500981
H 0	0.809417	1.684336	1.648508
H 0	-2.997099	0.132978	0.251822
H 0	-2.433042	1.656631	-0.418446
H 0	-1.702050	1.554589	1.937552
H 0	-0.967862	-0.019861	1.692659

TS-61+CP

B3LYP/6-31G(d) Geometry

C 0	1.466964	-0.434367	1.455158
C 0	2.077755	0.137073	0.328894
C 0	1.914916	-0.739500	-0.774593
C 0	1.006413	-1.704960	1.118276
C 0	1.688567	-2.108441	-0.157237
H 0	1.291774	0.067421	2.400942
H 0	2.479976	1.142914	0.274577
H 0	2.495976	-0.617722	-1.686164
H 0	0.487231	-2.388364	1.779697
H 0	2.674735	-2.531258	0.098668
H 0	1.163472	-2.840246	-0.768717
C 0	0.022819	-0.464995	-1.404499
C 0	-0.827013	-1.098652	-0.462732
C 0	-1.701938	-0.371395	0.483648

O 0	-2.448062	-0.929504	1.273262
C 0	-0.158812	1.033143	-1.640094
C 0	-1.747840	1.154666	0.339917
C 0	-0.560729	1.804526	-0.377854
Cl 0	-1.382143	-2.754258	-0.811666
H 0	0.173642	-1.027672	-2.324232
H 0	-0.945493	1.149878	-2.400942
H 0	0.753267	1.461919	-2.074031
H 0	-1.906526	1.581610	1.335760
H 0	-2.674735	1.344807	-0.222297
H 0	-0.807520	2.840246	-0.642145
H 0	0.291931	1.858261	0.304433

TS-62+CP

B3LYP/6-31G(d) Geometry

C 0	0.051801	2.117136	-0.717850
C 0	0.873412	1.612795	-1.727866
C 0	1.931940	0.900040	-1.134222
C 0	0.575473	1.720181	0.533931
C 0	2.031442	1.398046	0.284172
H 0	-0.904207	2.608384	-0.864686
H 0	0.666690	1.658761	-2.791751
H 0	2.773147	0.482288	-1.677578
H 0	0.196890	2.092946	1.479613
H 0	2.593031	2.346893	0.279937
H 0	2.521601	0.730468	0.991108
C 0	0.844938	-0.934393	-0.383038
C 0	0.068454	-0.358490	0.681364
C 0	-1.429104	-0.252911	0.517761
O 0	-2.118536	0.251867	1.390623
C 0	0.178781	-1.528709	-1.632458
C 0	-2.080799	-0.886885	-0.705150
C 0	-1.191870	-0.922920	-1.949667
C 0	2.049489	-1.632179	-0.024398
C 0	0.459187	-0.599403	2.136122
N 0	3.034032	-2.202437	0.229641
H 0	0.054828	-2.608384	-1.457494
H 0	0.848745	-1.438807	-2.494685
H 0	-3.034032	-0.379564	-0.884210
H 0	-2.329615	-1.916550	-0.401825
H 0	-1.674278	-1.514540	-2.736736
H 0	-1.076177	0.087832	-2.349769
H 0	1.533623	-0.510534	2.305638
H 0	0.172868	-1.617958	2.429890
H 0	-0.074953	0.090264	2.791751

TS-63+CP

B3LYP/6-31G(d) Geometry

C 0	-0.837784	-0.152152	-2.174020
C 0	-1.396698	1.004763	-1.620581
C 0	-1.904368	0.695770	-0.334687
C 0	-1.049666	-1.218547	-1.290788
C 0	-2.164760	-0.797505	-0.372823
H 0	-0.234237	-0.195236	-3.074617
H 0	-1.322586	2.002306	-2.040274
H 0	-2.558085	1.376997	0.205012
H 0	-0.765895	-2.247496	-1.480464
H 0	-3.123819	-0.964149	-0.892248
H 0	-2.224971	-1.306849	0.586679
C 0	-0.232357	0.561835	0.908403
C 0	0.388168	-0.667788	0.507309
C 0	1.650806	-0.670714	-0.287938
O 0	2.199814	-1.716675	-0.621056
C 0	0.525354	1.874448	0.670456
C 0	2.358889	0.653860	-0.566089
C 0	1.459846	1.889361	-0.541867
C 0	-0.945273	0.599147	2.258505
C 0	0.227542	-1.945095	1.316529
H 0	1.126031	2.063935	1.575976
H 0	-0.186904	2.707985	0.610449
H 0	2.907433	0.555905	-1.508838
H 0	3.123819	0.735034	0.222405
H 0	2.071815	2.800075	-0.521277
H 0	0.875812	1.934454	-1.464013
H 0	-0.215045	0.502135	3.074617
H 0	-1.680129	-0.199340	2.386661
H 0	-1.462334	1.555157	2.398753
H 0	-0.794091	-2.134029	1.652392
H 0	0.851999	-1.897026	2.221720
H 0	0.576902	-2.800075	0.735254

TS-64+CP

B3LYP/6-31G(d) Geometry

C 0	1.286806	-1.502224	-0.056843
C 0	0.278058	-0.877968	-1.009714
O 0	1.375927	-0.706215	1.134583
C 0	2.736192	-1.379488	-0.583166
C 0	2.086483	0.426656	0.676400
C 0	0.296011	0.529256	-1.089608
O 0	3.145062	-0.080463	-0.142082
C 0	1.182901	1.302996	-0.212399
O 0	1.298939	2.520768	-0.224675
H 0	1.021266	-2.520768	0.235640
H 0	0.106059	-1.440897	-1.926783
H 0	2.808634	-1.442700	-1.673815
H 0	3.385619	-2.138945	-0.129920
H 0	2.498553	0.980673	1.522164
H 0	-0.070693	1.053099	-1.965854
C 0	-1.589492	-1.362826	-0.243777
C 0	-1.509648	-0.952657	1.101131
C 0	-2.298594	-0.237614	-0.977895
C 0	-1.894963	0.929720	-0.116503
C 0	-1.650638	0.443925	1.162036
H 0	-1.713964	-2.403779	-0.531994
H 0	-1.234988	-1.586148	1.936527
H 0	-2.079541	-0.145359	-2.043543
H 0	-3.385619	-0.390412	-0.872852
H 0	-2.071760	1.968093	-0.371941
H 0	-1.480186	1.052096	2.043543

TS-65+CP

B3LYP/6-31G(d) Geometry

C 0	-1.293635	-1.585416	0.720847
C 0	-0.246947	-0.619489	1.261851
O 0	-1.383969	-1.452330	-0.705475
C 0	-2.728096	-1.176963	1.128119
C 0	-2.041692	-0.212160	-0.838193
C 0	-0.259144	0.694539	0.723289
O 0	-3.107154	-0.232458	0.120142
C 0	-1.114765	0.954562	-0.451174
O 0	-1.223637	2.042025	-1.003881
C 0	0.086579	1.919619	1.543227
H 0	-1.062415	-2.629067	0.947815
H 0	-0.090325	-0.700335	2.339396
H 0	-2.781178	-0.709017	2.116630
H 0	-3.409207	-2.036555	1.095284

H 0	-2.446762	-0.103292	-1.846007
H 0	0.725352	1.679161	2.398334
H 0	-0.833130	2.371579	1.940721
H 0	0.572177	2.691822	0.940404
C 0	1.524658	-1.477298	0.764018
C 0	1.401562	-1.757865	-0.617180
C 0	2.342553	-0.199152	0.841785
C 0	1.932614	0.446932	-0.453058
C 0	1.596047	-0.569744	-1.338370
H 0	1.635409	-2.267244	1.503910
H 0	1.052488	-2.691822	-1.041108
H 0	2.216229	0.399757	1.742868
H 0	3.409207	-0.471483	0.774193
H 0	2.159473	1.471015	-0.726321
H 0	1.404532	-0.442838	-2.398334

TS-66+CP

B3LYP/6-31G(d) Geometry

C 0	-1.287132	0.771083	0.460401
C 0	-0.277065	0.636280	-0.683545
O 0	-1.377460	-0.457515	1.194913
C 0	-2.749293	0.890802	-0.035472
C 0	-2.098934	-1.281387	0.303453
C 0	-0.289116	-0.630617	-1.324617
O 0	-3.160912	-0.469614	-0.206035
C 0	-1.204393	-1.690001	-0.880733
O 0	-1.337649	-2.776262	-1.427784
C 0	-0.114807	1.895996	-1.524414
H 0	-1.012148	1.565120	1.159641
H 0	-2.858249	1.429414	-0.981025
H 0	-3.377182	1.369873	0.726268
H 0	-2.506339	-2.144821	0.833075
H 0	0.065062	-0.731804	-2.346758
H 0	0.097782	2.776262	-0.905829
H 0	-1.028351	2.108355	-2.094200
H 0	0.694294	1.793179	-2.253141
C 0	1.588651	0.639931	0.278026
C 0	1.441021	-0.292510	1.327082
C 0	2.294298	-0.116237	-0.835333
C 0	1.773157	-1.502775	-0.567235
C 0	1.515421	-1.588420	0.800597
H 0	1.773385	1.695740	0.460496
H 0	1.163489	-0.051529	2.346758
H 0	2.148845	0.259774	-1.848533
H 0	3.377182	-0.101005	-0.628431
H 0	1.913207	-2.347818	-1.231689
H 0	1.277400	-2.498508	1.340031

TS-67+CP

B3LYP/6-31G(d) Geometry

C 0	-1.294739	0.667787	0.670209
C 0	-0.261775	0.639330	-0.462594
O 0	-1.549465	-0.670853	1.109591
C 0	-2.695223	1.066809	0.158579
C 0	-2.313432	-1.196865	0.042033
C 0	-0.307537	-0.481427	-1.337669
O 0	-3.217936	-0.167249	-0.353067
C 0	-1.384392	-1.491720	-1.147150
O 0	-1.561922	-2.440891	-1.889001
C 0	0.130540	1.919585	-0.966399
N 0	0.446960	2.976329	-1.344340
H 0	-0.960127	1.256514	1.525669
H 0	-2.675857	1.816972	-0.636581
H 0	-3.326436	1.419457	0.983261
H 0	-2.859348	-2.083880	0.370112
H 0	0.010223	-0.362739	-2.368859
C 0	1.744349	0.213318	0.561335
C 0	1.381473	-0.911696	1.313440
C 0	2.261281	-0.292590	-0.763547
C 0	1.474920	-1.580000	-0.868290
C 0	1.230352	-2.003267	0.451200
H 0	2.018199	1.176983	0.977531
H 0	1.134802	-0.912261	2.368859
H 0	2.181228	0.400082	-1.602848
H 0	3.326436	-0.549173	-0.644522
H 0	1.537674	-2.254614	-1.715576
H 0	0.843648	-2.976329	0.733157

TS-68+CP

B3LYP/6-31G(d) Geometry

C 0	1.326388	-0.931803	-1.043757
C 0	0.176367	0.047919	-1.267486
O 0	1.459955	-1.204966	0.356176
C 0	2.702001	-0.290817	-1.344038
C 0	2.035985	-0.007740	0.831087
C 0	0.146097	1.136911	-0.362328
O 0	3.066439	0.320950	-0.100353
C 0	1.024590	1.162454	0.816652
O 0	1.093170	2.051515	1.648322
Cl 0	-0.457047	2.713260	-0.896748
H 0	1.167381	-1.880477	-1.561661
H 0	-0.006418	0.287892	-2.314280
H 0	2.663688	0.464028	-2.135853
H 0	3.446656	-1.053486	-1.601731
H 0	2.460856	-0.158396	1.824775
C 0	-1.480517	-1.042741	-1.017394
C 0	-1.275466	-1.732447	0.202957
C 0	-2.409685	0.111872	-0.676663
C 0	-2.044752	0.330104	0.762290
C 0	-1.559821	-0.864169	1.270997
H 0	-1.564194	-1.574154	-1.963245
H 0	-0.826248	-2.713260	0.303457
H 0	-2.349534	0.990946	-1.317683
H 0	-3.446656	-0.260408	-0.720688
H 0	-2.329263	1.201580	1.340003
H 0	-1.341206	-1.063479	2.314280

TS-69+CP

B3LYP/6-31G(d) Geometry

C 0	1.304914	0.667034	-1.104459
C 0	0.213200	0.644673	-0.024315
O 0	1.578816	-0.667998	-1.540315
C 0	2.679002	1.056536	-0.522257
C 0	2.270338	-1.202584	-0.433399
C 0	0.233777	-0.434673	0.922590
O 0	3.162079	-0.182341	0.018109
C 0	1.287205	-1.484147	0.712206
O 0	1.427886	-2.450638	1.440739
C 0	-0.188614	1.949035	0.413454
C 0	-0.101547	-0.213260	2.389085
N 0	-0.510560	3.023532	0.731405
H 0	1.014652	1.262084	-1.971892
H 0	2.625285	1.808181	0.269930
H 0	3.355963	1.402168	-1.312976
H 0	2.824764	-2.095860	-0.728126
H 0	-0.994185	0.399611	2.531407

H 0	0.730498	0.305356	2.882875
H 0	-0.232997	-1.172137	2.894389
C 0	-1.646252	0.185518	-1.187873
C 0	-1.246622	-0.978691	-1.867601
C 0	-2.308661	-0.267563	0.088623
C 0	-1.545002	-1.550679	0.322478
C 0	-1.192664	-2.032952	-0.953246
H 0	-1.874126	1.131414	-1.668653
H 0	-0.903695	-1.023950	-2.894389
H 0	-2.320044	0.457698	0.901692
H 0	-3.355963	-0.528408	-0.134382
H 0	-1.694379	-2.189710	1.186193
H 0	-0.801895	-3.023532	-1.158970

TS-70+CP

B3LYP/6-31G(d) Geometry

C 0	-1.294674	-1.169942	-0.612778
C 0	-0.227341	-0.734786	0.399930
O 0	-1.394510	-0.228171	-1.687801
C 0	-2.732752	-1.081194	-0.046294
C 0	-2.045106	0.853382	-1.062657
C 0	-0.221368	0.665674	0.708031
O 0	-3.109181	0.278109	-0.295986
C 0	-1.104915	1.561223	-0.074322
O 0	-1.209240	2.767808	0.109599
C 0	-0.053328	-1.741299	1.532722
C 0	0.132519	1.209116	2.077940
H 0	-1.068685	-2.149682	-1.042528
H 0	-2.803253	-1.292773	1.024667
H 0	-3.408292	-1.752250	-0.591392
H 0	-2.449580	1.538254	-1.810115
H 0	-0.022193	-2.767808	1.148330
H 0	-0.882945	-1.682079	2.249413
H 0	0.865818	-1.573341	2.099549
H 0	1.036756	0.771565	2.508989
H 0	-0.685139	1.013403	2.788120
H 0	0.254374	2.293158	2.023386
C 0	1.518434	-1.061114	-0.633642
C 0	1.330573	-0.446901	-1.896857
C 0	2.350246	-0.072033	0.163499
C 0	1.856240	1.214200	-0.437912
C 0	1.491114	0.936077	-1.754840
H 0	1.665756	-2.134537	-0.534623
H 0	0.963724	-0.941615	-2.788120
H 0	2.292734	-0.151794	1.247907
H 0	3.408292	-0.206839	-0.116359
H 0	2.074614	2.199758	-0.042614
H 0	1.247135	1.676437	-2.509004

P-1+CP

B3LYP/6-31G(d) Geometry

C 0	0.741280	1.428549	-0.048026
C 0	1.469223	0.906145	-1.044746
C 0	1.777124	-0.539500	-0.683439
C 0	0.426596	-1.323262	-0.812426
C 0	0.556793	0.340366	0.999237
C 0	-0.421034	-0.738429	0.376332
C 0	1.893525	-0.421926	0.854694
C 0	-1.718736	-0.193715	-0.020402
N 0	-2.751032	0.240301	-0.329610
H 0	0.258398	2.399142	-0.019267
H 0	1.704230	1.368251	-1.998227
H 0	2.609388	-1.006940	-1.214560
H 0	0.576773	-2.399142	-0.676040
H 0	-0.053466	-1.168803	-1.781264
H 0	0.258692	0.664019	1.998227
H 0	-0.607767	-1.519602	1.122553
H 0	2.751032	0.177193	1.173563
H 0	1.907629	-1.389933	1.370904

P-2+CP

B3LYP/6-31G(d) Geometry

C 0	1.898692	0.688182	-0.951995
C 0	1.117129	1.382810	-0.112321
C 0	0.619572	0.417194	0.954807
C 0	-0.411921	-0.578270	0.274316
C 0	1.925199	-0.752947	-0.465842
C 0	0.496855	-1.338639	-0.749193
C 0	1.841593	-0.526418	1.061085
C 0	-1.592350	0.114480	-0.357511
O 0	-2.742278	-0.016700	0.004393
H 0	2.344487	1.038465	-1.877792
H 0	0.802677	2.417059	-0.209209
H 0	0.242175	0.862258	1.877792
H 0	-0.805713	-1.257264	1.037054
H 0	2.742278	-1.375272	-0.838117
H 0	0.192682	-1.174822	-1.788802
H 0	0.461159	-2.417059	-0.562903
H 0	1.641902	-1.440494	1.633332
H 0	2.724446	-0.021700	1.465335
H 0	-1.339255	0.784831	-1.210342

P-3+CP

B3LYP/6-31G(d) Geometry

C 0	2.864137	-0.602952	-0.709500
C 0	2.891595	-0.589300	0.835503
C 0	1.590662	0.239905	0.952330
C 0	1.904106	1.378869	-0.006452
C 0	2.665585	0.878597	-0.990459
C 0	1.478674	-1.290413	-0.969314
C 0	0.593596	-0.762126	0.218430
C 0	-0.658066	-0.112285	-0.238729
O 0	-1.770979	-0.480529	0.150351
H 0	3.696823	-1.087508	-1.223890
H 0	3.756490	-0.057410	1.242065
H 0	2.822082	-1.585311	1.289012
H 0	1.252958	0.517590	1.952489
H 0	1.495335	2.381422	0.067608
H 0	3.000327	1.389619	-1.887554
H 0	1.073516	-1.030832	-1.952489
H 0	1.550094	-2.381422	-0.920783
H 0	0.324720	-1.571569	0.902867
H 0	-0.602691	0.726177	-0.947074
B 0	-3.151757	0.217524	-0.327399
H 0	-2.811470	1.101023	-1.088395
H 0	-3.756490	-0.694783	-0.838894
H 0	-3.638358	0.596064	0.711853

P-4+CP

B3LYP/6-31G(d) Geometry

C 0	1.240064	-0.357590	1.115892
C 0	0.518008	-1.348127	0.574137
C 0	0.327165	-1.019050	-0.902322
C 0	-0.629349	0.214258	-0.959854
C 0	1.544314	0.650422	0.016707
C 0	0.189201	1.363725	-0.317642

C 0	1.664958	-0.298581	-1.201449
N 0	-1.958881	-0.057791	-0.278630
O 0	-2.520989	0.870951	0.292126
O 0	-2.414218	-1.192995	-0.395967
H 0	1.478430	-0.217267	2.165373
H 0	0.041907	-2.179050	1.081657
H 0	0.029087	-1.839316	-1.554301
H 0	-0.925496	0.439608	-1.989220
H 0	2.372597	1.337408	0.202779
H 0	-0.312832	1.773539	0.559534
H 0	0.335458	2.179050	-1.033406
H 0	1.681861	0.225603	-2.165373
H 0	2.520989	-0.976232	-1.137532

P-5+CP

B3LYP/6-31G(d) Geometry

C 0	-1.622833	-0.627793	-0.947425
C 0	-0.887447	-1.426853	-0.162872
C 0	-0.520608	-0.633111	1.084712
C 0	0.503205	0.488580	0.675864
C 0	-1.746079	0.716470	-0.246251
C 0	-0.322987	1.379501	-0.303686
C 0	-1.786229	0.247661	1.228019
C 0	1.827299	0.003693	0.130122
F 0	1.726759	-0.636378	-1.055637
F 0	2.679053	1.041794	-0.057578
F 0	2.426675	-0.852656	0.993409
H 0	-1.968373	-0.834275	-1.955470
H 0	-0.511232	-2.416762	-0.396592
H 0	-0.205630	-1.211138	1.955470
H 0	0.765539	1.057495	1.574653
H 0	-2.552583	1.369909	-0.586731
H 0	0.085813	1.378389	-1.317372
H 0	-0.353557	2.416762	0.044783
H 0	-1.675385	1.062698	1.954337
H 0	-2.679053	-0.338039	1.464821

P-6+CP

B3LYP/6-31G(d) Geometry

C 0	1.222851	-0.333061	1.349003
C 0	2.047553	0.678416	1.039969
C 0	2.379323	0.562892	-0.441192
C 0	1.067254	0.940487	-1.215851
C 0	0.991786	-1.138658	0.077754
C 0	0.093218	-0.238226	-0.888043
C 0	2.371664	-0.974937	-0.600677
B 0	-1.344981	0.039150	-0.285409
C 0	-1.814162	1.492111	0.121868
C 0	-2.342122	-1.174158	-0.090106
H 0	0.711583	-0.500259	2.292737
H 0	2.342131	1.505764	1.678687
H 0	3.271470	1.097234	-0.777957
H 0	1.266309	1.000236	-2.292737
H 0	0.687433	1.917135	-0.901087
H 0	0.614648	-2.155129	0.210292
H 0	-0.057562	-0.845642	-1.795779
H 0	3.178654	-1.462807	-0.043780
H 0	2.386010	-1.309825	-1.645055
H 0	-1.801222	2.156367	-0.755737
H 0	-2.814519	1.543986	0.566751
H 0	-1.099144	1.939077	0.828124
H 0	-3.271470	-0.980418	-0.647827
H 0	-1.963908	-2.156367	-0.395822
H 0	-2.656629	-1.241074	0.962443

P-7+CP

B3LYP/6-31G(d) Geometry

C 0	0.809889	0.038432	1.426981
C 0	1.646790	0.985412	0.979172
C 0	1.995897	0.646558	-0.462743
C 0	0.700306	0.918254	-1.305720
C 0	0.589212	-0.948632	0.290690
C 0	-0.282666	-0.197761	-0.824686
C 0	1.974628	-0.897404	-0.392618
B 0	-1.706290	0.188884	-0.307008
Cl 0	-2.895358	-1.095467	-0.003937
Cl 0	-2.222467	1.846675	0.024696
H 0	0.283786	0.018649	2.376426
H 0	1.938564	1.898243	1.488995
H 0	2.895358	1.118132	-0.865764
H 0	0.907895	0.811555	-2.376426
H 0	0.317524	1.928546	-1.142090
H 0	0.191697	-1.928546	0.560791
H 0	-0.434490	-0.930907	-1.629800
H 0	2.768053	-1.305093	0.241634
H 0	1.997038	-1.385326	-1.374600

P-8+CP

B3LYP/6-31G(d) Geometry

C 0	-1.953232	0.778376	0.206154
C 0	-1.215549	1.066503	-0.875014
C 0	-0.228695	-0.079881	-1.078300
C 0	0.839938	0.010324	0.089626
C 0	-1.459409	-0.555179	0.750916
C 0	-0.037408	-0.290691	1.355188
C 0	-1.085307	-1.265516	-0.570082
C 0	1.517627	1.372960	0.166735
O 0	2.696460	1.599640	0.055914
Cl 0	2.118663	-1.264863	-0.154678
H 0	-2.696460	1.409264	0.683251
H 0	-1.233753	1.976444	-1.465848
H 0	0.234852	-0.162299	-2.061970
H 0	-2.132071	-1.081409	1.431653
H 0	-0.040045	0.545733	2.061970
H 0	0.354357	-1.166459	1.876912
H 0	-0.518241	-2.190863	-0.434796
H 0	-1.951376	-1.446729	-1.212857
H 0	0.787289	2.190863	0.346952

P-9+CP

B3LYP/6-31G(d) Geometry

C 0	2.046705	-1.177067	0.323030
C 0	1.286750	-1.382480	-0.762028
C 0	0.579983	-0.070384	-1.082665
C 0	-0.520573	0.196522	0.045241
C 0	1.856255	0.273414	0.742964
C 0	0.398620	0.393204	1.309472
C 0	1.678221	0.929601	-0.643642
C 0	-1.419518	-1.015393	0.225646
O 0	-2.621979	-1.017202	0.067786
C 0	-1.384737	1.423197	-0.274781
H 0	2.615168	-1.916029	0.879069
H 0	1.113392	-2.322754	-1.275785
H 0	0.179661	0.029647	-2.094360
H 0	2.621979	0.690484	1.401617
H 0	0.209019	-0.347670	2.094360

H 0 0.223811 1.382224 1.747204
H 0 1.349388 1.972932 -0.602138
H 0 2.575305 0.854623 -1.265739
H 0 -0.892679 -1.945167 0.531697
H 0 -1.963961 1.262414 -1.189254
H 0 -0.775853 2.322754 -0.403011
H 0 -2.101617 1.608994 0.531552

P-10+CP

B3LYP/6-31G(d) Geometry
C 0 -1.933929 -1.062798 -0.974983
C 0 -1.193782 -1.930155 -0.269787
C 0 -0.660993 -1.189913 0.950362
C 0 0.419006 -0.141928 0.463062
C 0 -1.891344 0.271566 -0.246659
C 0 -0.428482 0.830382 -0.439718
C 0 -1.838476 -0.222127 1.217413
C 0 1.590826 -0.752866 -0.259441
O 0 2.750214 -0.621776 0.072761
C 0 -0.261771 2.302682 -0.052102
H 0 -2.390720 -1.224835 -1.946388
H 0 -0.933831 -2.948116 -0.541858
H 0 -0.318550 -1.808229 1.783251
H 0 0.817875 0.393663 1.331255
H 0 -2.671849 0.990913 -0.508184
H 0 -0.140425 0.719622 -1.492895
H 0 -1.604341 0.562254 1.946388
H 0 -2.750214 -0.745083 1.521879
H 0 1.324248 -1.351837 -1.160116
H 0 0.785383 2.615358 -0.137896
H 0 -0.579108 2.487802 0.980792
H 0 -0.858699 2.948116 -0.707395

P-11+CP

B3LYP/6-31G(d) Geometry
C 0 0.492433 -1.830986 -0.933100
C 0 1.579215 -1.553959 -0.198562
C 0 1.135580 -0.682539 0.969022
C 0 0.757099 0.746530 0.396569
C 0 -0.691047 -1.144821 -0.271953
C 0 -0.474759 0.408697 -0.525250
C 0 -0.284328 -1.245611 1.213785
C 0 1.899150 1.419531 -0.331419
O 0 2.526110 2.354596 0.112586
C 0 -1.657279 1.197502 -0.179242
N 0 -2.608501 1.799951 0.106594
H 0 0.451377 -2.354596 -1.882554
H 0 2.608501 -1.814477 -0.422404
H 0 1.813351 -0.625135 1.822496
H 0 0.463884 1.397247 1.224411
H 0 -1.685619 -1.492636 -0.554569
H 0 -0.246873 0.591076 -1.581838
H 0 -0.895879 -0.629596 1.882554
H 0 -0.266900 -2.278577 1.572436
H 0 2.155644 0.977521 -1.320873

P-12+CP

B3LYP/6-31G(d) Geometry
C 0 2.799360 0.029358 0.805664
C 0 2.825675 0.874309 -0.488088
C 0 1.555932 0.205826 -1.068550
C 0 1.923116 -1.264243 -0.896581
C 0 2.667420 -1.367066 0.213407
C 0 1.392115 0.408627 1.377011
C 0 0.512282 0.569374 0.078754
C 0 -0.657912 -0.363270 0.100056
O 0 -1.832232 -0.013645 0.023608
Cl 0 -0.069857 2.276518 -0.131497
H 0 3.609934 0.180050 1.521496
H 0 3.704294 0.674008 -1.106908
H 0 2.722491 1.950502 -0.323058
H 0 1.209143 0.518717 -2.053694
H 0 1.559256 -2.067917 -1.528222
H 0 3.036835 -2.276518 0.675905
H 0 0.998530 -0.356247 2.053694
H 0 1.407785 1.356445 1.918977
H 0 -0.427087 -1.432012 0.199653
B 0 -3.071089 -1.074977 0.060594
H 0 -3.622031 -0.874507 -0.994015
H 0 -2.538897 -2.160701 0.171892
H 0 -3.704294 -0.709043 1.020279

P-13+CP

B3LYP/6-31G(d) Geometry
C 0 2.789003 -0.237924 0.813796
C 0 2.881112 0.506300 -0.535445
C 0 1.560479 -0.098148 -1.071577
C 0 1.823871 -1.574543 -0.804363
C 0 2.552849 -1.657226 0.317722
C 0 1.413742 0.291641 1.345642
C 0 0.534025 0.442829 0.038194
C 0 -0.654410 -0.456055 0.131436
O 0 -1.812791 -0.048462 0.000595
C 0 0.093575 1.888263 -0.234134
H 0 3.611088 -0.102601 1.520323
H 0 3.742161 0.195217 -1.133793
H 0 2.876774 1.596827 -0.443482
H 0 1.253722 0.167523 -2.085506
H 0 1.404587 -2.393112 -1.380643
H 0 2.848460 -2.557714 0.846447
H 0 0.975257 -0.386038 2.085506
H 0 1.517448 1.271375 1.823653
H 0 -0.501556 -1.524395 0.331902
H 0 0.955740 2.557714 -0.290381
H 0 -0.566020 2.250070 0.560787
H 0 -0.459772 1.958911 -1.175706
B 0 -3.112267 -1.012297 0.101264
H 0 -3.637191 -0.873907 -0.978217
H 0 -2.665284 -2.120712 0.317708
H 0 -3.742161 -0.527359 1.011020

P-14+CP

B3LYP/6-31G(d) Geometry
C 0 -2.882568 0.116237 -0.291078
C 0 -2.899808 -0.321514 1.190705
C 0 -1.567170 -1.099424 1.078959
C 0 -1.847661 -1.945655 -0.154868
C 0 -2.636932 -1.224959 -0.964430
C 0 -1.520189 0.905651 -0.370288
C 0 -0.620996 0.101580 0.653949
C 0 0.663523 -0.330186 0.056822
O 0 1.753829 0.070289 0.479010
C 0 -1.623341 2.392465 -0.019496
H 0 -3.735723 0.692760 -0.656940
H 0 -3.742301 -0.976291 1.430374
H 0 -2.866029 0.508894 1.904984
H 0 -1.213516 -1.627813 1.966530

H	0	-1.406342	-2.916519	-0.355231
H	0	-2.963322	-1.484170	-1.966530
H	0	-1.114039	0.820995	-1.385392
H	0	-0.397334	0.719494	1.529082
H	0	0.656035	-1.021100	-0.797670
H	0	-0.636017	2.868072	-0.025201
H	0	-2.062010	2.546724	0.973059
H	0	-2.250326	2.916519	-0.749865
B	0	3.170253	-0.379016	-0.161685
H	0	2.882062	-1.136853	-1.066376
H	0	3.658535	0.670248	-0.509414
H	0	3.742301	-0.890293	0.771848

P-15+CP

B3LYP/6-31G(d) Geometry

C	0	-2.838498	-0.459046	-0.335753
C	0	-2.700364	-0.790698	1.165082
C	0	-1.225652	-1.238352	1.037097
C	0	-1.324212	-2.192073	-0.144743
C	0	-2.284373	-1.729495	-0.958071
C	0	-1.693734	0.629558	-0.499046
C	0	-0.592167	0.126813	0.516732
C	0	0.745984	-0.061597	-0.104504
O	0	1.773379	0.361885	0.429074
C	0	-2.155837	1.978944	-0.173141
N	0	-2.549908	3.037481	0.096900
H	0	-3.808113	-0.113561	-0.696272
H	0	-3.353591	-1.611045	1.473712
H	0	-2.848328	0.070840	1.825487
H	0	-0.726267	-1.611291	1.932543
H	0	-0.665849	-3.037481	-0.315150
H	0	-2.566825	-2.113597	-1.932543
H	0	-1.322379	0.640030	-1.529492
H	0	-0.486104	0.817485	1.356607
H	0	0.834526	-0.617371	-1.048612
B	0	3.257116	0.113665	-0.186391
H	0	3.065352	-0.514640	-1.207222
H	0	3.677769	1.234502	-0.336436
H	0	3.808113	-0.496746	0.698251

P-16+CP

B3LYP/6-31G(d) Geometry

C	0	-1.329467	0.772841	-0.908892
C	0	-2.029990	0.466070	0.191553
C	0	-1.444666	-0.812579	0.771780
C	0	-0.054052	-0.431975	1.378356
C	0	-0.272054	-0.303444	-1.087309
C	0	0.800693	-0.071965	0.088395
C	0	-1.008889	-1.536414	-0.523215
C	0	1.308725	1.307050	0.107158
C	0	1.935027	-0.995930	-0.072130
N	0	1.693107	2.402141	0.119580
N	0	2.801840	-1.755372	-0.212625
H	0	-1.401704	1.668583	-1.515001
H	0	-2.801840	1.063618	0.665371
H	0	-2.078418	-1.367666	1.466483
H	0	0.401445	-1.276691	1.901884
H	0	-0.103687	0.414150	2.066141
H	0	0.201637	-0.383840	-2.066141
H	0	-1.853546	-1.828335	-1.152562
H	0	-0.359326	-2.402141	-0.353157

P-17+CP

B3LYP/6-31G(d) Geometry

C	0	0.650442	-0.670007	1.169546
C	0	0.650515	0.670118	1.169520
C	0	0.762831	1.128278	-0.275994
C	0	-0.617696	0.794088	-0.973198
C	0	0.762706	-1.128237	-0.275950
C	0	-0.617787	-0.793926	-0.973163
C	0	1.635035	-0.000039	-0.868767
C	0	-1.761164	1.438376	-0.330745
C	0	-1.761324	-1.438071	-0.330690
N	0	-2.649416	-1.991459	0.172050
N	0	-2.649223	1.991728	0.172094
H	0	0.481267	-1.330072	2.012728
H	0	0.481416	1.330235	2.012674
H	0	1.078303	2.159399	-0.443939
H	0	-0.590285	1.139236	-2.012728
H	0	1.078062	-2.159399	-0.443854
H	0	-0.590425	-1.139121	-2.012678
H	0	2.649416	-0.000088	-0.462029
H	0	1.678289	-0.000063	-1.964795

P-18+CP

B3LYP/6-31G(d) Geometry

C	0	1.934870	-1.123066	-0.111543
C	0	1.038793	-1.540053	-1.016373
C	0	-0.345557	-1.295156	-0.438928
C	0	-0.544134	0.278079	-0.466388
C	0	1.162111	-0.595098	1.087843
C	0	0.483473	0.761061	0.641461
C	0	-0.074938	-1.521096	1.065145
C	0	-1.916556	0.671196	-0.146250
C	0	1.426581	1.767638	0.158940
N	0	2.186132	2.559549	-0.221034
N	0	-3.010980	0.956755	0.117984
H	0	3.010980	-1.059309	-0.227737
H	0	1.232163	-1.887113	-2.025842
H	0	-1.175854	-1.836833	-0.894172
H	0	-0.288179	0.686864	-1.447391
H	0	1.711553	-0.500483	2.025842
H	0	-0.062954	1.187744	1.488995
H	0	0.178500	-2.559549	1.292671
H	0	-0.892367	-1.189300	1.715642

P-19+CP

B3LYP/6-31G(d) Geometry

C	0	-0.494871	-2.039954	-0.138619
C	0	-1.346364	-1.452466	-0.990230
C	0	-1.850664	-0.176363	-0.332174
C	0	-0.637186	0.827679	-0.340377
C	0	-0.429011	-1.170348	1.108918
C	0	0.330751	0.158564	0.713685
C	0	-1.873393	-0.623413	1.148746
C	0	-1.010153	2.268150	0.019863
C	0	1.689582	-0.060531	0.221949
N	0	2.769937	-0.236243	-0.167808
H	0	0.130195	-2.907573	-0.319093
H	0	-1.558669	-1.745079	-2.013624
H	0	-2.769937	0.250496	-0.741433
H	0	-0.167258	0.826112	-1.328452
H	0	-0.035244	-1.637849	2.013624
H	0	0.402391	0.799431	1.601536
H	0	-2.611258	-1.406331	1.344739

H 0 -2.014602 0.197278 1.861792
H 0 -1.508271 2.330018 0.994838
H 0 -0.120566 2.907573 0.058630
H 0 -1.689788 2.689774 -0.729649

P-20+CP

B3LYP/6-31G(d) Geometry
C 0 0.928782 -1.482977 -0.799998
C 0 1.668126 -1.408481 0.314784
C 0 1.641805 0.038225 0.788559
C 0 0.199348 0.311896 1.329557
C 0 0.393137 -0.085947 -1.084635
C 0 -0.698329 0.224030 0.033251
C 0 1.575713 0.768854 -0.572662
C 0 -1.678392 -0.868965 0.123071
C 0 -1.471137 1.531623 -0.245396
N 0 -2.476558 -1.711071 0.184862
H 0 0.643992 -2.374668 -1.347335
H 0 2.117407 -2.231066 0.861805
H 0 2.433915 0.337184 1.479246
H 0 0.128320 1.316587 1.760991
H 0 -0.102573 -0.404911 2.096655
H 0 0.027137 0.101225 -2.096655
H 0 2.476558 0.627001 -1.176190
H 0 1.359511 1.839872 -0.490434
H 0 -2.046553 1.454381 -1.173728
H 0 -2.169423 1.750506 0.568997
H 0 -0.779802 2.374668 -0.335967

P-21+CP

B3LYP/6-31G(d) Geometry
C 0 1.102823 -1.962715 -1.016111
C 0 1.999504 -1.195640 -0.380054
C 0 1.323748 -0.636505 0.865934
C 0 0.242057 0.429074 0.407494
C 0 -0.190289 -1.911490 -0.213859
C 0 -0.739029 -0.449561 -0.432724
C 0 0.383418 -1.812550 1.219137
C 0 0.836845 1.590394 -0.354132
O 0 0.942236 2.711843 0.089544
C 0 -2.189756 -0.258607 -0.039146
F 0 -2.581446 1.020152 -0.234942
F 0 -2.433711 -0.554611 1.259796
F 0 -2.999377 -1.047754 -0.782374
H 0 1.212885 -2.447924 -1.980534
H 0 2.999377 -0.937733 -0.713471
H 0 1.981662 -0.259393 1.651056
H 0 -0.248859 0.836543 1.295888
H 0 -0.924336 -2.692176 -0.419793
H 0 -0.700354 -0.189365 -1.496365
H 0 -0.362386 -1.569509 1.980534
H 0 0.934842 -2.711843 1.508290
H 0 1.207877 1.343374 -1.375187

P-22+CP

B3LYP/6-31G(d) Geometry
C 0 0.881948 -2.038260 0.423290
C 0 1.829965 -1.378261 1.104012
C 0 2.337435 -0.255149 0.209746
C 0 1.171829 0.805646 0.137029
C 0 0.748862 -1.367982 -0.938132
C 0 0.077476 0.061784 -0.703329
C 0 2.215879 -0.940263 -1.171062
B 0 -1.409892 -0.063110 -0.174266
C 0 -1.812685 0.355357 1.295786
C 0 -2.523116 -0.630431 -1.145424
C 0 1.607301 2.141977 -0.475914
H 0 0.241315 -2.834870 0.790416
H 0 2.116610 -1.522189 2.141482
H 0 3.309607 0.169529 0.476098
H 0 0.814033 1.005053 1.153489
H 0 0.267120 -1.956766 -1.722176
H 0 0.026328 0.522085 -1.704518
H 0 2.894869 -1.792542 -1.279575
H 0 2.341956 -0.260650 -2.021800
H 0 -1.607826 1.424192 1.460078
H 0 -2.861864 0.171578 1.554159
H 0 -1.179914 -0.171033 2.025391
H 0 -3.309607 0.129454 -1.277238
H 0 -2.178022 -0.930812 -2.141482
H 0 -3.037000 -1.487669 -0.685517
H 0 2.017673 2.012117 -1.484837
H 0 2.376450 2.627781 0.137307
H 0 0.760169 2.834870 -0.554116

P-23+CP

B3LYP/6-31G(d) Geometry
C 0 0.582936 -1.553825 1.148470
C 0 1.524104 -0.644597 1.438265
C 0 2.016139 -0.056893 0.123930
C 0 0.842504 0.847411 -0.417598
C 0 0.439429 -1.591247 -0.366152
C 0 -0.240442 -0.213597 -0.818930
C 0 1.896860 -1.299135 -0.788014
B 0 -1.705179 -0.071240 -0.293273
C 0 1.256809 1.754695 -1.581723
Cl 0 -2.190326 1.026053 1.005830
Cl 0 -2.983090 -1.080071 -1.004157
H 0 -0.050016 -2.094082 1.845540
H 0 1.812043 -0.287619 2.422154
H 0 2.983090 0.452392 0.155192
H 0 0.478499 1.483262 0.395309
H 0 -0.045781 -2.471752 -0.791802
H 0 -0.308262 -0.264918 -1.915780
H 0 2.584244 -2.101174 -0.501479
H 0 2.009082 -1.084591 -1.857030
H 0 1.665260 1.180484 -2.422154
H 0 0.402321 2.329422 -1.958927
H 0 2.022980 2.471752 -1.263700

P-24+CP

B3LYP/6-31G(d) Geometry
C 0 -0.734301 1.534741 -0.978402
C 0 -1.748806 1.241284 -0.153899
C 0 -1.147090 0.676180 1.130112
C 0 -0.548279 -0.715984 0.766065
C 0 0.562292 1.181962 -0.260454
C 0 0.582045 -0.389952 -0.228451
C 0 0.169100 1.490690 1.205191
N 0 -1.564875 -1.680027 0.195094
N 0 1.941664 -0.876795 0.239566
O 0 -1.154125 -2.554992 -0.560309
O 0 -2.724613 -1.548509 0.571621
O 0 2.810539 -0.914448 -0.623280
O 0 2.107913 -1.148913 1.427575
H 0 -0.791361 1.866332 -2.009471

H 0	-2.810539	1.286244	-0.364865
H 0	-1.789098	0.659074	2.009471
H 0	-0.144023	-1.232008	1.640437
H 0	1.481274	1.612813	-0.659950
H 0	0.455211	-0.843292	-1.208133
H 0	0.884221	1.113780	1.943576
H 0	-0.013068	2.554992	1.373089

P-25+CP

B3LYP/6-31G(d) Geometry

C 0	1.340897	0.533424	1.123438
C 0	0.014000	0.726239	1.163700
C 0	-0.469809	0.856821	-0.270266
C 0	1.759231	0.531100	-0.336626
C 0	0.751185	1.544155	-0.918626
C 0	-0.347322	-0.580346	-0.953900
C 0	1.213839	-0.811681	-0.985737
C 0	-1.263637	-1.559225	-0.270956
C 0	1.958469	-2.019513	-0.395514
O 0	2.975392	-2.399288	-0.933536
O 0	1.552773	-2.557218	0.763271
O 0	-1.078318	-2.117472	0.800414
O 0	-2.420525	-1.713167	-0.943287
H 0	1.998034	0.305504	1.955359
H 0	-0.630931	0.687546	2.034479
H 0	-1.451028	1.311262	-0.422367
H 0	2.818831	0.685386	-0.545272
H 0	0.904994	2.557218	-0.536220
H 0	0.721405	1.561715	-2.014343
H 0	-0.700687	-0.491518	-1.983911
H 0	1.518392	-0.818985	-2.034479
H 0	0.643787	-2.260021	1.001563
H 0	-2.975392	-2.315901	-0.411206

P-26+CP

B3LYP/6-31G(d) Geometry

C 0	-1.995293	-0.586454	0.294325
C 0	-1.043131	-0.719229	1.227718
C 0	0.268307	-0.981063	0.508044
C 0	0.676620	0.407834	-0.189924
C 0	-1.333685	-0.753198	-1.064214
C 0	-0.461881	0.539333	-1.316556
C 0	-0.220581	-1.767772	-0.724861
C 0	1.998617	0.291869	-0.825839
C 0	0.712667	1.508545	0.781635
C 0	-1.229370	1.780813	-1.282869
N 0	-1.872705	2.746833	-1.287565
N 0	3.030493	0.153252	-1.338961
N 0	0.755664	2.349558	1.579549
H 0	-3.030493	-0.302267	0.444381
H 0	-1.135368	-0.562988	2.296063
H 0	1.089722	-1.393115	1.094593
H 0	-1.987764	-0.977537	-1.908179
H 0	0.021868	0.470819	-2.296063
H 0	-0.620281	-2.746833	-0.450793
H 0	0.535354	-1.885931	-1.508896

P-27+CP

B3LYP/6-31G(d) Geometry

C 0	0.925892	-0.287359	1.339852
C 0	1.577704	0.644186	0.630638
C 0	1.544336	0.213896	-0.829218
C 0	0.073013	0.386662	-1.353914
C 0	0.443782	-1.349976	0.360896
C 0	-0.724708	-0.689289	-0.494102
C 0	1.603100	-1.320888	-0.661342
C 0	-1.726567	-0.084539	0.396802
N 0	-2.543800	0.360622	1.092588
C 0	-1.458132	-1.719322	-1.381852
C 0	-0.461990	1.817927	-1.326277
H 0	0.670752	-0.259663	2.393451
H 0	1.974944	1.585897	0.994555
H 0	2.287831	0.674104	-1.485640
H 0	0.050881	0.034920	-2.393451
H 0	0.162665	-2.315139	0.788780
H 0	2.543800	-1.668035	-0.224680
H 0	1.407085	-1.875121	-1.586071
H 0	-1.977130	-2.463832	-0.769219
H 0	-2.201641	-1.225838	-2.016691
H 0	-0.748483	-2.240351	-2.031328
H 0	0.159203	2.463832	-1.958397
H 0	-1.488680	1.868703	-1.705399
H 0	-0.464808	2.230371	-0.312760

P-28+CP

B3LYP/6-31G(d) Geometry

C 0	-0.877438	-1.808499	0.010397
C 0	-1.663655	-1.202593	-0.888963
C 0	-1.687497	0.280553	-0.551607
C 0	-0.269988	0.852052	-0.930921
C 0	-0.369335	-0.736339	0.964299
C 0	0.672045	0.160677	0.161664
C 0	-1.590015	0.210840	0.988633
C 0	1.688466	-0.677452	-0.491994
N 0	2.512094	-1.324354	-0.995390
C 0	-0.230261	2.382541	-0.975971
C 0	1.416858	1.130662	1.106655
H 0	-0.549672	-2.842216	0.015125
H 0	-2.114289	-1.643884	-1.772271
H 0	-2.512094	0.859994	-0.975326
H 0	0.012909	0.484461	-1.921766
H 0	0.026508	-1.083081	1.921766
H 0	-2.465742	-0.255533	1.448775
H 0	-1.403727	1.176904	1.469778
H 0	-0.557130	2.842216	-0.037211
H 0	-0.898695	2.740649	-1.767452
H 0	0.773776	2.757244	-1.202978
H 0	2.013529	0.561881	1.827113
H 0	2.097013	1.785653	0.554323
H 0	0.716829	1.757057	1.665270

P-29+CP

B3LYP/6-31G(d) Geometry

C 0	-1.922770	-0.998576	0.058391
C 0	-1.012410	-1.252904	1.008246
C 0	0.362717	-1.092911	0.380714
C 0	0.583527	0.467609	0.138282
C 0	-1.166924	-0.666319	-1.219517
C 0	-0.497129	0.750204	-1.009208
C 0	0.074043	-1.571770	-1.059033
C 0	1.930400	0.678445	-0.414893
C 0	0.436699	1.325720	1.408130
C 0	-1.458746	1.803942	-0.693004
N 0	-2.235151	2.633917	-0.454029
N 0	2.999052	0.834182	-0.843258
H 0	-2.999052	-0.933922	0.173377

H 0	-1.194689	-1.444492	2.060015
H 0	1.200521	-1.551272	0.909511
H 0	-1.728612	-0.730525	-2.152986
H 0	0.019359	1.043877	-1.928960
H 0	-0.179404	-2.633917	-1.103629
H 0	0.880670	-1.355154	-1.768012
H 0	1.178702	1.020390	2.152986
H 0	0.590552	2.385493	1.186282
H 0	-0.562209	1.207948	1.834163

P-30+CP

B3LYP/6-31G(d) Geometry

C 0	-0.706332	1.601786	0.844240
C 0	-0.690028	0.358392	1.342794
C 0	-0.717377	-0.607716	0.166651
C 0	0.710815	-0.517803	-0.531686
C 0	-0.757011	1.484576	-0.671272
C 0	0.652017	0.952720	-1.149628
C 0	-1.586342	0.192561	-0.828834
C 0	1.777039	-0.695510	0.464177
C 0	1.756815	1.844789	-0.806398
N 0	2.613550	2.588425	-0.559278
N 0	2.609262	-0.906063	1.245993
C 0	0.908843	-1.585174	-1.629846
H 0	-0.591521	2.533046	1.387110
H 0	-0.555462	0.063390	2.377142
H 0	-1.006499	-1.637850	0.384694
H 0	-1.080307	2.368857	-1.223426
H 0	0.642181	0.856347	-2.241631
H 0	-2.613550	0.311397	-0.475057
H 0	-1.598954	-0.207776	-1.848428
H 0	0.112133	-1.525556	-2.377142
H 0	1.868625	-1.446277	-2.137466
H 0	0.898673	-2.588425	-1.193119

P-31+CP

B3LYP/6-31G(d) Geometry

C 0	1.823439	-0.828332	1.088242
C 0	1.230527	-1.905558	0.553824
C 0	0.726110	-1.507734	-0.827717
C 0	-0.487333	-0.513807	-0.648087
C 0	1.706327	0.305545	0.079876
C 0	0.186047	0.758880	0.037294
C 0	1.828791	-0.502363	-1.233393
C 0	-1.650362	-1.112469	0.102130
O 0	-2.807260	-1.026983	-0.254865
C 0	-0.362982	1.098314	1.435036
C 0	-0.000096	1.999808	-0.854778
H 0	2.229430	-0.732147	2.090087
H 0	1.063734	-2.868518	1.025662
H 0	0.516630	-2.327359	-1.519578
H 0	-0.873671	-0.227896	-1.632336
H 0	2.394050	1.144470	0.220126
H 0	1.596459	0.065551	-2.140340
H 0	2.807260	-0.979150	-1.344933
H 0	-1.389615	-1.664212	1.032618
H 0	-0.262497	0.268794	2.140340
H 0	-1.423439	1.372865	1.384798
H 0	0.178391	1.956937	1.851666
H 0	-1.063509	2.249434	-0.950345
H 0	0.396132	1.853059	-1.864628
H 0	0.507263	2.868518	-0.416844

P-32+CP

B3LYP/6-31G(d) Geometry

C 0	0.606853	1.372778	1.038900
C 0	1.745604	1.073977	0.397757
C 0	1.382225	0.658324	-1.020251
C 0	0.687947	-0.761889	-0.944829
C 0	-0.533034	1.165502	0.058163
C 0	-0.655340	-0.426416	-0.152960
C 0	0.147343	1.552754	-1.269907
C 0	1.596685	-1.817026	-0.337287
O 0	2.198101	-2.615541	-1.018883
C 0	-0.795336	-1.125039	1.134767
C 0	-1.827053	-0.740865	-0.985463
N 0	-2.745055	-0.946486	-1.665516
N 0	-0.905097	-1.654062	2.162008
H 0	0.479060	1.616866	2.087129
H 0	2.745055	1.037642	0.817823
H 0	2.183930	0.681761	-1.760096
H 0	0.438089	-1.097743	-1.953906
H 0	-1.493982	1.618336	0.303412
H 0	-0.427968	1.283165	-2.162008
H 0	0.401326	2.615541	-1.301232
H 0	1.721983	-1.788120	0.763616

P-33+CP

B3LYP/6-31G(d) Geometry

C 0	1.900054	-0.669909	-0.547713
C 0	1.900054	0.669908	-0.547714
C 0	0.469744	1.127616	-0.767725
C 0	-0.321713	0.817412	0.593947
C 0	0.469744	-1.127617	-0.767725
C 0	-0.321713	-0.817412	0.593948
C 0	-0.075363	0.000000	-1.665960
C 0	-1.679723	1.375490	0.522245
C 0	0.356684	1.398314	1.759103
C 0	0.356684	-1.398313	1.759103
N 0	0.906018	-1.896181	2.651382
C 0	-1.679723	-1.375490	0.522246
N 0	-2.729299	1.859981	0.422433
N 0	0.906019	1.896182	2.651381
N 0	-2.729299	-1.859981	0.422434
H 0	2.729299	-1.332240	-0.328765
H 0	2.729299	1.332239	-0.328765
H 0	0.316271	2.159774	-1.083179
H 0	0.316270	-2.159774	-1.083179
H 0	0.395712	-0.000001	-2.651382
H 0	-1.164107	0.000000	-1.780192

P-34+CP

B3LYP/6-31G(d) Geometry

C 0	2.050716	-0.620578	-0.752064
C 0	1.196652	-0.720307	-1.779150
C 0	-0.193281	-0.905215	-1.197564
C 0	-0.615583	0.507432	-0.560532
C 0	1.239947	-0.720062	0.531451
C 0	0.429966	0.640007	0.680525
C 0	0.125666	-1.691912	0.087969
C 0	-2.009062	0.439168	-0.093994
C 0	-0.524455	1.587437	-1.551920
C 0	1.326019	1.792688	0.520045
N 0	2.060662	2.689839	0.463534
C 0	-0.253090	0.768422	2.059176
N 0	-3.109460	0.340875	0.262133

N 0	-0.471594	2.410555	-2.368000
H 0	3.109460	-0.392469	-0.794826
H 0	1.408255	-0.590772	-2.833997
H 0	-0.966797	-1.290990	-1.862291
H 0	1.791953	-0.959937	1.442094
H 0	0.512690	-2.689839	-0.130979
H 0	-0.716397	-1.774869	0.781689
H 0	-0.896755	-0.089222	2.266748
H 0	0.517281	0.823194	2.833997
H 0	-0.860963	1.675232	2.117897

P-35+CP

B3LYP/6-31G(d) Geometry

C 0	0.201729	2.051660	0.495092
C 0	1.398359	1.790043	-0.048531
C 0	1.176732	0.854754	-1.229479
C 0	0.791059	-0.587298	-0.667381
C 0	-0.836462	1.306626	-0.323880
C 0	-0.646686	-0.259258	-0.000220
C 0	-0.197635	1.363372	-1.723267
C 0	1.828468	-1.022642	0.376550
O 0	2.614667	-1.922972	0.192403
C 0	-0.714440	-0.507796	1.449343
C 0	-1.735717	-1.022377	-0.629783
N 0	-2.614667	-1.582196	-1.141118
C 0	0.736096	-1.638145	-1.782143
N 0	-0.776598	-0.679547	2.595782
H 0	-0.010673	2.604965	1.402502
H 0	2.369031	2.101693	0.322435
H 0	1.985351	0.795826	-1.960638
H 0	-1.875791	1.617587	-0.213640
H 0	-0.684057	0.722478	-2.463811
H 0	-0.146588	2.386601	-2.104648
H 0	1.853600	-0.430627	1.311011
H 0	1.742188	-1.781277	-2.183427
H 0	0.069925	-1.344223	-2.595782
H 0	0.398826	-2.604965	-1.398228

P-36+CP

B3LYP/6-31G(d) Geometry

C 0	-2.054393	-0.922399	-0.915872
C 0	-1.346643	-1.923781	-0.374785
C 0	-0.639097	-1.368609	0.855223
C 0	0.517997	-0.378322	0.389203
C 0	-1.823496	0.311815	-0.057435
C 0	-0.338183	0.819364	-0.290386
C 0	-1.709408	-0.357457	1.329837
C 0	1.424904	-1.060621	-0.627355
O 0	2.636495	-0.991326	-0.625001
C 0	-0.031708	1.035418	-1.785833
C 0	-0.134039	2.179612	0.405425
C 0	1.392866	0.042186	1.582001
H 0	-2.621638	-0.943296	-1.840803
H 0	-1.226996	-2.930258	-0.762826
H 0	-0.292325	-2.107902	1.582430
H 0	-2.559876	1.113254	-0.167726
H 0	-1.376873	0.310524	2.129448
H 0	-2.636495	-0.850410	1.637335
H 0	0.907724	-1.661863	-1.403987
H 0	-0.216430	0.143476	-2.390179
H 0	1.012452	1.334362	-1.936075
H 0	-0.663691	1.839321	-2.183469
H 0	0.901383	2.525392	0.314533
H 0	-0.390025	2.167542	1.467990
H 0	-0.771220	2.930258	-0.077759
H 0	1.912229	-0.833957	1.983717
H 0	0.807173	0.485625	2.390179
H 0	2.163981	0.754831	1.279409

P-37+CP

B3LYP/6-31G(d) Geometry

C 0	-2.760129	0.617017	0.124895
C 0	-2.545914	1.028158	-1.343009
C 0	-1.013050	1.155051	-1.194278
C 0	-0.932796	2.019703	0.056153
C 0	-1.965761	1.691996	0.844401
C 0	-1.872013	-0.723807	0.167327
C 0	-0.622790	-0.350561	-0.794790
C 0	0.682102	-0.311885	-0.039476
O 0	1.731475	-0.679044	-0.568178
C 0	-1.492872	-1.061679	1.548227
C 0	-2.656447	-1.848081	-0.366713
C 0	-0.490305	-1.251402	-2.030749
N 0	-3.314237	-2.704752	-0.791383
N 0	-1.202739	-1.303522	2.645814
H 0	-3.778075	0.433700	0.469597
H 0	-3.013316	1.989987	-1.568424
H 0	-2.877649	0.283172	-2.071365
H 0	-0.442583	1.492764	-2.061167
H 0	-0.122894	2.704752	0.283710
H 0	-2.173209	2.042439	1.848710
H 0	0.723722	0.102260	0.974282
H 0	0.342051	-0.901600	-2.645814
H 0	-1.398909	-1.244242	-2.635181
H 0	-0.280545	-2.286635	-1.747065
B 0	3.194407	-0.529708	0.138593
H 0	2.962992	-0.031767	1.218768
H 0	3.597750	-1.665927	0.156924
H 0	3.778075	0.180517	-0.645485

P-38+CP

B3LYP/6-31G(d) Geometry

C 0	-2.029454	-1.062782	-0.308705
C 0	-1.232869	-1.658323	0.588579
C 0	0.201885	-1.457966	0.128209
C 0	0.563989	0.077999	0.354963
C 0	-1.135249	-0.451610	-1.378102
C 0	-0.401813	0.800113	-0.724862
C 0	0.011868	-1.486109	-1.402636
C 0	0.380860	0.542455	1.813185
C 0	-1.379321	1.679742	-0.068276
N 0	-2.156400	2.397790	0.411227
C 0	1.977360	0.273778	-0.001311
C 0	0.334774	1.649906	-1.785345
N 0	3.104480	0.401222	-0.252804
H 0	-3.104480	-0.931659	-0.255321
H 0	-1.525359	-2.122062	1.524275
H 0	0.951900	-2.124962	0.557876
H 0	-1.613697	-0.197855	-2.326335
H 0	-0.322181	-2.461696	-1.765025
H 0	0.896902	-1.174155	-1.965717
H 0	1.043785	-0.028817	2.471219
H 0	0.622103	1.603591	1.923618
H 0	-0.652206	0.391842	2.133098
H 0	1.032676	1.040243	-2.363591
H 0	-0.394721	2.091625	-2.471219

H 0 0.901094 2.461696 -1.320159

P-39+CP

B3LYP/6-31G(d) Geometry

C 0 0.696457 0.669637 -1.646346
C 0 0.696457 -0.669637 -1.646346
C 0 0.713713 -1.125336 -0.195082
C 0 -0.720295 -0.810190 0.419717
C 0 0.713713 1.125336 -0.195082
C 0 -0.720295 0.810190 0.419717
C 0 1.557805 0.000000 0.438898
C 0 -1.771142 -1.381459 -0.435446
C 0 -1.771142 1.381459 -0.435445
N 0 -2.587061 1.903996 -1.075614
N 0 -2.587063 -1.903995 -1.075614
C 0 -0.888458 -1.452823 1.815531
C 0 -0.888458 1.452822 1.815531
H 0 0.583491 1.330776 -2.497912
H 0 0.583491 -1.330776 -2.497912
H 0 1.019310 -2.157488 -0.010564
H 0 1.019310 2.157487 -0.010564
H 0 2.587063 0.000000 0.071028
H 0 1.570808 0.000000 1.533099
H 0 -0.091078 -1.149798 2.497912
H 0 -1.850052 -1.190194 2.264835
H 0 -0.853777 -2.541930 1.716076
H 0 -0.091078 1.149798 2.497912
H 0 -0.853776 2.541930 1.716076
H 0 -1.850052 1.190194 2.264835

P-40+CP

B3LYP/6-31G(d) Geometry

C 0 0.760557 -1.954255 -0.028350
C 0 1.579480 -1.253441 0.766919
C 0 1.741313 0.129961 0.153052
C 0 0.381383 0.921954 0.348509
C 0 0.371811 -1.047591 -1.187022
C 0 -0.603603 0.074537 -0.615163
C 0 1.676826 -0.238519 -1.346155
C 0 -0.069205 0.943839 1.819110
C 0 -1.708296 -0.556104 0.123650
N 0 -2.609122 -1.052545 0.664499
C 0 0.556233 2.385835 -0.099457
C 0 -1.256968 0.873477 -1.768799
H 0 0.346806 -2.940880 0.148803
H 0 1.979928 -1.558539 1.728043
H 0 2.609122 0.704306 0.489771
H 0 -0.034669 -1.540262 -2.073647
H 0 2.513676 -0.867202 -1.663119
H 0 1.598753 0.617995 -2.022563
H 0 0.688260 1.449231 2.430986
H 0 -1.010419 1.492881 1.935807
H 0 -0.220604 -0.059291 2.223317
H 0 0.936663 2.489471 -1.119022
H 0 -0.386073 2.940880 -0.033825
H 0 1.270659 2.881456 0.568098
H 0 -0.503429 1.306310 -2.430986
H 0 -1.890338 0.208447 -2.364667
H 0 -1.887832 1.683042 -1.390454

P-41+CP

B3LYP/6-31G(d) Geometry

C 0 0.996859 0.021249 1.222297
C 0 0.638743 -1.183595 0.755667
C 0 0.622589 -1.105218 -0.765663
C 0 -0.583084 -0.187337 -1.191363
C 0 1.220334 0.936878 0.024657
C 0 -0.168037 1.227016 -0.648772
C 0 1.780923 -0.094567 -0.991690
C 0 -1.463201 1.299857 0.214449
C 0 -1.830452 -0.109756 -0.290452
O 0 -2.755781 -0.852670 -0.084583
H 0 1.031293 0.336543 2.260280
H 0 0.315712 -2.044393 1.331866
H 0 0.671616 -2.056758 -1.298430
H 0 -0.805280 -0.277638 -2.260280
H 0 1.823259 1.829166 0.210138
H 0 -0.079768 2.016802 -1.399111
H 0 1.832802 0.287604 -2.018769
H 0 2.755781 -0.497802 -0.698831
H 0 -2.186754 2.056758 -0.111138
H 0 -1.338904 1.383760 1.299201

P-42+CP

B3LYP/6-31G(d) Geometry

C 0 1.392449 -1.525153 -0.208172
C 0 0.866440 -0.950931 -1.299217
C 0 0.465555 0.470751 -0.926051
C 0 -0.773335 0.402825 0.052192
C 0 1.345384 -0.502432 0.922188
C 0 -0.152813 -0.279627 1.333063
C 0 1.579895 0.795763 0.106972
C 0 -1.515410 1.731057 0.184937
C 0 -1.164234 -1.458775 1.227759
C 0 -1.707192 -0.823719 -0.064939
O 0 -2.574672 -1.127306 -0.844613
H 0 1.709625 -2.557405 -0.099574
H 0 0.660632 -1.418326 -2.256526
H 0 0.330316 1.166334 -1.757843
H 0 2.017345 -0.689246 1.763702
H 0 -0.224929 0.302005 2.256526
H 0 1.396101 1.711944 0.680928
H 0 2.574672 0.843322 -0.347687
H 0 -2.058260 1.953692 -0.740833
H 0 -0.822855 2.557405 0.383408
H 0 -2.247943 1.705143 1.000421
H 0 -1.919473 -1.485631 2.022333
H 0 -0.749228 -2.464987 1.109929

P-43+CP

B3LYP/6-31G(d) Geometry

C 0 1.000821 -1.114663 1.088461
C 0 0.581408 -1.961452 0.137774
C 0 0.603286 -1.212136 -1.189458
C 0 -0.533168 -0.122618 -1.159981
C 0 1.300263 0.222524 0.421324
C 0 -0.057269 0.884109 -0.040977
C 0 1.826008 -0.287949 -0.948421
C 0 -1.351578 0.579011 0.787397
C 0 -1.789887 -0.394304 -0.319546
O 0 -2.764899 -1.084121 -0.481731
C 0 0.107589 2.351107 -0.428750
H 0 1.036439 -1.296646 2.157895
H 0 0.198327 -2.967624 0.272005
H 0 0.605260 -1.829264 -2.090107
H 0 -0.728345 0.286959 -2.157895

H 0	1.950274	0.900766	0.981142
H 0	1.935578	0.498987	-1.703806
H 0	2.764899	-0.844311	-0.863258
H 0	-2.034098	1.431667	0.890682
H 0	-1.219503	0.120018	1.772315
H 0	-0.799429	2.741226	-0.906670
H 0	0.939037	2.499013	-1.127524
H 0	0.305028	2.967624	0.457415

P-44+CP

B3LYP/6-31G(d) Geometry

C 0	-1.212258	-0.983378	1.097093
C 0	-2.039531	-0.786366	0.060714
C 0	-1.184851	-0.630257	-1.191227
C 0	-0.427903	0.744000	-1.086779
C 0	0.212489	-0.968674	0.563585
C 0	0.564025	0.518234	0.130370
C 0	-0.014945	-1.588472	-0.839808
C 0	-0.083878	1.726755	0.892530
C 0	-1.068031	1.887672	-0.279467
O 0	-1.985193	2.635033	-0.492452
C 0	1.981783	0.668813	-0.156365
N 0	3.116499	0.780430	-0.383814
H 0	-1.478776	-1.058467	2.145994
H 0	-3.116499	-0.660397	0.091939
H 0	-1.691297	-0.780279	-2.145994
H 0	0.019616	1.048973	-2.037448
H 0	0.974768	-1.424214	1.197733
H 0	0.849869	-1.493394	-1.506301
H 0	-0.329717	-2.635033	-0.790971
H 0	0.579162	2.590562	1.008161
H 0	-0.539718	1.495774	1.859711

P-45+CP

B3LYP/6-31G(d) Geometry

C 0	-1.048426	0.352707	-1.263626
C 0	-1.741542	0.598212	-0.143329
C 0	-1.217611	-0.339326	0.941264
C 0	0.236581	0.109890	1.320763
C 0	-0.061395	-0.770519	-0.962685
C 0	1.029709	-0.185798	-0.001999
C 0	-0.885360	-1.583808	0.073545
C 0	0.640834	1.612209	1.246410
C 0	1.396195	1.323161	-0.063223
Cl 0	2.480283	-1.263277	0.118247
O 0	2.047293	1.983284	-0.824715
H 0	-1.094153	0.892395	-2.203400
H 0	-2.480283	1.377826	0.011855
H 0	-1.873013	-0.493716	1.801476
H 0	0.603333	-0.416436	2.203400
H 0	0.354352	-1.297554	-1.821670
H 0	-1.773325	-2.045700	-0.368438
H 0	-0.294516	-2.342152	0.598766
H 0	1.319488	1.937784	2.043000
H 0	-0.168968	2.342152	1.153118

P-46+CP

B3LYP/6-31G(d) Geometry

C 0	1.458399	-1.350551	-0.998680
C 0	2.145530	-0.771832	-0.003916
C 0	1.159981	-0.442992	1.109939
C 0	0.235121	0.741420	0.626770
C 0	-0.000933	-1.421251	-0.571747
C 0	-0.588877	0.053182	-0.563141
C 0	0.172570	-1.630267	0.953478
C 0	-0.023738	1.105880	-1.576009
C 0	0.823808	1.692938	-0.436868
O 0	1.620044	2.592871	-0.375244
C 0	-2.036187	0.048496	-0.433307
C 0	-0.504779	1.445099	1.760069
N 0	-3.193664	0.043111	-0.321780
H 0	1.832978	-1.644924	-1.973356
H 0	3.193664	-0.492094	-0.002591
H 0	1.589050	-0.272340	2.099640
H 0	-0.630747	-2.132174	-1.109479
H 0	-0.757802	-1.514223	1.520438
H 0	0.631629	-2.592871	1.197398
H 0	-0.772759	1.814539	-1.945371
H 0	0.535894	0.706282	-2.426477
H 0	0.207228	2.035633	2.346858
H 0	-0.991233	0.724646	2.426477
H 0	-1.277227	2.123760	1.383445

P-47+CP

B3LYP/6-31G(d) Geometry

C 0	-0.872794	-1.781244	0.111833
C 0	-1.407621	-1.099866	-0.910864
C 0	-1.339946	0.382699	-0.564541
C 0	0.166129	0.858941	-0.600353
C 0	-0.447198	-0.768108	1.166520
C 0	0.793757	0.048146	0.621583
C 0	-1.556191	0.298081	0.968878
C 0	0.284835	2.379800	-0.616505
C 0	1.130187	0.123357	-1.588663
C 0	1.688272	-0.675967	-0.403081
C 0	1.564277	0.762504	1.728768
O 0	2.549892	-1.512988	-0.293546
H 0	-0.677253	-2.847140	0.165269
H 0	-1.744776	-1.501291	-1.861260
H 0	-2.015259	1.034315	-1.126538
H 0	-0.297582	-1.159817	2.175677
H 0	-2.549892	-0.072461	1.240124
H 0	-1.364270	1.239082	1.497266
H 0	-0.298185	2.847140	0.185335
H 0	-0.083222	2.780364	-1.569575
H 0	1.324874	2.708213	-0.504867
H 0	1.891224	0.773659	-2.038621
H 0	0.678528	-0.478605	-2.383476
H 0	2.094651	0.025307	2.342242
H 0	0.895117	1.332975	2.383476
H 0	2.313053	1.455101	1.328073

P-48+CP

B3LYP/6-31G(d) Geometry

C 0	1.275300	0.292565	1.173583
C 0	0.851184	-0.978824	1.119179
C 0	0.818159	-1.387317	-0.347269
C 0	-0.353344	-0.578591	-1.039194
C 0	1.537401	0.752246	-0.254333
C 0	0.153749	0.892381	-0.992479
C 0	2.028861	-0.579291	-0.876590
C 0	-0.954970	1.737935	-0.301074
C 0	-1.680246	-0.611091	-0.282707
O 0	-2.420069	-1.569991	-0.211948
C 0	-1.923688	0.749053	0.377809
H 0	1.339076	0.925405	2.053311

H 0	0.490566	-1.590977	1.939681
H 0	0.786887	-2.458973	-0.550903
H 0	-0.508954	-0.962500	-2.053311
H 0	2.184568	1.626301	-0.365101
H 0	0.347691	1.277201	-1.999200
H 0	2.096436	-0.554499	-1.971136
H 0	2.979869	-0.921581	-0.455880
H 0	-1.491774	2.321124	-1.057858
H 0	-0.532919	2.458973	0.407392
H 0	-1.704195	0.631726	1.446604
H 0	-2.979869	1.025970	0.298354

P-49+CP

B3LYP/6-31G(d) Geometry

C 0	-1.392696	-1.113964	0.646846
C 0	-0.868724	-0.131165	1.393580
C 0	-0.643849	1.066513	0.479081
C 0	0.541612	0.698549	-0.514021
C 0	-1.535844	-0.583829	-0.774561
C 0	-0.100674	-0.420759	-1.397086
C 0	-1.855690	0.900331	-0.471544
C 0	0.844365	-1.653593	-1.350556
C 0	1.714961	0.022469	0.215855
O 0	2.484050	0.597474	0.958157
C 0	1.775499	-1.464661	-0.137375
C 0	1.057598	1.931635	-1.268408
H 0	-1.603994	-2.132793	0.956453
H 0	-0.555055	-0.183658	2.431203
H 0	-0.506702	2.031195	0.972294
H 0	-2.233567	-1.125734	-1.418867
H 0	-0.222083	-0.078749	-2.431203
H 0	-1.822738	1.547026	-1.355993
H 0	-2.812785	1.034842	0.042555
H 0	1.438749	-1.691468	-2.270638
H 0	0.283413	-2.593392	-1.302648
H 0	1.427732	-2.022828	0.740298
H 0	2.812785	-1.767680	-0.314739
H 0	1.589587	2.593392	-0.577100
H 0	0.236344	2.491706	-1.728533
H 0	1.756459	1.649231	-2.065199

P-50+CP

B3LYP/6-31G(d) Geometry

C 0	1.161812	-1.043286	1.160666
C 0	0.534651	-1.964531	0.415214
C 0	0.602671	-1.500677	-1.034059
C 0	-0.321130	-0.222306	-1.183178
C 0	1.652774	0.051284	0.221778
C 0	0.394475	0.857483	-0.307210
C 0	1.986883	-0.810545	-1.023262
C 0	-0.636330	1.275034	0.797725
C 0	-1.726051	-0.406244	-0.619873
O 0	-2.621301	-1.020718	-1.161544
C 0	0.840573	2.096278	-1.098963
C 0	-1.824965	0.296799	0.735111
H 0	1.237721	-1.016055	2.243136
H 0	-0.010456	-2.836889	0.761432
H 0	0.412285	-2.260352	-1.794343
H 0	-0.387956	0.047248	-2.243136
H 0	2.445003	0.695653	0.613617
H 0	2.198179	-0.232587	-1.929392
H 0	2.805416	-1.514204	-0.841860
H 0	-0.987963	2.293158	0.594656
H 0	-0.171658	1.300132	1.789121
H 0	-0.014916	2.577440	-1.588769
H 0	1.573412	1.854550	-1.876102
H 0	1.297144	2.836889	-0.430015
H 0	-1.756679	-0.478641	1.508423
H 0	-2.805416	0.771438	0.844461

P-51+CP

B3LYP/6-31G(d) Geometry

C 0	0.193753	1.443100	1.067257
C 0	1.081780	1.684838	0.091839
C 0	0.472648	1.193622	-1.214294
C 0	0.435694	-0.385971	-1.153874
C 0	-1.025763	0.797837	0.426921
C 0	-0.611587	-0.675614	-0.021041
C 0	-1.020500	1.503886	-0.950239
C 0	0.113382	-1.556515	1.060159
C 0	1.747978	-1.029001	-0.708630
O 0	2.746078	-1.094386	-1.391762
C 0	-1.797486	-1.368083	-0.530395
N 0	-2.746078	-1.912286	-0.924230
C 0	1.615996	-1.546983	0.724539
H 0	0.327055	1.596078	2.133079
H 0	2.090984	2.069302	0.197521
H 0	0.922273	1.572461	-2.133079
H 0	0.143051	-0.787122	-2.128524
H 0	-1.950489	0.820528	1.006573
H 0	-1.704512	1.055326	-1.678979
H 0	-1.217533	2.576891	-0.870052
H 0	-0.277418	-2.576891	1.018163
H 0	-0.096232	-1.177332	2.064581
H 0	2.177294	-0.861664	1.371219
H 0	2.091881	-2.528699	0.812070

P-52+CP

B3LYP/6-31G(d) Geometry

C 0	0.956862	-0.014436	1.450407
C 0	1.709010	0.412756	0.426047
C 0	1.381341	-0.460809	-0.780788
C 0	-0.070666	-0.109031	-1.266299
C 0	0.110919	-1.179571	0.942223
C 0	-0.933542	-0.548746	-0.047161
C 0	1.099753	-1.808777	-0.069783
C 0	-0.407880	1.379424	-1.554435
C 0	-1.621460	0.726369	0.493137
Cl 0	-2.229577	-1.758941	-0.488324
O 0	-2.374938	0.757438	1.436958
C 0	-1.155072	1.931516	-0.323368
H 0	0.865867	0.425240	2.437933
H 0	2.374938	1.269755	0.413598
H 0	2.119109	-0.463834	-1.587070
H 0	-0.297062	-0.727306	-2.138066
H 0	-0.346213	-1.817915	1.698109
H 0	1.984983	-2.226670	0.418969
H 0	0.640875	-2.563297	-0.717277
H 0	-1.051882	1.439457	-2.437933
H 0	0.493855	1.957704	-1.781995
H 0	-2.014478	2.563297	-0.571035
H 0	-0.502465	2.527427	0.326034

P-53+CP

B3LYP/6-31G(d) Geometry

C 0	0.533371	1.767164	0.943577
C 0	1.398482	1.665935	-0.075715
C 0	0.694768	0.916702	-1.199294
C 0	0.525737	-0.597922	-0.744397
C 0	-0.764542	1.103850	0.507729
C 0	-0.516206	-0.469911	0.442249
C 0	-0.749113	1.435796	-1.002088
C 0	0.142057	-1.110003	1.714948
C 0	1.811203	-1.134102	-0.090242
O 0	2.818993	-1.402712	-0.707753
C 0	-1.795050	-1.125810	0.162371
C 0	0.140139	-1.500434	-1.924263
N 0	-2.818993	-1.637029	-0.040705
C 0	1.642799	-1.271494	1.421239
H 0	0.721439	2.173248	1.931982
H 0	2.441570	1.964488	-0.089948
H 0	1.140485	1.003968	-2.191754
H 0	-1.658782	1.364986	1.077178
H 0	-1.506145	0.896739	-1.580957
H 0	-0.837623	2.508844	-1.195533
H 0	-0.312025	-2.086507	1.905686
H 0	-0.053124	-0.492022	2.596392
H 0	0.999454	-1.583336	-2.596392
H 0	-0.130091	-2.508844	-1.593479
H 0	-0.710361	-1.096045	-2.480919
H 0	2.246030	-0.487162	1.892648
H 0	2.053015	-2.230466	1.753958

P-54+CP

B3LYP/6-31G(d) Geometry

C 0	-0.516405	-2.043137	-0.093516
C 0	-1.263172	-1.447610	-1.034361
C 0	-1.723322	-0.108622	-0.473394
C 0	-0.478478	0.871526	-0.389037
C 0	-0.466110	-1.105282	1.105029
C 0	0.412193	0.166482	0.711712
C 0	-1.883872	-0.495885	1.016656
C 0	-0.962584	2.289363	-0.047584
C 0	0.387218	0.925906	-1.691115
C 0	1.702819	-0.263582	-0.004348
C 0	0.781649	0.974155	1.963502
O 0	2.669621	-0.739178	0.555256
C 0	1.596614	-0.006418	-1.505350
H 0	0.042400	-2.969623	-0.178951
H 0	-1.445823	-1.795322	-2.046382
H 0	-2.586697	0.343302	-0.970676
H 0	-0.156666	-1.551328	2.052694
H 0	-2.669621	-1.240709	1.177895
H 0	-2.049064	0.352220	1.688625
H 0	-1.606014	2.319557	0.837352
H 0	-1.538761	2.695447	-0.888557
H 0	-0.121877	2.969623	0.129509
H 0	0.738600	1.953052	-1.844940
H 0	-0.207453	0.667707	-2.574363
H 0	1.482292	0.389524	2.567703
H 0	-0.096210	1.208150	2.574363
H 0	1.275330	1.918924	1.710170
H 0	2.539975	0.403124	-1.881722
H 0	1.452250	-0.976571	-1.995257

P-55+CP

B3LYP/6-31G(d) Geometry

C 0	-0.553942	0.670534	1.167692
C 0	-0.553941	-0.670535	1.167692
C 0	-0.690982	-1.132130	-0.276950
C 0	-0.690983	1.132127	-0.276951
C 0	-1.585754	-0.000002	-0.842471
C 0	0.659024	-0.771215	-1.014823
C 0	0.659024	0.771213	-1.014823
C 0	1.920991	-1.153399	-0.265162
C 0	1.920990	1.153398	-0.265162
O 0	2.348001	2.242866	-0.010726
O 0	2.348003	-2.242866	-0.010726
O 0	2.588790	0.000000	0.139414
H 0	-0.380712	1.330199	2.011114
H 0	-0.380710	-1.330199	2.011115
H 0	-1.008966	-2.163632	-0.432848
H 0	-1.008967	2.163630	-0.432849
H 0	-2.588790	-0.000002	-0.406080
H 0	-1.658939	-0.000002	-1.936789
H 0	0.682771	-1.222260	-2.011115
H 0	0.682770	1.222258	-2.011115

P-56+CP

B3LYP/6-31G(d) Geometry

C 0	0.537598	-1.089933	1.024657
C 0	0.973304	0.167329	1.190354
C 0	1.244603	0.746872	-0.191669
C 0	-0.140305	0.954415	-0.911687
C 0	0.508691	-1.371186	-0.471059
C 0	-0.653697	-0.497135	-1.082867
C 0	1.724229	-0.528910	-0.930330
C 0	-1.958192	-0.559768	-0.304226
O 0	-2.674071	-1.515000	-0.139857
C 0	-1.263010	1.657946	-0.121431
O 0	-2.238139	0.658202	0.238031
H 0	0.160992	-1.764358	1.786101
H 0	1.036191	0.720840	2.121571
H 0	1.897640	1.622348	-0.229171
H 0	0.022720	1.450068	-1.873196
H 0	0.468217	-2.419957	-0.768495
H 0	-0.841753	-0.785695	-2.121571
H 0	2.674071	-0.911515	-0.544527
H 0	1.789737	-0.408221	-2.018749
H 0	-1.776085	2.419957	-0.717070
H 0	-0.911700	2.119928	0.805990

P-57+CP

B3LYP/6-31G(d) Geometry

C 0	-1.482205	1.180368	0.868098
C 0	-1.645346	-0.116812	1.165576
C 0	-1.599179	-0.897998	-0.140771
C 0	-0.121025	-0.860005	-0.676628
C 0	-1.329210	1.288740	-0.643988
C 0	0.068819	0.670350	-0.996646
C 0	-2.255165	0.132680	-1.092696
C 0	1.241734	1.359263	-0.310501
O 0	1.190787	2.534631	0.005371
C 0	0.968670	-1.439142	0.231177
C 0	2.509348	0.539362	-0.051477
C 0	2.352237	-0.977618	-0.251776
H 0	-1.366166	2.009303	1.557133
H 0	-1.698838	-0.560893	2.154631

H 0	-2.029783	-1.902853	-0.117761
H 0	-0.094970	-1.417371	-1.622421
H 0	-1.496953	2.276251	-1.075181
H 0	0.256367	0.790436	-2.075017
H 0	-3.307122	0.319595	-0.856631
H 0	-2.156535	-0.126157	-2.154631
H 0	0.905244	-2.534631	0.241212
H 0	0.820231	-1.101031	1.266031
H 0	2.804902	0.765274	0.980948
H 0	3.307122	0.951791	-0.683959
H 0	2.470086	-1.238205	-1.312873
H 0	3.151001	-1.503862	0.284107

P-58+CP

B3LYP/6-31G(d) Geometry

C 0	-1.489774	-0.890125	-1.582432
C 0	-1.669031	0.437253	-1.530131
C 0	-1.620178	0.847474	-0.063579
C 0	-0.137346	0.688024	0.435373
C 0	-1.317090	-1.386654	-0.151562
C 0	0.091580	-0.874005	0.340119
C 0	-2.260600	-0.402992	0.582628
C 0	1.213032	-1.294548	-0.616497
O 0	1.153492	-2.341792	-1.236094
C 0	0.912070	1.536001	-0.295330
C 0	2.452421	-0.401179	-0.729937
C 0	2.321294	0.974807	-0.061016
C 0	0.476781	-1.490247	1.707162
H 0	-1.375252	-1.510068	-2.464139
H 0	-1.742665	1.123562	-2.367815
H 0	-2.059204	1.818985	0.180447
H 0	-0.108846	0.967804	1.497548
H 0	-1.471083	-2.455378	0.005476
H 0	-3.308032	-0.539353	0.297264
H 0	-2.178051	-0.425213	1.675390
H 0	0.846136	2.578231	0.041904
H 0	0.709031	1.539598	-1.375328
H 0	2.639203	-0.288882	-1.805751
H 0	3.308032	-0.968157	-0.339833
H 0	2.510532	0.898169	1.018586
H 0	3.084998	1.653501	-0.459163
H 0	-0.283162	-1.270075	2.464139
H 0	1.430412	-1.093875	2.077114
H 0	0.573565	-2.578231	1.621814

P-59+CP

B3LYP/6-31G(d) Geometry

C 0	1.272300	-1.793523	0.790951
C 0	1.620525	-0.609113	1.313614
C 0	1.800726	0.368030	0.157768
C 0	0.364459	0.682250	-0.445151
C 0	1.233072	-1.628647	-0.722606
C 0	-0.013645	-0.723677	-1.059090
C 0	2.371920	-0.602062	-0.907273
C 0	-1.331083	-1.388847	-0.659505
O 0	-1.556095	-2.536657	-1.001874
C 0	-0.646266	1.179311	0.615609
C 0	-2.351098	-0.609903	0.164693
C 0	-2.101303	0.900826	0.215047
C 0	0.471217	1.751699	-1.551659
H 0	0.981700	-2.693680	1.322622
H 0	1.676725	-0.347731	2.365617
H 0	2.380861	1.268775	0.378445
H 0	1.263635	-2.546650	-1.310126
H 0	-0.072001	-0.634834	-2.153522
H 0	3.348817	-1.005156	-0.624046
H 0	2.433348	-0.184112	-1.917376
H 0	-0.495183	2.253844	0.782843
H 0	-0.461060	0.684578	1.576544
H 0	-2.294610	-1.023786	1.183244
H 0	-3.348817	-0.865144	-0.210014
H 0	-2.325769	1.353787	-0.759939
H 0	-2.788180	1.365307	0.932838
H 0	1.135864	1.445681	-2.365617
H 0	0.855648	2.693680	-1.141190
H 0	-0.508344	1.962770	-1.997517

P-60+CP

B3LYP/6-31G(d) Geometry

C 0	1.263646	-1.980412	0.246356
C 0	1.559568	-1.007903	1.120553
C 0	1.727730	0.282084	0.332299
C 0	0.280691	0.720021	-0.175362
C 0	1.226125	-1.353994	-1.141288
C 0	-0.056916	-0.452329	-1.192979
C 0	2.321387	-0.273938	-0.983611
C 0	-1.353918	-1.213772	-0.925623
O 0	-1.447909	-2.388942	-1.227841
C 0	-0.795155	0.888034	0.921904
C 0	-2.535848	-0.470025	-0.303646
C 0	-2.198273	0.904161	0.299913
C 0	0.398568	1.994968	-0.900705
N 0	0.488268	3.008652	-1.462333
H 0	0.998129	-3.008652	0.463630
H 0	1.592107	-1.081144	2.202525
H 0	2.264017	1.093451	0.828540
H 0	1.301831	-2.041570	-1.983497
H 0	-0.164907	-0.031916	-2.202525
H 0	3.316641	-0.703364	-0.840469
H 0	2.349670	0.457090	-1.799358
H 0	-0.604560	1.805642	1.489313
H 0	-0.713226	0.046977	1.620945
H 0	-2.941144	-1.144479	0.460803
H 0	-3.316641	-0.391254	-1.071943
H 0	-2.245543	1.687960	-0.466428
H 0	-2.946308	1.167874	1.055672

P-61+CP

B3LYP/6-31G(d) Geometry

C 0	-1.679368	0.008880	1.198540
C 0	-1.964070	-1.018552	0.386773
C 0	-1.751183	-0.542911	-1.045961
C 0	-0.208879	-0.353130	-1.265656
C 0	-1.281080	1.193898	0.321084
C 0	0.113148	0.811239	-0.260334
C 0	-2.186343	0.937271	-0.907565
C 0	1.179817	0.496108	0.800577
O 0	1.066994	0.910074	1.936864
C 0	0.694933	-1.577786	-1.080191
C 0	2.370489	-0.357711	0.370856
C 0	2.160268	-1.134925	-0.941952
Cl 0	0.862902	2.253902	-1.167250
H 0	-1.624749	0.010134	2.280483
H 0	-2.214047	-2.033950	0.676825
H 0	-2.230500	-1.134199	-1.830359
H 0	-0.053852	0.027605	-2.280483

H	0	-1.302644	2.175165	0.793084
H	0	-3.247698	1.047683	-0.668405
H	0	-1.935817	1.554984	-1.776530
H	0	0.573294	-2.253902	-1.935384
H	0	0.398601	-2.141350	-0.184518
H	0	2.560029	-1.040690	1.207564
H	0	3.247698	0.299093	0.311942
H	0	2.429612	-0.506943	-1.800371
H	0	2.831873	-2.000703	-0.964604

P-62+CP

B3LYP/6-31G(d) Geometry

C	0	-1.179317	-2.066185	-0.728185
C	0	-1.549427	-1.159621	-1.643207
C	0	-1.787502	0.152911	-0.912982
C	0	-0.366774	0.710415	-0.448593
C	0	-1.158367	-1.369675	0.626267
C	0	0.079161	-0.389647	0.632485
C	0	-2.327987	-0.376081	0.433567
C	0	1.378060	-1.117440	0.253492
O	0	1.524709	-2.295242	0.523699
C	0	0.663092	0.888418	-1.590773
C	0	2.513147	-0.322728	-0.394079
C	0	2.084082	1.011092	-1.028309
C	0	-0.570602	2.028952	0.170703
C	0	0.340529	0.174623	2.049768
N	0	-0.735240	3.085524	0.626209
H	0	-0.853625	-3.085524	-0.898600
H	0	-1.597612	-1.288415	-2.719373
H	0	-2.380183	0.904652	-1.438468
H	0	-1.184049	-2.022842	1.499316
H	0	-3.290983	-0.882234	0.324507
H	0	-2.408490	0.391295	1.210535
H	0	0.397134	1.765031	-2.191690
H	0	0.606261	0.012386	-2.248213
H	0	2.953897	-0.991363	-1.142880
H	0	3.290983	-0.176607	0.367519
H	0	2.116364	1.825267	-0.293364
H	0	2.786759	1.286869	-1.822342
H	0	-0.545442	0.672092	2.453209
H	0	1.154930	0.907089	2.056381
H	0	0.613087	-0.647625	2.719373

P-63+CP

B3LYP/6-31G(d) Geometry

C	0	-1.348258	-1.815868	-1.083321
C	0	-1.616261	-0.647905	-1.683159
C	0	-1.703349	0.414996	-0.596084
C	0	-0.246900	0.680184	-0.023662
C	0	-1.258750	-1.547545	0.413601
C	0	0.074241	-0.732453	0.665392
C	0	-2.320038	-0.433115	0.542265
C	0	1.273282	-1.489022	0.067753
O	0	1.301434	-2.707415	0.081948
C	0	0.781226	1.033226	-1.123921
C	0	2.467906	-0.707743	-0.481462
C	0	2.223938	0.796337	-0.657479
C	0	-0.307624	1.868178	0.960788
C	0	0.389705	-0.664704	2.180504
H	0	-1.131055	-2.769477	-1.550680
H	0	-1.673453	-0.454618	-2.749758
H	0	-2.223363	1.337361	-0.871670
H	0	-1.354458	-2.420874	1.060496
H	0	-3.326600	-0.788362	0.302243
H	0	-2.342027	0.062109	1.518167
H	0	0.641396	2.077804	-1.431112
H	0	0.605244	0.417527	-2.015181
H	0	2.710223	-1.176551	-1.443611
H	0	3.326600	-0.913905	0.171353
H	0	2.411115	1.329289	0.283423
H	0	2.936385	1.204908	-1.383939
H	0	-1.020256	1.717322	1.775522
H	0	-0.618532	2.769477	0.418853
H	0	0.665204	2.083185	1.415748
H	0	-0.445026	-0.246225	2.749758
H	0	1.275184	-0.054502	2.393110
H	0	0.580677	-1.675939	2.554324

P-64+CP

B3LYP/6-31G(d) Geometry

C	0	1.241738	-1.481764	0.085345
C	0	0.004025	-1.129725	-0.752094
O	0	1.483193	-0.490157	1.101431
C	0	2.548633	-1.374170	-0.717420
C	0	2.014469	0.584794	0.359412
C	0	-0.119765	0.402339	-1.084403
O	0	2.872319	0.020894	-0.633433
C	0	-1.402178	-1.446170	-0.124849
C	0	0.862630	1.309071	-0.348892
C	0	-1.570112	-0.634512	1.152656
C	0	-2.291171	-0.621085	-1.089189
C	0	-1.624392	0.721696	-0.714581
O	0	0.744549	2.517328	-0.314415
C	0	-1.720446	0.650293	0.802608
H	0	1.128866	-2.444506	0.591817
H	0	0.074917	-1.700349	-1.687098
H	0	2.444676	-1.656546	-1.769564
H	0	3.350467	-1.966920	-0.259830
H	0	2.570036	1.257637	1.017377
H	0	0.035230	0.575659	-2.156718
H	0	-1.608907	-2.517328	-0.047672
H	0	-1.476674	-1.034116	2.156718
H	0	-3.350467	-0.652020	-0.817752
H	0	-2.172146	-0.899270	-2.143915
H	0	-1.999464	1.630816	-1.185626
H	0	-1.767007	1.512414	1.458808

P-65+CP

B3LYP/6-31G(d) Geometry

C	0	-1.251695	-1.486168	-0.041521
C	0	0.005374	-0.870729	0.589069
O	0	-1.485574	-0.958675	-1.361238
C	0	-2.548444	-1.050532	0.657815
C	0	-1.972070	0.333739	-1.084863
C	0	0.156379	0.686832	0.366988
O	0	-2.836042	0.217684	0.049679
C	0	1.382733	-1.428437	0.079642
C	0	-0.794881	1.240409	-0.702136
C	0	1.527273	-1.119803	-1.405569
C	0	2.321487	-0.349635	0.670705
C	0	1.663795	0.798434	-0.128599
O	0	-0.647073	2.336894	-1.204444
C	0	1.715067	0.201181	-1.527945
C	0	-0.080139	1.507286	1.652012
H	0	-1.162198	-2.572031	-0.137650

H 0	-0.046937	-1.072936	1.667523
H 0	-2.444533	-0.917106	1.738734
H 0	-3.368495	-1.750277	0.454786
H 0	-2.515573	0.724738	-1.948449
H 0	1.563128	-2.465726	0.376621
H 0	1.397211	-1.842015	-2.204166
H 0	3.368495	-0.502178	0.392851
H 0	2.245195	-0.247198	1.759560
H 0	2.073308	1.803266	-0.013994
H 0	1.763249	0.779504	-2.443923
H 0	0.614164	1.206281	2.443923
H 0	-1.102448	1.376306	2.023238
H 0	0.067852	2.572031	1.445475

P-66+CP

B3LYP/6-31G(d) Geometry

C 0	1.224003	-0.827744	0.438465
C 0	0.021343	-0.725417	-0.542104
O 0	1.458970	0.422377	1.116448
C 0	2.604953	-1.004927	-0.214139
C 0	2.075934	1.200432	0.118639
C 0	-0.066457	0.687443	-1.239965
O 0	2.951765	0.330641	-0.604942
C 0	-1.383526	-0.779064	0.198487
C 0	1.007087	1.701789	-0.858733
C 0	-1.429164	0.306313	1.267172
C 0	-2.296318	-0.119736	-0.868774
C 0	-1.515525	1.209900	-0.851925
O 0	1.012130	2.837807	-1.289195
C 0	-1.516691	1.488211	0.643340
C 0	0.106948	-1.885197	-1.557611
H 0	1.028269	-1.580521	1.208045
H 0	2.634368	-1.647569	-1.094402
H 0	3.324606	-1.376703	0.526649
H 0	2.629862	2.025552	0.573468
H 0	-0.019996	0.576918	-2.330476
H 0	-1.647832	-1.788585	0.528083
H 0	-1.301450	0.134750	2.330476
H 0	-3.324606	-0.002183	-0.515003
H 0	-2.305748	-0.619076	-1.842662
H 0	-1.857004	2.017830	-1.500321
H 0	-1.470291	2.475493	1.090224
H 0	0.303719	-2.837807	-1.048345
H 0	0.902362	-1.728208	-2.293068
H 0	-0.825451	-2.003798	-2.114686

P-67+CP

B3LYP/6-31G(d) Geometry

C 0	-1.253495	0.559535	0.690831
C 0	0.003024	0.602817	-0.232702
O 0	-1.535508	-0.791186	1.069116
C 0	-2.566270	0.931888	-0.017099
C 0	-2.135614	-1.323585	-0.094901
C 0	0.052954	-0.589512	-1.278263
O 0	-2.953726	-0.298161	-0.647641
C 0	1.403345	0.422353	0.513038
C 0	-1.034069	-1.650461	-1.109475
C 0	1.399830	-0.917064	1.232610
C 0	2.295784	0.080394	-0.705548
C 0	1.500718	-1.195255	-1.055384
O 0	-1.017056	-2.689236	-1.735626
C 0	1.482819	-1.878444	0.303199
C 0	0.026015	1.905891	-0.910675
N 0	0.041687	2.950235	-1.420545
H 0	-1.077872	1.135383	1.602523
H 0	-2.470047	1.710986	-0.775787
H 0	-3.325603	1.226981	0.716808
H 0	-2.725963	-2.206797	0.160159
H 0	-0.028632	-0.203771	-2.300123
H 0	1.671892	1.297915	1.108091
H 0	1.259348	-1.042723	2.300123
H 0	3.325603	-0.139307	-0.411684
H 0	2.290845	0.845217	-1.489440
H 0	1.835432	-1.795052	-1.901779
H 0	1.421396	-2.950235	0.456157

P-68+CP

B3LYP/6-31G(d) Geometry

C 0	1.269920	-1.061756	-1.037254
C 0	-0.010591	-0.237785	-1.228578
O 0	1.506342	-1.336154	0.356184
C 0	2.544993	-0.276452	-1.394290
C 0	1.994995	-0.099382	0.826969
C 0	-0.172478	0.923886	-0.180582
O 0	2.860759	0.413480	-0.175528
C 0	-1.380994	-0.987729	-1.086349
C 0	0.809623	0.860724	1.008864
C 0	-1.505743	-1.524384	0.335971
C 0	-2.326374	0.236709	-1.001178
C 0	-1.668252	0.779774	0.286657
O 0	0.634035	1.490141	2.027601
C 0	-1.693358	-0.476959	1.149708
Cl 0	0.098557	2.561757	-0.977057
H 0	1.202630	-2.023810	-1.552595
H 0	0.023912	0.196249	-2.233084
H 0	2.401081	0.453885	-2.195320
H 0	3.370581	-0.949621	-1.653703
H 0	2.529316	-0.239657	1.769576
H 0	-1.561922	-1.703671	-1.892555
H 0	-1.371217	-2.561757	0.621584
H 0	-3.370581	-0.045583	-0.841630
H 0	-2.251411	0.915621	-1.857403
H 0	-2.059986	1.692225	0.734137
H 0	-1.727625	-0.475260	2.233084

P-69+CP

B3LYP/6-31G(d) Geometry

C 0	1.270092	0.534023	-1.235500
C 0	-0.024291	0.582725	-0.365526
O 0	1.571056	-0.814600	-1.602836
C 0	2.550502	0.909785	-0.473307
C 0	2.109814	-1.344058	-0.409994
C 0	-0.104322	-0.568415	0.749031
O 0	2.910079	-0.320198	0.175412
C 0	-1.377394	0.342122	-1.177012
C 0	0.962577	-1.659816	0.554501
C 0	-1.328238	-1.033466	-1.823851
C 0	-2.331968	0.057832	0.005993
C 0	-1.545743	-1.187243	0.467321
O 0	0.906439	-2.714818	1.152454
C 0	-1.458087	-1.943628	-0.849676
C 0	-0.099903	1.933101	0.208533
C 0	0.018346	-0.069395	2.202562
N 0	-0.147402	3.021812	0.612560
H 0	1.130166	1.110156	-2.153237
H 0	2.419354	1.690488	0.278447

H 0	3.342066	1.203865	-1.172518
H 0	2.705355	-2.232988	-0.630222
H 0	-1.619306	1.181788	-1.832562
H 0	-1.133901	-1.213697	-2.874848
H 0	-3.342066	-0.191507	-0.329858
H 0	-2.382688	0.867474	0.741175
H 0	-1.926624	-1.744043	1.324307
H 0	-1.388847	-3.021812	-0.940039
H 0	-0.778190	0.636984	2.452398
H 0	0.978832	0.425280	2.378547
H 0	-0.048974	-0.929466	2.874848

P-70+CP

B3LYP/6-31G(d) Geometry

C 0	-1.247130	-0.927836	-0.722103
C 0	0.019925	-0.778006	0.162924
O 0	-1.483427	0.240368	-1.528611
C 0	-2.585678	-0.972493	0.036607
C 0	-2.000704	1.152163	-0.592258
C 0	0.160824	0.681063	0.805737
O 0	-2.874193	0.413803	0.267732
C 0	1.364342	-0.869757	-0.678674
C 0	-0.860010	1.699886	0.269807
C 0	1.366279	0.190827	-1.772895
C 0	2.360501	-0.214517	0.310776
C 0	1.613124	1.132901	0.315020
O 0	-0.779900	2.885134	0.527995
C 0	1.532373	1.381965	-1.183216
C 0	0.007992	-1.947481	1.174544
C 0	0.065725	0.734909	2.343937
H 0	-1.129197	-1.773134	-1.406991
H 0	-2.569002	-1.492497	0.995160
H 0	-3.365758	-1.413614	-0.596995
H 0	-2.540360	1.953682	-1.102535
H 0	1.582438	-1.891804	-1.004026
H 0	1.165596	-0.000778	-2.821185
H 0	3.365758	-0.127950	-0.111760
H 0	2.426656	-0.698291	1.289461
H 0	2.019970	1.944156	0.920903
H 0	1.490712	2.361324	-1.647202
H 0	-0.223055	-2.885134	0.652083
H 0	-0.734440	-1.821921	1.966613
H 0	0.975945	-2.085123	1.660702
H 0	0.837944	0.124160	2.821185
H 0	-0.912094	0.392835	2.699822
H 0	0.192852	1.771207	2.669806

TS-1+CH

B3LYP/6-31G(d) Geometry

C 0	0.331026	-1.351324	0.774833
C 0	0.908767	-0.216113	1.371979
C 0	1.450834	0.765034	0.541886
C 0	0.374896	-1.480444	-0.598319
C 0	2.185232	0.320708	-0.714493
C 0	1.512373	-0.900450	-1.406504
H 0	-0.322853	-1.992820	1.359451
H 0	0.705390	0.002557	2.417643
H 0	1.830567	1.676670	1.001027
H 0	-0.224550	-2.248467	-1.081966
H 0	3.205223	0.049339	-0.413960
H 0	2.289809	1.158278	-1.413385
H 0	2.259548	-1.695328	-1.541996
H 0	1.172081	-0.650426	-2.417643
C 0	-0.286807	1.554548	-0.348966
C 0	-1.003426	0.561486	-1.026216
C 0	-2.211531	0.028612	-0.493867
N 0	-3.205223	-0.401172	-0.059048
H 0	0.299526	2.248467	-0.944546
H 0	-0.719735	1.982166	0.548890
H 0	-0.841846	0.396376	-2.086143

TS-2+CH

B3LYP/6-31G(d) Geometry

C 0	0.567178	-0.943566	1.172556
C 0	1.391318	0.194972	1.231646
C 0	1.734163	0.830927	0.036460
C 0	0.221272	-1.451373	-0.063008
C 0	2.016328	-0.019763	-1.193749
C 0	1.161633	-1.321117	-1.237965
H 0	0.054088	-1.286467	2.067965
H 0	1.529019	0.710209	2.179656
H 0	2.306462	1.755632	0.096241
H 0	-0.562886	-2.200238	-0.140997
H 0	3.080194	-0.287179	-1.171743
H 0	1.873271	0.573782	-2.103985
H 0	0.610385	-1.404546	-2.179656
H 0	1.830427	-2.193723	-1.209646
C 0	-0.122653	1.621185	-0.525023
C 0	-1.005206	0.597081	-0.876161
C 0	-2.134224	0.223998	-0.028686
O 0	-3.080194	-0.468401	-0.374257
H 0	0.343319	2.200238	-1.318305
H 0	-0.333966	2.193388	0.375029
H 0	-1.034537	0.219573	-1.894608
H 0	-2.083862	0.643719	1.004182

TS-3+CH

B3LYP/6-31G(d) Geometry

C 0	1.428321	-1.313914	1.057986
C 0	2.418103	-0.337197	1.286364
C 0	2.894207	0.416834	0.204539
C 0	1.063591	-1.614861	-0.232438
C 0	3.048076	-0.273706	-1.146463
C 0	1.988912	-1.386390	-1.397600
H 0	0.848719	-1.703246	1.891020
H 0	2.621111	-0.008994	2.303212
H 0	3.660310	1.160319	0.420675
H 0	0.172176	-2.210670	-0.415014
H 0	4.051317	-0.715676	-1.168929
H 0	3.026569	0.469673	-1.951146
H 0	1.406645	-1.192162	-2.303212
H 0	2.499822	-2.342987	-1.584210
C 0	1.346832	1.655864	-0.099737
C 0	0.296765	1.000086	-0.766037
C 0	-0.858380	0.516399	-0.100529
O 0	-1.842059	0.024684	-0.712049
B 0	-3.040946	-0.669691	0.061211
H 0	1.950542	2.342987	-0.689218
H 0	1.166521	2.005933	0.913210
H 0	0.313600	0.902218	-1.847756
H 0	-0.912075	0.582766	0.993904
H 0	-2.892502	-1.855154	-0.179649
H 0	-4.051317	-0.220171	-0.429942
H 0	-2.892137	-0.398187	1.241311

TS-4+CH

B3LYP/6-31G(d) Geometry

C 0	-0.166123	0.310655	1.414059
C 0	-0.675505	-0.976408	1.140150
C 0	-1.270677	-1.208707	-0.100345
C 0	-0.281261	1.294464	0.460306
C 0	-2.081214	-0.077687	-0.717237
C 0	-1.393515	1.306329	-0.560558
H 0	0.499179	0.450797	2.260747
H 0	-0.396822	-1.807228	1.782126
H 0	-1.631377	-2.213009	-0.316523
H 0	0.291616	2.213009	0.568163
H 0	-3.051874	-0.060525	-0.205064
H 0	-2.297512	-0.286744	-1.770664
H 0	-1.019702	1.681468	-1.520270
H 0	-2.138143	2.046639	-0.235516
C 0	0.392491	-1.203200	-1.352557
C 0	1.143444	-0.045812	-1.193082
N 0	2.272216	-0.061718	-0.319097
O 0	2.398318	-1.027333	0.454619
O 0	3.051874	0.900560	-0.364076
H 0	-0.197354	-1.288380	-2.260747
H 0	0.821188	-2.123602	-0.975544
H 0	1.119205	0.821115	-1.835719

TS-5+CH

B3LYP/6-31G(d) Geometry

C 0	-0.532232	0.848972	1.079975
C 0	-1.148836	-0.398327	1.286826
C 0	-1.632832	-1.089741	0.185333
C 0	-0.437663	1.333922	-0.212813
C 0	-2.249149	-0.312307	-0.963575
C 0	-1.533166	1.046979	-1.218577
H 0	0.066027	1.291237	1.871949
H 0	-1.021973	-0.907521	2.239522
H 0	-2.000583	-2.105511	0.319982
H 0	0.174523	2.209978	-0.408769
H 0	-3.299754	-0.124119	-0.704869
H 0	-2.271578	-0.923056	-1.873066
H 0	-1.138953	1.103032	-2.239522
H 0	-2.267086	1.860639	-1.142204
C 0	0.295428	-1.536052	-0.844225
C 0	0.965832	-0.343070	-1.070156
C 0	2.222768	-0.044298	-0.318642
F 0	3.299754	-0.656537	-0.884473
F 0	2.168938	-0.471571	0.964754
F 0	2.527166	1.277620	-0.294568
H 0	-0.246188	-2.004521	-1.658950
H 0	0.650517	-2.209978	-0.073221
H 0	0.926474	0.131944	-2.045006

TS-6+CH

B3LYP/6-31G(d) Geometry

C 0	-0.816328	-0.421293	1.596756
C 0	-1.703046	-1.268245	0.912980
C 0	-2.183150	-0.869638	-0.338681
C 0	-0.525787	0.821047	1.063668
C 0	-2.487417	0.603540	-0.575532
C 0	-1.567600	1.553943	0.245511
H 0	-0.232682	-0.809285	2.427553
H 0	-1.811042	-2.303090	1.229903
H 0	-2.829894	-1.561613	-0.876213
H 0	0.243647	1.436078	1.523534
H 0	-3.532407	0.774495	-0.286893
H 0	-2.428060	0.830966	-1.645998
H 0	-1.096226	2.303090	-0.397322
H 0	-2.183389	2.121437	0.959405
C 0	-0.471063	-1.074229	-1.518394
C 0	0.405725	-0.030336	-1.205581
B 0	1.635542	-0.094764	-0.284526
C 0	2.100599	-1.448743	0.413710
C 0	2.603144	1.167373	-0.173284
H 0	-1.068598	-1.009451	-2.427553
H 0	-0.204663	-2.091441	-1.244607
H 0	0.201627	0.911120	-1.721096
H 0	2.927154	-1.876669	-0.176372
H 0	2.511562	-1.284247	1.418857
H 0	1.331737	-2.226417	0.487508
H 0	3.532407	0.959475	-0.727178
H 0	2.189504	2.096726	-0.585453
H 0	2.921800	1.365221	0.859826

TS-7+CH

B3LYP/6-31G(d) Geometry

C 0	0.449098	-0.480937	-1.637391
C 0	1.267241	-1.302517	-0.840605
C 0	1.754611	-0.803954	0.372434
C 0	0.234065	0.824963	-1.258158
C 0	2.135000	0.669168	0.455818
C 0	1.253420	1.583899	-0.443819
H 0	-0.145074	-0.923266	-2.431752
H 0	1.314194	-2.369395	-1.044905
H 0	2.374770	-1.468033	0.972824
H 0	-0.517820	1.419215	-1.771456
H 0	3.182417	0.752468	0.140273
H 0	2.106340	1.005247	1.498404
H 0	0.764497	2.369395	0.139856
H 0	1.896752	2.113369	-1.162564
C 0	0.073005	-0.851047	1.535550
C 0	-0.816169	0.160371	1.142128
B 0	-2.054974	-0.034999	0.305690
Cl 0	-2.548103	-1.644446	-0.310589
Cl 0	-3.182417	1.322614	-0.008121
H 0	0.670198	-0.688617	2.431752
H 0	-0.223794	-1.885436	1.388166
H 0	-0.632572	1.157664	1.538406

TS-8+CH

B3LYP/6-31G(d) Geometry

C 0	-1.491613	1.347077	-0.440436
C 0	-2.063362	0.727424	0.685308
C 0	-1.724086	-0.608740	0.957566
C 0	-0.763290	0.592169	-1.331892
C 0	-1.584267	-1.562049	-0.226042
C 0	-0.987819	-0.884504	-1.492964
H 0	-1.494994	2.431576	-0.520988
H 0	-2.527445	1.337589	1.456983
H 0	-2.173935	-1.059003	1.842267
H 0	-0.166054	1.086551	-2.094526
H 0	-2.588755	-1.940131	-0.451928
H 0	-0.984307	-2.431576	0.060427
H 0	-0.057372	-1.371538	-1.799873
H 0	-1.676920	-1.012990	-2.341175
C 0	0.137368	-0.421589	1.628447
C 0	1.086651	-0.164584	0.623461
C 0	1.629140	1.163202	0.352096

O 0	2.588755	1.431963	-0.350536
Cl 0	1.935592	-1.513824	-0.121069
H 0	0.172645	-1.405567	2.089542
H 0	-0.018941	0.382834	2.341175
H 0	1.069935	1.956313	0.897420

TS-9+CH

B3LYP/6-31G(d) Geometry

C 0	-0.963618	-1.550431	0.479840
C 0	-1.700955	-1.144962	-0.645173
C 0	-1.744445	0.223528	-0.948648
C 0	-0.433613	-0.588871	1.315598
C 0	-1.875679	1.208817	0.205861
C 0	-1.115097	0.746153	1.482624
H 0	-0.660713	-2.589930	0.582645
H 0	-1.981300	-1.878159	-1.398044
H 0	-2.269840	0.519320	-1.856128
H 0	0.292458	-0.871725	2.074051
H 0	-2.944233	1.304277	0.435178
H 0	-1.543530	2.204264	-0.109175
H 0	-0.398913	1.501901	1.816860
H 0	-1.830009	0.638561	2.311772
C 0	0.167547	0.568088	-1.563118
C 0	1.105629	0.524899	-0.515338
C 0	1.934602	-0.670425	-0.344408
O 0	2.944233	-0.726251	0.346162
C 0	1.587697	1.770407	0.187220
H 0	-0.068288	1.546774	-1.978790
H 0	0.212473	-0.217870	-2.311772
H 0	1.594377	-1.557809	-0.924616
H 0	0.865737	2.589930	0.117632
H 0	2.524731	2.112716	-0.273282
H 0	1.821314	1.582501	1.239351

TS-10+CH

B3LYP/6-31G(d) Geometry

C 0	-0.260890	-2.315742	0.204373
C 0	0.050357	-1.418480	1.240895
C 0	0.849964	-0.302592	0.940070
C 0	0.215742	-2.070886	-1.065002
C 0	1.975983	-0.541611	-0.060156
C 0	1.498469	-1.314492	-1.314385
H 0	-1.043353	-3.053504	0.356345
H 0	-0.491431	-1.476223	2.180077
H 0	1.110393	0.355807	1.768357
H 0	-0.184767	-2.636585	-1.904179
H 0	2.742662	-1.132586	0.457416
H 0	2.458294	0.398241	-0.344064
H 0	2.270284	-2.042060	-1.606672
H 0	1.387467	-0.651774	-2.180077
C 0	-0.387153	0.967425	-0.022440
C 0	-1.014747	0.297155	-1.094398
C 0	-2.247999	-0.412212	-0.858194
O 0	-2.739044	-0.575769	0.261354
C 0	0.496166	2.169006	-0.310120
H 0	-1.042650	1.092953	0.836613
H 0	-0.672355	0.425634	-2.117895
H 0	-2.742662	-0.842378	-1.756293
H 0	1.094434	2.034671	-1.217635
H 0	-0.134943	3.053504	-0.463652
H 0	1.176721	2.397791	0.517621

TS-11+CH

B3LYP/6-31G(d) Geometry

C 0	0.492386	-1.831429	-0.543040
C 0	-0.656900	-1.639243	-1.318522
C 0	-1.733005	-0.958915	-0.753621
C 0	0.508399	-1.317594	0.755513
C 0	-2.044342	-1.141970	0.716194
C 0	-0.764594	-1.347179	1.577991
H 0	1.416575	-2.160841	-1.011628
H 0	-0.621286	-1.813584	-2.391542
H 0	-2.570220	-0.671060	-1.385758
H 0	1.442460	-1.318696	1.312463
H 0	-2.684732	-2.030098	0.796560
H 0	-2.645914	-0.304994	1.082454
H 0	-0.711968	-0.616938	2.391542
H 0	-0.803517	-2.332089	2.062218
C 0	-0.690331	1.072013	-0.554549
C 0	0.418208	0.872965	0.295918
C 0	1.783681	0.914326	-0.257415
O 0	2.790220	1.095470	0.401210
C 0	-1.838418	1.781296	-0.090957
N 0	-2.790220	2.332089	0.295409
H 0	-0.506351	1.158940	-1.622164
H 0	0.336437	1.147977	1.343610
H 0	1.838957	0.753268	-1.358765

TS-12+CH

B3LYP/6-31G(d) Geometry

C 0	-1.719413	-1.606397	-0.158169
C 0	-2.592796	-0.886082	-1.000492
C 0	-2.813758	0.482338	-0.769212
C 0	-1.210934	-1.017219	0.972238
C 0	-2.821118	0.951512	0.684081
C 0	-1.789180	0.220240	1.586197
H 0	-1.355185	-2.582794	-0.466363
H 0	-2.913564	-1.332231	-1.939393
H 0	-3.565317	0.961076	-1.396241
H 0	-0.405680	-1.510728	1.512837
H 0	-3.833578	0.761214	1.061605
H 0	-2.672076	2.033764	0.737767
H 0	-0.972534	0.888269	1.884222
H 0	-2.264366	-0.075804	2.533409
C 0	-1.224978	1.281374	-1.626270
C 0	-0.072821	1.246804	-0.812064
C 0	0.841981	0.166054	-0.814080
O 0	1.862422	0.092112	-0.083609
B 0	2.665783	-1.273149	0.029215
Cl 0	0.247964	2.582794	0.277478
H 0	-1.671286	2.260350	-1.782125
H 0	-1.179596	0.686763	-2.533409
H 0	0.643007	-0.649219	-1.518832
H 0	2.253887	-1.756714	1.073265
H 0	3.833578	-0.970982	0.086771
H 0	2.358649	-1.935553	-0.948244

TS-13+CH

B3LYP/6-31G(d) Geometry

C 0	-1.494618	-1.935985	-0.217976
C 0	-2.421385	-1.328526	-1.086283
C 0	-2.826790	-0.005623	-0.834434
C 0	-1.123746	-1.292209	0.938881
C 0	-3.019287	0.400786	0.623624
C 0	-1.986508	-0.247315	1.588973

H 0	-0.962438	-2.830081	-0.532531
H 0	-2.619061	-1.778502	-2.056527
H 0	-3.569028	0.412214	-1.513824
H 0	-0.272114	-1.659351	1.507357
H 0	-4.030023	0.084461	0.908719
H 0	-3.005926	1.491362	0.717724
H 0	-1.357668	0.505917	2.073264
H 0	-2.517196	-0.741830	2.416568
C 0	-1.262593	1.025787	-1.461236
C 0	-0.182454	1.027993	-0.545296
C 0	0.853316	0.062239	-0.681697
O 0	1.891356	0.075785	0.035041
B 0	2.939379	-1.112980	-0.006261
C 0	-0.002739	2.116990	0.482425
H 0	-1.807036	1.964528	-1.557852
H 0	-1.107631	0.533542	-2.416568
H 0	0.770767	-0.712788	-1.451588
H 0	2.739909	-1.714130	1.036006
H 0	4.030023	-0.589542	-0.037435
H 0	2.672427	-1.774549	-0.996187
H 0	-0.927307	2.677719	0.650237
H 0	0.758722	2.830081	0.138206
H 0	0.362052	1.726462	1.437154

TS-14+CH

B3LYP/6-31G(d) Geometry

C 0	1.146028	-2.144885	0.953118
C 0	2.325662	-1.468192	1.303109
C 0	2.965121	-0.668372	0.337233
C 0	0.731768	-2.135668	-0.361545
C 0	2.986500	-1.181318	-1.099982
C 0	1.702245	-1.962876	-1.497765
H 0	0.484167	-2.523573	1.727804
H 0	2.592879	-1.364005	2.352359
H 0	3.889643	-0.183869	0.647690
H 0	-0.275388	-2.462741	-0.610513
H 0	3.857292	-1.841142	-1.191155
H 0	3.163204	-0.352936	-1.794032
H 0	1.196283	-1.504233	-2.352359
H 0	1.975721	-2.974797	-1.833428
C 0	1.785868	0.931206	0.298241
C 0	0.637514	0.620842	-0.473519
C 0	-0.611821	0.265903	0.085795
O 0	-1.656021	0.120886	-0.606957
B 0	-2.975268	-0.491771	0.021705
C 0	2.736874	1.994831	-0.235001
H 0	1.600341	1.034012	1.366401
H 0	0.669177	0.747896	-1.553464
H 0	-0.692985	0.130096	1.171636
H 0	-2.995501	-1.636615	-0.402276
H 0	-3.889643	0.175760	-0.404620
H 0	-2.838770	-0.439888	1.233676
H 0	2.247833	2.974797	-0.187599
H 0	3.004306	1.815118	-1.281821
H 0	3.658219	2.054226	0.352394

TS-15+CH

B3LYP/6-31G(d) Geometry

C 0	0.769244	-1.963405	0.677248
C 0	1.919616	-1.535455	1.347544
C 0	2.840192	-0.733315	0.652470
C 0	0.626476	-1.648133	-0.668186
C 0	3.103275	-1.040148	-0.812568
C 0	1.832518	-1.530299	-1.564278
H 0	-0.074871	-2.361061	1.235015
H 0	1.977980	-1.619358	2.430175
H 0	3.695020	-0.344334	1.202067
H 0	-0.339426	-1.782289	-1.149137
H 0	3.869146	-1.824358	-0.837959
H 0	3.547096	-0.169535	-1.304991
H 0	1.606340	-0.901120	-2.430175
H 0	2.010707	-2.535232	-1.973505
C 0	1.722988	1.035798	0.500769
C 0	0.612127	0.827079	-0.359039
C 0	-0.707886	0.657633	0.156865
O 0	-1.724025	0.674597	-0.572310
B 0	-3.179967	0.336274	-0.002939
C 0	2.787002	1.882419	0.033827
N 0	3.669755	2.535232	-0.351434
H 0	1.510812	1.159344	1.559999
H 0	0.703380	1.039300	-1.419073
H 0	-0.845058	0.495709	1.234399
H 0	-3.473788	-0.690696	-0.581134
H 0	-3.869146	1.273366	-0.330405
H 0	-3.040055	0.202493	1.199831

TS-16+CH

B3LYP/6-31G(d) Geometry

C 0	0.892683	-1.412299	-0.835190
C 0	1.235476	-1.513963	0.532317
C 0	1.245552	-0.359209	1.329333
C 0	0.718002	-0.182238	-1.411063
C 0	1.683008	0.945553	0.662420
C 0	1.188537	1.100687	-0.799891
H 0	0.648716	-2.311548	-1.393340
H 0	1.277012	-2.495739	0.998253
H 0	1.611458	-0.479114	2.349195
H 0	0.301889	-0.121612	-2.414771
H 0	2.780238	0.948812	0.678176
H 0	1.366566	1.804785	1.263155
H 0	2.001529	1.492771	-1.428767
H 0	0.390622	1.850556	-0.879462
C 0	-0.636952	-0.126219	1.782165
C 0	-1.511015	0.090087	0.682353
C 0	-2.216919	-1.003728	0.108691
C 0	-1.783268	1.400347	0.216292
N 0	-2.780238	-1.930744	-0.321899
N 0	-1.952059	2.495739	-0.153433
H 0	-0.459203	0.741431	2.414771
H 0	-0.801254	-1.040876	2.343988

TS-17+CH

B3LYP/6-31G(d) Geometry

C 0	-0.459817	0.700527	1.235613
C 0	-0.459876	-0.700676	1.235536
C 0	-0.789373	-1.363433	0.056849
C 0	-0.789307	1.363437	0.057012
C 0	-1.838384	-0.778683	-0.866118
C 0	-1.838430	0.778849	-0.865929
H 0	0.016349	1.240650	2.049097
H 0	0.016225	-1.240930	2.048970
H 0	-0.647347	-2.440509	0.002171
H 0	-0.647211	2.440509	0.002443
H 0	-2.813738	-1.142118	-0.517146
H 0	-1.722571	-1.176378	-1.880446
H 0	-2.813740	1.142137	-0.516681

H 0	-1.722825	1.176795	-1.880181
C 0	0.989350	-0.705957	-1.185936
C 0	0.989332	0.705992	-1.185922
C 0	2.006018	-1.459477	-0.518023
C 0	2.006005	1.459532	-0.518039
N 0	2.813735	2.103129	0.019333
N 0	2.813740	-2.103060	0.019378
H 0	0.556200	-1.201490	-2.049097
H 0	0.556135	1.201525	-2.049061

TS-18+CH

B3LYP/6-31G(d) Geometry

C 0	-0.187508	-1.459485	1.254780
C 0	0.721272	-1.643979	0.204411
C 0	0.368629	-1.183147	-1.065209
C 0	-1.424831	-0.894875	0.972349
C 0	-1.073327	-1.269891	-1.527361
C 0	-2.090921	-1.182678	-0.353631
H 0	0.149429	-1.559534	2.283869
H 0	1.754684	-1.898771	0.421631
H 0	1.122175	-1.197152	-1.850135
H 0	-2.080876	-0.606973	1.790905
H 0	-1.190381	-2.232292	-2.041876
H 0	-1.277917	-0.504122	-2.283869
H 0	-2.870845	-0.444257	-0.558347
H 0	-2.606858	-2.145881	-0.242301
C 0	0.379305	0.985014	-0.620850
C 0	-0.592368	1.225425	0.378439
C 0	1.764407	1.145191	-0.291347
C 0	-1.849946	1.793825	0.026607
N 0	-2.891382	2.232292	-0.260807
N 0	2.891382	1.264662	-0.024430
H 0	0.124912	1.224926	-1.649339
H 0	-0.261167	1.420572	1.391841

TS-19+CH

B3LYP/6-31G(d) Geometry

C 0	0.064146	-2.307964	0.379203
C 0	0.748783	-1.527049	1.322955
C 0	1.505543	-0.448806	0.863133
C 0	0.178840	-1.978757	-0.961795
C 0	2.277603	-0.631922	-0.432921
C 0	1.457248	-1.391054	-1.514260
H 0	-0.719281	-2.986155	0.705820
H 0	0.494271	-1.611379	2.377000
H 0	1.973506	0.204767	1.597943
H 0	-0.492904	-2.442419	-1.680981
H 0	3.177791	-1.211109	-0.189581
H 0	2.635354	0.328769	-0.814433
H 0	1.239532	-0.751209	-2.377000
H 0	2.061133	-2.218949	-1.911603
C 0	-0.046734	0.891355	0.197093
C 0	-0.842455	0.203915	-0.739676
C 0	0.770910	2.086191	-0.251365
C 0	-2.125117	-0.299611	-0.378545
N 0	-3.177791	-0.702524	-0.077433
H 0	-0.469517	0.991057	1.192822
H 0	-0.697770	0.396007	-1.799563
H 0	1.140964	1.966864	-1.275076
H 0	0.142088	2.986155	-0.236903
H 0	1.627805	2.279407	0.402900

TS-20+CH

B3LYP/6-31G(d) Geometry

C 0	0.566250	-1.638652	-0.709676
C 0	1.166001	-1.625573	0.561560
C 0	1.436037	-0.384439	1.149867
C 0	0.374745	-0.445060	-1.372593
C 0	1.949092	0.736936	0.255631
C 0	1.303611	0.723349	-1.160523
H 0	0.082198	-2.543339	-1.067437
H 0	1.158598	-2.527641	1.168794
H 0	1.842356	-0.379928	2.160773
H 0	-0.250464	-0.421487	-2.262556
H 0	3.034285	0.606222	0.160997
H 0	1.804389	1.707343	0.744532
H 0	0.788870	1.665136	-1.375072
H 0	2.096634	0.652276	-1.919241
C 0	-0.453118	0.290227	1.581803
C 0	-1.254634	0.479111	0.439560
C 0	-2.221316	-0.522011	0.114127
C 0	-1.506442	1.856102	-0.145131
N 0	-3.034285	-1.317649	-0.147206
H 0	-0.093401	1.190577	2.076792
H 0	-0.714873	-0.512190	2.262556
H 0	-0.695813	2.543339	0.116142
H 0	-1.609936	1.839200	-1.234962
H 0	-2.436664	2.278572	0.258982

TS-21+CH

B3LYP/6-31G(d) Geometry

C 0	2.067079	-0.658903	-0.540518
C 0	1.051907	-1.252883	-1.304778
C 0	-0.176936	-1.500555	-0.694619
C 0	1.802934	-0.339456	0.785430
C 0	-0.168262	-1.961548	0.751546
C 0	0.873512	-1.196043	1.615729
H 0	2.948840	-0.253359	-1.030871
H 0	1.146879	-1.292576	-2.387685
H 0	-1.002246	-1.857525	-1.303683
H 0	2.497804	0.296131	1.329206
H 0	0.089751	-3.028520	0.734384
H 0	-1.165285	-1.896225	1.189807
H 0	0.384193	-0.594068	2.387685
H 0	1.498717	-1.919716	2.156719
C 0	-0.825863	0.604238	-0.432909
C 0	0.112129	1.275016	0.361314
C 0	1.091115	2.197503	-0.226295
O 0	1.724701	3.028520	0.401100
C 0	-2.223699	0.441524	0.094245
F 0	-2.948840	1.566987	-0.113103
F 0	-2.252784	0.197270	1.427018
F 0	-2.907626	-0.561616	-0.508844
H 0	-0.827950	0.809200	-1.500122
H 0	-0.077922	1.412005	1.421187
H 0	1.223022	2.089968	-1.327652

TS-22+CH

B3LYP/6-31G(d) Geometry

C 0	0.447469	-2.055383	0.946246
C 0	1.560480	-1.308920	1.348699
C 0	2.234011	-0.539315	0.388652
C 0	0.108764	-2.084111	-0.399604
C 0	2.396914	-1.113385	-1.012407
C 0	1.200927	-2.007902	-1.445800

H 0	-0.240384	-2.446622	1.691232
H 0	1.740138	-1.134641	2.407259
H 0	3.074678	0.062346	0.730936
H 0	-0.812554	-2.572598	-0.706494
H 0	3.317179	-1.711413	-1.016094
H 0	2.561787	-0.306859	-1.734591
H 0	0.790827	-1.684903	-2.407259
H 0	1.558099	-3.036589	-1.604183
C 0	0.883811	1.016859	0.064612
C 0	-0.137443	0.462908	-0.730307
B 0	-1.508881	-0.061347	-0.284549
C 0	-2.018480	0.045088	1.222925
C 0	-2.576757	-0.486987	-1.393227
C 0	1.811580	2.075539	-0.511067
H 0	0.637702	1.192792	1.110450
H 0	0.075149	0.477781	-1.804344
H 0	-2.688532	0.916592	1.299470
H 0	-2.625654	-0.819062	1.524745
H 0	-1.234505	0.183914	1.976269
H 0	-3.317179	0.320332	-1.509175
H 0	-2.150221	-0.667992	-2.388522
H 0	-3.158240	-1.374464	-1.106451
H 0	1.284270	3.036589	-0.565225
H 0	2.132233	1.827780	-1.529269
H 0	2.704566	2.229866	0.104593

TS-23+CH

B3LYP/6-31G(d) Geometry

C 0	0.255482	-1.330623	1.326408
C 0	1.260402	-0.357220	1.421614
C 0	1.876664	0.099356	0.246341
C 0	-0.027291	-1.882826	0.092212
C 0	2.138446	-0.912468	-0.862888
C 0	1.041355	-2.009729	-0.965750
H 0	-0.409620	-1.503951	2.167197
H 0	1.381929	0.199332	2.347886
H 0	2.653949	0.853344	0.359196
H 0	-0.905066	-2.512888	-0.026687
H 0	3.104997	-1.384286	-0.647008
H 0	2.264473	-0.400093	-1.822250
H 0	0.588587	-2.034442	-1.961273
H 0	1.502437	-2.999625	-0.829254
C 0	0.430638	1.308866	-0.542581
C 0	-0.559584	0.463906	-1.091675
B 0	-1.888285	0.120713	-0.476808
Cl 0	-2.424924	0.785080	1.103221
Cl 0	-3.104997	-0.836552	-1.389276
C 0	1.267654	2.172612	-1.474800
H 0	0.149175	1.823525	0.374031
H 0	-0.377166	0.111185	-2.107571
H 0	0.651474	2.999625	-1.848305
H 0	1.620540	1.613158	-2.347886
H 0	2.134437	2.611950	-0.970263

TS-24+CH

B3LYP/6-31G(d) Geometry

C 0	1.036808	1.302740	0.314111
C 0	0.036956	1.165152	1.292865
C 0	-1.234861	0.776053	0.900349
C 0	0.729581	0.974340	-1.002173
C 0	-1.761916	1.190135	-0.452960
C 0	-0.660404	1.217193	-1.550606
H 0	2.072211	1.419228	0.620061
H 0	0.315069	1.153906	2.343340
H 0	-1.970912	0.504110	1.653296
H 0	1.534265	0.917045	-1.731961
H 0	-2.181661	2.197077	-0.323426
H 0	-2.599425	0.557948	-0.759323
H 0	-0.888176	0.499354	-2.343340
H 0	-0.645143	2.204273	-2.030723
C 0	-0.562683	-1.409389	0.278261
C 0	0.455819	-1.240212	-0.651588
N 0	1.813750	-1.493137	-0.204863
O 0	2.039816	-1.486058	1.009879
O 0	2.662704	-1.671360	-1.080778
N 0	-1.870194	-1.820167	-0.179152
O 0	-2.662704	-2.204273	0.684230
O 0	-2.132279	-1.741491	-1.386765
H 0	-0.366223	-1.686633	1.301186
H 0	0.313322	-1.433405	-1.704462

TS-25+CH

B3LYP/6-31G(d) Geometry

C 0	0.050309	-1.660357	1.224886
C 0	0.783357	-0.466185	1.278921
C 0	1.459318	-0.047539	0.144353
C 0	0.005852	-2.360075	0.011539
C 0	2.040739	-1.045960	-0.828187
C 0	1.260508	-2.391582	-0.845313
H 0	-0.652760	-1.900025	2.017643
H 0	0.636954	0.217397	2.110445
H 0	1.867157	0.959918	0.104959
H 0	-0.627700	-3.240981	-0.056481
H 0	3.079041	-1.231040	-0.518390
H 0	2.110436	-0.607605	-1.829029
H 0	1.899413	-3.187244	-0.442095
H 0	1.015803	-2.692096	-1.869314
C 0	-0.564231	0.184563	-1.239140
C 0	-1.186290	-1.081278	-1.140819
C 0	-0.913550	1.392647	-0.514169
C 0	-2.521116	-1.463587	-0.529317
O 0	-3.079041	-2.466264	-0.930136
O 0	-3.026876	-0.740717	0.471528
O 0	-1.650329	1.496157	0.471591
O 0	-0.308563	2.496041	-1.019535
H 0	0.055554	0.361584	-2.110445
H 0	-1.037095	-1.704654	-2.017945
H 0	-2.514733	0.100915	0.609953
H 0	-0.612339	3.240981	-0.468554

TS-26+CH

B3LYP/6-31G(d) Geometry

C 0	-0.527471	-1.112543	1.388783
C 0	0.019694	-1.987043	0.435993
C 0	-0.265394	-1.767548	-0.926975
C 0	-1.443721	-0.162514	0.994001
C 0	-1.665667	-1.278519	-1.285903
C 0	-2.265544	-0.287574	-0.251067
H 0	-0.117470	-1.087087	2.394159
H 0	0.828965	-2.654350	0.718869
H 0	0.155944	-2.480853	-1.634307
H 0	-1.715900	0.631667	1.686017
H 0	-2.298242	-2.171886	-1.350749
H 0	-1.667814	-0.833610	-2.286758
H 0	-3.265913	-0.626504	0.056832
H 0	-2.426095	0.704695	-0.688178

C 0	0.904921	-0.230365	-1.356196
C 0	0.605482	0.954137	-0.601262
C 0	2.223817	-0.808357	-1.227639
C 0	1.367329	1.321331	0.544800
C 0	-0.290485	1.910512	-1.145019
N 0	1.997156	1.613211	1.481395
N 0	-1.061931	2.654350	-1.608278
N 0	3.265913	-1.315220	-1.142103
H 0	0.576864	-0.182039	-2.394159

TS-27+CH

B3LYP/6-31G(d) Geometry

C 0	0.642413	-0.035494	1.466188
C 0	1.021816	1.095841	0.725532
C 0	1.221437	0.940709	-0.652552
C 0	0.626370	-1.265637	0.839084
C 0	1.920051	-0.318797	-1.145384
C 0	1.597834	-1.566731	-0.274310
H 0	0.183260	0.086078	2.443734
H 0	0.890996	2.087420	1.151089
H 0	1.442590	1.834727	-1.235077
H 0	0.163024	-2.114689	1.336541
H 0	3.000124	-0.128258	-1.120168
H 0	1.672831	-0.498545	-2.198489
H 0	1.237738	-2.398381	-0.887270
H 0	2.523389	-1.932293	0.193783
C 0	-0.707589	0.616828	-1.323342
C 0	-1.200419	-0.620377	-0.840350
C 0	-2.179395	-0.618535	0.202322
C 0	-1.195243	-1.866719	-1.708820
N 0	-3.000124	-0.637427	1.032120
C 0	-1.408164	1.913779	-0.965695
H 0	-0.360118	0.569033	-2.356336
H 0	-0.385570	-1.827791	-2.443734
H 0	-1.090122	-2.786369	-1.124265
H 0	-2.139079	-1.947314	-2.265865
H 0	-0.808184	2.786369	-1.244714
H 0	-2.368190	1.983041	-1.494078
H 0	-1.624868	1.969596	0.104609

TS-28+CH

B3LYP/6-31G(d) Geometry

C 0	-0.495466	-2.069434	-0.328268
C 0	-1.107020	-1.244440	-1.282502
C 0	-1.403782	0.075103	-0.918714
C 0	-0.290235	-1.570946	0.946597
C 0	-1.936362	0.320076	0.485064
C 0	-1.259454	-0.587281	1.552185
H 0	0.001613	-2.982854	-0.642593
H 0	-1.097625	-1.534310	-2.330716
H 0	-1.815489	0.731826	-1.684109
H 0	0.349090	-2.118501	1.635761
H 0	-3.013497	0.111952	0.462488
H 0	-1.845076	1.377573	0.752044
H 0	-0.768260	0.004917	2.330716
H 0	-2.031208	-1.167962	2.077904
C 0	0.519091	0.913714	-0.806454
C 0	1.278078	0.252958	0.196561
C 0	0.200537	2.392506	-0.683235
C 0	2.219733	-0.730253	-0.242067
C 0	1.606095	0.894537	1.532659
N 0	3.013497	-1.510073	-0.594525
H 0	0.768658	0.624062	-1.822616
H 0	-0.207846	2.666649	0.293701
H 0	1.115916	2.982854	-0.825374
H 0	-0.516111	2.710871	-1.447047
H 0	0.765982	1.472688	1.925835
H 0	1.884520	0.146141	2.280666
H 0	2.455053	1.586311	1.433318

TS-29+CH

B3LYP/6-31G(d) Geometry

C 0	-0.600432	-1.253189	1.353985
C 0	0.253540	-1.898513	0.451022
C 0	0.043428	-1.691270	-0.915813
C 0	-1.635841	-0.475853	0.849640
C 0	-1.377187	-1.579827	-1.436851
C 0	-2.335115	-0.888804	-0.424261
H 0	-0.328998	-1.192608	2.404954
H 0	1.184985	-2.336034	0.799555
H 0	0.777160	-2.083179	-1.617304
H 0	-2.204424	0.159550	1.525217
H 0	-1.726639	-2.601120	-1.635356
H 0	-1.390311	-1.067214	-2.404954
H 0	-2.845642	-0.032605	-0.873884
H 0	-3.128411	-1.591095	-0.134694
C 0	0.561671	0.422514	-1.053527
C 0	-0.205700	1.175065	-0.119378
C 0	1.978517	0.305489	-0.864595
C 0	-1.305315	1.923065	-0.644562
N 0	-2.213982	2.527058	-1.056404
N 0	3.128411	0.198522	-0.715660
C 0	0.440044	1.735401	1.136325
H 0	0.259060	0.463372	-2.096142
H 0	1.068296	2.601120	0.890241
H 0	-0.311811	2.057749	1.861193
H 0	1.082974	0.984594	1.602769

TS-30+CH

B3LYP/6-31G(d) Geometry

C 0	0.408633	0.305924	1.509906
C 0	0.430287	1.584238	0.940888
C 0	0.738446	1.693935	-0.418237
C 0	0.758869	-0.778836	0.713487
C 0	1.788962	0.782177	-1.022342
C 0	1.838958	-0.610057	-0.329873
H 0	-0.084897	0.147592	2.464566
H 0	-0.034604	2.416646	1.461199
H 0	0.616633	2.661329	-0.901317
H 0	0.594576	-1.785971	1.090004
H 0	2.759630	1.281382	-0.908733
H 0	1.632280	0.684894	-2.102742
H 0	1.803591	-1.421285	-1.062316
H 0	2.801175	-0.725186	0.187408
C 0	-1.022229	0.686303	-1.244818
C 0	-1.067549	-0.655010	-0.776440
C 0	-2.011110	1.647878	-0.853334
C 0	-2.031234	-1.013381	0.226402
N 0	-2.801175	-1.361120	1.028164
N 0	-2.795178	2.454746	-0.554797
C 0	-0.707780	-1.785391	-1.729806
H 0	-0.662940	0.822042	-2.262425
H 0	0.033283	-1.458003	-2.464566
H 0	-0.316540	-2.661329	-1.203911
H 0	-1.601080	-2.106652	-2.280342

TS-31+CH

B3LYP/6-31G(d) Geometry

C	0	0.634224	-1.901425	0.598452
C	0	0.587278	-0.715160	1.341676
C	0	0.834198	0.494755	0.676596
C	0	0.955947	-1.827813	-0.747333
C	0	1.942578	0.486611	-0.366834
C	0	1.912098	-0.779654	-1.266152
H	0	0.204442	-2.811479	1.006707
H	0	0.142863	-0.720099	2.333247
H	0	0.759147	1.413701	1.256276
H	0	0.814806	-2.704502	-1.376273
H	0	2.893075	0.514535	0.181384
H	0	1.920428	1.397546	-0.971058
H	0	2.915119	-1.229871	-1.293462
H	0	1.678006	-0.530856	-2.306942
C	0	-0.916846	0.750097	-0.460309
C	0	-0.971182	-0.368389	-1.335343
C	0	-1.949360	0.887759	0.653700
C	0	-1.826674	-1.536920	-1.194818
O	0	-2.480335	-1.871584	-0.211505
C	0	-0.608570	2.089587	-1.124621
H	0	-0.557444	-0.239804	-2.333247
H	0	-1.657694	1.674895	1.359067
H	0	-2.915119	1.179947	0.218427
H	0	-2.106498	-0.049109	1.183505
H	0	-1.852938	-2.169582	-2.113087
H	0	0.065740	1.991456	-1.980780
H	0	-1.544917	2.527357	-1.496211
H	0	-0.176752	2.811479	-0.421728

TS-32+CH

B3LYP/6-31G(d) Geometry

C	0	-0.202600	-1.438183	0.736566
C	0	0.782287	-0.675341	1.380597
C	0	1.787466	-0.094780	0.633631
C	0	-0.206212	-1.480651	-0.675516
C	0	2.224035	-0.631728	-0.695872
C	0	1.155836	-1.539513	-1.363050
H	0	-1.066343	-1.789569	1.295789
H	0	0.660942	-0.409257	2.426672
H	0	2.424577	0.657293	1.094000
H	0	-0.977743	-2.084040	-1.151216
H	0	3.146458	-1.206250	-0.525272
H	0	2.523356	0.195789	-1.349019
H	0	1.056436	-1.300720	-2.426672
H	0	1.479070	-2.586482	-1.313302
C	0	-0.131886	1.376427	-0.680787
C	0	-0.904018	0.279312	-1.189563
C	0	-2.333004	0.127306	-0.756266
O	0	-3.146458	-0.499422	-1.401216
C	0	0.832202	2.005692	-1.512835
C	0	-0.513066	2.053628	0.516231
N	0	1.642916	2.468334	-2.213730
N	0	-0.849233	2.586482	1.497866
H	0	-0.784172	0.100556	-2.257010
H	0	-2.600753	0.607626	0.206101

TS-33+CH

B3LYP/6-31G(d) Geometry

C	0	0.040198	-0.695715	-1.962385
C	0	0.040212	0.695636	-1.962427
C	0	-0.685255	1.357667	-0.959366
C	0	-0.685289	-1.357671	-0.959289
C	0	-1.996223	0.777086	-0.487148
C	0	-1.996253	-0.777031	-0.487129
H	0	0.752533	-1.241745	-2.573789
H	0	0.752556	1.241615	-2.573866
H	0	-0.563422	2.432598	-0.848601
H	0	-0.563485	-2.432598	-0.848463
H	0	-2.764829	1.151349	-1.176160
H	0	-2.257444	1.179018	0.495944
H	0	-2.764845	-1.151281	-1.176163
H	0	-2.257526	-1.178928	0.495963
C	0	0.625515	0.728822	0.772218
C	0	0.625478	-0.728769	0.772264
C	0	-0.121344	1.413676	1.789402
C	0	1.818976	1.413792	0.349467
C	0	1.818909	-1.413828	0.349574
C	0	-0.121425	-1.413517	1.789488
N	0	2.764753	-1.986991	-0.010176
N	0	-0.761971	-1.986811	2.573866
N	0	2.764845	1.986882	-0.010332
N	0	-0.761853	1.987053	2.573749

TS-34+CH

B3LYP/6-31G(d) Geometry

C	0	-0.638388	-1.210827	1.814640
C	0	0.016760	-2.044998	0.902337
C	0	-0.174166	-1.812488	-0.479421
C	0	-1.529378	-0.263446	1.342746
C	0	-1.588564	-1.434952	-0.907612
C	0	-2.270084	-0.423651	0.051078
H	0	-0.315864	-1.184365	2.851248
H	0	0.829326	-2.681489	1.240398
H	0	0.334962	-2.494849	-1.158414
H	0	-1.863071	0.529469	2.008725
H	0	-2.161035	-2.370510	-0.921849
H	0	-1.600488	-1.062255	-1.935020
H	0	-2.413284	0.556697	-0.417728
H	0	-3.284458	-0.769753	0.298952
C	0	0.955118	-0.195293	-0.815840
C	0	0.510619	0.916249	0.005517
C	0	2.252992	-0.743866	-0.458019
C	0	1.162001	1.237655	1.232124
C	0	-0.340558	1.908155	-0.548386
N	0	1.697835	1.497041	2.234598
N	0	-1.079412	2.681489	-1.016983
N	0	3.284458	-1.226433	-0.226274
C	0	0.830141	-0.025672	-2.335703
H	0	-0.131031	0.413116	-2.608753
H	0	1.616545	0.651017	-2.686319
H	0	0.951209	-0.981662	-2.851248

TS-35+CH

B3LYP/6-31G(d) Geometry

C	0	0.093774	-1.314495	1.248598
C	0	1.224865	-0.604189	1.651958
C	0	2.046663	-0.049830	0.677473
C	0	-0.193017	-1.380040	-0.136993
C	0	2.215445	-0.690513	-0.670812
C	0	1.012759	-1.595518	-1.045456
H	0	-0.650491	-1.615381	1.981557
H	0	1.346291	-0.319130	2.692814
H	0	2.787792	0.692248	0.965844
H	0	-1.089642	-1.922019	-0.432698

H	0	3.133971	-1.293508	-0.631327
H	0	2.409478	0.076910	-1.427843
H	0	0.739480	-1.470325	-2.095406
H	0	1.294706	-2.649267	-0.928563
C	0	0.177606	1.450243	-0.171951
C	0	-0.817093	0.488295	-0.606285
C	0	-2.072570	0.405889	0.223890
O	0	-3.133971	0.024117	-0.220980
C	0	0.997199	2.109984	-1.133403
C	0	0.055852	2.116664	1.089375
C	0	-1.091586	0.387692	-2.099602
N	0	1.691603	2.599405	-1.932932
N	0	-0.052363	2.649267	2.120729
H	0	-1.964171	0.691751	1.288298
H	0	-0.176676	0.424326	-2.692814
H	0	-1.717773	1.234051	-2.403513
H	0	-1.647451	-0.522280	-2.335205

TS-36+CH

B3LYP/6-31G(d) Geometry

C	0	-0.996511	-1.629252	-1.381496
C	0	-1.712028	-0.427110	-1.374463
C	0	-1.683296	0.345936	-0.198095
C	0	-0.429491	-2.071676	-0.195134
C	0	-1.826573	-0.400168	1.122937
C	0	-1.121496	-1.785834	1.113114
H	0	-0.736481	-2.105422	-2.324387
H	0	-2.037850	0.014020	-2.312767
H	0	-2.193982	1.308223	-0.224604
H	0	0.284189	-2.891525	-0.209264
H	0	-2.899834	-0.541686	1.300606
H	0	-1.468938	0.215183	1.953891
H	0	-0.423283	-1.888453	1.948232
H	0	-1.870230	-2.578266	1.258974
C	0	0.271391	1.036691	-0.172150
C	0	1.112698	-0.063979	0.199582
C	0	1.942332	-0.778141	-0.781651
O	0	2.899834	-1.488415	-0.490870
C	0	0.126706	2.164654	0.848639
C	0	0.401323	1.613855	-1.582557
C	0	1.578077	-0.248540	1.627312
H	0	1.672824	-0.635860	-1.845660
H	0	1.080149	2.703020	0.941711
H	0	-0.143974	1.821097	1.849163
H	0	-0.625745	2.891525	0.524614
H	0	0.354965	0.857743	-2.366895
H	0	1.360195	2.140521	-1.685875
H	0	-0.395780	2.341600	-1.773236
H	0	0.784232	-0.117930	2.366895
H	0	2.360901	0.486420	1.867497
H	0	2.029625	-1.235192	1.750617

TS-37+CH

B3LYP/6-31G(d) Geometry

C	0	-0.794157	1.188269	1.239667
C	0	-1.965118	0.610574	1.710743
C	0	-2.912974	0.180827	0.762735
C	0	-0.644283	1.338099	-0.154220
C	0	-3.153795	1.017167	-0.472571
C	0	-1.866216	1.742893	-0.949724
H	0	0.055461	1.335917	1.901699
H	0	-2.041917	0.290419	2.745379
H	0	-3.751023	-0.423761	1.102019
H	0	0.317612	1.664377	-0.542911
H	0	-3.920551	1.757081	-0.209470
H	0	-3.595476	0.404562	-1.264396
H	0	-1.701451	1.605724	-2.020655
H	0	-1.973735	2.825937	-0.802712
C	0	-1.698844	-1.437932	-0.170927
C	0	-0.555659	-0.802935	-0.806898
C	0	0.737219	-0.903714	-0.144084
O	0	1.794297	-0.669014	-0.755198
C	0	-2.735833	-1.957156	-1.022236
C	0	-1.497514	-2.217291	1.026525
C	0	-0.511155	-0.686442	-2.316701
N	0	-3.599030	-2.327614	-1.709470
N	0	-1.336542	-2.825937	2.004690
H	0	0.790071	-1.158182	0.920247
H	0	-1.494281	-0.485824	-2.745379
H	0	-0.155365	-1.633242	-2.741468
H	0	0.191049	0.088607	-2.630912
B	0	3.227845	-0.590871	-0.013232
H	0	3.543300	0.568155	-0.177578
H	0	3.920551	-1.365843	-0.626064
H	0	3.004560	-0.893686	1.141668

TS-38+CH

B3LYP/6-31G(d) Geometry

C	0	-0.728198	-1.558802	1.561888
C	0	0.218401	-2.089379	0.680877
C	0	0.133897	-1.729429	-0.667567
C	0	-1.682643	-0.678602	1.050142
C	0	-1.241127	-1.593415	-1.286707
C	0	-2.261765	-0.920737	-0.326301
H	0	-0.576863	-1.642101	2.634993
H	0	1.113281	-2.570206	1.065981
H	0	0.938728	-2.026492	-1.336652
H	0	-2.317820	-0.127316	1.740439
H	0	-1.577963	-2.610582	-1.527095
H	0	-1.189671	-1.067724	-2.243878
H	0	-2.656042	0.012506	-0.739608
H	0	-3.131322	-1.578671	-0.198885
C	0	0.655411	0.456367	-0.500560
C	0	-0.210711	1.005547	0.505203
C	0	0.531683	0.890705	-1.957282
C	0	2.018539	0.210524	-0.105396
C	0	-1.240255	1.897407	0.060138
N	0	-2.098266	2.610582	-0.278642
N	0	3.131322	0.014581	0.177497
C	0	0.333561	1.319054	1.892519
H	0	-0.511179	1.048041	-2.239178
H	0	1.057068	1.842265	-2.105824
H	0	0.978349	0.157600	-2.634993
H	0	0.985991	2.200770	1.857164
H	0	-0.475750	1.522870	2.598793
H	0	0.929541	0.484446	2.268424

TS-39+CH

B3LYP/6-31G(d) Geometry

C	0	-0.439893	-0.698253	-1.734964
C	0	-0.440092	0.698156	-1.735008
C	0	-0.730394	1.355488	-0.536898
C	0	-0.729931	-1.355556	-0.536756
C	0	-1.791511	0.777743	0.373713
C	0	-1.791310	-0.778053	0.373722
H	0	0.014371	-1.239762	-2.559462

H 0	0.014012	1.239742	-2.559545
H 0	-0.584404	2.432301	-0.483298
H 0	-0.583739	-2.432340	-0.483127
H 0	-2.760380	1.142379	0.007603
H 0	-1.695806	1.178488	1.387070
H 0	-1.695635	-1.178756	1.387103
H 0	-2.760033	-1.142944	0.007487
C 0	1.113408	0.718062	0.638134
C 0	1.113476	-0.717902	0.638055
C 0	2.028880	1.392159	-0.245845
C 0	2.029125	-1.391782	-0.245938
N 0	2.760380	-1.992760	-0.924241
N 0	2.760041	1.993290	-0.924120
C 0	0.896221	1.486596	1.936268
C 0	0.896590	-1.486515	1.936211
H 0	0.069532	1.084846	2.525239
H 0	0.693327	2.542130	1.735809
H 0	1.798798	1.436735	2.559545
H 0	0.069746	-1.085079	2.525185
H 0	0.694100	-2.542130	1.735771
H 0	1.799150	-1.436283	2.559476

TS-40+CH

B3LYP/6-31G(d) Geometry

C 0	-0.671982	-1.828930	-1.039034
C 0	-1.001169	-0.578560	-1.576250
C 0	-1.126418	0.501714	-0.691307
C 0	-0.601619	-1.955162	0.340777
C 0	-1.835593	0.251710	0.630745
C 0	-1.545301	-1.162226	1.210206
H 0	-0.274484	-2.610013	-1.681613
H 0	-0.893892	-0.404455	-2.643755
H 0	-1.295794	1.489593	-1.118197
H 0	-0.168343	-2.854834	0.771937
H 0	-2.912420	0.351278	0.444892
H 0	-1.589997	1.033577	1.355450
H 0	-1.173356	-1.107396	2.237579
H 0	-2.484190	-1.730827	1.273087
C 0	0.901894	0.776119	-0.091735
C 0	1.273251	-0.380526	0.665338
C 0	0.764888	2.097920	0.653105
C 0	2.162098	-1.330343	0.065022
C 0	1.360051	-0.364299	2.184248
N 0	2.912420	-2.102619	-0.385367
C 0	1.562512	0.962314	-1.451711
H 0	0.204714	2.027505	1.587598
H 0	1.764649	2.478968	0.906322
H 0	0.281942	2.854834	0.026004
H 0	0.514894	0.153587	2.643755
H 0	1.396467	-1.379702	2.589846
H 0	2.273690	0.151165	2.514028
H 0	1.044113	1.726117	-2.042001
H 0	2.602123	1.293655	-1.319172
H 0	1.590590	0.035245	-2.027314

TS-41+CH

B3LYP/6-31G(d) Geometry

C 0	0.499910	-0.610626	1.270650
C 0	0.875243	0.747556	1.219622
C 0	1.216035	1.298668	-0.013292
C 0	0.619694	-1.373900	0.128963
C 0	1.985753	0.460790	-1.023357
C 0	1.709770	-1.064374	-0.874114
H 0	-0.050221	-0.988105	2.128956
H 0	0.663339	1.395949	2.066242
H 0	1.410214	2.369305	-0.058128
H 0	0.183579	-2.369305	0.097197
H 0	3.056004	0.649457	-0.871300
H 0	1.763735	0.802651	-2.041619
H 0	1.486529	-1.521523	-1.843253
H 0	2.621329	-1.562951	-0.514271
C 0	-0.674377	1.201506	-1.006963
C 0	-0.977198	-0.141583	-1.303392
C 0	-1.847567	1.339385	-0.023938
C 0	-2.155495	-0.137159	-0.412170
O 0	-3.056004	-0.902328	-0.146940
H 0	-0.307577	1.962697	-1.687839
H 0	-0.704229	-0.790493	-2.128956
H 0	-2.642340	2.035479	-0.316628
H 0	-1.583092	1.513497	1.026355

TS-42+CH

B3LYP/6-31G(d) Geometry

C 0	-0.731669	-1.014452	1.403906
C 0	-1.175031	-1.597488	0.199004
C 0	-1.321918	-0.767913	-0.917997
C 0	-0.654701	0.357237	1.489317
C 0	-1.911680	0.623331	-0.724968
C 0	-1.596444	1.216630	0.678584
H 0	-0.297201	-1.638990	2.180716
H 0	-1.143502	-2.677286	0.078416
H 0	-1.585721	-1.243331	-1.862091
H 0	-0.161629	0.819916	2.340979
H 0	-2.999211	0.549745	-0.849552
H 0	-1.562746	1.290649	-1.522337
H 0	-1.220501	2.240596	0.601739
H 0	-2.529101	1.292294	1.256792
C 0	0.638222	-0.236659	-1.300633
C 0	1.136817	0.728081	-0.387603
C 0	1.605195	-1.324748	-0.803411
C 0	2.097753	-0.238077	0.187545
O 0	2.999211	-0.179672	0.998059
C 0	1.200868	2.224968	-0.392994
H 0	0.384457	-0.046658	-2.340979
H 0	2.383461	-1.625294	-1.514824
H 0	1.149721	-2.221783	-0.364988
H 0	0.380194	2.677286	-0.958517
H 0	1.198599	2.642104	0.619902
H 0	2.139886	2.550475	-0.862649

TS-43+CH

B3LYP/6-31G(d) Geometry

C 0	0.516392	-1.874702	0.749722
C 0	0.848380	-0.653385	1.364265
C 0	1.125385	0.444942	0.550647
C 0	0.598147	-1.959471	-0.628845
C 0	1.904817	0.228960	-0.737950
C 0	1.671177	-1.179098	-1.355795
H 0	0.008247	-2.648632	1.319423
H 0	0.651648	-0.512585	2.424378
H 0	1.287976	1.408374	1.030499
H 0	0.175091	-2.820652	-1.140119
H 0	2.970883	0.347690	-0.505871
H 0	1.671754	1.016465	-1.462507
H 0	1.444603	-1.109572	-2.424378

H 0	2.597521	-1.766746	-1.284066
C 0	-0.845327	0.771580	-0.326892
C 0	-1.032200	-0.294052	-1.246432
C 0	-1.938503	0.223825	0.617583
C 0	-2.148012	-0.862538	-0.469978
O 0	-2.970883	-1.738292	-0.632296
C 0	-0.674334	2.240497	-0.626251
H 0	-0.773027	-0.390029	-2.297176
H 0	-2.812666	0.873412	0.752650
H 0	-1.602334	-0.134558	1.597514
H 0	0.113037	2.432916	-1.362409
H 0	-1.610401	2.635953	-1.044258
H 0	-0.450991	2.820652	0.275288

TS-44+CH

B3LYP/6-31G(d) Geometry

C 0	-0.134201	-2.234345	0.535440
C 0	0.641770	-1.415099	1.372647
C 0	1.493481	-0.485223	0.793077
C 0	0.009676	-2.095826	-0.843784
C 0	2.182951	-0.786949	-0.519889
C 0	1.389328	-1.795204	-1.400072
H 0	-0.972754	-2.791079	0.945597
H 0	0.418576	-1.364656	2.435568
H 0	1.971067	0.263946	1.419967
H 0	-0.675643	-2.630278	-1.497829
H 0	3.165647	-1.213205	-0.278722
H 0	2.392315	0.144237	-1.055936
H 0	1.323254	-1.446006	-2.435568
H 0	1.928082	-2.751337	-1.438551
C 0	-0.213593	0.811289	-0.205737
C 0	-0.777774	-0.055391	-1.180259
C 0	-1.463838	0.773072	0.694400
C 0	-2.070293	-0.100989	-0.436726
O 0	-3.165647	-0.562327	-0.642973
C 0	0.674942	1.899345	-0.389188
N 0	1.412781	2.791079	-0.536611
H 0	-0.583540	-0.123093	-2.246063
H 0	-1.983261	1.728568	0.827347
H 0	-1.341318	0.282835	1.667106

TS-45+CH

B3LYP/6-31G(d) Geometry

C 0	-1.302445	-0.917668	1.085589
C 0	-1.704193	-1.139444	-0.251580
C 0	-1.453013	-0.136369	-1.197768
C 0	-0.890737	0.332732	1.468811
C 0	-1.641878	1.318436	-0.772993
C 0	-1.313674	1.569993	0.726630
H 0	-1.193979	-1.760470	1.763890
H 0	-1.976915	-2.141026	-0.573659
H 0	-1.764914	-0.343602	-2.221063
H 0	-0.431243	0.472964	2.444586
H 0	-2.689176	1.580928	-0.966257
H 0	-1.040511	1.975017	-1.411158
H 0	-0.555036	2.350364	0.837120
H 0	-2.205909	1.957851	1.240944
C 0	0.534772	-0.242604	-1.415645
C 0	1.279087	0.400451	-0.398411
C 0	1.101687	-1.609346	-0.980512
C 0	1.869721	-0.836308	0.130542
O 0	2.689176	-1.140528	0.965664
Cl 0	1.813266	2.050702	-0.234420
H 0	0.480122	0.102453	-2.444586
H 0	1.788150	-2.068194	-1.700264
H 0	0.368930	-2.350364	-0.639495

TS-46+CH

B3LYP/6-31G(d) Geometry

C 0	-0.202494	-2.304470	-0.832539
C 0	-0.983497	-1.420538	-1.592027
C 0	-1.550867	-0.321411	-0.946548
C 0	-0.122563	-2.099822	0.541980
C 0	-1.360767	-1.594720	1.255011
C 0	-2.081641	-0.466587	0.466491
H 0	0.474905	-2.996013	-1.326976
H 0	-0.943658	-1.457557	-2.677761
H 0	-2.019039	0.455792	-1.546201
H 0	0.585167	-2.685490	1.123876
H 0	-1.129695	-1.280252	2.275924
H 0	-2.033580	-2.457441	1.354626
H 0	-2.025779	0.495458	0.986969
H 0	-3.151293	-0.701516	0.396005
C 0	0.367444	0.706144	-0.369361
C 0	0.996811	-0.070566	0.657242
C 0	-0.261797	1.969168	-0.198596
C 0	1.441726	0.358822	-1.418967
C 0	2.103988	-0.443251	-0.271929
C 0	1.071376	0.143005	2.141026
O 0	3.151293	-1.034498	-0.153147
N 0	-0.793601	2.996013	-0.046175
H 0	2.059230	1.201686	-1.748945
H 0	1.102023	-0.211446	-2.290965
H 0	1.309855	-0.780629	2.677761
H 0	0.143307	0.557899	2.544586
H 0	1.873610	0.859262	2.362518

TS-47+CH

B3LYP/6-31G(d) Geometry

C 0	-0.777926	-1.850597	-1.009356
C 0	-1.142384	-0.622240	-1.589651
C 0	-1.198153	0.504345	-0.759081
C 0	-0.670903	-1.925088	0.365598
C 0	-1.803032	0.344994	0.630446
C 0	-1.575388	-1.073631	1.224471
H 0	-0.405515	-2.658100	-1.634957
H 0	-1.118787	-0.506486	-2.670299
H 0	-1.403643	1.463571	-1.231767
H 0	-0.216657	-2.799609	0.825139
H 0	-2.880774	0.534075	0.550308
H 0	-1.416182	1.117598	1.304060
H 0	-1.202843	-1.020087	2.251100
H 0	-2.538823	-1.599981	1.289467
C 0	0.827870	0.762686	-0.256199
C 0	1.195834	-0.220167	0.715538
C 0	1.703607	0.096386	-1.340896
C 0	2.075945	-0.921394	-0.237805
O 0	2.880774	-1.828455	-0.161668
C 0	0.800067	2.258109	-0.031761
C 0	1.286367	-0.182273	2.210935
H 0	2.566692	0.692517	-1.664691
H 0	1.185963	-0.294472	-2.225072
H 0	0.136999	2.546319	0.791513
H 0	1.808040	2.612098	0.225578
H 0	0.481825	2.799609	-0.928733

H 0	0.484681	0.404780	2.670299
H 0	1.274122	-1.188051	2.644227
H 0	2.238203	0.278819	2.513242

TS-48+CH

B3LYP/6-31G(d) Geometry

C 0	0.763202	-0.607500	1.248472
C 0	1.082089	0.749283	1.065797
C 0	1.434081	1.179719	-0.216568
C 0	0.900971	-1.468896	0.175673
C 0	2.296528	0.269043	-1.078385
C 0	2.004041	-1.241500	-0.834131
H 0	0.222656	-0.923000	2.137702
H 0	0.818385	1.473274	1.833215
H 0	1.592387	2.246350	-0.371794
H 0	0.477747	-2.468916	0.229000
H 0	3.346205	0.476860	-0.835956
H 0	2.176220	0.525563	-2.137702
H 0	1.782389	-1.760637	-1.772002
H 0	2.907517	-1.724018	-0.435014
C 0	-0.378913	0.947704	-1.278771
C 0	-0.698045	-0.416954	-1.319145
C 0	-1.467640	1.707202	-0.515643
C 0	-1.904452	-0.694569	-0.520427
C 0	-2.263117	0.607964	0.215194
O 0	-2.529590	-1.741452	-0.458866
H 0	0.094466	1.432657	-2.128987
H 0	-0.366360	-1.115206	-2.077711
H 0	-2.108961	2.229845	-1.238253
H 0	-1.065575	2.468916	0.160309
H 0	-1.947449	0.512837	1.262075
H 0	-3.346205	0.760456	0.216521

TS-49+CH

B3LYP/6-31G(d) Geometry

C 0	-0.778398	-0.634955	1.510572
C 0	-1.131051	-1.613391	0.566177
C 0	-1.381812	-1.194473	-0.750962
C 0	-0.840842	0.694600	1.143435
C 0	-2.175644	0.091165	-0.950627
C 0	-1.888766	1.147335	0.155857
H 0	-0.290102	-0.925263	2.437971
H 0	-0.952352	-2.663570	0.783339
H 0	-1.585448	-1.969462	-1.489833
H 0	-0.392631	1.453964	1.779651
H 0	-3.241469	-0.167522	-0.936779
H 0	-1.977377	0.502548	-1.947470
H 0	-1.623457	2.116421	-0.274588
H 0	-2.808518	1.326455	0.731589
C 0	0.450745	-0.594294	-1.421657
C 0	0.885715	0.574931	-0.759570
C 0	1.422448	-1.740769	-1.118888
C 0	1.986064	0.240719	0.168228
C 0	2.176339	-1.281909	0.143616
O 0	2.672530	1.037146	0.793106
C 0	0.757946	1.989099	-1.255988
H 0	0.066242	-0.509459	-2.437971
H 0	2.120275	-1.843052	-1.961092
H 0	0.924882	-2.708569	-0.996602
H 0	1.738811	-1.714253	1.051731
H 0	3.241469	-1.531461	0.147401
H 0	-0.115708	2.132911	-1.898280
H 0	1.645732	2.249178	-1.849805
H 0	0.721076	2.708569	-0.432119

TS-50+CH

B3LYP/6-31G(d) Geometry

C 0	0.576381	-1.882196	0.721645
C 0	0.928700	-0.679478	1.351415
C 0	1.406792	0.364364	0.553735
C 0	0.734867	-1.973075	-0.655714
C 0	2.358471	-0.010358	-0.571766
C 0	1.915219	-1.300279	-1.322032
H 0	-0.025513	-2.617483	1.250190
H 0	0.615359	-0.494838	2.376348
H 0	1.595058	1.327794	1.025165
H 0	0.272441	-2.797908	-1.192633
H 0	3.342289	-0.181220	-0.116030
H 0	2.493769	0.822561	-1.266849
H 0	1.698465	-1.098569	-2.376348
H 0	2.745044	-2.020631	-1.323858
C 0	-0.363066	0.910880	-0.598224
C 0	-0.718149	-0.252318	-1.313187
C 0	-1.431315	1.164214	0.482039
C 0	-1.945474	-0.860010	-0.769164
C 0	-2.264735	-0.128557	0.543944
O 0	-2.610902	-1.755958	-1.264009
C 0	0.193698	2.133490	-1.301533
H 0	-0.434055	-0.437436	-2.343525
H 0	-2.059998	2.004992	0.154590
H 0	-1.004973	1.452707	1.448257
H 0	-1.963146	-0.768660	1.382481
H 0	-3.342289	0.036672	0.635698
H 0	0.851456	1.873042	-2.135568
H 0	0.742834	2.797908	-0.624204
H 0	-0.638882	2.717800	-1.717283

TS-51+CH

B3LYP/6-31G(d) Geometry

C 0	-0.048850	-2.106870	0.499026
C 0	0.663598	-1.258994	1.356878
C 0	1.550177	-0.343061	0.798738
C 0	0.143012	-1.960570	-0.878698
C 0	2.338880	-0.726230	-0.433694
C 0	1.544642	-1.669209	-1.384595
H 0	-0.892459	-2.679974	0.875561
H 0	0.374238	-1.178973	2.402173
H 0	1.988947	0.427896	1.428374
H 0	-0.513580	-2.500991	-1.556965
H 0	3.243968	-1.241120	-0.085059
H 0	2.688592	0.169851	-0.953915
H 0	1.510867	-1.266389	-2.402173
H 0	2.062321	-2.634214	-1.459782
C 0	-0.064955	0.950719	-0.330366
C 0	-0.654421	0.022999	-1.221185
C 0	-1.072358	1.369233	0.758480
C 0	-2.068834	-0.213148	-0.822557
C 0	-2.278508	0.433521	0.552831
O 0	-2.910300	-0.807527	-1.468382
C 0	0.906622	1.900122	-0.761627
N 0	1.706312	2.679974	-1.097117
H 0	-0.382957	-0.037007	-2.269252
H 0	-1.356763	2.415860	0.595776
H 0	-0.649107	1.308199	1.764579
H 0	-3.243968	0.946711	0.579455
H 0	-2.316558	-0.361133	1.307624

TS-52+CH

B3LYP/6-31G(d) Geometry

C 0	-0.953288	-0.782106	1.398620
C 0	-1.323169	-1.366414	0.173764
C 0	-1.354647	-0.546312	-0.970231
C 0	-0.813966	0.585388	1.476773
C 0	-1.926330	0.860950	-0.807859
C 0	-1.593345	1.498294	0.571678
H 0	-0.631178	-1.411452	2.224991
H 0	-1.333220	-2.448876	0.074039
H 0	-1.629121	-1.031187	-1.907503
H 0	-0.344669	1.032397	2.349972
H 0	-3.014269	0.787355	-0.923897
H 0	-1.573229	1.504550	-1.621126
H 0	-1.066876	2.448876	0.451184
H 0	-2.526484	1.744461	1.100002
C 0	0.548785	-0.177323	-1.374234
C 0	1.157784	0.671944	-0.424826
C 0	1.303525	-1.512664	-1.333197
C 0	2.114822	-0.040409	0.437893
C 0	2.016015	-1.520113	0.034217
O 0	2.876519	0.431410	1.263152
Cl 0	1.280881	2.405911	-0.603891
H 0	0.305292	0.239455	-2.349972
H 0	2.043389	-1.517317	-2.143879
H 0	0.650396	-2.378353	-1.483503
H 0	3.014269	-1.966537	0.013815
H 0	1.431963	-2.061666	0.787973

TS-53+CH

B3LYP/6-31G(d) Geometry

C 0	0.079907	-2.197184	-0.846002
C 0	-0.712792	-1.413826	-1.689655
C 0	-1.518257	-0.429105	-1.104184
C 0	-0.018796	-1.987018	0.530915
C 0	-2.219475	-0.740545	0.203914
C 0	-1.392910	-1.704970	1.100884
H 0	0.894048	-2.790593	-1.254741
H 0	-0.528991	-1.411013	-2.761260
H 0	-2.024967	0.285193	-1.750035
H 0	0.703850	-2.460888	1.190962
H 0	-3.179857	-1.209283	-0.045378
H 0	-2.468528	0.187448	0.727264
H 0	-1.325241	-1.336048	2.126868
H 0	-1.906209	-2.673786	1.166963
C 0	0.077919	0.896913	-0.304778
C 0	0.766347	0.160222	0.705932
C 0	1.007950	1.151498	-1.510164
C 0	2.125965	-0.182966	0.197304
C 0	2.215679	0.226928	-1.275855
O 0	3.027030	-0.665553	0.859839
C 0	-0.827452	1.944537	0.056945
C 0	0.606122	0.381481	2.189429
N 0	-1.577712	2.790593	0.339793
H 0	1.319256	2.203051	-1.498786
H 0	0.509270	0.975736	-2.466946
H 0	3.179857	0.707328	-1.465766
H 0	2.174951	-0.671097	-1.902341
H 0	-0.424439	0.609881	2.470877
H 0	0.959433	-0.480973	2.761260
H 0	1.222841	1.237239	2.494082

TS-54+CH

B3LYP/6-31G(d) Geometry

C 0	-0.678716	-1.723435	-1.363796
C 0	-1.077415	-0.442276	-1.766453
C 0	-1.373554	0.496935	-0.761233
C 0	-0.713166	-2.032267	-0.013057
C 0	-2.188682	-0.004389	0.426173
C 0	-1.813169	-1.455417	0.842622
H 0	-0.168220	-2.381121	-2.063298
H 0	-0.909872	-0.120225	-2.791211
H 0	-1.621581	1.507867	-1.083418
H 0	-0.215393	-2.928751	0.348338
H 0	-3.245157	0.025282	0.132475
H 0	-2.097329	0.680737	1.273870
H 0	-1.555016	-1.516147	1.903080
H 0	-2.689396	-2.108233	0.718968
C 0	0.477827	0.896104	0.099944
C 0	0.900151	-0.274238	0.792912
C 0	1.423562	1.113394	-1.098613
C 0	1.986984	-0.946240	0.051132
C 0	2.177861	-0.213812	-1.282543
O 0	2.668906	-1.879159	0.453366
C 0	0.125097	2.161681	0.864662
C 0	0.806994	-0.503150	2.276172
H 0	2.129882	1.912925	-0.833404
H 0	0.898258	1.445455	-2.000188
H 0	1.756879	-0.817771	-2.094143
H 0	3.245157	-0.093114	-1.491849
H 0	-0.581315	1.993917	1.682127
H 0	-0.294774	2.928751	0.204256
H 0	1.037297	2.581555	1.310778
H 0	-0.146136	-0.184253	2.707694
H 0	1.595543	0.065896	2.791211
H 0	0.975963	-1.557220	2.515098

TS-55+CH

B3LYP/6-31G(d) Geometry

C 0	0.290076	-0.701548	1.251250
C 0	0.290077	0.701547	1.251250
C 0	0.667576	1.365713	0.088641
C 0	0.667575	-1.365713	0.088640
C 0	1.753592	0.779115	-0.789851
C 0	1.753592	-0.779115	-0.789851
H 0	-0.216343	-1.241185	2.046966
H 0	-0.216342	1.241184	2.046967
H 0	0.514609	2.440355	0.022554
H 0	0.514609	-2.440355	0.022552
H 0	2.713418	1.142073	-0.399160
H 0	1.679588	1.175137	-1.808156
H 0	1.679589	-1.175137	-1.808156
H 0	2.713418	-1.142072	-0.399159
C 0	-1.025879	0.696916	-1.266148
C 0	-1.025879	-0.696915	-1.266148
C 0	-2.152341	-1.141792	-0.416482
C 0	-2.152341	1.141792	-0.416482
O 0	-2.713418	0.000000	0.167974
O 0	-2.580425	2.242387	-0.193712
O 0	-2.580425	-2.242387	-0.193712
H 0	-0.648460	1.343297	-2.046967
H 0	-0.648461	-1.343296	-2.046967

TS-56+CH

B3LYP/6-31G(d) Geometry

C 0	0.270525	-0.607558	1.244395
C 0	0.624373	0.751388	1.185602
C 0	1.033473	1.278608	-0.038676
C 0	0.426078	-1.380407	0.107565
C 0	1.566380	-1.094208	-0.845464
C 0	1.884355	0.426387	-0.966510
H 0	-0.315275	-0.977040	2.081948
H 0	0.346156	1.413732	2.001779
H 0	1.203842	2.352451	-0.108505
H 0	-0.012734	-2.374370	0.071197
H 0	1.368686	-1.536214	-1.827654
H 0	2.450476	-1.618801	-0.457311
H 0	1.776169	0.769498	-2.002500
H 0	2.935927	0.597059	-0.703844
C 0	-0.798438	1.121728	-1.174971
C 0	-1.118754	-0.229978	-1.281910
C 0	-2.315831	-0.508329	-0.466227
O 0	-2.935927	-1.533293	-0.311874
C 0	-1.902328	1.756508	-0.348003
O 0	-2.665459	0.661744	0.179489
H 0	-0.338814	1.685589	-1.980010
H 0	-0.836470	-0.899481	-2.081948
H 0	-2.559933	2.374370	-0.975797
H 0	-1.556054	2.363289	0.492360

TS-57+CH

B3LYP/6-31G(d) Geometry

C 0	-0.941269	0.519789	1.372285
C 0	-1.234492	-0.791128	0.962392
C 0	-1.563762	-1.005333	-0.380933
C 0	-1.102718	1.546095	0.458182
C 0	-2.225169	1.463237	-0.552043
C 0	-2.449064	0.016192	-1.081255
H 0	-0.398570	0.689945	2.299573
H 0	-0.960836	-1.630402	1.597403
H 0	-1.699169	-2.033429	-0.715159
H 0	-0.691861	2.530732	0.664359
H 0	-2.059818	2.166492	-1.373985
H 0	-3.137161	1.807301	-0.043779
H 0	-2.298146	-0.033037	-2.166406
H 0	-3.493124	-0.273274	-0.909109
C 0	0.248707	-0.570972	-1.375461
C 0	0.495576	0.804394	-1.210044
C 0	1.693115	1.333825	-0.536411
O 0	1.947585	2.534326	-0.513064
C 0	1.278674	-1.576410	-0.881424
C 0	2.682062	0.321819	0.045859
C 0	2.080268	-1.061713	0.321576
H 0	-0.251435	-0.859251	-2.299573
H 0	0.018363	1.520991	-1.870480
H 0	1.971171	-1.784071	-1.713041
H 0	0.801473	-2.534326	-0.640784
H 0	3.134624	0.760185	0.941877
H 0	3.493124	0.236628	-0.693772
H 0	2.875119	-1.774784	0.572835
H 0	1.423920	-1.007677	1.196483

TS-58+CH

B3LYP/6-31G(d) Geometry

C 0	-0.893222	-0.647530	1.523800
C 0	-1.155374	-1.713055	0.649649
C 0	-1.491810	-1.400717	-0.679759
C 0	-1.137218	0.641582	1.087778
C 0	-2.283307	0.893176	0.138264
C 0	-2.464909	-0.249302	-0.901695
H 0	-0.333213	-0.820526	2.440406
H 0	-0.847007	-2.721393	0.913721
H 0	-1.620264	-2.234176	-1.370471
H 0	-0.758077	1.489769	1.651911
H 0	-2.178600	1.864735	-0.350289
H 0	-3.191546	0.970755	0.753384
H 0	-2.372765	0.130319	-1.925650
H 0	-3.480816	-0.654932	-0.820348
C 0	0.231420	-0.619309	-1.454027
C 0	0.514058	0.645422	-0.877210
C 0	1.662251	0.831891	0.038659
O 0	1.953198	1.938636	0.487869
C 0	1.263866	-1.737510	-1.346383
C 0	2.603353	-0.347004	0.298345
C 0	2.034168	-1.733001	-0.020434
C 0	0.057373	1.925502	-1.546897
H 0	-0.234742	-0.564256	-2.440406
H 0	1.978054	-1.606367	-2.174929
H 0	0.791565	-2.714949	-1.506090
H 0	2.962517	-0.277699	1.331058
H 0	3.480816	-0.147993	-0.336046
H 0	2.844898	-2.471346	-0.060675
H 0	1.369776	-2.051630	0.787227
H 0	-0.825498	1.772292	-2.173757
H 0	0.859411	2.301519	-2.198214
H 0	-0.140292	2.721393	-0.824851

TS-59+CH

B3LYP/6-31G(d) Geometry

C 0	0.712274	-1.346140	1.278709
C 0	1.078453	-0.026143	1.571843
C 0	1.566263	0.767812	0.528776
C 0	0.887300	-1.798266	-0.024912
C 0	2.106883	-1.350018	-0.801341
C 0	2.527851	0.106179	-0.445780
H 0	0.090037	-1.905883	1.973491
H 0	0.767692	0.426919	2.510326
H 0	1.754573	1.821971	0.726791
H 0	0.418908	-2.726245	-0.342111
H 0	1.944287	-1.471417	-1.877070
H 0	2.925452	-2.036648	-0.545020
H 0	2.655309	0.712673	-1.345929
H 0	3.511848	0.086044	0.040219
C 0	-0.209300	0.991512	-0.753594
C 0	-0.519248	-0.331255	-1.153093
C 0	-1.774112	-1.020849	-0.793140
O 0	-2.090590	-2.091033	-1.303015
C 0	-1.203675	1.712822	0.158499
C 0	-2.731167	-0.307660	0.162058
C 0	-2.069981	0.780641	1.014509
C 0	0.403621	1.913921	-1.799084
H 0	-0.092973	-0.701889	-2.081584
H 0	-1.867962	2.306532	-0.491674
H 0	-0.684392	2.442812	0.792159
H 0	-3.234224	-1.064394	0.773660
H 0	-3.511848	0.136857	-0.474289
H 0	-2.836787	1.367970	1.534798
H 0	-1.456632	0.316173	1.791636
H 0	1.036215	1.375915	-2.510326

H 0	0.992496	2.726245	-1.355993
H 0	-0.402214	2.384660	-2.379723

TS-60+CH

B3LYP/6-31G(d) Geometry

C 0	0.321466	-1.916794	0.624213
C 0	0.919428	-0.890100	1.362411
C 0	1.718344	0.031459	0.689048
C 0	0.535376	-1.937992	-0.759792
C 0	1.922637	-1.589773	-1.269715
C 0	2.589038	-0.445682	-0.451532
H 0	-0.471983	-2.515559	1.065362
H 0	0.598367	-0.696219	2.383228
H 0	2.054772	0.926754	1.207571
H 0	-0.042338	-2.626322	-1.371534
H 0	1.890698	-1.345530	-2.336332
H 0	2.528519	-2.501119	-1.186171
H 0	2.876307	0.392797	-1.091442
H 0	3.521770	-0.814350	-0.004153
C 0	0.004267	0.982059	-0.635402
C 0	-0.456207	-0.134434	-1.388862
C 0	-1.872202	-0.598832	-1.298468
O 0	-2.302984	-1.449251	-2.063326
C 0	-0.912938	1.646891	0.397599
C 0	-2.779765	0.074827	-0.275375
C 0	-2.023352	0.714034	0.894246
C 0	0.915771	1.881763	-1.275088
N 0	1.659400	2.626322	-1.777906
H 0	-0.042373	-0.274224	-2.383228
H 0	-1.372640	2.526278	-0.078523
H 0	-0.325851	2.032041	1.238088
H 0	-3.521770	-0.657695	0.058733
H 0	-3.337278	0.847868	-0.826661
H 0	-2.717926	1.281184	1.524780
H 0	-1.595150	-0.068252	1.528070

TS-61+CH

B3LYP/6-31G(d) Geometry

C 0	-0.925200	-0.909380	1.489009
C 0	-1.124945	-1.647852	0.311360
C 0	-1.449232	-0.940364	-0.864821
C 0	-1.241724	0.432415	1.501574
C 0	-2.324943	0.974275	0.612629
C 0	-2.464235	0.193211	-0.725368
H 0	-0.381211	-1.349964	2.321745
H 0	-0.790105	-2.680349	0.255166
H 0	-1.579289	-1.536946	-1.768398
H 0	-0.906407	1.063032	2.321294
H 0	-2.168175	2.040677	0.432859
H 0	-3.264048	0.904855	1.181685
H 0	-2.386697	0.876687	-1.577020
H 0	-3.461351	-0.259621	-0.781885
C 0	0.214321	-0.002968	-1.369708
C 0	0.507934	1.075799	-0.498049
C 0	1.625283	1.097954	0.464031
O 0	1.881835	2.057107	1.179126
C 0	1.292716	-1.075921	-1.528450
C 0	2.583394	-0.099851	0.430272
C 0	2.054400	-1.375738	-0.232529
Cl 0	-0.112811	2.680349	-0.917128
H 0	-0.213362	0.312242	-2.321745
H 0	2.002003	-0.711603	-2.286730
H 0	0.854449	-1.996445	-1.933689
H 0	2.926336	-0.284527	1.453767
H 0	3.461351	0.271458	-0.119202
H 0	2.888057	-2.056425	-0.445813
H 0	1.398499	-1.906411	0.462878

TS-62+CH

B3LYP/6-31G(d) Geometry

C 0	-0.187145	-1.804643	-1.322305
C 0	-0.821616	-0.753156	-1.984740
C 0	-1.635058	0.100589	-1.226700
C 0	-0.453778	-1.974878	0.040601
C 0	-1.882687	-1.760836	0.493574
C 0	-2.526658	-0.507899	-0.162014
H 0	0.643191	-2.327829	-1.791236
H 0	-0.508125	-0.467483	-2.985691
H 0	-2.009326	1.013658	-1.685590
H 0	0.147045	-2.674165	0.615808
H 0	-1.950143	-1.721184	1.582672
H 0	-2.439090	-2.658812	0.193129
H 0	-2.799650	0.247338	0.580492
H 0	-3.465166	-0.795291	-0.653085
C 0	-0.068050	1.000173	0.095658
C 0	0.436134	-0.075652	0.905440
C 0	1.851695	-0.541362	0.714162
O 0	2.331090	-1.401886	1.440628
C 0	0.850834	1.723466	-0.904596
C 0	2.736923	0.154012	-0.315603
C 0	1.986906	0.853618	-1.449747
C 0	-0.987496	1.914467	0.718691
C 0	-0.027322	-0.224296	2.346214
N 0	-1.737747	2.674165	1.186042
H 0	1.290908	2.584375	-0.379187
H 0	0.257147	2.142437	-1.724317
H 0	3.465166	-0.575975	-0.683854
H 0	3.314718	0.895181	0.258737
H 0	2.677999	1.484174	-2.021899
H 0	1.594742	0.112700	-2.150244
H 0	-1.077209	0.042383	2.478221
H 0	0.558916	0.449080	2.985691
H 0	0.147048	-1.237739	2.712006

TS-63+CH

B3LYP/6-31G(d) Geometry

C 0	0.697106	0.512770	-2.010987
C 0	1.065542	-0.788644	-1.653133
C 0	1.511670	-1.000952	-0.333401
C 0	0.920726	1.535730	-1.100858
C 0	2.154750	1.480925	-0.236832
C 0	2.492700	0.031361	0.214297
H 0	0.070900	0.682777	-2.884292
H 0	0.768842	-1.629207	-2.275070
H 0	1.736925	-2.027535	-0.045086
H 0	0.455108	2.506672	-1.247493
H 0	2.063482	2.158398	0.615399
H 0	2.984558	1.878570	-0.838942
H 0	2.561826	-0.033949	1.303579
H 0	3.486493	-0.241320	-0.161451
C 0	-0.195585	-0.731993	0.817061
C 0	-0.509389	0.666439	0.789635
C 0	-1.702413	1.185274	0.073750
O 0	-2.027805	2.369958	0.136781
C 0	-1.212912	-1.703962	0.198140
C 0	-2.645351	0.206255	-0.625791

C 0	-2.043189	-1.156895	-0.966342
C 0	0.323674	-1.315091	2.132572
C 0	-0.056168	1.590061	1.903024
H 0	-1.904267	-1.989737	1.007928
H 0	-0.707449	-2.632503	-0.098011
H 0	-3.063267	0.706747	-1.505870
H 0	-3.486493	0.079845	0.073241
H 0	-2.841087	-1.870367	-1.209014
H 0	-1.424951	-1.075286	-1.862382
H 0	-0.477338	-1.292021	2.884292
H 0	1.172609	-0.775872	2.556219
H 0	0.618718	-2.362679	2.005902
H 0	0.957032	1.387927	2.255359
H 0	-0.722891	1.477313	2.771805
H 0	-0.131397	2.632503	1.588298

TS-64+CH

B3LYP/6-31G(d) Geometry

C 0	1.479453	-1.442093	-0.207832
C 0	0.372663	-0.857934	-1.071284
O 0	1.674511	-0.610260	0.946453
C 0	2.868518	-1.320013	-0.878710
C 0	2.322692	0.514559	0.388175
C 0	0.353684	0.543367	-1.179911
O 0	3.303853	-0.005998	-0.514457
C 0	1.325694	1.353082	-0.433882
O 0	1.430754	2.570406	-0.505076
H 0	1.259904	-2.454592	0.138283
H 0	0.112374	-1.442635	-1.953140
H 0	2.833435	-1.412671	-1.969111
H 0	3.568250	-2.061019	-0.472233
H 0	2.807454	1.099023	1.172634
H 0	-0.129168	1.035854	-2.016728
C 0	-1.416087	-1.492209	-0.143171
C 0	-1.283546	-0.934475	1.130607
C 0	-2.406871	-0.868534	-1.115750
C 0	-1.336934	0.465041	1.253546
C 0	-2.539646	0.673020	-0.935743
C 0	-1.624669	1.219711	0.135274
H 0	-1.293430	-2.570406	-0.245064
H 0	-0.887017	-1.527707	1.949577
H 0	-3.382507	-1.337999	-0.939438
H 0	-2.135846	-1.120582	-2.147906
H 0	-0.940612	0.938885	2.147906
H 0	-2.381952	1.199362	-1.882445
H 0	-3.568250	0.914612	-0.632305
H 0	-1.466748	2.295074	0.150540

TS-65+CH

B3LYP/6-31G(d) Geometry

C 0	1.509638	-1.544403	-0.682025
C 0	0.382927	-0.686394	-1.245664
O 0	1.680852	-1.258580	0.714069
C 0	2.895077	-1.124868	-1.226540
C 0	2.293864	0.010779	0.673670
C 0	0.375379	0.674015	-0.846472
O 0	3.303910	-0.077926	-0.338943
C 0	1.300741	1.096316	0.220534
O 0	1.412175	2.246825	0.629287
C 0	-0.113536	1.782809	-1.748827
H 0	1.316107	-2.614857	-0.785440
H 0	0.166323	-0.874709	-2.299849
H 0	2.860552	-0.751937	-2.255689
H 0	3.612138	-1.952984	-1.164612
H 0	2.751467	0.242692	1.637093
H 0	-0.850086	1.432350	-2.477808
H 0	0.734299	2.198682	-2.311831
H 0	-0.535984	2.614857	-1.179158
C 0	-1.292241	-1.664118	-0.640633
C 0	-1.138494	-1.725164	0.754290
C 0	-2.386310	-0.758425	-1.195022
C 0	-1.239585	-0.526009	1.478957
C 0	-2.594231	0.526422	-0.341996
C 0	-1.644820	0.616970	0.825457
H 0	-1.159579	-2.592216	-1.197892
H 0	-0.684256	-2.594524	1.219657
H 0	-3.316941	-1.338475	-1.209798
H 0	-2.172854	-0.505375	-2.239835
H 0	-0.814690	-0.466594	2.477808
H 0	-2.536774	1.427760	-0.957843
H 0	-3.612138	0.525234	0.074531
H 0	-1.535367	1.585988	1.306292

TS-66+CH

B3LYP/6-31G(d) Geometry

C 0	1.435230	-0.898080	0.306104
C 0	0.334688	-0.671543	-0.734750
O 0	1.615985	0.282605	1.102156
C 0	2.848773	-1.015480	-0.319282
C 0	2.286461	1.142129	0.205097
C 0	0.319611	0.631285	-1.291084
O 0	3.286838	0.342636	-0.430187
C 0	1.314053	1.635259	-0.881276
O 0	1.442986	2.740616	-1.390202
C 0	0.063270	-1.861675	-1.642162
H 0	1.205163	-1.728309	0.978398
H 0	2.863903	-1.487196	-1.305891
H 0	3.523607	-1.562366	0.350998
H 0	2.753371	1.966210	0.748040
H 0	-0.112935	0.792943	-2.274385
H 0	-0.291159	-2.740616	-1.090498
H 0	0.977363	-2.159753	-2.171733
H 0	-0.675851	-1.618475	-2.409913
C 0	-1.442668	-0.803862	0.518616
C 0	-1.226083	0.229524	1.435575
C 0	-2.533890	-0.586525	-0.518033
C 0	-1.267401	1.547763	0.962407
C 0	-2.525250	0.857170	-1.098271
C 0	-1.544091	1.757360	-0.380972
H 0	-1.330350	-1.830912	0.865008
H 0	-0.792905	0.024461	2.409913
H 0	-3.491952	-0.765573	-0.013697
H 0	-2.475733	-1.332349	-1.315228
H 0	-0.843172	2.348000	1.563605
H 0	-2.329680	0.857928	-2.175653
H 0	-3.523607	1.300966	-0.980764
H 0	-1.360752	2.734088	-0.821779

TS-67+CH

B3LYP/6-31G(d) Geometry

C 0	-1.502591	0.750961	0.479347
C 0	-0.403781	0.613813	-0.581054
O 0	-1.818655	-0.546004	0.998428
C 0	-2.860015	1.143671	-0.142591
C 0	-2.534641	-1.129347	-0.072287
C 0	-0.420040	-0.571694	-1.364537

O 0	-3.388754	-0.111921	-0.590838
C 0	-1.547211	-1.528539	-1.180149
O 0	-1.716032	-2.518319	-1.870404
C 0	0.049361	1.838234	-1.155865
N 0	0.419472	2.853245	-1.596135
H 0	-1.205730	1.394210	1.308854
H 0	-2.773657	1.831284	-0.988283
H 0	-3.526330	1.572954	0.615504
H 0	-3.120953	-1.978847	0.284070
H 0	-0.029122	-0.533991	-2.376667
C 0	1.534919	0.347807	0.777644
C 0	1.129586	-0.840142	1.373873
C 0	2.524807	0.313984	-0.363677
C 0	0.996435	-1.978786	0.569997
C 0	2.353963	-0.942575	-1.266534
C 0	1.230537	-1.850648	-0.801731
H 0	1.489655	1.274641	1.346215
H 0	0.712344	-0.839940	2.376667
H 0	3.526330	0.306217	0.086849
H 0	2.468479	1.237693	-0.946392
H 0	0.479218	-2.853245	0.956150
H 0	2.209036	-0.658030	-2.313886
H 0	3.275282	-1.538654	-1.243006
H 0	0.982054	-2.682925	-1.455974

TS-68+CH

B3LYP/6-31G(d) Geometry

C 0	1.575284	-0.915882	-1.009498
C 0	0.391505	0.020768	-1.258875
O 0	1.734951	-1.114539	0.399816
C 0	2.930338	-0.260908	-1.370789
C 0	2.307406	0.112583	0.800331
C 0	0.394668	1.167777	-0.422660
O 0	3.327910	0.389103	-0.157246
C 0	1.288301	1.274718	0.731415
O 0	1.378014	2.221900	1.498039
Cl 0	-0.305778	2.675194	-1.001709
H 0	1.429827	-1.893344	-1.475705
H 0	0.207157	0.224796	-2.315043
H 0	2.851753	0.469570	-2.182702
H 0	3.680121	-1.016788	-1.632695
H 0	2.744301	0.021066	1.795848
C 0	-1.178851	-1.102463	-1.048943
C 0	-1.012676	-1.722058	0.207177
C 0	-2.358097	-0.137651	-1.190922
C 0	-1.227891	-0.953105	1.365606
C 0	-2.630510	0.700019	0.089592
C 0	-1.779869	0.299102	1.258024
H 0	-1.040192	-1.744903	-1.920348
H 0	-0.499106	-2.675194	0.287053
H 0	-3.239671	-0.746635	-1.424129
H 0	-2.203817	0.522199	-2.050969
H 0	-0.821149	-1.291503	2.315043
H 0	-2.509771	1.770014	-0.105322
H 0	-3.680121	0.579194	0.397548
H 0	-1.776543	0.965473	2.117717

TS-69+CH

B3LYP/6-31G(d) Geometry

C 0	1.453544	0.661650	-0.962562
C 0	0.318836	0.538070	0.069313
O 0	1.738788	-0.624142	-1.520126
C 0	2.808105	0.987241	-0.298223
C 0	2.399884	-1.266839	-0.452330
C 0	0.321245	-0.632634	0.901178
O 0	3.289598	-0.301364	0.109498
C 0	1.391720	-1.643779	0.642922
O 0	1.539432	-2.654878	1.310474
C 0	-0.046784	1.795843	0.653274
C 0	-0.107600	-0.560506	2.354151
N 0	-0.344476	2.836250	1.086766
H 0	1.196466	1.342166	-1.775913
H 0	2.724888	1.644804	0.571506
H 0	3.503629	1.425193	-1.024363
H 0	2.955710	-2.133091	-0.816322
H 0	-0.932472	0.137156	2.511888
H 0	0.736223	-0.209612	2.962815
H 0	-0.382710	-1.547461	2.732434
C 0	-1.466065	0.399754	-1.258080
C 0	-1.105761	-0.746172	-1.976731
C 0	-2.536785	0.288986	-0.190876
C 0	-1.024236	-1.952689	-1.278889
C 0	-2.521739	-1.094437	0.518259
C 0	-1.358998	-1.955804	0.075897
H 0	-1.392126	1.370358	-1.745621
H 0	-0.659125	-0.662147	-2.962815
H 0	-3.503629	0.433464	-0.689441
H 0	-2.446851	1.112536	0.523944
H 0	-0.495849	-2.795245	-1.717532
H 0	-2.539941	-0.986073	1.605235
H 0	-3.434634	-1.648443	0.261206
H 0	-1.139896	-2.836250	0.674600

TS-70+CH

B3LYP/6-31G(d) Geometry

C 0	-1.481108	-1.112873	-0.618205
C 0	-0.354948	-0.734958	0.357911
O 0	-1.609808	-0.134432	-1.656091
C 0	-2.892975	-1.018699	0.013989
C 0	-2.218444	0.934416	-0.969243
C 0	-0.313717	0.659169	0.695415
O 0	-3.267740	0.348024	-0.191913
C 0	-1.232332	1.589520	0.011223
O 0	-1.336950	2.783508	0.275554
C 0	-0.214091	-1.760666	1.480735
C 0	0.172673	1.148224	2.040056
H 0	-1.296398	-2.082088	-1.089589
H 0	-2.921161	-1.252968	1.081831
H 0	-3.598187	-1.671806	-0.515028
H 0	-2.636052	1.653147	-1.676491
H 0	-0.233443	-2.783508	1.086275
H 0	-1.035613	-1.668730	2.202050
H 0	0.711247	-1.642452	2.047909
H 0	1.048021	0.608108	2.407989
H 0	-0.620243	1.024250	2.793353
H 0	0.397214	2.216520	1.997848
C 0	1.317803	-1.190220	-0.728057
C 0	1.115820	-0.526281	-1.955612
C 0	2.473606	-0.675507	0.127011
C 0	1.188935	0.870869	-1.957735
C 0	2.605558	0.873655	0.100128
C 0	1.585977	1.518598	-0.801435
H 0	1.224750	-2.276807	-0.733711
H 0	0.655124	-1.040491	-2.793353
H 0	3.389835	-1.124427	-0.274939
H 0	2.395260	-1.041109	1.155160

H 0	0.737712	1.430247	-2.773362
H 0	2.557872	1.300348	1.105281
H 0	3.598187	1.149333	-0.284841
H 0	1.436860	2.590823	-0.701315

P-1+CH

B3LYP/6-31G(d) Geometry

C 0	-0.361530	0.540020	1.169894
C 0	-1.004498	-0.633499	1.146245
C 0	-1.343160	-1.132146	-0.240541
C 0	-0.016205	-1.266188	-1.036201
C 0	-0.117168	1.141976	-0.194620
C 0	0.714203	0.120027	-1.049144
C 0	2.096303	0.022127	-0.568513
N 0	3.191334	-0.051738	-0.188199
C 0	-1.484878	1.307281	-0.912101
C 0	-2.220837	-0.061467	-0.946307
H 0	-0.032693	1.039600	2.076522
H 0	-1.260018	-1.203209	2.035792
H 0	-1.858877	-2.097333	-0.219426
H 0	-0.221359	-1.587557	-2.063690
H 0	0.618192	-2.028018	-0.575797
H 0	0.412190	2.097333	-0.143387
H 0	0.762332	0.502955	-2.076522
H 0	-1.323106	1.694358	-1.925969
H 0	-2.075975	2.056557	-0.376571
H 0	-2.416742	-0.375243	-1.979108
H 0	-3.191334	0.005567	-0.444443

P-2+CH

B3LYP/6-31G(d) Geometry

C 0	-1.349782	-1.022538	0.851246
C 0	-0.612476	0.002042	1.298356
C 0	-0.089499	0.914301	0.212034
C 0	0.776602	0.078522	-0.798148
C 0	-1.487786	-1.078343	-0.652520
C 0	-0.056662	-1.156973	-1.254403
C 0	2.087082	-0.329937	-0.162396
O 0	3.171828	0.110075	-0.476167
C 0	-1.309323	1.449958	-0.591230
C 0	-2.134249	0.250455	-1.135737
H 0	-1.810942	-1.766031	1.496502
H 0	-0.408933	0.193439	2.348837
H 0	0.500448	1.745688	0.610185
H 0	1.027667	0.722790	-1.647788
H 0	-2.081951	-1.936467	-0.982682
H 0	0.420653	-2.089519	-0.928111
H 0	-0.106316	-1.192099	-2.348837
H 0	1.993491	-1.083368	0.653594
H 0	-0.955076	2.089519	-1.408516
H 0	-1.919992	2.077493	0.066151
H 0	-2.162028	0.259986	-2.232454
H 0	-3.171828	0.302202	-0.790221

P-3+CH

B3LYP/6-31G(d) Geometry

C 0	-2.418823	-1.145331	-0.672574
C 0	-1.090691	0.803921	0.385554
C 0	-1.517277	-0.264106	1.366143
C 0	-2.214857	-1.268096	0.819558
C 0	-1.017361	-1.071879	-1.338360
C 0	-0.223954	0.145557	-0.754844
C 0	1.094799	-0.289995	-0.220961
O 0	2.159028	0.185921	-0.626131
C 0	-2.363867	1.363120	-0.310361
C 0	-3.153424	0.193637	-0.961104
H 0	-2.980132	-1.988884	-1.085750
H 0	-0.528341	1.612690	0.861510
H 0	-1.279244	-0.190788	2.423877
H 0	-2.606714	-2.110927	1.382757
H 0	-0.480728	-2.011719	-1.164189
H 0	-1.110884	-0.957782	-2.423877
H 0	-0.033126	0.897319	-1.527299
H 0	1.128924	-1.059252	0.563732
H 0	-2.073583	2.110927	-1.057802
H 0	-2.972999	1.878585	0.438557
H 0	-3.236904	0.333350	-2.045702
H 0	-4.172925	0.145289	-0.566197
B 0	3.607686	-0.265073	-0.055790
H 0	3.366082	-1.106412	0.785973
H 0	4.172925	-0.673552	-1.042200
H 0	4.065119	0.769291	0.369245

P-4+CH

B3LYP/6-31G(d) Geometry

C 0	-0.876496	-1.113108	0.975948
C 0	-0.188725	-0.031569	1.361186
C 0	0.101019	0.949130	0.248018
C 0	0.877148	0.203123	-0.876948
C 0	-1.220789	-1.141854	-0.495550
C 0	0.106759	-1.057889	-1.302092
C 0	-2.054596	0.129486	-0.820500
N 0	2.289747	-0.091709	-0.370677
O 0	3.014931	0.892847	-0.242265
O 0	2.614995	-1.242449	-0.101541
C 0	-1.248869	1.387242	-0.389935
H 0	-1.163833	-1.918901	1.646003
H 0	0.150782	0.149780	2.376799
H 0	0.679837	1.815225	0.575807
H 0	1.060720	0.892475	-1.703982
H 0	-1.769817	-2.045508	-0.776670
H 0	0.723008	-1.938211	-1.110023
H 0	-0.105717	-1.021665	-2.376799
H 0	-2.275402	0.155709	-1.894676
H 0	-3.014931	0.084112	-0.297398
H 0	-1.053861	2.045508	-1.245640
H 0	-1.804462	1.977109	0.345274

P-5+CH

B3LYP/6-31G(d) Geometry

C 0	-1.092218	-0.529247	1.187240
C 0	-0.418464	0.626223	1.211260
C 0	0.004999	1.128869	-0.151225
C 0	0.884705	0.052015	-0.858953
C 0	-1.255995	-1.123063	-0.193134
C 0	0.165562	-1.325150	-0.789193
C 0	2.298259	-0.008735	-0.314113
F 0	2.356104	-0.371056	0.986344
F 0	3.045564	-0.903312	-1.006185
F 0	2.919339	1.191715	-0.419138
C 0	-1.278602	1.274715	-1.017533
C 0	-2.009711	-0.095894	-1.084853
H 0	-1.477050	-1.027298	2.073411
H 0	-0.192195	1.183781	2.115737
H 0	0.544658	2.078140	-0.099460
H 0	1.009375	0.357103	-1.904965

H 0	-1.790417	-2.078140	-0.173457
H 0	0.727500	-2.021856	-0.160069
H 0	0.099484	-1.770732	-1.788101
H 0	-1.009165	1.627976	-2.020729
H 0	-1.922321	2.039117	-0.571271
H 0	-2.046609	-0.469929	-2.115737
H 0	-3.045564	-0.001795	-0.743358

P-6+CH

B3LYP/6-31G(d) Geometry

C 0	-0.810255	-0.207944	1.383678
C 0	-1.554709	-1.215560	0.910116
C 0	-1.887647	-1.103608	-0.559806
C 0	-0.547644	-1.029247	-1.346645
C 0	-0.469244	0.849254	0.358166
C 0	0.311576	0.168644	-0.841013
C 0	-2.647877	0.232941	-0.787005
B 0	1.810141	-0.105149	-0.390186
C 0	2.343672	-1.562149	-0.092233
C 0	2.798650	1.120656	-0.234737
C 0	-1.807657	1.404371	-0.207390
H 0	-0.480717	-0.128904	2.417323
H 0	-1.896940	-2.053347	1.513172
H 0	-2.488978	-1.948788	-0.911708
H 0	-0.765516	-0.919270	-2.417323
H 0	-0.017092	-1.980302	-1.230940
H 0	0.120998	1.665000	0.787699
H 0	0.350653	0.941035	-1.626015
H 0	-3.632071	0.185847	-0.308553
H 0	-2.821989	0.369255	-1.861853
H 0	2.348842	-2.154478	-1.020683
H 0	3.355156	-1.600448	0.328048
H 0	1.663023	-2.096978	0.585131
H 0	3.632071	0.993549	-0.944203
H 0	2.361177	2.110265	-0.411371
H 0	3.273112	1.123270	0.757339
H 0	-1.591932	2.154478	-0.978224
H 0	-2.353578	1.915604	0.593721

P-7+CH

B3LYP/6-31G(d) Geometry

C 0	0.463619	0.307280	1.399170
C 0	1.208964	1.289797	0.878488
C 0	1.541785	1.110480	-0.584663
C 0	0.202786	1.011402	-1.368917
C 0	0.120758	-0.795350	0.424870
C 0	-0.654920	-0.163545	-0.808614
B 0	-2.138668	0.147677	-0.403133
Cl 0	-3.279530	-1.196774	-0.185833
Cl 0	-2.766124	1.773355	-0.108852
C 0	1.450611	-1.379182	-0.129000
C 0	2.297632	-0.236563	-0.753941
H 0	0.128921	0.277505	2.433058
H 0	1.546955	2.157020	1.440081
H 0	2.142728	1.937866	-0.975781
H 0	0.413442	0.847152	-2.433058
H 0	-0.328585	1.964152	-1.291547
H 0	-0.476445	-1.588583	0.883224
H 0	-0.711882	-0.966895	-1.557267
H 0	1.226574	-2.157020	-0.869269
H 0	1.992402	-1.863888	0.690302
H 0	2.475665	-0.419115	-1.821108
H 0	3.279530	-0.172807	-0.273551

P-8+CH

B3LYP/6-31G(d) Geometry

C 0	-1.780145	1.230256	0.164502
C 0	-1.040990	1.228889	-0.951497
C 0	-0.146638	0.014034	-1.110539
C 0	0.823424	-0.026576	0.124337
C 0	-1.546296	0.035783	1.061603
C 0	-0.037988	-0.000744	1.427314
C 0	1.750813	1.191687	0.078855
O 0	2.948678	1.182491	-0.049472
Cl 0	1.863495	-1.527086	0.054263
C 0	-1.070813	-1.236484	-1.076700
C 0	-1.872279	-1.251053	0.251884
H 0	-2.493001	2.009981	0.419314
H 0	-1.078818	2.002907	-1.713274
H 0	0.439928	0.040032	-2.032853
H 0	-2.144400	0.078229	1.977103
H 0	0.217268	0.879337	2.029822
H 0	0.191567	-0.881026	2.032853
H 0	1.187073	2.144344	0.176440
H 0	-0.473776	-2.144344	-1.190702
H 0	-1.742873	-1.177357	-1.938660
H 0	-1.609542	-2.128879	0.853902
H 0	-2.948678	-1.302701	0.059518

P-9+CH

B3LYP/6-31G(d) Geometry

C 0	1.519191	-1.516494	0.142860
C 0	0.789123	-1.380040	-0.970813
C 0	0.128469	-0.025762	-1.121515
C 0	-0.828869	0.233028	0.111391
C 0	1.500781	-0.303542	1.044293
C 0	0.020257	-0.006262	1.409032
C 0	-1.940429	-0.809637	0.052192
O 0	-3.121161	-0.563203	-0.066042
C 0	-1.457448	1.633421	0.077672
C 0	1.273369	1.028485	-1.098850
C 0	2.048290	0.911151	0.242108
H 0	2.077076	-2.413680	0.398740
H 0	0.689365	-2.149542	-1.732132
H 0	-0.444008	0.054869	-2.051705
H 0	2.086429	-0.455692	1.956739
H 0	-0.380922	-0.843824	1.993339
H 0	-0.037659	0.880501	2.051705
H 0	-1.589846	-1.862696	0.126817
H 0	-1.950073	1.825187	-0.881330
H 0	-0.709908	2.413680	0.247012
H 0	-2.222301	1.722042	0.855258
H 0	0.873119	2.036843	-1.241600
H 0	1.935375	0.829595	-1.947937
H 0	1.929151	1.820658	0.844340
H 0	3.121161	0.785908	0.063080

P-10+CH

B3LYP/6-31G(d) Geometry

C 0	-1.473743	-0.923563	-1.430746
C 0	-0.851718	-1.915893	-0.781784
C 0	-0.254747	-1.510745	0.547658
C 0	0.762760	-0.337964	0.336565
C 0	-1.416874	0.410933	-0.723475
C 0	0.094773	0.768954	-0.547657
C 0	2.046515	-0.821939	-0.296204

O 0	3.150899	-0.680373	0.183642
C 0	0.354269	2.177084	-0.000173
C 0	-1.404718	-0.937682	1.424604
C 0	-2.079259	0.243145	0.673246
H 0	-1.971613	-1.042525	-2.389823
H 0	-0.793322	-2.938908	-1.144418
H 0	0.233131	-2.347133	1.058812
H 0	1.029700	0.072460	1.317598
H 0	-1.917874	1.201536	-1.292739
H 0	0.536689	0.725089	-1.553029
H 0	1.915243	-1.331064	-1.279325
H 0	1.430697	2.376492	0.054157
H 0	-0.053709	2.309061	1.008536
H 0	-0.095744	2.938908	-0.648031
H 0	-0.999119	-0.611076	2.389823
H 0	-2.127206	-1.733742	1.632368
H 0	-1.987402	1.174103	1.243683
H 0	-3.150899	0.060827	0.543440

P-11+CH

B3LYP/6-31G(d) Geometry

C 0	0.512074	-2.062173	0.315833
C 0	0.831777	-1.225718	1.309985
C 0	0.890027	0.229674	0.909084
C 0	-0.531179	0.606794	0.354724
C 0	0.273863	-1.382763	-1.014204
C 0	-0.880185	-0.337394	-0.835307
C 0	1.923337	0.382318	-0.240348
C 0	1.555395	-0.590123	-1.395293
C 0	-0.599841	2.019788	-0.028943
C 0	-2.211043	-1.042506	-0.641181
N 0	-0.632294	3.139714	-0.336288
O 0	-2.922417	-0.943228	0.332706
H 0	0.429965	-3.139714	0.428451
H 0	1.036118	-1.540946	2.329363
H 0	1.139619	0.885607	1.747268
H 0	-1.276647	0.440389	1.141029
H 0	0.010907	-2.092547	-1.805684
H 0	-0.961494	0.225654	-1.775826
H 0	2.922417	0.164942	0.149269
H 0	1.932969	1.421224	-0.587571
H 0	2.367967	-1.298649	-1.584310
H 0	1.382038	-0.042475	-2.329363
H 0	-2.502152	-1.700177	-1.490596

P-12+CH

B3LYP/6-31G(d) Geometry

C 0	2.349592	-0.235836	1.080539
C 0	3.118660	0.860125	0.290810
C 0	1.080945	0.289488	-1.110375
C 0	1.494732	-1.161142	-0.956909
C 0	2.163309	-1.429708	0.171246
C 0	0.947953	0.325261	1.435380
C 0	0.160970	0.654249	0.116956
C 0	-1.084659	-0.187975	0.067230
O 0	-2.227917	0.255178	0.031815
Cl 0	-0.314014	2.411299	0.053878
C 0	2.374872	1.148812	-1.039679
H 0	2.879503	-0.492304	2.002662
H 0	4.143156	0.525028	0.102077
H 0	3.183582	1.766330	0.904216
H 0	0.536946	0.479019	-2.039315
H 0	1.273710	-1.892800	-1.729097
H 0	2.553819	-2.411299	0.425200
H 0	0.394726	-0.402874	2.039315
H 0	1.032090	1.236621	2.032488
H 0	-0.934830	-1.275855	0.072758
H 0	2.124829	2.208021	-1.135351
H 0	2.993527	0.881988	-1.901810
B 0	-3.546941	-0.708289	-0.003202
H 0	-4.085445	-0.380286	-1.031774
H 0	-3.099703	-1.836781	0.014470
H 0	-4.143156	-0.372750	0.990596

P-13+CH

B3LYP/6-31G(d) Geometry

C 0	2.343754	-0.467836	1.070084
C 0	1.076866	0.087553	-1.109588
C 0	1.427205	-1.376084	-0.947419
C 0	2.095655	-1.661926	0.176683
C 0	0.969771	0.156873	1.430603
C 0	0.185171	0.552596	0.120873
C 0	-1.075001	-0.258476	0.080957
O 0	-2.198158	0.248492	0.018556
C 0	-0.149366	2.051216	0.074498
C 0	2.417350	0.876972	-1.074673
C 0	3.150988	0.586552	0.262219
H 0	2.875831	-0.738702	1.987284
H 0	0.540201	0.287196	-2.042607
H 0	1.167628	-2.108966	-1.706770
H 0	2.440714	-2.657745	0.441669
H 0	0.396090	-0.550515	2.040959
H 0	1.108976	1.055324	2.042607
H 0	-0.999624	-1.353678	0.111496
H 0	0.748819	2.657745	0.214880
H 0	-0.857716	2.310148	0.867086
H 0	-0.609698	2.328286	-0.879525
H 0	2.239286	1.947998	-1.209859
H 0	3.019628	0.550217	-1.928127
H 0	3.250840	1.499656	0.862212
H 0	4.163799	0.214826	0.078004
B 0	-3.568077	-0.621699	-0.019247
H 0	-4.074436	-0.284527	-1.062969
H 0	-3.204848	-1.779458	0.027274
H 0	-4.163799	-0.231826	0.956661

P-14+CH

B3LYP/6-31G(d) Geometry

C 0	2.383958	0.293295	0.778608
C 0	1.113433	-1.415356	-0.681456
C 0	1.547538	-1.949524	0.664695
C 0	2.218310	-1.067130	1.415765
C 0	0.951648	0.853970	0.504267
C 0	0.218360	-0.141530	-0.473600
C 0	-1.111336	-0.500325	0.084706
O 0	-2.168267	-0.130966	-0.436297
C 0	0.917390	2.292183	-0.025205
C 0	2.380577	-0.931675	-1.441461
C 0	3.140875	0.101660	-0.565724
H 0	2.925178	0.989674	1.427638
H 0	0.574483	-2.160373	-1.274901
H 0	1.341113	-2.973756	0.963217
H 0	2.615083	-1.288357	2.403103
H 0	0.429893	0.849066	1.470492
H 0	0.052166	0.341392	-1.442882
H 0	-1.162085	-1.101329	1.004079

H 0	-0.116053	2.635851	-0.146500
H 0	1.411951	2.383263	-0.998562
H 0	1.416657	2.973756	0.673115
H 0	2.084370	-0.495761	-2.403103
H 0	3.011071	-1.798140	-1.663447
H 0	3.236253	1.061522	-1.084498
H 0	4.158499	-0.241606	-0.355371
B 0	-3.627995	-0.489857	0.169481
H 0	-3.402786	-1.151061	1.163113
H 0	-4.111065	0.597999	0.377280
H 0	-4.158499	-1.088790	-0.735722

P-15+CH

B3LYP/6-31G(d) Geometry

C 0	-2.535957	-0.173112	-0.874038
C 0	-0.873506	-1.423640	0.663612
C 0	-1.216511	-2.157121	-0.612507
C 0	-2.084728	-1.513856	-1.402631
C 0	-1.239993	0.700042	-0.703319
C 0	-0.264950	-0.013296	0.304407
C 0	1.098931	-0.188155	-0.276239
O 0	2.115385	0.065897	0.371595
C 0	-1.555578	2.062796	-0.262907
N 0	-1.831689	3.133171	0.092653
C 0	-2.192193	-1.146793	1.439283
C 0	-3.180340	-0.374390	0.523614
H 0	-3.224194	0.336943	-1.552726
H 0	-0.165059	-1.971988	1.290555
H 0	-0.795392	-3.133171	-0.836557
H 0	-2.450035	-1.901557	-2.349372
H 0	-0.762639	0.782511	-1.687468
H 0	-0.162494	0.564747	1.227056
H 0	1.209005	-0.591733	-1.293314
H 0	-1.969370	-0.578258	2.349372
H 0	-2.615841	-2.105119	1.754243
H 0	-3.435596	0.601123	0.951451
H 0	-4.116939	-0.926600	0.405023
B 0	3.618072	-0.187910	-0.196485
H 0	4.070315	-0.970775	0.604430
H 0	3.453406	-0.628295	-1.315470
H 0	4.116939	0.908944	-0.137213

P-16+CH

B3LYP/6-31G(d) Geometry

C 0	0.712862	-1.317777	-0.981580
C 0	1.428795	-1.382896	0.146814
C 0	1.265605	-0.189064	1.059583
C 0	-0.232539	-0.064341	1.439782
C 0	-0.109986	-0.059174	-1.125625
C 0	-1.102605	-0.009001	0.117968
C 0	-2.026733	-1.156710	0.050628
C 0	-1.908535	1.226004	0.075550
N 0	-2.740939	-2.069776	-0.003498
N 0	-2.511837	2.216970	0.036989
C 0	0.833618	1.169225	-1.033804
C 0	1.670505	1.087389	0.272493
H 0	0.699601	-2.087162	-1.747325
H 0	2.074739	-2.216970	0.406372
H 0	1.859221	-0.281707	1.974120
H 0	-0.402919	0.843537	2.026353
H 0	-0.549928	-0.915716	2.046101
H 0	-0.697927	-0.038265	-2.046101
H 0	0.248022	2.093490	-1.074793
H 0	1.480617	1.162778	-1.915860
H 0	1.501086	1.970855	0.899185
H 0	2.740939	1.053014	0.048185

P-17+CH

B3LYP/6-31G(d) Geometry

C 0	0.554564	-0.668905	1.177817
C 0	0.554566	0.668911	1.177815
C 0	0.636209	1.291582	-0.196202
C 0	-0.590849	0.790944	-1.038654
C 0	0.636208	-1.291582	-0.196197
C 0	-0.590849	-0.790945	-1.038652
C 0	-1.833766	1.399010	-0.554784
C 0	-1.833767	-1.399010	-0.554783
N 0	-2.793053	-1.933925	-0.179320
N 0	-2.793051	1.933926	-0.179318
C 0	1.916828	-0.776752	-0.905913
C 0	1.916828	0.776747	-0.905918
H 0	0.489231	-1.279512	2.073113
H 0	0.489234	1.279522	2.073107
H 0	0.622653	2.383999	-0.163547
H 0	-0.458460	1.130429	-2.073113
H 0	0.622650	-2.383999	-0.163537
H 0	-0.458458	-1.130432	-2.073110
H 0	1.955029	-1.171506	-1.928529
H 0	2.793052	-1.168275	-0.380965
H 0	1.955026	1.171495	-1.928537
H 0	2.793053	1.168273	-0.380974

P-18+CH

B3LYP/6-31G(d) Geometry

C 0	-0.616880	-1.851506	0.456134
C 0	0.330593	-1.595909	1.365292
C 0	1.395043	-0.627357	0.904816
C 0	0.658508	0.712314	0.543182
C 0	-0.428810	-1.130068	-0.858376
C 0	-0.405981	0.413765	-0.585451
C 0	1.599859	1.756792	0.127201
C 0	-1.731376	0.918390	-0.215643
N 0	-2.785618	1.306071	0.078238
N 0	2.362805	2.565673	-0.208061
C 0	0.965071	-1.503362	-1.433332
C 0	2.062312	-1.189727	-0.378967
H 0	-1.457269	-2.519005	0.621179
H 0	0.353806	-2.029374	2.361073
H 0	2.142317	-0.425354	1.676714
H 0	0.143098	1.071192	1.439266
H 0	-1.220152	-1.354984	-1.578094
H 0	-0.108392	0.921433	-1.510146
H 0	1.140687	-0.945657	-2.361073
H 0	0.964547	-2.565673	-1.694818
H 0	2.785618	-0.463191	-0.765054
H 0	2.623432	-2.091785	-0.118028

P-19+CH

B3LYP/6-31G(d) Geometry

C 0	0.459258	-1.955817	0.610452
C 0	1.099173	-1.087198	1.401739
C 0	1.354303	0.262508	0.768343
C 0	-0.036772	0.862220	0.387158
C 0	0.148394	-1.423156	-0.769973
C 0	-0.718817	-0.123530	-0.630676
C 0	0.018550	2.296603	-0.149187

C 0	-2.100565	-0.431586	-0.249957
N 0	-3.194883	-0.676442	0.053493
C 0	1.484188	-0.988263	-1.432932
C 0	2.204632	0.036583	-0.513235
H 0	0.185188	-2.965069	0.903762
H 0	1.405274	-1.306215	2.421358
H 0	1.867499	0.947543	1.451661
H 0	-0.635499	0.872063	1.303981
H 0	-0.375008	-2.152672	-1.394059
H 0	-0.762197	0.352588	-1.619764
H 0	0.578397	2.365117	-1.089206
H 0	-0.991397	2.678815	-0.337194
H 0	0.497203	2.965069	0.575905
H 0	1.280453	-0.557214	-2.421358
H 0	2.104942	-1.875008	-1.593894
H 0	2.362952	0.987365	-1.034098
H 0	3.194883	-0.329657	-0.224634

P-20+CH

B3LYP/6-31G(d) Geometry

C 0	0.422851	-1.360262	-0.971449
C 0	1.087409	-1.625772	0.158945
C 0	1.285110	-0.427082	1.060283
C 0	-0.109851	0.152054	1.417932
C 0	0.007927	0.087426	-1.122334
C 0	-0.920046	0.453516	0.102969
C 0	-2.116226	-0.407834	0.039594
C 0	-1.409331	1.919399	0.057690
N 0	-3.075966	-1.060335	-0.012748
C 0	1.298437	0.950343	-1.062620
C 0	2.058050	0.657394	0.260100
H 0	0.185189	-2.099810	-1.730476
H 0	1.458443	-2.611000	0.428387
H 0	1.823785	-0.682248	1.978426
H 0	0.011797	1.080290	1.989553
H 0	-0.656717	-0.549195	2.053914
H 0	-0.536711	0.268868	-2.053914
H 0	-1.922087	2.135417	-0.885684
H 0	-2.109662	2.113917	0.876189
H 0	-0.568365	2.611000	0.163006
H 0	1.056786	2.014155	-1.156124
H 0	1.915276	0.695760	-1.930180
H 0	2.146558	1.564482	0.871253
H 0	3.075966	0.310180	0.056081

P-21+CH

B3LYP/6-31G(d) Geometry

C 0	1.208436	-1.315184	-1.426334
C 0	2.008414	-0.453551	-0.786433
C 0	1.456441	0.048178	0.530362
C 0	0.071017	0.745462	0.282654
C 0	-0.098196	-1.594798	-0.715793
C 0	-0.805399	-0.209344	-0.575187
C 0	0.274353	2.097505	-0.375960
O 0	0.317676	3.143667	0.230050
C 0	-2.232456	-0.267653	-0.060488
F 0	-2.814102	0.951621	-0.146469
F 0	-2.325125	-0.653146	1.235397
F 0	-2.985627	-1.126302	-0.784253
C 0	1.178740	-1.186044	1.435192
C 0	0.244710	-2.175980	0.685874
H 0	1.452296	-1.787039	-2.374382
H 0	2.985627	-0.145831	-1.148826
H 0	2.129880	0.749678	1.030902
H 0	-0.386079	0.935852	1.258735
H 0	-0.738709	-2.280083	-1.276802
H 0	-0.906892	0.201580	-1.587926
H 0	0.420919	2.070094	-1.480609
H 0	0.723219	-0.851439	2.374382
H 0	2.131302	-1.661950	1.689134
H 0	-0.670175	-2.360573	1.254086
H 0	0.736433	-3.143667	0.546620

P-22+CH

B3LYP/6-31G(d) Geometry

C 0	0.734750	-1.903265	0.908450
C 0	1.553818	-0.962784	1.395586
C 0	1.926162	0.111288	0.398424
C 0	0.591681	0.777000	-0.072901
C 0	0.376824	-1.719922	-0.549743
C 0	-0.309267	-0.305870	-0.746084
B 0	-1.832677	-0.410315	-0.306980
C 0	-2.366216	0.232618	1.034487
C 0	-2.844132	-1.190746	-1.240355
C 0	0.805895	1.998897	-0.976172
C 0	1.707747	-1.706717	-1.354522
C 0	2.625788	-0.580495	-0.805298
H 0	0.367179	-2.748933	1.485377
H 0	1.923955	-0.949115	2.418071
H 0	2.585624	0.868705	0.837682
H 0	0.100051	1.137260	0.838741
H 0	-0.273718	-2.519939	-0.918051
H 0	-0.301218	-0.141216	-1.836894
H 0	-2.263750	1.328226	0.998701
H 0	-3.413439	0.004628	1.263558
H 0	-1.747614	-0.083279	1.886940
H 0	-3.430904	-1.927464	-0.673350
H 0	-3.587645	-0.471674	-1.621566
H 0	-2.399300	-1.693075	-2.107411
H 0	1.274692	1.729909	-1.930273
H 0	1.441859	2.748933	-0.489349
H 0	-0.151560	2.480092	-1.211898
H 0	1.487067	-1.552510	-2.418071
H 0	2.194805	-2.684519	-1.266072
H 0	2.850312	0.158072	-1.583227
H 0	3.587645	-0.988688	-0.477133

P-23+CH

B3LYP/6-31G(d) Geometry

C 0	0.440461	-0.717120	1.691475
C 0	1.274709	0.326459	1.614737
C 0	1.647906	0.721064	0.203797
C 0	0.317653	1.072355	-0.538606
C 0	0.072097	-1.315931	0.353670
C 0	-0.593354	-0.196855	-0.556393
B 0	-2.099572	-0.017337	-0.158693
C 0	0.531698	1.647814	-1.944983
Cl 0	-2.710687	1.315827	0.828308
Cl 0	-3.287059	-1.235154	-0.672071
C 0	1.390062	-1.737773	-0.354172
C 0	2.326121	-0.503689	-0.471598
H 0	0.062466	-1.130020	2.623282
H 0	1.649282	0.869063	2.479064
H 0	2.318392	1.587364	0.183555
H 0	-0.166870	1.851491	0.059664
H 0	-0.594401	-2.177945	0.449979
H 0	-0.598184	-0.619599	-1.572191

H 0	0.996536	0.922377	-2.623282
H 0	-0.423314	1.947883	-2.393116
H 0	1.174128	2.535977	-1.912413
H 0	1.156534	-2.153753	-1.341929
H 0	1.865384	-2.535977	0.226079
H 0	2.548761	-0.278448	-1.520498
H 0	3.287059	-0.697436	0.016060

P-24+CH

B3LYP/6-31G(d) Geometry

C 0	0.074838	1.294820	1.390554
C 0	1.127620	1.370402	0.567731
C 0	0.887903	0.776620	-0.804733
C 0	0.462786	-0.696830	-0.622624
C 0	-1.149842	0.642043	0.784505
C 0	-0.704468	-0.790891	0.365441
N 0	1.637479	-1.566985	-0.167701
N 0	-1.902999	-1.530429	-0.218050
O 0	1.392186	-2.537462	0.540758
O 0	2.745551	-1.264618	-0.594337
O 0	-2.745551	-1.887954	0.596289
O 0	-1.985067	-1.679631	-1.435896
C 0	-0.329593	1.502384	-1.450185
C 0	-1.546818	1.442726	-0.486527
H 0	0.064438	1.669485	2.409976
H 0	2.081054	1.816960	0.832771
H 0	1.764334	0.828007	-1.450370
H 0	0.176557	-1.139536	-1.580911
H 0	-1.981181	0.562843	1.488309
H 0	-0.439371	-1.378793	1.241883
H 0	-0.569408	1.030877	-2.409976
H 0	-0.045499	2.537462	-1.660799
H 0	-2.410595	0.978768	-0.973913
H 0	-1.855786	2.446259	-0.180145

P-25+CH

B3LYP/6-31G(d) Geometry

C 0	-0.931303	0.506607	1.125629
C 0	-0.767767	-0.821503	1.174929
C 0	-0.707293	-1.488594	-0.178008
C 0	-1.012839	1.069333	-0.272044
C 0	0.482739	-0.863432	-1.005368
C 0	0.306149	0.700730	-1.048299
C 0	1.774008	-1.419523	-0.449160
C 0	1.414389	1.670178	-0.592941
O 0	1.656712	2.655940	-1.252783
O 0	2.003880	1.484380	0.600032
O 0	2.252590	-1.178304	0.647372
O 0	2.338401	-2.318110	-1.278968
C 0	-2.194433	0.383435	-1.009958
C 0	-2.011790	-1.157172	-0.951570
H 0	-0.991755	1.145589	2.001822
H 0	-0.680149	-1.393107	2.093989
H 0	-0.572454	-2.572414	-0.105891
H 0	-1.135030	2.155705	-0.282706
H 0	0.405897	-1.236463	-2.029791
H 0	0.157527	0.979683	-2.093989
H 0	1.864539	0.568745	0.927793
H 0	3.134661	-2.655940	-0.824501
H 0	-2.231269	0.737878	-2.046716
H 0	-3.134661	0.682717	-0.536202
H 0	-1.961158	-1.589204	-1.958303
H 0	-2.854846	-1.633726	-0.441694

P-26+CH

B3LYP/6-31G(d) Geometry

C 0	0.671784	-1.812247	0.444231
C 0	0.607408	-0.768529	1.278019
C 0	0.565076	0.576675	0.592486
C 0	-0.737178	0.582856	-0.325160
C 0	0.697413	-1.439707	-1.019461
C 0	-0.603540	-0.632010	-1.357776
C 0	-0.833261	1.852355	-1.069979
C 0	-1.921741	0.478038	0.546091
C 0	-1.779238	-1.504066	-1.392242
N 0	-2.679808	-2.233237	-1.456220
N 0	-0.864458	2.848485	-1.664699
N 0	-2.827545	0.429273	1.268990
C 0	1.901819	-0.494924	-1.274083
C 0	1.810323	0.724836	-0.318337
H 0	0.699726	-2.848485	0.766158
H 0	0.571372	-0.848102	2.359702
H 0	0.488277	1.409161	1.295254
H 0	0.742046	-2.313344	-1.674467
H 0	-0.492484	-0.202831	-2.359702
H 0	1.902917	-0.173473	-2.322152
H 0	2.827545	-1.053488	-1.109633
H 0	1.755678	1.665239	-0.876111
H 0	2.692578	0.786983	0.324849

P-27+CH

B3LYP/6-31G(d) Geometry

C 0	0.498724	-0.222341	1.352628
C 0	0.939246	0.933651	0.843148
C 0	1.078066	0.933899	-0.662716
C 0	-0.305110	0.618246	-1.312399
C 0	0.216285	-1.287788	0.315608
C 0	-0.876575	-0.713327	-0.669706
C 0	-2.088674	-0.459707	0.134346
N 0	-3.058146	-0.309955	0.756662
C 0	-1.279753	-1.729446	-1.764747
C 0	-1.258789	1.816884	-1.263226
C 0	1.534400	-1.546493	-0.463365
C 0	2.058539	-0.207443	-1.049306
H 0	0.340048	-0.405351	2.411357
H 0	1.189743	1.804167	1.443356
H 0	1.443912	1.893421	-1.043617
H 0	-0.115348	0.390792	-2.370011
H 0	-0.156384	-2.214205	0.763383
H 0	-1.644570	-2.662402	-1.322107
H 0	-2.077327	-1.319173	-2.392705
H 0	-0.428430	-1.961149	-2.411357
H 0	-0.823892	2.662402	-1.809145
H 0	-2.224983	1.582977	-1.723480
H 0	-1.452032	2.136115	-0.234286
H 0	1.377605	-2.291210	-1.250563
H 0	2.260394	-1.979563	0.231977
H 0	2.140261	-0.262697	-2.142176
H 0	3.058146	0.021183	-0.665914

P-28+CH

B3LYP/6-31G(d) Geometry

C 0	-0.508795	-1.808713	-0.416641
C 0	-1.190885	-1.129495	-1.345153
C 0	-1.311916	0.351486	-1.064853
C 0	0.137878	0.930538	-0.982934

C 0	-0.035118	-0.962591	0.744149
C 0	0.911318	0.177447	0.190553
C 0	2.113854	-0.466617	-0.369781
N 0	3.074840	-0.961302	-0.796249
C 0	0.171328	2.463099	-0.916030
C 0	1.397815	1.096427	1.337946
C 0	-1.294291	-0.311153	1.378088
C 0	-2.033924	0.525613	0.299671
H 0	-0.308333	-2.875351	-0.459496
H 0	-1.610699	-1.578245	-2.241647
H 0	-1.859845	0.875252	-1.855578
H 0	0.628722	0.650961	-1.920371
H 0	0.512664	-1.548851	1.488317
H 0	-0.306481	2.868993	-0.019004
H 0	-0.356045	2.875351	-1.784134
H 0	1.197998	2.842778	-0.948301
H 0	1.847639	0.493788	2.134053
H 0	2.155045	1.801574	0.984873
H 0	0.574998	1.671080	1.768809
H 0	-1.021348	0.303439	2.241647
H 0	-1.935366	-1.113181	1.757173
H 0	-2.063235	1.585644	0.576529
H 0	-3.074840	0.201357	0.201437

P-29+CH

B3LYP/6-31G(d) Geometry

C 0	-0.035085	-2.000771	0.408352
C 0	0.639552	-1.301191	1.327593
C 0	1.361706	-0.089701	0.784504
C 0	0.280160	0.873471	0.150066
C 0	0.054604	-1.433329	-0.988797
C 0	-0.494567	0.036241	-0.965633
C 0	0.961046	2.005487	-0.503135
C 0	-0.641898	1.449858	1.248057
C 0	-1.949952	0.040418	-0.788441
N 0	-3.104923	0.017813	-0.670947
N 0	1.501549	2.900591	-1.009213
C 0	1.549782	-1.355868	-1.399674
C 0	2.340970	-0.568983	-0.320658
H 0	-0.604643	-2.900591	0.620723
H 0	0.686980	-1.565111	2.380180
H 0	1.898839	0.459825	1.562938
H 0	-0.518884	-2.014663	-1.715575
H 0	-0.297942	0.486605	-1.945381
H 0	-0.044187	2.003580	1.978970
H 0	-1.386243	2.129959	0.825852
H 0	-1.166970	0.640399	1.760872
H 0	1.635142	-0.872368	-2.380180
H 0	1.939089	-2.372356	-1.510094
H 0	2.858117	0.290846	-0.758424
H 0	3.104923	-1.200649	0.142247

P-30+CH

B3LYP/6-31G(d) Geometry

C 0	-0.587110	1.326439	1.131946
C 0	-0.599198	0.033827	1.474843
C 0	-0.643284	-0.921518	0.302401
C 0	0.645220	-0.658954	-0.575563
C 0	-0.632877	1.572962	-0.358247
C 0	0.597454	0.864203	-1.026524
C 0	1.814237	-0.955030	0.273284
C 0	1.833902	1.611100	-0.779872
N 0	2.789318	2.248783	-0.611655
N 0	2.716690	-1.267217	0.933537
C 0	0.733847	-1.585308	-1.809640
C 0	-1.906551	0.896315	-0.931521
C 0	-1.917495	-0.601953	-0.524452
H 0	-0.545180	2.146891	1.841672
H 0	-0.564776	-0.327411	2.498006
H 0	-0.639271	-1.968341	0.619379
H 0	-0.611489	2.636435	-0.609824
H 0	0.441059	0.878627	-2.112583
H 0	-0.095379	-1.398241	-2.498006
H 0	1.670421	-1.414344	-2.349492
H 0	0.704446	-2.636435	-1.506334
H 0	-1.923432	1.009764	-2.022565
H 0	-2.789318	1.414027	-0.544841
H 0	-1.983057	-1.252262	-1.402733
H 0	-2.789233	-0.830244	0.096032

P-31+CH

B3LYP/6-31G(d) Geometry

C 0	1.254391	-0.554535	1.398085
C 0	0.830970	-1.746605	0.960115
C 0	0.381429	-1.749157	-0.483524
C 0	-0.765572	-0.700064	-0.670599
C 0	1.193146	0.544037	0.360310
C 0	-0.300239	0.709501	-0.107530
C 0	-2.048465	-1.214352	-0.052644
O 0	-3.120881	-1.227288	-0.619462
C 0	-1.148167	1.192123	1.089357
C 0	-0.432586	1.768181	-1.219076
C 0	1.577199	-1.278021	-1.358595
C 0	2.088450	0.087630	-0.827234
H 0	1.626586	-0.374551	2.403421
H 0	0.822330	-2.650743	1.563357
H 0	0.039836	-2.737331	-0.810370
H 0	-0.975703	-0.599783	-1.741742
H 0	1.549222	1.501876	0.756761
H 0	-1.953316	-1.614715	0.981786
H 0	-1.085576	0.512677	1.944403
H 0	-2.203756	1.296526	0.812902
H 0	-0.796631	2.176889	1.421363
H 0	-1.487106	1.907867	-1.484124
H 0	0.098886	1.487211	-2.133742
H 0	-0.041728	2.737331	-0.883968
H 0	1.252712	-1.200380	-2.403421
H 0	2.369190	-2.033285	-1.325189
H 0	2.092167	0.843697	-1.618613
H 0	3.120881	0.002788	-0.472983

P-32+CH

B3LYP/6-31G(d) Geometry

C 0	0.761302	-0.446085	1.365344
C 0	0.611467	-1.644966	0.789822
C 0	0.401400	-1.597435	-0.706014
C 0	-0.884098	-0.752531	-1.017991
C 0	0.687303	0.717866	0.406817
C 0	-0.746009	0.651089	-0.287058
C 0	-2.120510	-1.563764	-0.646342
O 0	-2.746967	-2.188723	-1.471004
C 0	-1.774517	0.862513	0.752862
C 0	-0.884519	1.740010	-1.272604
N 0	-0.953338	2.590584	-2.059295
N 0	-2.561258	1.040971	1.587142
C 0	1.609976	-0.861285	-1.346881

C 0	1.764571	0.537578	-0.693604
H 0	0.918979	-0.289736	2.427834
H 0	0.641497	-2.585740	1.331984
H 0	0.277755	-2.590584	-1.146766
H 0	-0.939074	-0.586283	-2.097024
H 0	0.786764	1.685435	0.903877
H 0	-2.382671	-1.603317	0.429613
H 0	1.453060	-0.774918	-2.427834
H 0	2.510739	-1.464485	-1.198557
H 0	1.675095	1.336751	-1.436538
H 0	2.746967	0.646860	-0.225322

P-33+CH

B3LYP/6-31G(d) Geometry

C 0	-0.579600	-1.841344	0.667917
C 0	-0.579728	-1.840783	-0.669043
C 0	-0.626192	-0.467041	-1.293060
C 0	0.675329	0.315941	-0.813707
C 0	-0.625877	-0.468108	1.293088
C 0	0.675593	0.315143	0.814060
C 0	0.660562	1.683064	-1.363754
C 0	1.861157	-0.364294	-1.363189
C 0	1.861490	-0.365860	1.362442
N 0	2.761439	-0.911315	1.850310
C 0	0.661284	1.681732	1.365437
N 0	0.610615	2.736245	-1.847824
N 0	2.761027	-0.909109	-1.851916
N 0	0.611714	2.734460	1.850531
C 0	-1.876746	0.286000	0.775864
C 0	-1.877004	0.286542	-0.774914
H 0	-0.539346	-2.736245	1.280262
H 0	-0.539621	-2.735175	-1.282143
H 0	-0.606287	-0.496203	-2.384526
H 0	-0.605707	-0.498169	2.384526
H 0	-1.890076	1.305385	1.173649
H 0	-2.761150	-0.222412	1.169555
H 0	-1.890674	1.306196	-1.171989
H 0	-2.761439	-0.221780	-1.168653

P-34+CH

B3LYP/6-31G(d) Geometry

C 0	-0.553251	-1.935007	-0.955056
C 0	-0.534198	-0.946425	-1.854778
C 0	-0.616007	0.437600	-1.257813
C 0	0.644331	0.617514	-0.298676
C 0	-0.641869	-1.468987	0.480845
C 0	0.631439	-0.584774	0.789495
C 0	0.571693	1.940039	0.351350
C 0	1.861037	0.623771	-1.131733
C 0	1.812477	-1.450128	0.623413
N 0	2.716112	-2.176702	0.568240
C 0	0.654748	-0.077718	2.249951
N 0	0.478951	2.989419	0.838408
N 0	2.788799	0.667100	-1.826977
C 0	-1.929940	-0.616945	0.628908
C 0	-1.902710	0.541930	-0.401495
H 0	-0.496450	-2.989419	-1.206360
H 0	-0.459272	-1.091836	-2.927589
H 0	-0.579161	1.227881	-2.010815
H 0	-0.646528	-2.304251	1.186486
H 0	-0.180758	0.593290	2.458007
H 0	0.594631	-0.934615	2.927589
H 0	1.582308	0.460194	2.462457
H 0	-2.027809	-0.236860	1.650175
H 0	-2.788799	-1.272075	0.456526
H 0	-1.946061	1.517999	0.092312
H 0	-2.762177	0.489077	-1.075850

P-35+CH

B3LYP/6-31G(d) Geometry

C 0	1.027679	-0.535239	1.639674
C 0	0.697179	-1.723005	1.120961
C 0	0.387059	-1.694618	-0.359550
C 0	-0.841319	-0.733812	-0.625347
C 0	1.010594	0.598227	0.644089
C 0	-0.467952	0.681051	0.053182
C 0	-2.042950	-1.384431	0.086603
O 0	-3.002434	-1.826428	-0.500520
C 0	-1.383570	1.037767	1.157775
C 0	-0.536223	1.794086	-0.913336
N 0	-0.543933	2.685801	-1.656222
C 0	-1.170739	-0.615006	-2.118897
N 0	-2.081529	1.328603	2.038460
C 0	1.649917	-1.143559	-1.078685
C 0	1.979483	0.264967	-0.519987
H 0	1.285332	-0.367335	2.680608
H 0	0.664011	-2.646222	1.692599
H 0	0.130693	-2.685801	-0.746648
H 0	1.252833	1.563325	1.094893
H 0	-1.953764	-1.480891	1.185889
H 0	-1.319830	-1.613962	-2.537730
H 0	-0.381080	-0.113121	-2.680608
H 0	-2.099730	-0.059106	-2.268721
H 0	1.495686	-1.115474	-2.160787
H 0	2.475415	-1.838003	-0.895148
H 0	1.901586	1.032719	-1.297001
H 0	3.002434	0.306707	-0.134958

P-36+CH

B3LYP/6-31G(d) Geometry

C 0	-1.389513	-0.469131	-1.567149
C 0	-0.848645	-1.657719	-1.275195
C 0	-0.287899	-1.751792	0.126910
C 0	0.831640	-0.653119	0.327123
C 0	-1.316761	0.532547	-0.438087
C 0	0.193624	0.779436	-0.063480
C 0	1.962088	-1.016531	-0.641153
O 0	3.140847	-1.030540	-0.357505
C 0	0.897949	1.426454	-1.279731
C 0	0.294212	1.811141	1.079546
C 0	1.421846	-0.722824	1.746956
C 0	-1.470349	-1.474624	1.097218
C 0	-2.084900	-0.090030	0.762362
H 0	-1.857566	-0.230606	-2.518811
H 0	-0.830548	-2.504323	-1.956875
H 0	0.141620	-2.739380	0.331126
H 0	-1.767204	1.492620	-0.715392
H 0	1.633142	-1.306609	-1.661579
H 0	0.809628	0.822643	-2.186968
H 0	1.962969	1.593218	-1.082157
H 0	0.446069	2.403446	-1.491220
H 0	1.338606	2.058858	1.297240
H 0	-0.168893	1.484976	2.013275
H 0	-0.203508	2.739380	0.772860
H 0	1.765007	-1.742248	1.955486
H 0	0.701213	-0.447676	2.518811

H 0	2.293879	-0.071586	1.839923
H 0	-1.133203	-1.521240	2.137180
H 0	-2.212472	-2.270221	0.973807
H 0	-2.049251	0.578173	1.628417
H 0	-3.140847	-0.189474	0.490531

P-37+CH

B3LYP/6-31G(d) Geometry

C 0	2.517730	0.104802	0.711655
C 0	3.246638	-0.670156	-0.416053
C 0	0.856479	-1.505092	-0.435828
C 0	1.007367	-1.718926	1.054195
C 0	1.868536	-0.885174	1.647730
C 0	1.351800	0.967344	0.049765
C 0	0.325907	-0.028236	-0.703105
C 0	-1.037959	0.008672	-0.046197
O 0	-2.066167	0.030600	-0.721274
C 0	0.693538	1.752696	1.113436
C 0	1.946862	1.945065	-0.881291
C 0	0.181562	0.270713	-2.202728
N 0	0.191489	2.360038	1.965668
N 0	2.461505	2.703702	-1.592801
C 0	2.263325	-1.672017	-1.072899
H 0	3.197289	0.790425	1.222526
H 0	4.100488	-1.190737	0.026650
H 0	3.651321	0.034373	-1.150016
H 0	0.146102	-2.204142	-0.886945
H 0	0.458045	-2.498242	1.574589
H 0	2.103007	-0.895331	2.707386
H 0	-1.124869	-0.062901	1.044023
H 0	1.148308	0.291624	-2.707386
H 0	-0.303171	1.237038	-2.365264
H 0	-0.442441	-0.494374	-2.671742
H 0	2.216514	-1.533588	-2.156342
H 0	2.584221	-2.703702	-0.901259
B 0	-3.565283	-0.094103	-0.086690
H 0	-3.385692	-0.180633	1.108403
H 0	-4.100488	0.916613	-0.468394
H 0	-3.978237	-1.095317	-0.622705

P-38+CH

B3LYP/6-31G(d) Geometry

C 0	-0.501516	1.836971	-0.460170
C 0	0.344650	1.511337	-1.442933
C 0	1.379613	0.480642	-1.054990
C 0	0.625182	-0.840032	-0.621902
C 0	-0.258901	1.095105	0.835133
C 0	-0.414947	-0.451598	0.549184
C 0	-0.046950	-1.497143	-1.851334
C 0	-1.803541	-0.663963	0.098162
N 0	-2.914925	-0.826405	-0.197359
C 0	1.626228	-1.802066	-0.127236
C 0	-0.247984	-1.294294	1.836687
N 0	2.434341	-2.562653	0.216390
C 0	1.192121	1.404772	1.290803
C 0	2.179617	1.039686	0.151416
H 0	-1.303416	2.562653	-0.557497
H 0	0.319591	1.944275	-2.438781
H 0	2.053069	0.234091	-1.880999
H 0	-0.976599	1.374040	1.612126
H 0	0.715697	-1.758449	-2.591844
H 0	-0.581033	-2.409740	-1.573008
H 0	-0.760454	-0.806553	-2.306223
H 0	0.760505	-1.205302	2.245139
H 0	-0.965094	-0.957283	2.591844
H 0	-0.435029	-2.353272	1.638266
H 0	1.432074	0.864401	2.211808
H 0	1.250332	2.470530	1.532330
H 0	2.914925	0.300702	0.485658
H 0	2.738983	1.920206	-0.178561

P-39+CH

B3LYP/6-31G(d) Geometry

C 0	0.519824	0.667949	-1.666681
C 0	0.519868	-0.668881	-1.666472
C 0	0.605561	-1.286975	-0.289400
C 0	-0.649114	-0.808259	0.548067
C 0	0.605542	1.286483	-0.289808
C 0	-0.649067	0.808001	0.547896
C 0	-1.842299	-1.350176	-0.129574
C 0	-1.842301	1.349844	-0.129711
N 0	-2.758147	1.861505	-0.627467
N 0	-2.758113	-1.861897	-0.627328
C 0	-0.652754	-1.437961	1.963010
C 0	-0.652488	1.437983	1.962714
C 0	1.909279	0.775493	0.377633
C 0	1.909239	-0.775745	0.377974
H 0	0.452085	1.280531	-2.560404
H 0	0.452158	-1.281747	-2.560003
H 0	0.593829	-2.380082	-0.325383
H 0	0.593780	2.379578	-0.326136
H 0	0.200614	-1.111819	2.560404
H 0	-1.568603	-1.188953	2.505243
H 0	-0.607080	-2.527628	1.871656
H 0	0.200899	1.111848	2.560086
H 0	-0.606685	2.527628	1.871147
H 0	-1.568313	1.189198	2.505088
H 0	2.009023	1.174103	1.392105
H 0	2.758121	1.165395	-0.192250
H 0	2.008808	-1.173902	1.392641
H 0	2.758147	-1.165945	-0.191608

P-40+CH

B3LYP/6-31G(d) Geometry

C 0	-0.434023	-1.909717	-0.834373
C 0	-0.934675	-0.918490	-1.579093
C 0	-1.155185	0.373005	-0.822849
C 0	0.220439	0.890173	-0.256834
C 0	-0.167962	-1.522059	0.602719
C 0	0.861184	-0.318338	0.598922
C 0	1.117691	1.299738	-1.443195
C 0	2.094685	-0.830735	-0.032130
N 0	3.083608	-1.259587	-0.465772
C 0	-0.002215	2.162084	0.588125
C 0	1.279649	0.055720	2.044286
C 0	-1.511733	-1.059390	1.226782
C 0	-2.138453	0.043899	0.334135
H 0	-0.215023	-2.907196	-1.203929
H 0	-1.182436	-1.015983	-2.632721
H 0	-1.577217	1.154217	-1.464886
H 0	0.260868	-2.346436	1.180812
H 0	0.645811	2.122804	-1.993520
H 0	2.098485	1.647220	-1.100889
H 0	1.282917	0.474198	-2.139912
H 0	-0.592389	1.998433	1.492685
H 0	0.950986	2.609170	0.889614

H 0	-0.532319	2.907196	-0.017069
H 0	0.435060	0.418354	2.632721
H 0	1.691105	-0.825282	2.547598
H 0	2.052624	0.829397	2.045600
H 0	-1.356913	-0.702778	2.250479
H 0	-2.174167	-1.927781	1.299653
H 0	-2.370671	0.941130	0.916430
H 0	-3.083608	-0.298952	-0.098836

P-41+CH

B3LYP/6-31G(d) Geometry

C 0	0.675069	0.518578	1.221127
C 0	0.366407	-0.776297	1.074293
C 0	0.321029	-1.256532	-0.360694
C 0	-0.688814	-0.382338	-1.151346
C 0	0.912905	1.264268	-0.074887
C 0	-0.338841	1.136789	-0.978593
C 0	-1.741588	1.409138	-0.353843
C 0	-2.052399	-0.091028	-0.498050
O 0	-3.001244	-0.777741	-0.216494
C 0	1.717051	-0.972425	-0.992853
C 0	2.067469	0.536290	-0.828650
H 0	0.762669	1.011691	2.185917
H 0	0.171562	-1.451937	1.902837
H 0	0.060431	-2.315975	-0.437148
H 0	-0.775958	-0.737752	-2.185917
H 0	1.166691	2.315975	0.095308
H 0	-0.171709	1.668133	-1.920877
H 0	-2.402661	2.045408	-0.954198
H 0	-1.756125	1.771190	0.680125
H 0	1.702385	-1.258248	-2.051702
H 0	2.467896	-1.600541	-0.502428
H 0	2.216037	1.009694	-1.807237
H 0	3.001244	0.658627	-0.270473

P-42+CH

B3LYP/6-31G(d) Geometry

C 0	-0.835067	-1.600210	0.389175
C 0	-0.420724	-0.761418	1.346875
C 0	-0.182150	0.660069	0.879923
C 0	0.871089	0.641277	-0.269368
C 0	-0.970339	-0.973869	-0.983396
C 0	0.384149	-0.347174	-1.396828
C 0	1.327020	2.033616	-0.713937
C 0	1.665655	-1.216697	-1.222615
C 0	2.069721	-0.311765	-0.048480
O 0	2.984051	-0.316109	0.736668
C 0	-1.531169	1.161597	0.279784
C 0	-1.980954	0.205741	-0.862750
H 0	-1.070035	-2.647065	0.563648
H 0	-0.277390	-1.047456	2.385386
H 0	0.152747	1.311030	1.693661
H 0	-1.308347	-1.696070	-1.734432
H 0	0.293351	0.116200	-2.385386
H 0	1.820021	2.555267	0.114408
H 0	0.486091	2.647065	-1.055674
H 0	2.045609	1.971246	-1.539859
H 0	2.372434	-1.163331	-2.059532
H 0	1.521544	-2.269909	-0.958902
H 0	-1.428413	2.189175	-0.085194
H 0	-2.279033	1.187412	1.079038
H 0	-2.028055	0.738828	-1.820920
H 0	-2.984051	-0.187389	-0.668097

P-43+CH

B3LYP/6-31G(d) Geometry

C 0	0.679622	-0.967581	1.306501
C 0	0.392327	-1.940753	0.433352
C 0	0.336262	-1.491903	-1.011662
C 0	-0.692593	-0.336490	-1.140432
C 0	0.904507	0.395939	0.683620
C 0	-0.363607	0.818878	-0.120176
C 0	2.086084	0.220616	-0.321000
C 0	-1.738405	0.577252	0.597818
C 0	-2.040519	-0.523735	-0.428266
O 0	-2.981831	-1.253311	-0.615186
C 0	-0.253196	2.218784	-0.726337
C 0	1.723007	-0.875448	-1.365293
H 0	0.772964	-1.125392	2.378024
H 0	0.218433	-2.976490	0.712247
H 0	0.081474	-2.309778	-1.691723
H 0	-0.788947	-0.026332	-2.189381
H 0	1.150200	1.154472	1.435682
H 0	2.315902	1.170595	-0.814440
H 0	2.981831	-0.063680	0.240319
H 0	-2.438436	1.420543	0.556009
H 0	-1.695043	0.214271	1.630120
H 0	-1.160995	2.473207	-1.286730
H 0	0.590848	2.308937	-1.418378
H 0	-0.126243	2.976490	0.057491
H 0	1.684262	-0.455265	-2.378024
H 0	2.480165	-1.666297	-1.376828

P-44+CH

B3LYP/6-31G(d) Geometry

C 0	0.426375	-1.406599	1.260513
C 0	-0.103688	-2.102303	0.246955
C 0	0.086309	-1.473781	-1.116900
C 0	-0.515778	-0.044912	-1.092264
C 0	1.134703	-0.132879	0.855038
C 0	0.120678	0.788711	0.095540
C 0	2.247203	-0.522976	-0.164113
C 0	-1.304239	0.980924	0.730074
C 0	-1.884114	0.133026	-0.412045
O 0	-2.991152	-0.254391	-0.676936
C 0	0.746303	2.044781	-0.304968
N 0	1.244642	3.046120	-0.621709
C 0	1.616240	-1.300890	-1.355246
H 0	0.387822	-1.723395	2.299098
H 0	-0.627957	-3.046120	0.367573
H 0	-0.376141	-2.060790	-1.915041
H 0	-0.451189	0.429374	-2.078013
H 0	1.558336	0.400325	1.710935
H 0	2.761833	0.379009	-0.512266
H 0	2.991152	-1.137773	0.351208
H 0	-1.666219	2.014384	0.734538
H 0	-1.435628	0.552420	1.728502
H 0	1.777784	-0.767090	-2.299098
H 0	2.076697	-2.288052	-1.462050

P-45+CH

B3LYP/6-31G(d) Geometry

C 0	-0.662187	-0.786480	1.272496
C 0	-1.247429	-1.325284	0.195759
C 0	-1.105659	-0.510852	-1.074146
C 0	0.397008	-0.278880	-1.363154

C 0	0.008838	0.552404	1.027599
C 0	1.059330	0.341472	-0.084805
C 0	-1.728856	0.892469	-0.800858
C 0	1.359018	-1.503182	-1.287333
C 0	1.967874	-0.917167	-0.004682
Cl 0	2.051949	1.842834	-0.372456
O 0	2.811209	-1.272863	0.771531
C 0	-1.078284	1.517258	0.466703
H 0	-0.669218	-1.235917	2.261365
H 0	-1.795799	-2.263382	0.214285
H 0	-1.590594	-0.989917	-1.930911
H 0	0.526134	0.329353	-2.261365
H 0	0.482876	0.953970	1.926188
H 0	-2.811209	0.790452	-0.673889
H 0	-1.567145	1.534331	-1.675245
H 0	2.084990	-1.561923	-2.106334
H 0	0.896945	-2.486626	-1.154235
H 0	-0.624867	2.486626	0.239591
H 0	-1.827373	1.684916	1.246914

P-46+CH

B3LYP/6-31G(d) Geometry

C 0	-0.692974	-1.527154	-1.481523
C 0	-0.157392	-2.174693	-0.439878
C 0	-0.065559	-1.355607	0.830434
C 0	0.787330	-0.080921	0.547849
C 0	-1.113053	-0.102878	-1.191658
C 0	0.133884	0.700984	-0.686319
C 0	-2.138484	-0.147500	-0.021138
C 0	1.458608	0.524677	-1.508681
C 0	2.018192	-0.316618	-0.355276
O 0	3.046492	-0.919292	-0.190233
C 0	-0.214860	2.094983	-0.436623
C 0	1.136981	0.721112	1.802745
N 0	-0.493079	3.206456	-0.239176
C 0	-1.513253	-0.902065	1.186361
H 0	-0.845979	-1.972446	-2.460723
H 0	0.181110	-3.206456	-0.474701
H 0	0.383290	-1.919583	1.653608
H 0	-1.542309	0.391587	-2.068081
H 0	-2.424067	0.873156	0.256353
H 0	-3.046492	-0.650138	-0.367653
H 0	2.015495	1.454268	-1.668715
H 0	1.360705	0.000835	-2.464109
H 0	1.757160	0.106381	2.464109
H 0	0.242588	1.032128	2.351550
H 0	1.701692	1.627055	1.558921
H 0	-1.502257	-0.269111	2.079590
H 0	-2.103339	-1.789051	1.437781

P-47+CH

B3LYP/6-31G(d) Geometry

C 0	-0.427542	-1.883317	-0.495729
C 0	-0.839790	-1.096777	-1.496996
C 0	-0.970901	0.367951	-1.132341
C 0	0.400573	0.910988	-0.619758
C 0	-0.170611	-1.154568	0.806351
C 0	0.892921	-0.035446	0.565354
C 0	-2.000809	0.432872	0.036189
C 0	0.360647	2.416360	-0.349872
C 0	1.633927	0.475015	-1.482939
C 0	2.055798	-0.467590	-0.351346
C 0	1.389709	0.597323	1.868097
O 0	2.973280	-1.236437	-0.202827
C 0	-1.509512	-0.465207	1.207356
H 0	-0.291629	-2.958077	-0.580658
H 0	-1.084780	-1.460691	-2.491644
H 0	-1.316051	0.970300	-1.980758
H 0	0.173888	-1.830943	1.595047
H 0	-2.973280	0.090848	-0.332271
H 0	-2.139714	1.467230	0.367718
H 0	-0.355815	2.688135	0.432408
H 0	0.077391	2.958077	-1.261447
H 0	1.341120	2.793567	-0.038630
H 0	2.364905	1.273158	-1.663818
H 0	1.426511	-0.024083	-2.435138
H 0	1.860176	-0.171283	2.491644
H 0	0.577135	1.054129	2.443272
H 0	2.141047	1.372643	1.683986
H 0	-1.373733	0.122110	2.122020
H 0	-2.248955	-1.238518	1.439954

P-48+CH

B3LYP/6-31G(d) Geometry

C 0	0.972684	0.449325	1.180643
C 0	0.661148	-0.853225	1.148880
C 0	0.608454	-1.446618	-0.241719
C 0	-0.419409	-0.625310	-1.084627
C 0	1.227713	1.062075	-0.178714
C 0	-0.028742	0.877689	-1.081522
C 0	-1.296097	1.666041	-0.624423
C 0	-1.826117	-0.713246	-0.479951
O 0	-2.488012	-1.727930	-0.421833
C 0	-2.241508	0.657743	0.050758
C 0	2.002348	-1.246769	-0.899681
C 0	2.384316	0.260081	-0.844573
H 0	1.063234	1.028635	2.096244
H 0	0.461842	-1.454700	2.032019
H 0	0.315670	-2.500068	-0.236158
H 0	-0.456604	-1.048546	-2.096244
H 0	1.487759	2.124159	-0.111841
H 0	0.251730	1.201831	-2.090589
H 0	-1.787002	2.101790	-1.502418
H 0	-1.034478	2.500068	0.035612
H 0	-2.095125	0.634522	1.138568
H 0	-3.306189	0.836930	-0.128108
H 0	1.970772	-1.607530	-1.935076
H 0	2.742501	-1.856728	-0.371294
H 0	2.565923	0.654507	-1.852162
H 0	3.306189	0.407240	-0.272625

P-49+CH

B3LYP/6-31G(d) Geometry

C 0	0.987420	1.202276	0.850575
C 0	0.639471	0.024516	1.384577
C 0	0.519223	-1.101884	0.379865
C 0	-0.543463	-0.675891	-0.695458
C 0	1.208696	1.163786	-0.646028
C 0	-0.077306	0.655040	-1.362901
C 0	-1.290459	1.630059	-1.306771
C 0	-1.861543	-0.324202	0.031049
O 0	-2.524402	-1.123505	0.658533
C 0	-2.198492	1.152448	-0.162241
C 0	-0.846328	-1.800248	-1.700799
C 0	1.907602	-1.249862	-0.304956
C 0	2.325304	0.114700	-0.921264

H 0	1.132646	2.111838	1.428287
H 0	0.460050	-0.136987	2.444233
H 0	0.202761	-2.038995	0.846932
H 0	1.496052	2.141882	-1.047480
H 0	0.192567	0.477392	-2.411387
H 0	-1.837289	1.581878	-2.256050
H 0	-0.967877	2.669622	-1.183131
H 0	-1.965122	1.661058	0.781525
H 0	-3.270256	1.283766	-0.342264
H 0	-1.260752	-2.669622	-1.180001
H 0	0.051894	-2.110170	-2.244738
H 0	-1.583990	-1.474325	-2.444233
H 0	1.875254	-2.034206	-1.068493
H 0	2.634838	-1.576505	0.445747
H 0	2.479197	0.025158	-2.004041
H 0	3.270256	0.464007	-0.492408

P-50+CH

B3LYP/6-31G(d) Geometry

C 0	0.921079	-0.725655	1.309231
C 0	0.527973	-1.852548	0.702136
C 0	0.487460	-1.760282	-0.807852
C 0	-0.449011	-0.573317	-1.207093
C 0	1.271540	0.402114	0.360709
C 0	0.014512	0.745559	-0.513879
C 0	2.416749	-0.139453	-0.545566
C 0	-1.193745	1.209224	0.383535
C 0	-1.885650	-0.841972	-0.752859
O 0	-2.618786	-1.675376	-1.242426
C 0	0.332114	1.849197	-1.538312
C 0	-2.233081	0.076041	0.415471
C 0	1.915721	-1.399840	-1.304515
H 0	1.019893	-0.619867	2.386780
H 0	0.261423	-2.767567	1.224752
H 0	0.123144	-2.679314	-1.275493
H 0	-0.445606	-0.490803	-2.301392
H 0	1.600160	1.300708	0.895467
H 0	2.759195	0.631992	-1.242477
H 0	3.273157	-0.387242	0.089890
H 0	-1.642882	2.109690	-0.050796
H 0	-0.854990	1.484818	1.387612
H 0	-0.561290	2.096523	-2.124259
H 0	1.113788	1.555862	-2.246370
H 0	0.661559	2.767567	-1.035385
H 0	-2.148391	-0.525710	1.329545
H 0	-3.273157	0.409742	0.345376
H 0	1.885880	-1.222529	-2.386780
H 0	2.587010	-2.248933	-1.138377

P-51+CH

B3LYP/6-31G(d) Geometry

C 0	0.583402	-1.197458	1.291949
C 0	0.012698	-1.983673	0.370414
C 0	0.162846	-1.485797	-1.050041
C 0	-0.444583	-0.049456	-1.133581
C 0	1.288546	0.015112	0.727650
C 0	0.234285	0.876972	-0.067337
C 0	-0.927994	1.433785	0.846136
C 0	-1.941189	-0.068766	-0.801761
O 0	-2.783799	-0.582118	-1.503868
C 0	0.921555	2.006593	-0.706812
N 0	1.463877	2.906968	-1.202657
C 0	-2.187919	0.609201	0.542640
C 0	1.680906	-1.369685	-1.361983
C 0	2.363809	-0.494157	-0.274728
H 0	0.583101	-1.408045	2.357988
H 0	-0.512985	-2.906968	0.598324
H 0	-0.347675	-2.124983	-1.775048
H 0	-0.317779	0.329005	-2.153372
H 0	1.744502	0.634228	1.505943
H 0	-1.101115	2.487542	0.610227
H 0	-0.634555	1.386245	1.898708
H 0	-2.337355	-0.189323	1.280116
H 0	-3.109304	1.198085	0.510855
H 0	1.814454	-0.931590	-2.357988
H 0	2.120711	-2.371697	-1.390075
H 0	2.886171	0.356673	-0.723974
H 0	3.109304	-1.071437	0.280562

P-52+CH

B3LYP/6-31G(d) Geometry

C 0	-0.705618	-0.547871	1.434955
C 0	-1.163212	-1.388519	0.497984
C 0	-1.233232	-0.793036	-0.892405
C 0	0.172745	-0.289186	-1.333180
C 0	-0.318252	0.822640	0.909522
C 0	0.757325	0.557978	-0.174061
C 0	-2.153801	0.460406	-0.803843
C 0	1.227144	-1.391598	-1.641784
C 0	1.940441	-0.262004	0.410910
O 0	2.584044	0.068218	1.378286
C 0	-1.569621	1.452893	0.240241
C 0	2.106038	-1.550148	-0.389853
Cl 0	1.474332	2.134465	-0.796517
H 0	-0.605459	-0.796109	2.487644
H 0	-1.500523	-2.400800	0.705849
H 0	-1.618899	-1.503210	-1.631423
H 0	0.027936	0.335385	-2.218695
H 0	0.101176	1.463885	1.687569
H 0	-3.164712	0.147372	-0.523598
H 0	-2.224229	0.931027	-1.791908
H 0	1.843295	-1.067946	-2.487644
H 0	0.748165	-2.330618	-1.938038
H 0	-1.289828	2.400800	-0.229579
H 0	-2.305665	1.683232	1.016958
H 0	3.164712	-1.731731	-0.600441
H 0	1.763076	-2.369619	0.254226

P-53+CH

B3LYP/6-31G(d) Geometry

C 0	-0.431152	-1.396323	-1.621798
C 0	0.212627	-1.986863	-0.607562
C 0	0.011633	-1.310440	0.731493
C 0	0.507710	0.176787	0.607125
C 0	-1.255958	-0.195473	-1.217669
C 0	-0.308051	0.877536	-0.553786
C 0	-2.279420	-0.677081	-0.150505
C 0	0.754937	1.459339	-1.561830
C 0	1.968167	0.144766	0.099692
O 0	2.888388	-0.301910	0.749158
C 0	-1.141483	1.988396	-0.074643
C 0	0.495262	0.905803	1.961506
N 0	-1.804180	2.876934	0.274475
C 0	2.078908	0.730289	-1.302843
C 0	-1.513301	-1.331563	1.031253

H 0	-0.412000	-1.751822	-2.648555
H 0	0.827440	-2.876934	-0.710159
H 0	0.581620	-1.796790	1.527718
H 0	-1.770250	0.264212	-2.067090
H 0	-2.886315	0.167829	0.190612
H 0	-2.961223	-1.392778	-0.619999
H 0	0.875374	2.531312	-1.379302
H 0	0.399594	1.350126	-2.590731
H 0	1.171137	0.388065	2.648555
H 0	0.842964	1.939713	1.862639
H 0	-0.504968	0.940709	2.400854
H 0	2.230421	-0.107404	-1.993499
H 0	2.961223	1.373468	-1.376901

P-54+CH

B3LYP/6-31G(d) Geometry

C 0	-0.408561	-1.822802	-1.190455
C 0	-0.861778	-0.698431	-1.758168
C 0	-1.252192	0.378444	-0.768373
C 0	-0.010606	0.772298	0.113337
C 0	-0.342990	-1.766255	0.320954
C 0	0.583032	-0.557030	0.728134
C 0	-2.362559	-0.252005	0.122235
C 0	-0.426006	1.832854	1.149710
C 0	1.131797	1.380153	-0.777757
C 0	1.942154	-0.771218	0.023210
C 0	0.851127	-0.551969	2.243757
O 0	2.712758	-1.666686	0.300897
C 0	-1.786990	-1.505899	0.834215
C 0	2.168322	0.282836	-1.053267
H 0	-0.106862	-2.709642	-1.741686
H 0	-0.984251	-0.563912	-2.830204
H 0	-1.631301	1.276630	-1.269424
H 0	0.071355	-2.683684	0.748923
H 0	-3.207379	-0.524244	-0.518918
H 0	-2.744490	0.474656	0.846196
H 0	-1.178697	1.478360	1.859795
H 0	-0.842486	2.709642	0.637093
H 0	0.435074	2.176813	1.732246
H 0	1.610605	2.204136	-0.235212
H 0	0.724089	1.812343	-1.698175
H 0	1.338790	-1.491132	2.522449
H 0	-0.065858	-0.446131	2.830204
H 0	1.523667	0.263216	2.532449
H 0	-1.784523	-1.376078	1.921677
H 0	-2.401058	-2.389018	0.628191
H 0	3.207379	0.627750	-1.033469
H 0	2.009308	-0.203743	-2.022769

P-55+CH

B3LYP/6-31G(d) Geometry

C 0	0.456004	-0.669598	1.171993
C 0	0.456005	0.669601	1.171992
C 0	0.550397	1.297273	-0.201445
C 0	0.550394	-1.297272	-0.201443
C 0	-0.637778	0.769692	-1.062570
C 0	-0.637779	-0.769691	-1.062569
C 0	-1.990293	1.148818	-0.479134
C 0	-1.990294	-1.148815	-0.479134
O 0	-2.434573	-2.240918	-0.269096
O 0	-2.434569	2.240921	-0.269096
O 0	-2.716119	0.000002	-0.185786
C 0	1.849270	-0.778385	-0.881970
C 0	1.849272	0.778382	-0.881970
H 0	0.396531	-1.278333	2.069691
H 0	0.396533	1.278339	2.069688
H 0	0.524474	2.389148	-0.168021
H 0	0.524470	-2.389148	-0.168017
H 0	-0.572773	1.196861	-2.069691
H 0	-0.572773	-1.196860	-2.069690
H 0	1.908859	-1.170850	-1.904390
H 0	2.716118	-1.167892	-0.339568
H 0	1.908863	1.170846	-1.904390
H 0	2.716119	1.167888	-0.339568

P-56+CH

B3LYP/6-31G(d) Geometry

C 0	0.255254	-0.807924	1.118811
C 0	0.604019	0.483339	1.185892
C 0	0.848740	1.133923	-0.158097
C 0	-0.436793	0.997019	-1.025593
C 0	0.172901	-1.359939	-0.286918
C 0	-0.841143	-0.492830	-1.089111
C 0	-2.240675	-0.558139	-0.487427
O 0	-2.909838	-1.543069	-0.303059
C 0	-1.689597	1.698966	-0.444341
O 0	-2.673225	0.687604	-0.158364
C 0	1.560651	-1.168816	-0.960152
C 0	1.968165	0.330880	-0.882262
H 0	0.045501	-1.428599	1.985425
H 0	0.717888	1.032539	2.116782
H 0	1.131960	2.187968	-0.064106
H 0	-0.223379	1.389297	-2.025737
H 0	-0.144288	-2.405602	-0.307841
H 0	-0.901055	-0.870079	-2.116782
H 0	-2.138789	2.405602	-1.149287
H 0	-1.479341	2.225854	0.491422
H 0	1.511112	-1.508477	-2.002015
H 0	2.297610	-1.800020	-0.453548
H 0	2.124068	0.746699	-1.885607
H 0	2.909838	0.451098	-0.337568

P-57+CH

B3LYP/6-31G(d) Geometry

C 0	-1.239099	1.218963	0.998085
C 0	-1.392859	-0.073378	1.311900
C 0	-1.345565	-1.009810	0.125548
C 0	0.019149	-0.839118	-0.609701
C 0	-1.039310	1.481464	-0.478035
C 0	0.217946	0.686299	-0.930813
C 0	1.500455	1.305413	-0.364623
O 0	1.532354	2.458629	0.025276
C 0	1.203239	-1.451336	0.152461
C 0	2.770023	0.452425	-0.345062
C 0	2.528496	-1.057198	-0.511165
C 0	-2.264898	0.912074	-1.243680
C 0	-2.466042	-0.582041	-0.863582
H 0	-1.246220	2.029408	1.721201
H 0	-1.549597	-0.438700	2.323770
H 0	-1.475692	-2.057541	0.419434
H 0	-0.058192	-1.379020	-1.563992
H 0	-0.896597	2.542633	-0.689693
H 0	0.323906	0.796219	-2.023019
H 0	1.091489	-2.542633	0.183745
H 0	1.199697	-1.101128	1.194867
H 0	3.261378	0.667848	0.611437

H 0	3.443672	0.843885	-1.119828
H 0	2.493295	-1.327767	-1.575651
H 0	3.367610	-1.615734	-0.080190
H 0	-2.105820	1.024274	-2.323770
H 0	-3.153084	1.500950	-0.992067
H 0	-2.432795	-1.222281	-1.754231
H 0	-3.443672	-0.737461	-0.395579

P-58+CH

B3LYP/6-31G(d) Geometry

C 0	-1.235965	-0.920226	-1.609894
C 0	-1.417265	0.405848	-1.621068
C 0	-1.378421	1.044170	-0.249749
C 0	-0.005467	0.725557	0.417179
C 0	-1.042382	-1.509840	-0.229237
C 0	0.222127	-0.836287	0.402958
C 0	1.465733	-1.264933	-0.401789
O 0	1.481364	-2.298043	-1.046392
C 0	1.144551	1.530741	-0.211195
C 0	2.729610	-0.404880	-0.315111
C 0	2.507428	1.005541	0.250481
C 0	0.492561	-1.366489	1.835450
C 0	-2.307491	-1.149730	0.597450
C 0	-2.492406	0.392415	0.614790
H 0	-1.228694	-1.545762	-2.497766
H 0	-1.583681	0.990510	-2.522323
H 0	-1.517006	2.130516	-0.294804
H 0	-0.074969	1.037937	1.469285
H 0	-0.891374	-2.590408	-0.268012
H 0	1.024692	2.590408	0.048124
H 0	1.089132	1.465524	-1.307354
H 0	3.123956	-0.355094	-1.337350
H 0	3.475407	-0.967197	0.262750
H 0	2.542728	0.994826	1.348393
H 0	3.316997	1.668851	-0.076205
H 0	-0.307277	-1.071879	2.522323
H 0	1.429272	-0.967026	2.241988
H 0	0.564196	-2.460139	1.837404

P-59+CH

B3LYP/6-31G(d) Geometry

C 0	-1.309204	1.770069	0.735770
C 0	-1.449202	0.591173	1.353107
C 0	-1.403055	-0.604689	0.424866
C 0	-0.018637	-0.622748	-0.325585
C 0	-1.119085	1.664994	-0.760966
C 0	0.132550	0.785675	-1.028277
C 0	1.428072	1.510494	-0.658432
O 0	1.459411	2.703041	-0.414412
C 0	1.117496	-0.831447	0.704887
C 0	2.690983	0.659720	-0.667182
C 0	2.530043	-0.672863	0.120021
C 0	0.025027	-1.762038	-1.362730
C 0	-2.351131	0.926621	-1.353333
C 0	-2.564500	-0.410306	-0.591670
H 0	-1.320752	2.731940	1.239723
H 0	-1.600357	0.478480	2.423807
H 0	-1.526370	-1.549771	0.967017
H 0	-0.982224	2.643644	-1.225775
H 0	0.207406	0.616485	-2.115411
H 0	1.017138	-1.825468	1.161241
H 0	0.990318	-0.101071	1.513893
H 0	3.508180	1.275148	-0.281925
H 0	2.921865	0.447053	-1.721047
H 0	2.772811	-1.524041	-0.525288
H 0	3.255904	-0.700824	0.940169
H 0	-0.711785	-1.626224	-2.160219
H 0	-0.169819	-2.731940	-0.887249
H 0	1.007134	-1.823897	-1.844834
H 0	-2.186786	0.746880	-2.423807
H 0	-3.235524	1.567195	-1.272771
H 0	-2.626797	-1.256833	-1.283004
H 0	-3.508180	-0.393133	-0.036904

P-60+CH

B3LYP/6-31G(d) Geometry

C 0	1.128909	-1.887335	0.496638
C 0	1.311941	-0.858957	1.333249
C 0	1.345603	0.493337	0.658152
C 0	-0.032377	0.704931	-0.085900
C 0	0.970417	-1.487916	-0.953265
C 0	-0.251866	-0.532316	-1.052335
C 0	-1.569742	-1.291864	-0.830648
O 0	-1.625894	-2.494212	-1.008367
C 0	-1.202757	0.868324	0.918947
C 0	-2.821980	-0.510461	-0.441415
C 0	-2.555796	0.864206	0.200330
C 0	0.038338	1.944119	-0.882522
N 0	0.079461	2.927372	-1.500738
C 0	2.237268	-0.702287	-1.386276
C 0	2.488680	0.466304	-0.393969
H 0	1.087965	-2.927372	0.806279
H 0	1.447065	-0.959805	2.406696
H 0	1.491706	1.312723	1.368913
H 0	0.796420	-2.349289	-1.599595
H 0	-0.317165	-0.157340	-2.084774
H 0	-1.062882	1.795032	1.486706
H 0	-1.154128	0.036305	1.632724
H 0	-3.384148	-1.165556	0.233558
H 0	-3.439312	-0.414643	-1.345321
H 0	-2.563804	1.657198	-0.557046
H 0	-3.359142	1.104816	0.905074
H 0	2.101069	-0.324087	-2.406696
H 0	3.093103	-1.384160	-1.410784

P-61+CH

B3LYP/6-31G(d) Geometry

C 0	1.329861	-0.073849	1.315239
C 0	1.566154	1.065677	0.654242
C 0	1.454910	0.941178	-0.849872
C 0	0.027433	0.434406	-1.214367
C 0	0.998825	-1.257595	0.425965
C 0	-0.270125	-0.837386	-0.349741
C 0	2.474288	-0.137864	-1.310467
C 0	-1.488262	-0.705284	0.595533
O 0	-1.456347	-1.171126	1.716309
C 0	-1.056706	1.515853	-1.071425
C 0	-2.724058	0.017033	0.068993
C 0	-2.460451	0.904423	-1.159294
Cl 0	-0.832959	-2.232628	-1.466166
C 0	2.180543	-1.464656	-0.558590
H 0	1.353225	-0.178193	2.395327
H 0	1.833350	2.002528	1.135913
H 0	1.642607	1.891424	-1.361502
H 0	0.042936	0.121384	-2.264011
H 0	0.790515	-2.158280	1.004207

H 0	3.491475	0.212239	-1.107094
H 0	2.393124	-0.277170	-2.395327
H 0	-0.909129	2.269577	-1.854614
H 0	-0.943508	2.034271	-0.108303
H 0	-3.099344	0.610306	0.911199
H 0	-3.491475	-0.740090	-0.135284
H 0	-2.543901	0.315536	-2.080911
H 0	-3.224168	1.688329	-1.216640
H 0	1.938340	-2.269577	-1.258793
H 0	3.052960	-1.790711	0.016214

P-62+CH

B3LYP/6-31G(d) Geometry

C 0	-1.081713	-1.956964	-0.850134
C 0	-1.307302	-0.957981	-1.710576
C 0	-1.381280	0.406646	-1.065189
C 0	-0.006051	0.681240	-0.332808
C 0	-0.941191	-1.516104	0.589778
C 0	0.272958	-0.529953	0.679719
C 0	1.562797	-1.305634	0.320841
O 0	1.617312	-2.514091	0.451800
C 0	1.136571	0.855789	-1.372248
C 0	2.804918	-0.526611	-0.109849
C 0	2.511096	0.862904	-0.699355
C 0	-0.116918	1.966921	0.380816
C 0	0.513446	-0.069993	2.140982
N 0	-0.196911	3.002293	0.902565
C 0	-2.257767	-0.791041	0.979100
C 0	-2.521456	0.373825	-0.012454
H 0	-1.001907	-3.002293	-1.132420
H 0	-1.443524	-1.088255	-2.780696
H 0	-1.550802	1.205564	-1.793987
H 0	-0.748320	-2.361227	1.252582
H 0	0.966314	1.779440	-1.936465
H 0	1.077154	0.023257	-2.084654
H 0	3.318370	-1.166482	-0.836067
H 0	3.474363	-0.464401	0.758718
H 0	2.532510	1.636366	0.078191
H 0	3.288768	1.133013	-1.422099
H 0	-0.323194	0.517770	2.525955
H 0	1.409232	0.553574	2.230761
H 0	0.645149	-0.949192	2.780696
H 0	-2.207380	-0.426130	2.010047
H 0	-3.073933	-1.519849	0.948447
H 0	-2.576384	1.335620	0.508339
H 0	-3.474363	0.239002	-0.533490

P-63+CH

B3LYP/6-31G(d) Geometry

C 0	-1.123444	-1.769102	-1.128418
C 0	-1.303740	-0.586019	-1.726058
C 0	-1.388449	0.580936	-0.766651
C 0	-0.053355	0.684359	0.066821
C 0	-0.999675	-1.685381	0.377394
C 0	0.231836	-0.763721	0.692546
C 0	-2.589944	0.279512	0.170617
C 0	1.488062	-1.458207	0.109340
O 0	1.527540	-2.667976	-0.027529
C 0	1.087202	1.124459	-0.888746
C 0	2.732534	-0.628100	-0.206566
C 0	2.481299	0.881295	-0.302609
C 0	-0.209652	1.792894	1.132059
C 0	0.531561	-0.754194	2.216158
C 0	-2.307318	-1.048158	0.921527
H 0	-1.050440	-2.717851	-1.651487
H 0	-1.414595	-0.455022	-2.799689
H 0	-1.544045	1.530884	-1.291957
H 0	-0.829032	-2.667258	0.822761
H 0	-3.494468	0.195757	-0.440664
H 0	-2.763763	1.104088	0.869261
H 0	0.950267	2.185332	-1.135959
H 0	1.008726	0.570061	-1.833772
H 0	3.115900	-1.021544	-1.155786
H 0	3.494468	-0.874625	0.545089
H 0	2.568067	1.353636	0.683981
H 0	3.250337	1.348323	-0.929204
H 0	-0.936507	1.550129	1.910088
H 0	-0.545740	2.717851	0.647579
H 0	0.737252	2.015194	1.634206
H 0	-0.298626	-0.349069	2.799689
H 0	1.420945	-0.161108	2.456728
H 0	0.711781	-1.779666	2.556425
H 0	-2.229611	-0.881328	2.001961
H 0	-3.129016	-1.758188	0.780085

P-64+CH

B3LYP/6-31G(d) Geometry

C 0	1.408934	-1.519441	0.007134
C 0	0.089233	-1.083962	-0.651906
O 0	1.829232	-0.571670	1.005091
C 0	2.612635	-1.479196	-0.950561
C 0	2.349443	0.476507	0.220536
C 0	0.060271	0.442971	-1.008476
O 0	3.073450	-0.124702	-0.853134
C 0	-1.177185	-1.411931	0.201141
C 0	1.186015	1.272969	-0.375957
C 0	-1.331301	-0.408567	1.322116
C 0	-2.403059	-1.246479	-0.741808
C 0	-1.320932	1.040598	-0.584062
O 0	1.169394	2.487074	-0.356151
C 0	-1.439696	0.860835	0.913049
C 0	-2.437532	0.213196	-1.275239
H 0	1.298871	-2.487074	0.505011
H 0	0.001357	-1.666430	-1.579607
H 0	2.352766	-1.702852	-1.990365
H 0	3.408542	-2.159145	-0.623201
H 0	3.006042	1.110058	0.821362
H 0	0.175840	0.567147	-2.094463
H 0	-1.118819	-2.441726	0.571377
H 0	-1.369329	-0.719509	2.362396
H 0	-3.316768	-1.480650	-0.186477
H 0	-2.335203	-1.965915	-1.567515
H 0	-1.359198	2.090202	-0.881957
H 0	-1.566957	1.709150	1.579411
H 0	-2.291078	0.238074	-2.362396
H 0	-3.408542	0.677993	-1.076331

P-65+CH

B3LYP/6-31G(d) Geometry

C 0	-1.414397	-1.422920	-0.025632
C 0	-0.096915	-0.811361	0.482844
O 0	-1.816500	-0.826997	-1.273085
C 0	-2.635664	-1.093368	0.848398
C 0	-2.323539	0.415809	-0.852102
C 0	-0.060730	0.763763	0.414684
O 0	-3.074397	0.175252	0.341283

C 0	1.153647	-1.380242	-0.260896
C 0	-1.156529	1.346056	-0.503517
C 0	1.288338	-0.737091	-1.623264
C 0	2.402309	-0.974853	0.571283
C 0	1.326453	1.186311	-0.199915
O 0	-1.128396	2.493321	-0.902362
C 0	1.403287	0.595067	-1.589945
C 0	2.482702	0.575079	0.636559
C 0	-0.286831	1.407903	1.803042
H 0	-1.301289	-2.496471	-0.201537
H 0	-0.003269	-1.115407	1.535549
H 0	-2.401539	-1.001316	1.913462
H 0	-3.433974	-1.833641	0.716100
H 0	-2.960879	0.848388	-1.626725
H 0	1.078407	-2.471871	-0.323888
H 0	1.304856	-1.329767	-2.533510
H 0	3.299244	-1.394382	0.104564
H 0	2.331806	-1.408687	1.576915
H 0	1.382498	2.277046	-0.214192
H 0	1.518285	1.222163	-2.469286
H 0	2.436190	0.928501	1.672134
H 0	3.433974	0.932968	0.229732
H 0	0.443767	1.045468	2.533510
H 0	-1.288229	1.182740	2.183616
H 0	-0.196506	2.496471	1.729859

P-66+CH

B3LYP/6-31G(d) Geometry

C 0	1.360834	-0.957197	0.244559
C 0	0.064621	-0.700853	-0.583873
O 0	1.729360	0.212536	1.000931
C 0	2.668149	-1.163946	-0.539966
C 0	2.322977	1.027823	0.020483
C 0	0.049638	0.739066	-1.222849
O 0	3.107471	0.172383	-0.814762
C 0	-1.177714	-0.777889	0.390472
C 0	1.232739	1.646203	-0.858462
C 0	-1.192884	0.424262	1.313218
C 0	-2.501988	-0.685154	-0.423818
C 0	-1.272478	1.486150	-0.825730
O 0	1.307664	2.793930	-1.249074
C 0	-1.289949	1.599253	0.682252
C 0	-0.050288	-1.785875	-1.675497
C 0	-2.476901	0.614555	-1.270602
H 0	1.188182	-1.763876	0.963149
H 0	2.575160	-1.707721	-1.480417
H 0	3.405725	-1.672639	0.093928
H 0	2.946926	1.791940	0.490071
H 0	0.070127	0.651272	-2.317794
H 0	-1.141911	-1.722265	0.946231
H 0	-1.162613	0.311703	2.393219
H 0	-3.332410	-0.663980	0.288767
H 0	-2.654566	-1.569897	-1.049451
H 0	-1.279839	2.459300	-1.321152
H 0	-1.338118	2.561901	1.183243
H 0	-0.044531	-2.793930	-1.240085
H 0	0.772773	-1.725058	-2.393219
H 0	-0.971708	-1.681002	-2.252026
H 0	-2.386966	0.388437	-2.340809
H 0	-3.405725	1.180373	-1.144492

P-67+CH

B3LYP/6-31G(d) Geometry

C 0	-1.383104	0.863354	0.517065
C 0	-0.050656	0.697398	-0.286533
O 0	-1.824712	-0.409786	0.991821
C 0	-2.595736	1.305461	-0.322995
C 0	-2.419382	-0.974299	-0.157920
C 0	-0.099738	-0.531388	-1.282562
O 0	-3.135757	0.067642	-0.808699
C 0	1.184035	0.476212	0.682117
C 0	-1.318911	-1.453078	-1.108019
C 0	1.139995	-0.926603	1.244403
C 0	2.488306	0.582109	-0.158877
C 0	1.200811	-1.385464	-1.101778
O 0	-1.406538	-2.504349	-1.706766
C 0	1.199289	-1.893345	0.322236
C 0	0.159566	1.951454	-1.028718
N 0	0.301195	2.955106	-1.597167
C 0	2.430286	-0.461410	-1.307221
H 0	-1.212952	1.505866	1.384125
H 0	-2.346279	1.953796	-1.165867
H 0	-3.340571	1.802706	0.308842
H 0	-3.088924	-1.789149	0.125404
H 0	-0.140008	-0.163846	-2.315209
H 0	1.164160	1.243123	1.462667
H 0	1.098324	-1.101200	2.315209
H 0	3.334894	0.385593	0.505492
H 0	2.612721	1.596143	-0.550649
H 0	1.180424	-2.193955	-1.834768
H 0	1.204244	-2.955106	0.550170
H 0	2.353736	0.035925	-2.281458
H 0	3.340571	-1.068507	-1.329307

P-68+CH

B3LYP/6-31G(d) Geometry

C 0	1.407320	-1.188867	-1.064806
C 0	0.085455	-0.409136	-1.158166
O 0	1.793972	-1.375341	0.308759
C 0	2.624381	-0.421666	-1.617231
C 0	2.334316	-0.113559	0.633306
C 0	0.068964	0.861222	-0.243162
O 0	3.112424	0.301593	-0.477441
C 0	-1.170990	-1.265051	-0.807543
C 0	1.177253	0.871836	0.845867
C 0	-1.313486	-1.399498	0.693261
C 0	-2.409949	-0.475592	-1.318560
C 0	-1.319981	0.984783	0.445055
O 0	1.116610	1.593445	1.815532
C 0	-1.422749	-0.233940	1.340443
C 0	-2.444872	0.912079	-0.620259
Cl 0	0.411076	2.371209	-1.264006
H 0	1.297843	-2.181442	-1.510215
H 0	-0.024249	-0.086900	-2.199811
H 0	2.370252	0.281260	-2.415293
H 0	3.405651	-1.107009	-1.965224
H 0	2.950959	-0.184191	1.532041
H 0	-1.102076	-2.237016	-1.307850
H 0	-1.352202	-2.371209	1.176751
H 0	-3.316288	-1.048987	-1.099727
H 0	-2.353955	-0.364325	-2.408264
H 0	-1.350741	1.918067	1.008751
H 0	-1.537694	-0.134262	2.415293
H 0	-2.316050	1.722384	-1.344425

H 0 -3.405651 1.076436 -0.122985

P-69+CH

B3LYP/6-31G(d) Geometry

C 0 1.389577 0.852881 -1.076825
C 0 0.052520 0.672318 -0.282066
O 0 1.835093 -0.406029 -1.582375
C 0 2.598508 1.273240 -0.223876
C 0 2.405729 -1.001733 -0.438332
C 0 0.103651 -0.541497 0.759232
O 0 3.117122 0.021604 0.251729
C 0 -1.153401 0.412448 -1.278800
C 0 1.288464 -1.501035 0.480487
C 0 -1.086019 -1.003845 -1.803018
C 0 -2.483694 0.533975 -0.484162
C 0 -1.207319 -1.394503 0.552356
O 0 1.352055 -2.592551 1.007455
C 0 -1.162662 -1.944144 -0.855712
C 0 -0.188376 1.964123 0.382761
C 0 0.266304 -0.095261 2.229989
N 0 -0.347652 3.012099 0.859011
C 0 -2.464001 -0.493418 0.678818
H 0 1.220796 1.516714 -1.927890
H 0 2.348970 1.915641 0.623335
H 0 3.355023 1.768006 -0.843579
H 0 3.075778 -1.813422 -0.729289
H 0 -1.113048 1.158145 -2.079009
H 0 -1.016121 -1.206198 -2.867390
H 0 -3.310004 0.332720 -1.172356
H 0 -2.615822 1.554264 -0.111165
H 0 -1.212267 -2.187479 1.302702
H 0 -1.155676 -3.012099 -1.051890
H 0 -0.552168 0.552665 2.553434
H 0 1.204276 0.448048 2.381245
H 0 0.287257 -0.983826 2.867390
H 0 -2.472325 0.015058 1.648461
H 0 -3.355023 -1.128515 0.652869

P-70+CH

B3LYP/6-31G(d) Geometry

C 0 -1.382260 -1.079157 -0.544704
C 0 -0.054642 -0.739240 0.190487
O 0 -1.746165 -0.037162 -1.466895
C 0 -2.662530 -1.128294 0.313872
C 0 -2.295143 0.931124 -0.610730
C 0 -0.064016 0.741121 0.786757
O 0 -3.115699 0.232034 0.328277
C 0 1.125864 -0.803771 -0.863452
C 0 -1.190551 1.624887 0.190914
C 0 1.100366 0.398027 -1.784203
C 0 2.493596 -0.716075 -0.124895
C 0 1.281062 1.451050 0.351322
O 0 -1.235256 2.822414 0.393904
C 0 1.241996 1.570348 -1.156821
C 0 0.168021 -1.842734 1.249764
C 0 2.503313 0.574903 0.733941
C 0 -0.256971 0.815401 2.318633
H 0 -1.251130 -1.994747 -1.129210
H 0 -2.520225 -1.469219 1.340897
H 0 -3.420610 -1.758247 -0.167572
H 0 -2.888887 1.650624 -1.178575
H 0 1.055281 -1.746642 -1.418478
H 0 1.018849 0.285066 -2.861319
H 0 3.284389 -0.683961 -0.880815
H 0 2.682971 -1.605308 0.483960
H 0 1.325307 2.426987 0.839550
H 0 1.277199 2.534559 -1.655299
H 0 0.233093 -2.822414 0.758748
H 0 -0.644133 -1.893434 1.978508
H 0 1.089416 -1.703065 1.816122
H 0 2.480787 0.338443 1.804280
H 0 3.420610 1.148596 0.565172
H 0 0.546450 0.310539 2.861319
H 0 -1.208395 0.370407 2.628524
H 0 -0.270988 1.866009 2.622604

TS-1+BU

B3LYP/6-31G(d) Geometry

C 0 -0.283925 -1.433381 1.604729
C 0 -0.268171 1.449547 1.558008
C 0 0.869739 0.716032 1.800581
C 0 0.867482 -0.692017 1.846027
H 0 -0.219874 -2.518795 1.583799
H 0 -1.243068 -1.057151 1.947107
H 0 -0.209380 2.518795 1.377944
H 0 -1.254017 1.068370 1.795466
H 0 1.831739 1.222758 1.767274
H 0 1.828726 -1.202260 1.840130
C 0 -0.812733 -0.979355 -0.382479
C 0 -0.880507 0.399252 -0.611356
C 0 0.144962 1.073902 -1.335971
N 0 0.979185 1.613082 -1.947107
H 0 -1.749675 -1.521378 -0.293746
H 0 -0.004874 -1.538112 -0.841767
H 0 -1.831739 0.917366 -0.543744

TS-2+BU

B3LYP/6-31G(d) Geometry

C 0 -2.122930 0.614583 0.137538
C 0 -0.309749 -1.565665 0.719136
C 0 -1.171887 -1.592271 -0.351367
C 0 -2.081042 -0.550333 -0.622960
H 0 -2.801824 1.410211 -0.160682
H 0 -1.950146 0.565353 1.208171
H 0 0.489653 -2.293967 0.813059
H 0 -0.527087 -0.994771 1.613342
H 0 -1.029206 -2.354199 -1.115484
H 0 -2.590727 -0.560434 -1.584754
C 0 -0.244232 1.483153 -0.152933
C 0 0.783533 0.675181 0.337270
C 0 1.714721 -0.014196 -0.557021
O 0 2.801824 -0.464582 -0.231391
H 0 -0.538642 2.354199 0.426291
H 0 -0.318372 1.618993 -1.228988
H 0 1.095723 0.754051 1.376028
H 0 1.362197 -0.079381 -1.613342

TS-3+BU

B3LYP/6-31G(d) Geometry

C 0 3.099565 -0.346114 0.065591
C 0 0.915445 1.473358 0.809742
C 0 1.718697 1.676732 -0.280594
C 0 2.798328 0.831125 -0.622099
H 0 3.948128 -0.932653 -0.278746
H 0 2.947519 -0.391454 1.139941
H 0 -0.002858 2.036999 0.944168

H 0	1.217435	0.850768	1.643236
H 0	1.428883	2.438966	-1.000806
H 0	3.274443	0.994850	-1.587195
C 0	1.550711	-1.579278	-0.342565
C 0	0.384458	-1.177490	0.323767
C 0	-0.687462	-0.512330	-0.336668
O 0	-1.797627	-0.304598	0.211240
B 0	-2.917378	0.581673	-0.487677
H 0	2.082481	-2.438966	0.057738
H 0	1.562062	-1.526727	-1.427788
H 0	0.220651	-1.459362	1.361028
H 0	-0.554742	-0.191191	-1.377980
H 0	-2.906335	1.614178	0.158839
H 0	-2.559221	0.733712	-1.643236
H 0	-3.948128	-0.037368	-0.359155

TS-4+BU

B3LYP/6-31G(d) Geometry

C 0	-0.994488	1.461195	0.305802
C 0	-1.783925	0.376325	0.749554
C 0	-2.072740	-0.713192	-0.063546
C 0	-0.471032	1.522045	-0.959650
H 0	-0.637075	2.164385	1.053868
H 0	-1.981695	0.299864	1.816243
H 0	-2.643513	-1.542272	0.347175
H 0	-2.217279	-0.561255	-1.128998
H 0	0.264781	2.275664	-1.223535
H 0	-0.910049	0.982480	-1.790305
C 0	0.744347	-0.674829	-0.806625
C 0	-0.209315	-1.603390	-0.416066
N 0	1.631540	-0.132198	0.183378
O 0	1.326396	-0.274146	1.377687
O 0	2.643513	0.457515	-0.214490
H 0	1.092391	-0.514558	-1.816243
H 0	-0.587494	-2.275664	-1.180388
H 0	-0.122008	-2.011536	0.583057

TS-5+BU

B3LYP/6-31G(d) Geometry

C 0	1.329887	-1.426094	0.326797
C 0	2.083972	-0.326898	0.781535
C 0	2.271666	0.804109	0.008217
C 0	0.737061	-1.442068	-0.918765
H 0	1.034164	-2.177611	1.055512
H 0	2.329535	-0.282336	1.841085
H 0	2.765385	1.675283	0.431317
H 0	2.345025	0.725814	-1.070933
H 0	0.057697	-2.242298	-1.193464
H 0	1.175817	-0.905346	-1.751783
C 0	0.183147	1.510675	-0.340355
C 0	-0.612625	0.465657	-0.785667
C 0	-1.676712	-0.084210	0.110848
F 0	-1.255273	-0.213114	1.390085
F 0	-2.139182	-1.292022	-0.293157
F 0	-2.765385	0.733256	0.144873
H 0	0.545567	2.242298	-1.054577
H 0	0.078258	1.864539	0.678538
H 0	-0.848401	0.372737	-1.841085

TS-6+BU

B3LYP/6-31G(d) Geometry

C 0	1.296743	-1.665639	-0.058844
C 0	2.344440	-0.785818	0.266858
C 0	2.602510	0.379475	-0.450899
C 0	0.448828	-1.478657	-1.130678
H 0	1.046149	-2.438352	0.665478
H 0	2.827723	-0.913658	1.233858
H 0	3.402296	1.033788	-0.112100
H 0	2.444325	0.400053	-1.524291
H 0	-0.395068	-2.143290	-1.286763
H 0	0.746580	-0.900741	-1.996265
C 0	0.915922	1.597379	-0.133196
C 0	-0.187580	1.002785	-0.746096
B 0	-1.265267	0.133354	-0.066299
C 0	-2.572071	-0.276949	-0.883366
C 0	-1.246322	-0.148515	1.501889
H 0	1.408012	2.438352	-0.620486
H 0	0.972633	1.621240	0.951360
H 0	-0.290362	1.211322	-1.815638
H 0	-2.477829	-0.180005	-1.972606
H 0	-3.402296	0.379713	-0.578018
H 0	-2.911256	-1.297658	-0.659948
H 0	-1.920946	0.568667	1.996265
H 0	-0.266902	-0.042495	1.983262
H 0	-1.637260	-1.143577	1.752575

TS-7+BU

B3LYP/6-31G(d) Geometry

C 0	-1.030017	-0.247163	-1.576270
C 0	-2.034089	0.358591	-0.793606
C 0	-2.288152	0.001892	0.528885
C 0	-0.230633	-1.268589	-1.124571
H 0	-0.775379	0.228334	-2.520718
H 0	-2.480376	1.275429	-1.173781
H 0	-3.070747	0.532868	1.065427
H 0	-2.168131	-1.031667	0.838881
H 0	0.608368	-1.621553	-1.715735
H 0	-0.519782	-1.905016	-0.297846
C 0	-0.613945	0.604153	1.576920
C 0	0.498007	-0.154442	1.196962
B 0	1.586427	0.296872	0.246824
Cl 0	3.070747	-0.679478	0.017226
Cl 0	1.550165	1.905016	-0.542287
H 0	-1.102221	0.368292	2.520718
H 0	-0.638527	1.656799	1.311963
H 0	0.620161	-1.125503	1.677368

TS-8+BU

B3LYP/6-31G(d) Geometry

C 0	-1.256263	-1.271378	-0.139629
C 0	-0.246700	1.178926	-1.385291
C 0	-1.399415	1.140639	-0.647251
C 0	-1.922309	-0.044583	-0.081874
H 0	-1.731697	-2.124798	0.339294
H 0	-0.693303	-1.537447	-1.031294
H 0	0.203562	2.124798	-1.670414
H 0	0.178542	0.298971	-1.850253
H 0	-1.867683	2.081628	-0.363503
H 0	-2.759230	0.053681	0.607222
C 0	0.393191	-1.018533	0.961273
C 0	1.366037	-0.286944	0.274360
C 0	1.775743	1.069238	0.639969
O 0	2.759230	1.663465	0.235451
Cl 0	2.342948	-1.123802	-0.921800
H 0	0.548116	-2.089216	1.060119
H 0	-0.015220	-0.545200	1.850253

H 0 1.093392 1.514878 1.397516

TS-9+BU

B3LYP/6-31G(d) Geometry

C 0 -2.081809 -0.306056 -0.244938
C 0 -1.338676 -1.417090 0.205744
C 0 -0.280180 -1.306607 1.071918
C 0 -1.735752 1.005028 0.083824
H 0 -2.791627 -0.465642 -1.054494
H 0 -1.517813 -2.376055 -0.277537
H 0 0.368506 -2.152618 1.276277
H 0 -0.170547 -0.460322 1.737619
H 0 -2.330468 1.812889 -0.337013
H 0 -1.350700 1.226014 1.076043
C 0 1.104407 0.604497 -0.118201
C 0 0.087322 1.302535 -0.782268
C 0 1.732370 -0.549175 -0.771913
O 0 2.791627 -1.057491 -0.429973
C 0 1.787571 1.178435 1.096517
H 0 -0.156018 1.001212 -1.797951
H 0 0.019631 2.376055 -0.616067
H 0 1.183144 -0.922848 -1.665283
H 0 2.366872 0.408046 1.611468
H 0 2.489090 1.974199 0.810868
H 0 1.069118 1.621899 1.797951

TS-10+BU

B3LYP/6-31G(d) Geometry

C 0 -1.436985 -1.782215 -0.679609
C 0 -0.234236 -2.290890 -0.158194
C 0 0.400069 -1.710641 0.919935
C 0 -2.031610 -0.632707 -0.170066
H 0 -1.774849 -2.161468 -1.642506
H 0 0.303435 -3.035715 -0.741855
H 0 1.407046 -2.004147 1.200077
H 0 -0.154284 -1.172452 1.679277
H 0 -2.919417 -0.241915 -0.661397
H 0 -1.999083 -0.436026 0.897049
C 0 0.599754 0.588265 0.140271
C 0 -0.622221 0.934417 -0.456759
C 0 1.756024 0.174527 -0.656971
O 0 2.919417 0.224295 -0.290418
C 0 -1.442190 2.070712 0.128683
H 0 0.828109 0.951971 1.140671
H 0 -0.654303 0.862703 -1.542924
H 0 1.495919 -0.187899 -1.679277
H 0 -0.991409 3.035715 -0.136488
H 0 -2.471702 2.076391 -0.243020
H 0 -1.474969 2.016593 1.222830

TS-11+BU

B3LYP/6-31G(d) Geometry

C 0 -0.281622 1.743448 -0.649436
C 0 -1.460444 1.389417 0.025581
C 0 -1.465926 0.447727 1.047056
C 0 0.943951 1.181795 -0.328906
H 0 -0.372688 2.310310 -1.574128
H 0 -2.411271 1.702430 -0.400812
H 0 -2.406909 0.098332 1.461862
H 0 -0.612793 0.352268 1.710177
H 0 1.812703 1.369039 -0.953806
H 0 1.177663 0.900245 0.691106
C 0 -0.656654 -1.381798 0.069465
C 0 0.515840 -1.040612 -0.633539
C 0 -1.900458 -1.645895 -0.684442
O 0 -2.829029 -2.310310 -0.269962
C 0 1.789466 -1.472250 -0.147430
N 0 2.829029 -1.803784 0.260020
H 0 -0.568396 -1.905315 1.017394
H 0 0.453349 -0.909710 -1.710177
H 0 -1.931097 -1.178554 -1.695300

TS-12+BU

B3LYP/6-31G(d) Geometry

C 0 3.002408 0.724833 -0.145463
C 0 0.933247 -0.969605 -1.438279
C 0 1.937515 -1.464570 -0.656188
C 0 2.956161 -0.667544 -0.072187
H 0 3.847277 1.223886 0.323190
H 0 2.628168 1.235426 -1.029534
H 0 0.095559 -1.592251 -1.738684
H 0 0.966360 0.024038 -1.869831
H 0 1.898028 -2.512252 -0.364859
H 0 3.630235 -1.161115 0.625861
C 0 1.471484 1.342896 1.010838
C 0 0.269779 1.268520 0.298645
C 0 -0.686003 0.228190 0.488956
O 0 -1.798008 0.179009 -0.083919
B 0 -2.723335 -1.114437 0.047772
Cl 0 -0.082245 2.512252 -0.880907
H 0 1.913915 2.325012 1.148452
H 0 1.566488 0.685348 1.869831
H 0 -0.432723 -0.546555 1.222292
H 0 -2.559212 -1.681906 -1.018387
H 0 -2.288305 -1.743359 0.996980
H 0 -3.847277 -0.697106 0.188989

TS-13+BU

B3LYP/6-31G(d) Geometry

C 0 -3.044104 0.200561 0.065442
C 0 -0.881211 -1.421804 1.247819
C 0 -1.789590 -1.916781 0.352109
C 0 -2.858559 -1.160892 -0.184085
H 0 -3.901711 0.684811 -0.395682
H 0 -2.791053 0.606691 1.041461
H 0 0.013888 -1.979272 1.507405
H 0 -1.069874 -0.526368 1.827940
H 0 -1.607939 -2.900734 -0.075659
H 0 -3.434714 -1.614172 -0.988681
C 0 -1.504100 1.112181 -0.865609
C 0 -0.329253 1.005209 -0.102038
C 0 0.668826 0.056710 -0.484703
O 0 1.799736 -0.000153 0.064130
B 0 2.809278 -1.186240 -0.252044
C 0 -0.059560 1.936684 1.051685
H 0 -2.018079 2.071312 -0.855979
H 0 -1.538008 0.609932 -1.827940
H 0 0.465362 -0.621410 -1.321552
H 0 2.700560 -1.917698 0.718217
H 0 2.417751 -1.703308 -1.284267
H 0 3.901711 -0.674426 -0.329815
H 0 -0.975294 2.147920 1.618619
H 0 0.324140 2.900734 0.692314
H 0 0.691659 1.520756 1.727068

TS-14+BU

B3LYP/6-31G(d) Geometry

C 0	2.922417	0.745582	-0.049226
C 0	0.343971	1.778324	0.853750
C 0	1.001513	2.283789	-0.239783
C 0	2.265989	1.821967	-0.655907
H 0	3.897380	0.470617	-0.443870
H 0	2.842086	0.615195	1.026345
H 0	-0.699287	2.015024	1.040543
H 0	0.862515	1.254816	1.647755
H 0	0.461744	2.956450	-0.902981
H 0	2.637479	2.173351	-1.616829
C 0	1.841090	-0.900422	-0.465800
C 0	0.607440	-0.834950	0.218473
C 0	-0.614259	-0.465520	-0.406201
O 0	-1.733859	-0.618035	0.144973
B 0	-3.056525	-0.014900	-0.496342
C 0	2.836213	-1.969977	-0.035524
H 0	1.780550	-0.763535	-1.544389
H 0	0.537338	-1.219173	1.234587
H 0	-0.592094	-0.057872	-1.425043
H 0	-3.289497	0.960575	0.197289
H 0	-2.777241	0.275188	-1.647755
H 0	-3.897380	-0.876724	-0.386644
H 0	2.464832	-2.956450	-0.337619
H 0	2.962356	-1.984359	1.052503
H 0	3.818541	-1.829932	-0.495381

TS-15+BU

B3LYP/6-31G(d) Geometry

C 0	2.708490	0.815821	-0.310825
C 0	0.165885	1.164467	1.011706
C 0	0.522298	1.904369	-0.099216
C 0	1.766409	1.757529	-0.731818
H 0	3.624187	0.695251	-0.883471
H 0	2.826013	0.607565	0.747876
H 0	-0.856793	1.167040	1.376507
H 0	0.907983	0.775543	1.699021
H 0	-0.245781	2.487302	-0.602735
H 0	1.906014	2.236125	-1.699021
C 0	1.754510	-1.031354	-0.606421
C 0	0.563358	-1.119919	0.154908
C 0	-0.721752	-0.974762	-0.462482
O 0	-1.779891	-1.315164	0.104240
B 0	-3.218682	-1.023724	-0.538022
C 0	2.870204	-1.848451	-0.207360
N 0	3.784531	-2.487302	0.121780
H 0	1.649275	-0.931244	-1.683787
H 0	0.587704	-1.568628	1.143215
H 0	-0.782742	-0.550618	-1.473748
H 0	-3.703305	-0.220251	0.232473
H 0	-2.995775	-0.574769	-1.647452
H 0	-3.784531	-2.090639	-0.524568

TS-16+BU

B3LYP/6-31G(d) Geometry

C 0	1.368151	-1.525116	-0.810772
C 0	0.513842	-0.078862	1.601899
C 0	1.543291	0.338850	0.809239
C 0	1.994734	-0.373827	-0.330414
H 0	1.815941	-2.024093	-1.667394
H 0	0.912446	-2.210100	-0.100174
H 0	0.108768	0.568245	2.373750
H 0	0.123042	-1.088658	1.578456
H 0	1.964407	1.327022	0.980587
H 0	2.735867	0.111433	-0.962671
C 0	-0.355943	-0.936642	-1.583837
C 0	-1.236455	-0.357442	-0.640864
C 0	-1.432491	1.054826	-0.604917
C 0	-2.080561	-1.189810	0.150549
N 0	-1.588916	2.210100	-0.627530
N 0	-2.735867	-1.910146	0.792463
H 0	-0.603052	-1.941781	-1.915773
H 0	0.001198	-0.283968	-2.373750

TS-17+BU

B3LYP/6-31G(d) Geometry

C 0	-0.279164	-1.432240	1.534938
C 0	-0.279101	1.432246	1.534850
C 0	0.877663	0.702117	1.758372
C 0	0.877632	-0.702149	1.758408
H 0	-0.225473	-2.509914	1.410185
H 0	-1.242304	-1.057134	1.863816
H 0	-0.225359	2.509914	1.410058
H 0	-1.242255	1.057205	1.863764
H 0	1.835354	1.214949	1.711754
H 0	1.835300	-1.215026	1.711816
C 0	-0.875419	-0.705903	-0.522899
C 0	-0.875359	0.705904	-0.522911
C 0	0.092843	-1.454971	-1.265602
C 0	0.092963	1.454868	-1.265646
N 0	0.864365	2.088781	-1.863816
N 0	0.864192	-2.088966	-1.863754
H 0	-1.835354	-1.199266	-0.406346
H 0	-1.835261	1.199345	-0.406400

TS-18+BU

B3LYP/6-31G(d) Geometry

C 0	0.490947	-1.441953	1.459726
C 0	0.307024	1.424140	1.489640
C 0	1.504635	0.760271	1.723817
C 0	1.596431	-0.640819	1.683344
H 0	0.609539	-2.508491	1.290071
H 0	-0.492643	-1.145879	1.804478
H 0	0.300158	2.508491	1.419384
H 0	-0.638553	0.982485	1.786356
H 0	2.427813	1.334552	1.710473
H 0	2.588136	-1.085367	1.627875
C 0	-0.248249	-0.633233	-0.590766
C 0	-0.151780	0.775037	-0.569093
C 0	-1.537560	-1.242374	-0.513227
C 0	0.942652	1.399941	-1.252430
N 0	1.834794	1.903636	-1.804478
N 0	-2.588136	-1.737321	-0.421459
H 0	0.522093	-1.207768	-1.091110
H 0	-1.071197	1.352399	-0.547522

TS-19+BU

B3LYP/6-31G(d) Geometry

C 0	-1.373321	-1.099622	1.194967
C 0	0.297927	1.219088	1.401798
C 0	0.573288	0.062221	2.100842
C 0	-0.247046	-1.075726	2.009068
H 0	-1.932444	-2.026647	1.091764
H 0	-1.981948	-0.205831	1.097987
H 0	1.023457	2.026647	1.365452
H 0	-0.717000	1.495093	1.140308

H	0	1.551336	-0.046537	2.563885
H	0	0.136604	-2.014316	2.404340
C	0	-0.690716	-0.757045	-0.806512
C	0	0.255279	0.282725	-0.813980
C	0	-2.032264	-0.533571	-1.475728
C	0	1.650603	-0.008385	-0.855781
N	0	2.787717	-0.262543	-0.900767
H	0	-0.292302	-1.764432	-0.885372
H	0	-0.032492	1.262631	-1.184942
H	0	-1.936116	-0.642196	-2.563885
H	0	-2.412864	0.475982	-1.280264
H	0	-2.787717	-1.250886	-1.139562

TS-20+BU

B3LYP/6-31G(d) Geometry

C	0	-1.765720	-1.145205	1.164202
C	0	0.150365	0.990367	1.453838
C	0	0.275504	-0.197807	2.129541
C	0	-0.673215	-1.235124	2.024437
H	0	-2.437008	-1.997333	1.082779
H	0	-2.263679	-0.188201	1.033592
H	0	0.969126	1.703154	1.428729
H	0	-0.811785	1.366563	1.129861
H	0	1.219175	-0.419454	2.623713
H	0	-0.414000	-2.207375	2.438789
C	0	-0.960539	-1.060047	-0.727654
C	0	-0.123978	0.050843	-0.925636
C	0	1.287791	-0.160331	-1.001236
C	0	-0.661197	1.336786	-1.526482
N	0	2.437008	-0.332209	-1.107615
H	0	-1.947833	-1.017903	-1.182692
H	0	-0.511077	-2.046915	-0.727374
H	0	-1.694235	1.508610	-1.203202
H	0	-0.664728	1.283550	-2.623713
H	0	-0.063222	2.207375	-1.242904

TS-21+BU

B3LYP/6-31G(d) Geometry

C	0	0.928119	-2.077187	-0.660050
C	0	1.973271	-1.394140	-0.011508
C	0	1.745557	-0.532685	1.042444
C	0	-0.400132	-1.909915	-0.297521
H	0	1.153682	-2.576650	-1.600479
H	0	2.956643	-1.400560	-0.477543
H	0	2.540656	0.099485	1.425660
H	0	0.896380	-0.665094	1.702408
H	0	-1.180330	-2.373375	-0.892423
H	0	-0.669080	-1.740731	0.739363
C	0	0.221649	1.000151	0.053556
C	0	-0.748687	0.243162	-0.606885
C	0	1.315498	1.641992	-0.691866
O	0	1.979227	2.576650	-0.282444
C	0	-2.155680	0.293004	-0.079434
F	0	-2.193012	0.106176	1.263513
F	0	-2.735546	1.490310	-0.325550
F	0	-2.956643	-0.641981	-0.640362
H	0	0.000357	1.426388	1.027924
H	0	-0.702413	0.169273	-1.689627
H	0	1.496580	1.208671	-1.702408

TS-22+BU

B3LYP/6-31G(d) Geometry

C	0	-0.216020	2.213176	-0.304548
C	0	-1.497726	1.924392	0.186593
C	0	-2.274528	0.878891	-0.313722
C	0	0.374720	1.507740	-1.337090
H	0	0.401846	2.903530	0.266367
H	0	-1.799053	2.391553	1.122460
H	0	-3.242136	0.693101	0.146036
H	0	-2.246370	0.648491	-1.374251
H	0	1.401432	1.712399	-1.623587
H	0	-0.219553	1.008149	-2.091820
C	0	-1.290954	-0.915532	0.144815
C	0	-0.068818	-0.888285	-0.544987
B	0	1.303914	-0.434564	-0.017339
C	0	2.610938	-0.738815	-0.882853
C	0	1.506036	0.057657	1.485847
C	0	-2.378799	-1.891453	-0.277742
H	0	-1.248457	-0.734381	1.217340
H	0	-0.117813	-1.290787	-1.563446
H	0	2.416564	-0.946967	-1.943013
H	0	3.110436	-1.630413	-0.471776
H	0	3.356771	0.065785	-0.825487
H	0	1.844633	-0.797982	2.091820
H	0	0.605303	0.450218	1.972424
H	0	2.294468	0.816411	1.577683
H	0	-2.125766	-2.903530	0.063469
H	0	-2.477602	-1.930546	-1.368889
H	0	-3.356771	-1.640854	0.146507

TS-23+BU

B3LYP/6-31G(d) Geometry

C	0	0.377032	-2.238979	-0.243192
C	0	1.552554	-1.773794	0.371711
C	0	2.177015	-0.580318	0.005038
C	0	-0.242381	-1.570215	-1.274909
H	0	-0.151631	-3.062267	0.231469
H	0	1.860814	-2.255312	1.297552
H	0	3.078062	-0.293783	0.541371
H	0	2.179360	-0.281964	-1.039338
H	0	-1.215688	-1.884808	-1.637627
H	0	0.295073	-0.886204	-1.919370
C	0	0.926605	0.968255	0.525336
C	0	-0.269868	0.836994	-0.205626
B	0	-1.554556	0.218056	0.290274
Cl	0	-3.078062	0.382290	-0.642769
Cl	0	-1.687887	-0.519803	1.919370
C	0	1.855343	2.132633	0.212874
H	0	0.866189	0.715097	1.581766
H	0	-0.293491	1.323034	-1.182824
H	0	1.420694	3.062267	0.600606
H	0	1.991708	2.259500	-0.867151
H	0	2.841210	2.015279	0.673311

TS-24+BU

B3LYP/6-31G(d) Geometry

C	0	0.719683	1.804888	-0.838214
C	0	1.658506	1.387558	0.131158
C	0	1.314921	0.569982	1.190956
C	0	-0.616081	1.475288	-0.762805
H	0	1.104051	2.237979	-1.758734
H	0	2.712390	1.543613	-0.086022
H	0	2.088313	0.167767	1.839293
H	0	0.313373	0.569433	1.608865
H	0	-1.286375	1.690578	-1.589771
H	0	-1.097173	1.301047	0.193465

C 0 0.593134 -1.235718 0.058903
C 0 -0.459591 -0.866646 -0.762814
N 0 1.855546 -1.552803 -0.588377
N 0 -1.798671 -1.032863 -0.236639
O 0 2.652839 -2.237979 0.051841
O 0 2.053706 -1.094280 -1.717494
O 0 -1.941113 -1.024441 0.993869
O 0 -2.712390 -1.139112 -1.053535
H 0 0.446580 -1.749566 0.997136
H 0 -0.401218 -0.882605 -1.839293

TS-25+BU

B3LYP/6-31G(d) Geometry
C 0 0.655227 1.791487 0.884246
C 0 -0.749579 1.768953 0.924099
C 0 -1.511735 1.567186 -0.207694
C 0 1.357276 1.585944 -0.303621
H 0 1.197438 1.748383 1.825735
H 0 -1.233018 1.715016 1.896748
H 0 -2.582457 1.402065 -0.134457
H 0 -1.153756 1.842580 -1.192011
H 0 2.442080 1.542235 -0.283626
H 0 0.945038 1.960973 -1.235309
C 0 -0.509135 -0.554143 -0.922805
C 0 0.890226 -0.372432 -0.859801
C 0 -1.349255 -1.214497 0.066401
C 0 1.912700 -1.043440 0.042714
O 0 3.049492 -1.173060 -0.363752
O 0 1.564583 -1.415212 1.275145
O 0 -1.059212 -1.493762 1.232228
O 0 -2.576793 -1.519482 -0.417320
H 0 -0.974737 -0.450607 -1.896748
H 0 1.349751 -0.235703 -1.834779
H 0 0.579651 -1.372600 1.403692
H 0 -3.049492 -1.960973 0.312464

TS-26+BU

B3LYP/6-31G(d) Geometry
C 0 0.219589 -1.377808 1.675023
C 0 0.527135 1.505914 1.549246
C 0 1.577242 0.669637 1.834300
C 0 1.429545 -0.726780 1.950596
H 0 0.188308 -2.459697 1.779878
H 0 -0.716094 -0.886764 1.931182
H 0 0.700011 2.545889 1.289668
H 0 -0.504319 1.232099 1.731594
H 0 2.586962 1.073081 1.819151
H 0 2.331061 -1.328693 2.034788
C 0 -0.061736 -1.152885 -0.296214
C 0 -0.212709 0.219414 -0.670335
C 0 1.030397 -1.908190 -0.861544
C 0 0.787173 0.916347 -1.412862
C 0 -1.514703 0.795604 -0.581560
N 0 1.597803 1.476000 -2.034788
N 0 1.902897 -2.545889 -1.287906
N 0 -2.586962 1.236529 -0.460495
H 0 -0.992595 -1.715836 -0.262572

TS-27+BU

B3LYP/6-31G(d) Geometry
C 0 -1.738036 -0.542128 1.088962
C 0 0.360726 1.390727 1.394619
C 0 0.371858 0.196544 2.076617
C 0 -0.678296 -0.735799 1.974830
H 0 -2.495573 -1.318757 1.006485
H 0 -2.129008 0.460303 0.936416
H 0 1.248479 2.014823 1.355321
H 0 -0.565622 1.874487 1.112473
H 0 1.290637 -0.117713 2.568002
H 0 -0.531626 -1.722585 2.408746
C 0 -0.870118 -0.576589 -0.790679
C 0 -0.057147 0.566936 -0.955933
C 0 -0.272954 -1.965201 -0.887705
C 0 1.351963 0.404411 -1.134048
C 0 -0.657743 1.861695 -1.473975
N 0 2.495573 0.277380 -1.329573
H 0 -1.864408 -0.476333 -1.225987
H 0 0.619726 -2.058360 -0.262477
H 0 0.031042 -2.178383 -1.920529
H 0 -0.991839 -2.731419 -0.581130
H 0 -1.662117 2.012219 -1.060301
H 0 -0.754298 1.840870 -2.568002
H 0 -0.047152 2.731419 -1.215049

TS-28+BU

B3LYP/6-31G(d) Geometry
C 0 -1.459000 -1.206144 1.176196
C 0 0.323751 1.021335 1.437214
C 0 0.533592 -0.155211 2.120076
C 0 -0.348549 -1.245563 2.016199
H 0 -2.075713 -2.097364 1.085310
H 0 -2.017567 -0.279659 1.076106
H 0 1.093916 1.786421 1.405006
H 0 -0.670103 1.346961 1.156047
H 0 1.498473 -0.319426 2.594650
H 0 -0.025820 -2.205084 2.415393
C 0 -0.741415 -0.987436 -0.779118
C 0 0.151265 0.108344 -0.870364
C 0 -2.073840 -0.944171 -1.505827
C 0 1.549691 -0.193113 -0.879051
C 0 -0.254018 1.427768 -1.504673
N 0 2.687681 -0.447642 -0.918816
H 0 -0.267265 -1.964484 -0.780384
H 0 -1.915729 -0.946143 -2.592716
H 0 -2.654814 -0.047991 -1.264503
H 0 -2.687681 -1.815796 -1.260051
H 0 -1.217506 1.779760 -1.121071
H 0 -0.355810 1.326822 -2.594650
H 0 0.489836 2.205084 -1.312770

TS-29+BU

B3LYP/6-31G(d) Geometry
C 0 -1.408079 -0.536439 1.080209
C 0 0.399304 1.672976 0.997664
C 0 0.645297 0.559908 1.794243
C 0 -0.241941 -0.528104 1.824407
H 0 -2.010016 -1.437981 1.010871
H 0 -1.942998 0.380858 0.866845
H 0 1.156876 2.446920 0.909491
H 0 -0.617446 2.016304 0.836723
H 0 1.636569 0.431456 2.222343
H 0 0.097620 -1.454223 2.283772
C 0 -0.531305 -0.287294 -1.082088
C 0 0.347332 0.828491 -1.017779
C 0 -1.834339 -0.026869 -1.622502
C 0 0.015830 -1.693925 -1.264131

C 0 1.756464 0.618435 -1.183958
N 0 2.900111 0.449470 -1.320320
N 0 -2.900111 0.179274 -2.045996
H 0 -0.011480 1.773346 -1.415294
H 0 0.843836 -1.872124 -0.572900
H 0 0.399764 -1.824836 -2.283772
H 0 -0.756610 -2.446920 -1.092114

TS-30+BU

B3LYP/6-31G(d) Geometry

C 0 -1.804682 -0.548487 1.299985
C 0 0.145926 1.535901 1.343805
C 0 0.299038 0.385484 2.097165
C 0 -0.665610 -0.633802 2.091874
H 0 -2.471003 -1.403349 1.222868
H 0 -2.279205 0.411383 1.121961
H 0 0.967465 2.240413 1.252511
H 0 -0.838036 1.948626 1.152883
H 0 1.271622 0.169566 2.533116
H 0 -0.401894 -1.595502 2.524823
C 0 -0.951837 -0.419134 -0.718626
C 0 -0.087974 0.701853 -0.815858
C 0 -0.448391 -1.757980 -0.819234
C 0 1.323487 0.489866 -0.974893
C 0 -0.632393 1.979836 -1.438359
N 0 2.471003 0.366882 -1.129822
N 0 -0.068598 -2.855024 -0.898111
H 0 -1.950464 -0.291824 -1.128990
H 0 -1.671161 2.143895 -1.131690
H 0 -0.612929 1.910133 -2.533116
H 0 -0.044173 2.855024 -1.150740

TS-31+BU

B3LYP/6-31G(d) Geometry

C 0 -1.349997 1.855428 0.365881
C 0 -0.023069 2.283826 0.193620
C 0 0.770120 1.800341 -0.827966
C 0 -1.907895 0.864835 -0.436760
H 0 -1.862060 2.134424 1.284853
H 0 0.442067 2.858570 0.992387
H 0 1.836082 2.004131 -0.852688
H 0 0.341740 1.484596 -1.771594
H 0 -2.914302 0.518602 -0.213786
H 0 -1.649203 0.812078 -1.489107
C 0 0.586374 -0.581689 -0.505791
C 0 -0.722440 -0.887820 -0.066780
C 0 1.766004 -0.476412 0.356307
O 0 2.914302 -0.639682 -0.031854
C 0 -0.990235 -1.091633 1.418747
C 0 -1.524080 -1.820067 -0.969308
H 0 0.833874 -0.800743 -1.543690
H 0 1.564749 -0.246814 1.424530
H 0 -0.593618 -0.276773 2.029461
H 0 -2.065580 -1.164898 1.613113
H 0 -0.528693 -2.025854 1.767180
H 0 -1.203880 -2.858570 -0.807705
H 0 -2.597887 -1.776058 -0.758098
H 0 -1.370629 -1.592205 -2.029461

TS-32+BU

B3LYP/6-31G(d) Geometry

C 0 -0.226525 1.673519 0.181340
C 0 1.030186 1.350774 -0.363585
C 0 1.165551 0.486652 -1.460712
C 0 -1.406567 1.229497 -0.366050
H 0 -0.251111 2.154690 1.156292
H 0 1.918315 1.609728 0.208817
H 0 2.165619 0.259653 -1.821176
H 0 0.417343 0.530531 -2.248244
H 0 -2.344813 1.343519 0.168257
H 0 -1.491927 0.931627 -1.403319
C 0 0.555519 -1.318854 -0.867548
C 0 -0.763428 -1.307589 -0.319796
C 0 1.719006 -1.686393 0.005635
O 0 2.743326 -2.154690 -0.440462
C 0 -1.865980 -1.626813 -1.169455
C 0 -0.981007 -1.355432 1.093576
N 0 -2.743326 -1.862922 -1.899439
N 0 -1.129875 -1.407003 2.248244
H 0 0.635379 -1.742974 -1.866294
H 0 1.590302 -1.488342 1.088226

TS-33+BU

B3LYP/6-31G(d) Geometry

C 0 0.365185 -1.425344 1.480653
C 0 0.365045 1.425314 1.480893
C 0 1.532706 0.699358 1.703963
C 0 1.532771 -0.699321 1.703855
H 0 0.413337 -2.501310 1.341572
H 0 -0.594313 -1.054657 1.823958
H 0 0.413091 2.501310 1.342007
H 0 -0.594405 1.054467 1.824158
H 0 2.487641 1.217302 1.665835
H 0 2.487756 -1.217167 1.665658
C 0 -0.209852 -0.724530 -0.575075
C 0 -0.209958 0.724838 -0.574921
C 0 -1.476247 -1.408435 -0.559510
C 0 0.845862 -1.409102 -1.275420
C 0 0.845641 1.409720 -1.275143
N 0 -2.487447 -1.980227 -0.508832
C 0 -1.476465 1.408537 -0.559222
N 0 1.699920 -1.975650 -1.824158
N 0 1.699602 1.976514 -1.823777
N 0 -2.487756 1.980157 -0.508429

TS-34+BU

B3LYP/6-31G(d) Geometry

C 0 0.693898 -1.141724 1.539763
C 0 0.537562 1.733527 1.571928
C 0 1.746105 1.075061 1.553131
C 0 1.833714 -0.326602 1.580196
H 0 0.842152 -2.218363 1.544604
H 0 -0.200929 -0.821479 2.066886
H 0 0.479786 2.795630 1.353884
H 0 -0.356712 1.295040 1.996280
H 0 2.648444 1.640489 1.333508
H 0 2.803996 -0.782391 1.399113
C 0 -0.172268 -0.862936 -0.275493
C 0 -0.448090 0.538104 -0.480960
C 0 0.864270 -1.427249 -1.117799
C 0 0.361774 1.333089 -1.349871
C 0 -1.746453 1.043165 -0.167108
N 0 1.016912 1.976203 -2.066886
N 0 1.681270 -1.937404 -1.767960
N 0 -2.803996 1.436790 0.125254
C 0 -1.372628 -1.801241 -0.101726

H	0	-1.901964	-1.898766	-1.055457
H	0	-2.074293	-1.403405	0.635367
H	0	-1.048473	-2.795630	0.212756

TS-35+BU

B3LYP/6-31G(d) Geometry

C	0	-0.996408	2.051671	-0.694044
C	0	0.389474	2.014543	-0.896677
C	0	1.009437	0.924023	-1.526275
C	0	-1.823034	1.037690	-1.138150
H	0	-1.398628	2.794012	-0.009127
H	0	1.007574	2.743435	-0.377245
H	0	2.091889	0.929590	-1.624557
H	0	0.500480	0.454045	-2.363174
H	0	-2.858156	0.984118	-0.814539
H	0	-1.576951	0.430310	-2.000482
C	0	0.691802	-0.760551	-0.407600
C	0	-0.683175	-0.812273	0.022406
C	0	1.710892	-0.379647	0.634800
O	0	2.858156	-0.768670	0.606496
C	0	-1.564750	-1.782218	-0.553820
C	0	-1.065332	-0.315514	1.313169
C	0	1.165424	-1.820557	-1.387783
N	0	-2.273786	-2.560225	-1.053085
N	0	-1.359288	0.094241	2.363174
H	0	1.349077	0.303375	1.427570
H	0	2.171131	-1.588565	-1.743085
H	0	1.210449	-2.794012	-0.887070
H	0	0.488352	-1.916744	-2.240538

TS-36+BU

B3LYP/6-31G(d) Geometry

C	0	-1.995769	1.417063	-0.058326
C	0	-0.889396	2.282814	-0.021701
C	0	0.257914	2.041698	-0.745058
C	0	-1.948743	0.193841	-0.734774
H	0	-2.805688	1.592121	0.646897
H	0	-0.881905	3.076150	0.724098
H	0	1.158335	2.624681	-0.578563
H	0	0.239350	1.468740	-1.662684
H	0	-2.828790	-0.443673	-0.685061
H	0	-1.431617	0.132536	-1.689214
C	0	0.738006	-0.406713	-0.153758
C	0	-0.528692	-0.946260	0.220279
C	0	1.626337	0.256372	0.811967
O	0	2.828790	0.427285	0.639760
C	0	1.398398	-0.826841	-1.444723
C	0	-0.969534	-0.861348	1.679116
C	0	-0.914974	-2.280170	-0.423530
H	0	1.156333	0.577168	1.761538
H	0	2.296807	-0.228999	-1.611376
H	0	1.709402	-1.880187	-1.410430
H	0	0.729938	-0.724529	-2.310045
H	0	-0.907654	0.152828	2.079067
H	0	-2.007181	-1.196684	1.782116
H	0	-0.347748	-1.510263	2.310045
H	0	-0.252367	-3.076150	-0.056913
H	0	-1.940023	-2.561577	-0.161621
H	0	-0.835894	-2.264683	-1.513563

TS-37+BU

B3LYP/6-31G(d) Geometry

C	0	-2.805920	0.976936	-0.878999
C	0	-0.096927	1.110110	-1.750439
C	0	-0.655241	2.114305	-0.959503
C	0	-1.987887	2.063101	-0.549782
H	0	-3.794780	0.898756	-0.436133
H	0	-2.711129	0.488006	-1.843333
H	0	0.971301	1.103609	-1.947289
H	0	-0.700402	0.603451	-2.494948
H	0	0.003556	2.848671	-0.501668
H	0	-2.323701	2.756817	0.216375
C	0	-1.749357	-0.687274	0.035682
C	0	-0.468331	-0.837313	-0.617858
C	0	0.738267	-0.507197	0.123938
O	0	1.850766	-0.930504	-0.235498
C	0	-2.767662	-1.660794	-0.279753
C	0	-0.336257	-1.824892	-1.755049
C	0	-1.788477	-0.222882	1.403970
N	0	-3.595715	-2.427092	-0.561084
N	0	-1.817307	0.177409	2.494948
H	0	0.675876	0.137958	1.007398
H	0	-1.179673	-1.760012	-2.448947
H	0	-0.316278	-2.848671	-1.362362
H	0	0.596018	-1.662350	-2.298677
B	0	3.227520	-0.451680	0.460230
H	0	3.764428	0.168585	-0.433456
H	0	2.887015	0.225057	1.409098
H	0	3.794780	-1.480668	0.733690

TS-38+BU

B3LYP/6-31G(d) Geometry

C	0	-1.451671	-0.672662	1.276819
C	0	0.549552	1.345933	1.293474
C	0	0.676887	0.198241	2.064311
C	0	-0.318395	-0.790071	2.068813
H	0	-2.147421	-1.502708	1.192047
H	0	-1.890270	0.298163	1.076779
H	0	1.386493	2.033237	1.208623
H	0	-0.425131	1.794220	1.136205
H	0	1.643355	-0.035587	2.504989
H	0	-0.091584	-1.750266	2.527118
C	0	-0.525641	-0.564835	-0.788929
C	0	0.322004	0.588211	-0.816883
C	0	-1.817594	-0.427755	-1.402724
C	0	0.086352	-1.956287	-0.864868
C	0	1.730370	0.344647	-0.981649
C	0	-0.170908	1.892364	-1.433241
N	0	2.870852	0.168398	-1.139376
N	0	-2.870852	-0.334389	-1.891909
H	0	0.893703	-2.055615	-0.134494
H	0	0.514749	-2.133425	-1.858995
H	0	-0.662288	-2.728157	-0.670914
H	0	-1.190119	2.117410	-1.106134
H	0	-0.186229	1.816648	-2.527118
H	0	0.478675	2.728157	-1.161254

TS-39+BU

B3LYP/6-31G(d) Geometry

C	0	-1.516567	-0.648336	1.334675
C	0	0.310605	1.529530	1.336245
C	0	0.541687	0.394675	2.100354
C	0	-0.359353	-0.679328	2.099550
H	0	-2.129385	-1.541028	1.248022
H	0	-2.045278	0.284421	1.171835
H	0	1.083241	2.288282	1.250878

H	0	-0.699734	1.888209	1.172977
H	0	1.531520	0.238468	2.522032
H	0	-0.033778	-1.627315	2.520626
C	0	-0.739031	-0.377720	-0.767269
C	0	0.181041	0.718697	-0.766360
C	0	-2.101644	-0.220749	-1.433948
C	0	-0.201241	-1.710204	-0.854412
C	0	1.586722	0.420395	-0.852550
C	0	-0.209433	2.033947	-1.432303
N	0	2.732342	0.233291	-0.941639
N	0	0.181909	-2.805876	-0.944369
H	0	-1.989146	-0.129237	-2.522032
H	0	-2.628529	0.669185	-1.078290
H	0	-2.732342	-1.090709	-1.236524
H	0	-1.177598	2.398123	-1.077180
H	0	-0.279096	1.908156	-2.520548
H	0	0.537716	2.805876	-1.233609

TS-40+BU

B3LYP/6-31G(d) Geometry

C	0	-1.507917	-0.571848	1.176528
C	0	0.548014	1.389183	1.438309
C	0	0.608351	0.192343	2.118205
C	0	-0.423582	-0.757993	2.032931
H	0	-2.252807	-1.361052	1.105768
H	0	-1.919419	0.425343	1.047224
H	0	1.418534	2.035551	1.377494
H	0	-0.400241	1.858312	1.208270
H	0	1.548432	-0.104817	2.578505
H	0	-0.250084	-1.745698	2.454841
C	0	-0.716278	-0.548244	-0.768639
C	0	0.142285	0.586822	-0.869631
C	0	-2.057860	-0.472171	-1.491331
C	0	-0.068347	-1.923591	-0.838892
C	0	1.548203	0.369511	-1.024113
C	0	-0.359624	1.919803	-1.399773
N	0	2.690203	0.203547	-1.199156
H	0	-1.897586	-0.496492	-2.578505
H	0	-2.617925	0.439144	-1.264542
H	0	-2.690203	-1.328166	-1.236272
H	0	0.810284	-1.991142	-0.192820
H	0	0.263552	-2.135053	-1.864454
H	0	-0.775731	-2.707041	-0.547516
H	0	-1.284665	2.231563	-0.901678
H	0	-0.575045	1.864836	-2.476230
H	0	0.383994	2.707041	-1.251226

TS-41+BU

B3LYP/6-31G(d) Geometry

C	0	2.080181	-0.227701	-0.924864
C	0	1.506222	1.055749	-0.778830
C	0	0.956652	1.493354	0.401067
C	0	2.035327	-1.181461	0.082681
H	0	2.358888	-0.544634	-1.927977
H	0	1.342394	1.643377	-1.680076
H	0	0.381837	2.413437	0.441548
H	0	1.279643	1.098400	1.356674
H	0	2.430414	-2.174529	-0.118014
H	0	2.101009	-0.881484	1.123675
C	0	-0.656962	-0.343487	0.905450
C	0	-0.051446	-1.486557	0.351121
C	0	-1.501019	-0.135795	-0.291794
C	0	-0.803776	-1.344592	-0.981884
O	0	-2.430414	0.578210	-0.594435
H	0	-0.748739	0.010515	1.927977
H	0	0.189580	-2.413437	0.860406
H	0	-0.182399	-1.093336	-1.850947
H	0	-1.490592	-2.156366	-1.246877

TS-42+BU

B3LYP/6-31G(d) Geometry

C	0	-1.980742	-0.735389	-0.131704
C	0	-1.386440	-0.732423	1.152157
C	0	-0.478036	0.212530	1.551420
C	0	-1.597533	0.153269	-1.133254
H	0	-2.582618	-1.598963	-0.407396
H	0	-1.542820	-1.605405	1.783276
H	0	0.078702	0.097173	2.476286
H	0	-0.436979	1.192409	1.094410
H	0	-2.063014	0.053225	-2.111287
H	0	-1.340637	1.178538	-0.880336
C	0	1.223888	0.205859	-0.453319
C	0	0.384860	-0.302808	-1.471264
C	0	1.660602	-1.152226	-0.061722
C	0	0.709491	-1.765165	-1.126232
O	0	2.515470	-1.607489	0.668945
C	0	1.819933	1.553115	-0.198458
H	0	0.293043	0.100285	-2.476286
H	0	-0.129834	-2.354004	-0.733936
H	0	1.228806	-2.343334	-1.898823
H	0	1.070427	2.354004	-0.240674
H	0	2.582618	1.791525	-0.952939
H	0	2.305987	1.584813	0.781727

TS-43+BU

B3LYP/6-31G(d) Geometry

C	0	-2.051902	-0.734806	-0.837308
C	0	-1.546601	-1.922570	-0.269164
C	0	-1.007884	-1.954583	0.997911
C	0	-1.955515	0.490021	-0.192945
H	0	-2.317505	-0.749838	-1.892739
H	0	-1.402345	-2.781339	-0.921597
H	0	-0.470942	-2.829661	1.351442
H	0	-1.345949	-1.271637	1.768392
H	0	-2.293707	1.383393	-0.711538
H	0	-2.034669	0.547548	0.887706
C	0	0.673195	-0.241447	0.890781
C	0	0.188869	0.789605	0.048829
C	0	1.469643	-0.844531	-0.197653
C	0	0.890811	0.196089	-1.192181
O	0	2.317505	-1.705160	-0.286443
C	0	0.096134	2.260085	0.377080
H	0	0.790299	-0.283920	1.970679
H	0	0.229820	-0.204532	-1.970679
H	0	1.659431	0.826048	-1.657396
H	0	1.107795	2.679267	0.468720
H	0	-0.416756	2.431897	1.329844
H	0	-0.423578	2.829661	-0.399516

TS-44+BU

B3LYP/6-31G(d) Geometry

C	0	-0.880479	1.946437	-0.794522
C	0	-2.010297	1.536659	-0.058891
C	0	-1.903128	0.971568	1.202122
C	0	0.407245	1.776847	-0.323082

H 0	-1.024308	2.217042	-1.838724
H 0	-2.964854	1.477322	-0.577334
H 0	-2.779775	0.548762	1.684120
H 0	-1.111910	1.283445	1.875934
H 0	1.259093	1.980492	-0.964980
H 0	0.624519	1.795624	0.738275
C 0	-0.622754	-0.831895	0.908187
C 0	0.410271	-0.533085	-0.016236
C 0	-1.405102	-1.541343	-0.149039
C 0	-0.345348	-1.147013	-1.212172
O 0	-2.402955	-2.217042	-0.171948
C 0	1.812644	-0.522835	0.207832
N 0	2.964854	-0.519878	0.385445
H 0	-0.566066	-1.005862	1.978353
H 0	-0.678115	-0.437154	-1.978353
H 0	0.132513	-2.009617	-1.689024

TS-45+BU

B3LYP/6-31G(d) Geometry

C 0	1.811015	-0.371329	-0.284754
C 0	1.363039	-0.017366	1.013800
C 0	0.230777	-0.528341	1.582625
C 0	1.077698	-1.188074	-1.143903
H 0	2.651323	0.185749	-0.694330
H 0	1.876696	0.800559	1.515828
H 0	-0.165031	-0.118568	2.506816
H 0	-0.231593	-1.442690	1.235385
H 0	1.494266	-1.385722	-2.129063
H 0	0.505439	-2.020600	-0.742401
C 0	-1.540617	-0.206743	-0.495130
C 0	-0.601156	-0.129081	-1.539782
C 0	-1.523720	1.238032	-0.203905
C 0	-0.439480	1.385219	-1.315950
O 0	-2.154911	2.013166	0.473302
Cl 0	-2.651323	-1.480595	-0.082092
H 0	-0.698265	-0.611993	-2.506816
H 0	0.551221	1.703801	-0.970344
H 0	-0.769787	2.020600	-2.144198

TS-46+BU

B3LYP/6-31G(d) Geometry

C 0	-2.085623	1.467214	0.060197
C 0	-0.910614	2.103194	-0.384163
C 0	0.339823	1.763407	0.112799
C 0	-2.070949	0.522898	1.069738
H 0	-2.988925	1.584861	-0.534822
H 0	-0.967551	2.711130	-1.284746
H 0	1.232493	2.186293	-0.338776
H 0	0.464439	1.463942	1.147947
H 0	-2.960111	-0.060736	1.288616
H 0	-1.346978	0.586994	1.873416
C 0	0.419324	-0.398922	-0.390753
C 0	-0.538450	-1.110772	0.393209
C 0	1.833047	-0.451239	-0.223793
C 0	-0.352357	-0.625385	-1.706695
C 0	-1.315329	-1.464558	-0.830110
C 0	-0.391185	-1.837559	1.694920
O 0	-2.240542	-2.204565	-1.066888
N 0	2.988925	-0.502218	-0.082960
H 0	0.166303	-1.215386	-2.469432
H 0	-0.776258	0.278542	-2.160604
H 0	-1.360072	-2.195676	2.055055
H 0	0.062357	-1.208961	2.469432
H 0	0.260896	-2.711130	1.565563

TS-47+BU

B3LYP/6-31G(d) Geometry

C 0	-2.059938	-0.376825	-0.476448
C 0	-1.597581	-1.670395	-0.152471
C 0	-0.700430	-1.897835	0.861795
C 0	-1.543423	0.765367	0.130225
H 0	-2.659938	-0.262299	-1.377082
H 0	-1.828210	-2.481784	-0.840318
H 0	-0.225671	-2.867005	0.980702
H 0	-0.622561	-1.228242	1.708553
H 0	-1.910739	1.731814	-0.205916
H 0	-1.280411	0.746288	1.184441
C 0	1.160000	-0.228361	0.342280
C 0	0.483592	0.787166	-0.392360
C 0	1.484599	-0.982189	-0.883931
C 0	0.682056	0.039341	-1.728251
O 0	2.211441	-1.916031	-1.156928
C 0	1.799214	-0.221685	1.694720
C 0	0.694522	2.275550	-0.213164
H 0	-0.233996	-0.339814	-2.199330
H 0	1.289879	0.555986	-2.481339
H 0	1.109946	0.112444	2.481339
H 0	2.659938	0.462303	1.716519
H 0	2.165045	-1.219169	1.957187
H 0	1.732119	2.532631	-0.467998
H 0	0.522964	2.590616	0.822372
H 0	0.041096	2.867005	-0.861919

TS-48+BU

B3LYP/6-31G(d) Geometry

C 0	2.045460	-0.042688	-0.829004
C 0	1.423292	1.218804	-0.897397
C 0	0.860219	1.819462	0.207065
C 0	2.073574	-0.785745	0.348965
H 0	2.300394	-0.536496	-1.764854
H 0	1.212652	1.632548	-1.881949
H 0	0.231490	2.698670	0.105122
H 0	1.241221	1.631970	1.203432
H 0	2.503272	-1.784927	0.327143
H 0	2.197045	-0.277099	1.300315
C 0	-0.618956	0.061082	1.003675
C 0	0.052401	-1.155237	0.815408
C 0	-1.623102	0.271135	-0.057784
O 0	-2.503272	1.115050	-0.091677
C 0	-1.383215	-0.820817	-1.112848
C 0	-0.549388	-1.892794	-0.386322
H 0	-0.686055	0.593050	1.945765
H 0	0.385813	-1.737785	1.670320
H 0	-0.822585	-0.376512	-1.945765
H 0	-2.333392	-1.183055	-1.514915
H 0	0.205182	-2.358747	-1.027346
H 0	-1.198139	-2.698670	-0.017427

TS-49+BU

B3LYP/6-31G(d) Geometry

C 0	-2.096093	-0.149783	-0.351037
C 0	-1.388416	-0.911711	-1.301927
C 0	-0.462730	-1.862676	-0.945737
C 0	-1.826747	-0.243327	1.018598

H 0	-2.691606	0.687375	-0.709447
H 0	-1.461674	-0.617393	-2.347633
H 0	0.193328	-2.311775	-1.684955
H 0	-0.510816	-2.369540	0.008355
H 0	-2.383510	0.408225	1.689461
H 0	-1.612784	-1.217833	1.451518
C 0	0.984588	-0.562736	0.752365
C 0	0.081008	0.385119	1.271035
C 0	1.716099	0.007085	-0.396859
O 0	2.691606	-0.479258	-0.951170
C 0	1.494393	-1.776330	1.472843
C 0	1.084875	1.368858	-0.717623
C 0	0.257933	1.719244	0.534973
H 0	-0.081015	0.417838	2.347633
H 0	2.068261	-2.409079	0.789509
H 0	0.686222	-2.370944	1.918031
H 0	2.165417	-1.488444	2.294210
H 0	0.450545	1.268013	-1.606642
H 0	1.862929	2.099940	-0.955731
H 0	-0.694699	2.202612	0.296517
H 0	0.815809	2.409079	1.181569

TS-50+BU

B3LYP/6-31G(d) Geometry

C 0	-1.400583	1.539908	0.915751
C 0	-0.359987	2.256445	0.299066
C 0	0.034450	1.986260	-0.996721
C 0	-2.057630	0.502344	0.261055
H 0	-1.535492	1.654044	1.989884
H 0	0.279924	2.877029	0.923445
H 0	0.951664	2.407220	-1.397413
H 0	-0.679375	1.641499	-1.735643
H 0	-2.801286	-0.074469	0.805846
H 0	-2.257370	0.585044	-0.802414
C 0	0.467581	-0.329166	-0.907811
C 0	-0.566961	-0.983334	-0.208088
C 0	1.676235	-0.206821	-0.068873
O 0	2.801286	0.099863	-0.426817
C 0	-1.510242	-1.934375	-0.920323
C 0	1.257932	-0.585113	1.358975
C 0	-0.035533	-1.396801	1.175383
H 0	0.549384	-0.319087	-1.989884
H 0	-0.989468	-2.877029	-1.137594
H 0	-1.859463	-1.525743	-1.874692
H 0	-2.388374	-2.181350	-0.313727
H 0	1.067325	0.342138	1.915385
H 0	2.061877	-1.118641	1.873376
H 0	-0.763061	-1.246851	1.979159
H 0	0.191415	-2.472763	1.150106

TS-51+BU

B3LYP/6-31G(d) Geometry

C 0	0.200516	2.012753	0.714095
C 0	1.321295	1.962924	-0.131320
C 0	1.253410	1.377647	-1.390958
C 0	-1.026693	1.498127	0.329792
H 0	0.356044	2.280333	1.757662
H 0	2.299119	2.179841	0.293724
H 0	2.161716	1.224113	-1.966571
H 0	0.349373	1.476007	-1.983219
H 0	-1.841313	1.426535	1.044982
H 0	-1.339072	1.523143	-0.707216
C 0	0.613294	-0.666890	-1.017270
C 0	-0.480412	-0.712752	-0.123220
C 0	1.835384	-1.159763	-0.318301
O 0	2.892270	-1.459587	-0.836604
C 0	-1.806151	-0.978799	-0.586255
C 0	1.503992	-1.230591	1.176814
C 0	-0.033054	-1.252965	1.248620
N 0	-2.892270	-1.189770	-0.952055
H 0	0.503383	-0.830360	-2.083581
H 0	1.913520	-0.332439	1.657005
H 0	1.986927	-2.096614	1.636699
H 0	-0.436103	-0.675237	2.083581
H 0	-0.401986	-2.280333	1.359326

TS-52+BU

B3LYP/6-31G(d) Geometry

C 0	1.806599	-0.991239	-0.006413
C 0	1.199279	-0.886133	1.262455
C 0	-0.007493	-1.467802	1.557697
C 0	1.172481	-1.610953	-1.091832
H 0	2.687919	-0.382459	-0.198098
H 0	1.637627	-0.193190	1.978855
H 0	-0.536612	-1.229170	2.475316
H 0	-0.389283	-2.314332	1.004103
H 0	1.710363	-1.627047	-2.038010
H 0	0.592031	-2.514656	-0.918258
C 0	-1.434118	-0.716963	-0.551306
C 0	-0.430069	-0.524921	-1.516579
C 0	-1.755145	0.506448	0.202931
O 0	-2.687919	0.696442	0.961766
Cl 0	-2.512098	-2.088593	-0.575970
C 0	-0.704901	1.541801	-0.231100
C 0	-0.077718	0.969633	-1.521160
H 0	-0.536003	-1.027374	-2.475316
H 0	0.037462	1.655612	0.566856
H 0	-1.184407	2.514656	-0.371737
H 0	0.999979	1.146956	-1.584630
H 0	-0.535892	1.431168	-2.404459

TS-53+BU

B3LYP/6-31G(d) Geometry

C 0	0.188534	2.169179	0.104499
C 0	1.421004	1.867283	-0.493275
C 0	1.533420	0.881902	-1.462435
C 0	-0.967629	1.466090	-0.224609
H 0	0.184559	2.805653	0.987037
H 0	2.326461	2.270696	-0.044105
H 0	2.511582	0.550860	-1.798389
H 0	0.725191	0.712710	-2.163577
H 0	-1.881122	1.641820	0.337074
H 0	-1.135320	1.137371	-1.244880
C 0	0.632855	-1.013400	-0.525290
C 0	-0.454915	-0.599330	0.293918
C 0	1.828867	-1.221524	0.340798
O 0	2.856672	-1.783345	0.008634
C 0	0.487078	-1.801752	-1.800026
C 0	-1.779141	-1.066607	-0.000031
C 0	1.515338	-0.657004	1.728544
C 0	-0.018350	-0.539173	1.773337
N 0	-2.856672	-1.442228	-0.233314
H 0	1.460563	-1.919188	-2.283078
H 0	0.101696	-2.805653	-1.580827
H 0	-0.213125	-1.336515	-2.501784
H 0	2.001749	0.320522	1.830566

H 0	1.930841	-1.308773	2.501784
H 0	-0.456809	-1.392244	2.304755
H 0	-0.366629	0.367158	2.274765

TS-54+BU

B3LYP/6-31G(d) Geometry

C 0	1.912794	-1.325259	0.267886
C 0	0.917855	-2.226435	-0.151663
C 0	0.047153	-1.924528	-1.174719
C 0	2.018194	-0.044441	-0.284522
H 0	2.452721	-1.547172	1.186293
H 0	0.718718	-3.098683	0.468623
H 0	-0.827901	-2.538352	-1.364772
H 0	0.331214	-1.253703	-1.974089
H 0	2.785318	0.615626	0.114503
H 0	1.860681	0.080397	-1.352997
C 0	-0.787806	0.353993	-0.505252
C 0	0.299169	0.991019	0.150139
C 0	-1.664024	-0.311395	0.480156
O 0	-2.785318	-0.754437	0.274586
C 0	-1.315413	0.717424	-1.863255
C 0	-0.949367	-0.269690	1.835329
C 0	0.106452	0.836268	1.670507
C 0	0.783613	2.348820	-0.337372
H 0	-2.120145	0.032275	-2.144533
H 0	-0.542114	0.698595	-2.641711
H 0	-1.733698	1.734509	-1.860514
H 0	-0.483226	-1.245181	2.020417
H 0	-1.666000	-0.090133	2.641711
H 0	1.042817	0.626145	2.197358
H 0	-0.276348	1.787069	2.067995
H 0	-0.004982	3.098683	-0.186093
H 0	1.033127	2.345513	-1.403231
H 0	1.665892	2.685369	0.217172

TS-55+BU

B3LYP/6-31G(d) Geometry

C 0	1.490614	0.702429	-0.952430
C 0	1.489507	-0.703830	-0.951798
C 0	1.371848	-1.439634	0.216080
C 0	1.374540	1.439513	0.214700
H 0	1.358794	1.211701	-1.904402
H 0	1.356914	-1.213764	-1.903305
H 0	1.223391	-2.514425	0.169598
H 0	1.782907	-1.069368	1.149061
H 0	1.227265	2.514425	0.167376
H 0	1.784650	1.069311	1.148122
C 0	-0.601931	-0.696040	1.041759
C 0	-0.601541	0.697372	1.042077
C 0	-1.427669	1.142529	-0.105845
C 0	-1.428793	-1.139992	-0.106304
O 0	-1.781272	0.001485	-0.834209
O 0	-1.782547	2.240543	-0.437497
O 0	-1.784650	-2.237627	-0.438169
H 0	-0.482783	-1.338467	1.904132
H 0	-0.480999	1.339586	1.904402

TS-56+BU

B3LYP/6-31G(d) Geometry

C 0	1.283734	1.257979	-0.891199
C 0	1.925787	0.005577	-0.931552
C 0	2.027740	-0.805308	0.192133
C 0	0.777512	1.784028	0.278125
H 0	1.001957	1.717785	-1.836043
H 0	2.135528	-0.425876	-1.908376
H 0	2.455306	-1.800621	0.091078
H 0	2.167881	-0.362333	1.172985
H 0	0.133514	2.657765	0.260587
H 0	1.228710	1.554236	1.236462
C 0	-0.022407	-1.183824	0.733811
C 0	-0.672464	0.028051	0.957379
C 0	-1.652568	0.257056	-0.124881
O 0	-2.455306	1.145195	-0.278579
C 0	-0.674635	-1.797802	-0.494148
O 0	-1.516624	-0.771445	-1.035624
H 0	0.313588	-1.826651	1.540328
H 0	-0.780053	0.531223	1.908376
H 0	-1.300265	-2.657765	-0.216975
H 0	0.020264	-2.111253	-1.276654

TS-57+BU

B3LYP/6-31G(d) Geometry

C 0	1.607397	-1.105531	1.081851
C 0	2.282384	0.066071	0.694084
C 0	2.298588	0.497436	-0.632825
C 0	0.990068	-1.932122	0.168729
H 0	1.402120	-1.250468	2.141297
H 0	2.588573	0.761675	1.473168
H 0	2.783353	1.442922	-0.866861
H 0	2.378069	-0.238593	-1.427429
H 0	0.315897	-2.720554	0.487948
H 0	1.359849	-2.022681	-0.844724
C 0	0.307782	0.868150	-1.151118
C 0	-0.400842	-0.345900	-1.078412
C 0	-1.569328	-0.545492	-0.202929
O 0	-2.298859	-1.526027	-0.307912
C 0	-0.143218	2.038067	-0.286133
C 0	-1.918105	0.577336	0.776382
C 0	-0.779330	1.572607	1.029653
H 0	0.664486	1.149529	-2.141297
H 0	-0.353517	-1.042458	-1.911051
H 0	-0.882012	2.618893	-0.861105
H 0	0.691538	2.720554	-0.088207
H 0	-2.279610	0.121087	1.704478
H 0	-2.783353	1.098174	0.339036
H 0	-1.153139	2.437058	1.591970
H 0	-0.010170	1.103607	1.653227

TS-58+BU

B3LYP/6-31G(d) Geometry

C 0	-1.420424	-0.875314	-1.457270
C 0	-2.172607	-0.279732	-0.427259
C 0	-1.953477	-0.588660	0.922227
C 0	-0.489807	-1.859475	-1.223222
H 0	-1.459094	-0.417333	-2.444703
H 0	-2.765439	0.599774	-0.670620
H 0	-2.554906	-0.061976	1.661094
H 0	-1.763094	-1.624516	1.194907
H 0	0.201875	-2.174539	-1.998420
H 0	-0.562108	-2.517699	-0.368879
C 0	-0.093574	-0.004616	1.401264
C 0	0.838140	-0.880017	0.793385
C 0	1.839620	-0.394802	-0.178024
O 0	2.765439	-1.106291	-0.563834
C 0	-0.003981	1.492627	1.130549
C 0	1.798936	1.077735	-0.593001

C 0	0.485436	1.804022	-0.287927
C 0	1.120841	-2.219740	1.429337
H 0	-0.310252	-0.243051	2.444703
H 0	0.699258	1.924217	1.860091
H 0	-0.970947	1.975294	1.317117
H 0	2.062472	1.136829	-1.654759
H 0	2.629257	1.556715	-0.052328
H 0	0.616509	2.886527	-0.409415
H 0	-0.281286	1.500340	-1.006841
H 0	0.203732	-2.699664	1.795327
H 0	1.785748	-2.101783	2.296675
H 0	1.626082	-2.886527	0.727653

TS-59+BU

B3LYP/6-31G(d) Geometry

C 0	-0.728374	2.083748	0.484583
C 0	-1.684274	1.133484	0.878350
C 0	-2.130393	0.144254	0.004569
C 0	-0.229281	2.113630	-0.803539
H 0	-0.220060	2.655952	1.258807
H 0	-1.899978	1.032169	1.940512
H 0	-2.811139	-0.616279	0.380054
H 0	-2.283645	0.390400	-1.041073
H 0	0.640918	2.711994	-1.054480
H 0	-0.852328	1.834184	-1.644664
C 0	-0.416179	-1.018524	-0.591936
C 0	0.514563	-0.101717	-1.135862
C 0	1.851629	0.139890	-0.557925
O 0	2.727838	0.727710	-1.182743
C 0	-0.028892	-1.734644	0.701636
C 0	2.153535	-0.463523	0.814139
C 0	0.909958	-0.910828	1.589421
C 0	-1.179050	-1.891095	-1.581066
H 0	0.474826	0.100564	-2.204016
H 0	0.474288	-2.675841	0.422428
H 0	-0.925559	-2.030415	1.259102
H 0	2.756546	0.256051	1.378932
H 0	2.811139	-1.325414	0.624736
H 0	1.204207	-1.498745	2.467448
H 0	0.373557	-0.033917	1.966283
H 0	-1.487795	-1.326761	-2.467448
H 0	-2.071271	-2.344346	-1.134754
H 0	-0.534488	-2.711994	-1.924425

TS-60+BU

B3LYP/6-31G(d) Geometry

C 0	0.214453	2.175264	-0.156044
C 0	-0.868776	1.843340	0.670453
C 0	-1.906330	1.040299	0.220905
C 0	0.292549	1.706304	-1.464527
H 0	1.102149	2.607373	0.301841
H 0	-0.786774	2.050306	1.735971
H 0	-2.664102	0.684528	0.913537
H 0	-2.228750	1.081141	-0.812281
H 0	1.199825	1.849390	-2.043437
H 0	-0.613091	1.628105	-2.057341
C 0	-0.793355	-0.890662	-0.432828
C 0	0.238403	-0.452093	-1.306601
C 0	1.678387	-0.678979	-0.978015
O 0	2.546332	-0.509892	-1.820108
C 0	-0.435630	-1.516145	0.919128
C 0	2.020962	-1.205243	0.411831
C 0	0.908934	-1.006395	1.447447
C 0	-1.989040	-1.397082	-1.046428
N 0	-2.967366	-1.804469	-1.530925
H 0	0.045813	-0.497805	-2.374593
H 0	-0.382266	-2.607373	0.783539
H 0	-1.233121	-1.338715	1.646869
H 0	2.967366	-0.751441	0.724408
H 0	2.225969	-2.279083	0.283946
H 0	1.161661	-1.533528	2.374593
H 0	0.823178	0.054659	1.703952

TS-61+BU

B3LYP/6-31G(d) Geometry

C 0	1.185641	-1.215138	1.379788
C 0	1.829755	-1.388189	0.138146
C 0	1.157589	-1.857223	-1.003682
C 0	-0.121117	-1.570075	1.600772
H 0	1.706877	-0.638083	2.142402
H 0	2.814841	-0.942830	0.012786
H 0	1.751712	-1.957672	-1.910790
H 0	0.434806	-2.662661	-0.885359
H 0	-0.638777	-1.263908	2.504932
H 0	-0.630562	-2.309074	0.999120
C 0	-0.177826	-0.540940	-1.529636
C 0	-1.278929	-0.607177	-0.645539
C 0	-1.767158	0.498114	0.193917
O 0	-2.814841	0.455390	0.824370
C 0	0.493650	0.819991	-1.704361
C 0	-0.954909	1.797946	0.130459
C 0	0.466345	1.667162	-0.427472
Cl 0	-2.387061	-1.963605	-0.864639
H 0	-0.340012	-1.066620	-2.470344
H 0	-0.042783	1.350924	-2.504932
H 0	1.523447	0.688640	-2.056821
H 0	-0.959835	2.239814	1.132371
H 0	-1.547737	2.475619	-0.501549
H 0	0.876720	2.662661	-0.636710
H 0	1.119810	1.213540	0.323712

TS-62+BU

B3LYP/6-31G(d) Geometry

C 0	0.525452	2.003766	-1.301243
C 0	-0.686845	2.150124	-0.616293
C 0	-1.687764	1.181045	-0.704641
C 0	0.757866	0.915764	-2.129728
H 0	1.361548	2.640220	-1.016889
H 0	-0.755641	2.907958	0.161497
H 0	-2.573711	1.271290	-0.081530
H 0	-1.871374	0.682840	-1.651083
H 0	1.751334	0.720417	-2.521516
H 0	-0.051934	0.496837	-2.713450
C 0	-0.765967	-0.631164	0.035838
C 0	0.289097	-0.974606	-0.871986
C 0	1.699639	-1.047560	-0.378969
O 0	2.578162	-1.559303	-1.060989
C 0	-0.442330	-0.311361	1.503977
C 0	2.020257	-0.573816	1.036133
C 0	0.947606	0.303994	1.683521
C 0	-0.012313	-1.874779	-2.053918
C 0	-1.997316	-1.372468	-0.107430
N 0	-2.999502	-1.959119	-0.191199
H 0	-0.495910	-1.252944	2.070409
H 0	-1.214594	0.341499	1.923385
H 0	2.999502	-0.083729	1.013315

H 0	2.158793	-1.492725	1.625467
H 0	1.155681	0.423620	2.753374
H 0	0.968159	1.306770	1.248725
H 0	-0.928073	-1.576530	-2.574881
H 0	-0.160078	-2.907958	-1.714511
H 0	0.824943	-1.876628	-2.753374

TS-63+BU

B3LYP/6-31G(d) Geometry

C 0	0.798087	-2.230981	-0.819494
C 0	1.860337	-1.462783	-0.315185
C 0	2.052439	-0.129435	-0.705930
C 0	-0.057203	-1.754268	-1.787966
H 0	0.539460	-3.152107	-0.299010
H 0	2.393596	-1.834375	0.557609
H 0	2.885500	0.405096	-0.253872
H 0	1.908545	0.124959	-1.753867
H 0	-0.980029	-2.273556	-2.027504
H 0	0.266748	-1.025055	-2.517062
C 0	0.476243	0.991933	-0.119225
C 0	-0.636633	0.590694	-0.922269
C 0	-1.848631	-0.023494	-0.332985
O 0	-2.885500	-0.159281	-0.981125
C 0	0.368895	0.788977	1.396514
C 0	-1.856563	-0.366580	1.156804
C 0	-0.476472	-0.415882	1.813345
C 0	1.112691	2.346943	-0.449969
C 0	-0.829525	1.185073	-2.297529
H 0	-0.081670	1.702852	1.817326
H 0	1.373341	0.723153	1.833166
H 0	-2.407570	-1.304998	1.282494
H 0	-2.474772	0.409224	1.633191
H 0	-0.577685	-0.436910	2.905720
H 0	0.037488	-1.338321	1.531269
H 0	0.394141	3.152107	-0.246411
H 0	1.418011	2.435027	-1.495616
H 0	1.993009	2.527571	0.176028
H 0	0.083442	1.144830	-2.905720
H 0	-1.115338	2.244771	-2.231397
H 0	-1.634377	0.663796	-2.818372

TS-64+BU

B3LYP/6-31G(d) Geometry

C 0	-0.608564	-1.429594	-0.084920
C 0	0.273409	-0.823021	0.997616
O 0	-0.537215	-0.614813	-1.263338
C 0	-2.114158	-1.311451	0.253616
C 0	-1.308246	0.508255	-0.887513
C 0	0.268667	0.580811	1.074133
O 0	-2.468741	-0.013253	-0.232648
C 0	-0.542554	1.369474	0.134253
O 0	-0.709065	2.579751	0.190947
H 0	-0.311332	-2.444500	-0.355978
H 0	0.320374	-1.382518	1.931143
H 0	-2.324454	-1.380266	1.326059
H 0	-2.697840	-2.071147	-0.280924
H 0	-1.602004	1.077857	-1.771224
H 0	0.571959	1.089799	1.984020
C 0	2.197588	-1.499449	0.504577
C 0	2.452151	-0.955704	-0.751402
C 0	2.516498	0.436047	-0.959985
C 0	2.408310	1.339587	0.069450
H 0	2.106247	-2.579751	0.599454
H 0	2.602351	-1.017844	1.389740
H 0	2.361665	-1.595374	-1.626209
H 0	2.450321	0.797611	-1.984020
H 0	2.272585	2.399085	-0.122903
H 0	2.697840	1.082256	1.080929

TS-65+BU

B3LYP/6-31G(d) Geometry

C 0	-0.617303	-1.620367	0.314581
C 0	0.309206	-0.697498	1.094962
O 0	-0.555816	-1.287100	-1.077888
C 0	-2.109574	-1.338591	0.610687
C 0	-1.279554	-0.076034	-1.114009
C 0	0.318950	0.660892	0.704126
O 0	-2.444408	-0.294505	-0.308828
C 0	-0.482175	1.068383	-0.462784
O 0	-0.648993	2.227346	-0.826258
C 0	0.776967	1.741999	1.649026
H 0	-0.350623	-2.673953	0.423163
H 0	0.333259	-0.886924	2.169998
H 0	-2.292906	-1.007952	1.638678
H 0	-2.726683	-2.220381	0.398273
H 0	-1.574232	0.158932	-2.138232
H 0	1.687644	1.455777	2.190844
H 0	0.006355	1.949419	2.404897
H 0	0.957721	2.673953	1.108398
C 0	2.147157	-1.508041	0.879166
C 0	2.372516	-1.616764	-0.496396
C 0	2.462920	-0.484975	-1.331903
C 0	2.437777	0.797451	-0.849243
H 0	2.065705	-2.428742	1.454625
H 0	2.625720	-0.702994	1.432252
H 0	2.238963	-2.585950	-0.971170
H 0	2.376093	-0.643101	-2.404897
H 0	2.331749	1.647601	-1.515826
H 0	2.726683	1.031392	0.166574

TS-66+BU

B3LYP/6-31G(d) Geometry

C 0	-0.634595	-0.849658	-0.666615
C 0	0.271951	-0.688036	0.556400
O 0	-0.541851	0.316416	-1.495252
C 0	-2.142822	-0.818545	-0.314109
C 0	-1.288434	1.260444	-0.757071
C 0	0.311753	0.623193	1.084310
O 0	-2.464372	0.575730	-0.317012
C 0	-0.506530	1.696123	0.494265
O 0	-0.656631	2.809575	0.976783
C 0	0.297869	-1.860316	1.526473
H 0	-0.365282	-1.719122	-1.270377
H 0	-2.379651	-1.251697	0.662516
H 0	-2.731351	-1.329356	-1.086290
H 0	-1.562453	2.105781	-1.391046
H 0	0.592139	0.776420	2.123400
H 0	0.520492	-2.809575	1.026124
H 0	-0.670398	-1.972760	2.031022
H 0	1.048585	-1.705530	2.308399
C 0	2.185253	-1.083239	-0.333458
C 0	2.408902	-0.058163	-1.247467
C 0	2.481577	1.285239	-0.841678
C 0	2.382315	1.647773	0.484808
H 0	2.074187	-2.100215	-0.703545
H 0	2.630269	-1.024579	0.654796

H 0	2.288973	-0.263537	-2.308399
H 0	2.389772	2.055294	-1.604779
H 0	2.241914	2.684591	0.773892
H 0	2.731351	0.990081	1.272128

TS-67+BU

B3LYP/6-31G(d) Geometry

C 0	0.682788	0.732138	-0.792565
C 0	-0.241257	0.627712	0.427289
O 0	0.894478	-0.580641	-1.320623
C 0	2.123782	1.121929	-0.398104
C 0	1.772819	-1.147473	-0.368209
C 0	-0.099173	-0.531406	1.231831
O 0	2.713922	-0.131304	-0.028770
C 0	0.988154	-1.498674	0.905033
O 0	1.287149	-2.447147	1.607190
C 0	-0.618816	1.862038	1.046109
N 0	-0.926654	2.879064	1.524992
H 0	0.267354	1.362321	-1.579196
H 0	2.174738	1.819128	0.442965
H 0	2.662109	1.541196	-1.256553
H 0	2.281936	-2.014706	-0.793286
H 0	-0.343965	-0.469128	2.287732
C 0	-2.293198	0.428912	-0.648183
C 0	-2.167186	-0.828765	-1.211570
C 0	-1.928293	-1.968542	-0.426870
C 0	-1.798184	-1.887710	0.953117
H 0	-2.349080	1.311339	-1.279980
H 0	-2.713922	0.558941	0.341789
H 0	-2.036972	-0.913765	-2.287732
H 0	-1.611527	-2.879064	-0.930718
H 0	-1.470585	-2.751937	1.522960
H 0	-2.387989	-1.169430	1.513045

TS-68+BU

B3LYP/6-31G(d) Geometry

C 0	0.737825	-0.775513	-0.797849
C 0	-0.409365	0.143994	-1.211389
O 0	0.752604	-0.907577	0.626271
C 0	2.121103	-0.127160	-1.047557
C 0	1.269409	0.343657	1.026614
C 0	-0.567863	1.277212	-0.386093
O 0	2.373725	0.601476	0.159282
C 0	0.239869	1.479649	0.819660
O 0	0.248931	2.472469	1.529664
Cl 0	-1.472919	2.647146	-1.012523
H 0	0.641360	-1.772530	-1.232778
H 0	-0.476645	0.327122	-2.283784
H 0	2.133532	0.550728	-1.907315
H 0	2.896967	-0.891291	-1.175666
H 0	1.609865	0.299860	2.062248
C 0	-2.045591	-0.946184	-1.215405
C 0	-2.108861	-1.608507	0.018370
C 0	-2.299654	-0.931737	1.243582
C 0	-2.535080	0.412443	1.328201
H 0	-1.912226	-1.564206	-2.102128
H 0	-2.699561	-0.093865	-1.389390
H 0	-1.788992	-2.647146	0.064668
H 0	-2.100529	-1.488085	2.157138
H 0	-2.508929	0.927353	2.283784
H 0	-2.896967	0.994503	0.491753

TS-69+BU

B3LYP/6-31G(d) Geometry

C 0	0.681687	0.720818	-1.209374
C 0	-0.294870	0.632540	-0.024570
O 0	0.919393	-0.594971	-1.712094
C 0	2.104922	1.129556	-0.770737
C 0	1.763733	-1.138381	-0.718854
C 0	-0.146967	-0.491395	0.849438
O 0	2.703063	-0.115879	-0.387925
C 0	0.960683	-1.446495	0.553371
O 0	1.293835	-2.350824	1.302159
C 0	-0.623651	1.904572	0.560760
C 0	-0.560343	-0.395169	2.302069
N 0	-0.880004	2.951345	1.002526
H 0	0.287833	1.337172	-2.018400
H 0	2.120305	1.827885	0.071102
H 0	2.663362	1.558104	-1.611328
H 0	2.281605	-2.019358	-1.102162
H 0	-1.549468	0.059259	2.418705
H 0	0.150489	0.230409	2.856987
H 0	-0.556764	-1.384833	2.762865
C 0	-2.210757	0.459209	-1.051857
C 0	-2.070634	-0.718169	-1.782520
C 0	-1.824262	-1.942598	-1.147564
C 0	-1.752622	-2.039316	0.232032
H 0	-2.296908	1.408919	-1.573871
H 0	-2.703063	0.446779	-0.084809
H 0	-1.916924	-0.656144	-2.856987
H 0	-1.472907	-2.773329	-1.755405
H 0	-1.401411	-2.951345	0.704653
H 0	-2.371151	-1.407255	0.857601

TS-70+BU

B3LYP/6-31G(d) Geometry

C 0	-0.650504	-1.101136	-0.860140
C 0	0.300039	-0.754868	0.292526
O 0	-0.547256	-0.119935	-1.896609
C 0	-2.146432	-0.953572	-0.486364
C 0	-1.235808	0.971293	-1.326439
C 0	0.366413	0.635997	0.610769
O 0	-2.428674	0.423282	-0.754936
C 0	-0.422327	1.596559	-0.181715
O 0	-0.563292	2.783067	0.096664
C 0	0.240424	-1.750231	1.452409
C 0	0.836798	1.109417	1.963144
H 0	-0.420221	-2.078228	-1.292249
H 0	-2.367395	-1.182292	0.560566
H 0	-2.770602	-1.584561	-1.131111
H 0	-1.493445	1.701558	-2.095373
H 0	0.204300	-2.783067	1.087743
H 0	-0.652469	-1.582289	2.067012
H 0	1.106472	-1.661295	2.113719
H 0	1.793240	0.659212	2.258224
H 0	0.110552	0.849900	2.747186
H 0	0.938588	2.196684	1.959033
C 0	2.096843	-1.326178	-0.427990
C 0	2.311274	-0.693951	-1.659805
C 0	2.427941	0.703065	-1.761193
C 0	2.433087	1.521401	-0.657610
H 0	2.007888	-2.411139	-0.430861
H 0	2.624100	-0.950572	0.446293
H 0	2.146660	-1.258358	-2.574428
H 0	2.320989	1.150751	-2.747186

H 0 2.327993 2.597448 -0.755180
H 0 2.770602 1.171681 0.308473

P-1+BU
B3LYP/6-31G(d) Geometry
C 0 -1.470781 1.227799 -0.101928
C 0 -2.165122 0.090702 0.000199
C 0 -1.527117 -1.274628 0.061025
C 0 -0.043446 -1.243389 -0.334317
C 0 0.664544 -0.042317 0.335357
C 0 0.036040 1.291056 -0.136024
C 0 2.110796 -0.061592 0.084465
N 0 3.252526 -0.076397 -0.127344
H 0 -1.996978 2.179038 -0.161109
H 0 -3.252526 0.129229 0.042614
H 0 -2.066017 -1.966397 -0.600158
H 0 -1.640511 -1.690639 1.074445
H 0 0.451366 -2.179038 -0.053920
H 0 0.051977 -1.141287 -1.422320
H 0 0.522339 -0.123231 1.422320
H 0 0.385524 1.523477 -1.152478
H 0 0.396400 2.110500 0.498493

P-2+BU
B3LYP/6-31G(d) Geometry
C 0 -1.131056 1.310538 -0.089357
C 0 -1.981075 0.278950 -0.070974
C 0 -1.536635 -1.162862 -0.024111
C 0 -0.047868 -1.315096 -0.369087
C 0 0.795014 -0.250627 0.370753
C 0 0.369307 1.166702 -0.031217
C 0 2.270768 -0.508315 0.153368
O 0 3.053959 0.273625 -0.339944
H 0 -1.521350 2.325941 -0.144595
H 0 -3.053959 0.464949 -0.093867
H 0 -2.139339 -1.762013 -0.720276
H 0 -1.737150 -1.582065 0.974784
H 0 0.091735 -1.183469 -1.450274
H 0 0.300696 -2.325941 -0.121473
H 0 0.617969 -0.396265 1.450274
H 0 0.819052 1.421134 -1.001516
H 0 0.789542 1.894393 0.675444
H 0 2.613205 -1.518576 0.479939

P-3+BU
B3LYP/6-31G(d) Geometry
C 0 -2.574525 -1.162425 0.097472
C 0 -0.670764 1.171487 0.005028
C 0 -2.168234 1.312556 0.124085
C 0 -3.015550 0.279480 0.150276
C 0 -1.070152 -1.317957 0.363447
C 0 -0.272666 -0.246023 -0.428659
C 0 1.187786 -0.528531 -0.320858
O 0 1.993439 0.268575 0.164206
H 0 -3.134760 -1.751640 0.835566
H 0 -2.831255 -1.595625 -0.881901
H 0 -0.185844 1.416591 0.960241
H 0 -0.279116 1.902440 -0.713891
H 0 -2.554903 2.328131 0.186563
H 0 -4.086392 0.464385 0.215726
H 0 -0.736571 -2.328131 0.096903
H 0 -0.866804 -1.181516 1.432869
H 0 -0.523267 -0.391897 -1.493435
H 0 1.567064 -1.498780 -0.675684
B 0 3.582942 -0.039671 0.304426
H 0 3.770304 0.057215 1.493435
H 0 3.722788 -1.155612 -0.152659
H 0 4.086392 0.848579 -0.340246

P-4+BU
B3LYP/6-31G(d) Geometry
C 0 1.320971 1.204639 -0.079475
C 0 1.996617 0.051912 -0.091134
C 0 1.333687 -1.301150 -0.024831
C 0 -0.145774 -1.205982 0.381244
C 0 -0.819066 -0.056383 -0.378180
C 0 -0.185373 1.292655 -0.022796
N 0 -2.297716 -0.039972 -0.045157
O 0 -3.083419 -0.316562 -0.947051
O 0 -2.612773 0.229247 1.112436
H 0 1.859195 2.149728 -0.117482
H 0 3.083419 0.067146 -0.152163
H 0 1.863493 -1.942160 0.692021
H 0 1.429412 -1.807492 -0.997706
H 0 -0.663149 -2.149728 0.175478
H 0 -0.233197 -1.006597 1.454753
H 0 -0.790198 -0.233710 -1.454753
H 0 -0.518881 1.588973 0.980400
H 0 -0.545645 2.066713 -0.712852

P-5+BU
B3LYP/6-31G(d) Geometry
C 0 1.248901 1.219648 0.057469
C 0 1.935815 0.079432 -0.059080
C 0 1.284902 -1.280049 -0.113264
C 0 -0.186639 -1.234050 0.323476
C 0 -0.904889 -0.036684 -0.322463
C 0 -0.257045 1.290904 0.113020
C 0 -2.391217 -0.048219 -0.022291
F 0 -3.022861 1.008096 -0.586417
F 0 -2.643558 0.002671 1.308070
F 0 -2.987707 -1.167139 -0.496451
H 0 1.781520 2.167804 0.111725
H 0 3.022861 0.111244 -0.117050
H 0 1.836285 -1.982537 0.526051
H 0 1.364789 -1.688019 -1.133314
H 0 -0.244770 -1.131087 1.414084
H 0 -0.694270 -2.167804 0.059985
H 0 -0.825532 -0.125672 -1.414084
H 0 -0.583468 1.543579 1.132894
H 0 -0.618124 2.106289 -0.525801

P-6+BU
B3LYP/6-31G(d) Geometry
C 0 -1.739445 -1.230422 0.418880
C 0 -2.508673 -0.253680 -0.070376
C 0 -1.956502 1.032632 -0.631943
C 0 -0.480745 1.236866 -0.253899
C 0 0.344384 -0.047403 -0.464938
C 0 -0.230069 -1.184926 0.433470
B 0 1.904807 0.034196 -0.184947
C 0 2.868558 -1.036588 -0.833473
C 0 2.502901 1.159956 0.751001
H 0 -2.203543 -2.124223 0.836097
H 0 -3.591882 -0.372165 -0.067830
H 0 -2.560044 1.880290 -0.277395

H	0	-2.068327	1.033101	-1.728377
H	0	-0.061669	2.067294	-0.836966
H	0	-0.420957	1.538935	0.801194
H	0	0.190683	-0.381633	-1.505123
H	0	0.111773	-1.067298	1.476262
H	0	0.167899	-2.155391	0.106781
H	0	2.371437	-1.873745	-1.336985
H	0	3.591882	-1.437278	-0.110128
H	0	3.480691	-0.519347	-1.591479
H	0	1.997249	1.163043	1.728377
H	0	2.300972	2.155391	0.327497
H	0	3.581207	1.082184	0.929523

P-7+BU

B3LYP/6-31G(d) Geometry

C	0	-1.466901	-0.888172	0.917896
C	0	-2.221496	-0.146382	0.102516
C	0	-1.655401	0.872437	-0.854346
C	0	-0.187136	1.202330	-0.546274
C	0	0.625275	-0.084237	-0.284453
C	0	0.041281	-0.828829	0.956451
B	0	2.166258	0.114732	-0.074805
Cl	0	3.304005	-1.179871	-0.482777
Cl	0	2.838557	1.588232	0.637094
H	0	-1.939911	-1.589200	1.604722
H	0	-3.304005	-0.266273	0.117481
H	0	-2.257683	1.790617	-0.816101
H	0	-1.752060	0.502031	-1.887389
H	0	0.249436	1.774763	-1.373329
H	0	-0.136074	1.846583	0.340275
H	0	0.489460	-0.758854	-1.142641
H	0	0.363173	-0.335357	1.887389
H	0	0.450314	-1.846583	1.002951

P-8+BU

B3LYP/6-31G(d) Geometry

C	0	-1.079973	-1.144907	-0.722515
C	0	-1.761812	-0.254281	0.004017
C	0	-1.122969	0.690433	0.987480
C	0	0.355484	0.351256	1.273602
C	0	1.072810	-0.083072	-0.001740
C	0	0.420203	-1.315874	-0.635167
Cl	0	2.841493	-0.490702	0.378545
C	0	1.220073	1.051644	-1.021555
O	0	0.917079	2.201457	-0.808646
H	0	-1.603125	-1.798699	-1.417691
H	0	-2.841493	-0.181357	-0.117358
H	0	-1.681819	0.676815	1.932840
H	0	-1.197294	1.716968	0.606315
H	0	0.418305	-0.472828	1.992591
H	0	0.864033	1.214903	1.709719
H	0	0.674448	-2.201457	-0.037574
H	0	0.848221	-1.493137	-1.630780
H	0	1.655633	0.733791	-1.992591

P-9+BU

B3LYP/6-31G(d) Geometry

C	0	1.171309	0.976758	0.827438
C	0	1.878161	0.414007	-0.156255
C	0	1.312802	-0.629580	-1.085570
C	0	0.012544	-1.240352	-0.540696
C	0	-0.955696	-0.171070	0.017466
C	0	-0.271998	0.653833	1.123770
C	0	-2.239685	-0.849146	0.546536
C	0	-1.402802	0.727214	-1.134410
O	0	-1.438333	1.936588	-1.123535
H	0	1.639951	1.723879	1.466403
H	0	2.910945	0.717704	-0.320693
H	0	2.051193	-1.425317	-1.253620
H	0	1.137757	-0.182646	-2.077792
H	0	0.249181	-1.936588	0.274519
H	0	-0.488051	-1.829738	-1.321072
H	0	-0.338099	0.108445	2.077792
H	0	-0.831962	1.586303	1.266175
H	0	-1.982187	-1.602601	1.299770
H	0	-2.790019	-1.354467	-0.256848
H	0	-2.910945	-0.117018	1.009556
H	0	-1.750580	0.161022	-2.032501

P-10+BU

B3LYP/6-31G(d) Geometry

C	0	1.570461	-1.413879	-0.208210
C	0	1.950318	-0.134221	-0.201377
C	0	0.984424	1.017839	-0.114815
C	0	-0.486718	0.625212	-0.363831
C	0	-0.801160	-0.698819	0.358720
C	0	0.130681	-1.848221	-0.118855
C	0	-2.222027	-1.198511	0.188558
O	0	-3.010110	-0.820884	-0.651535
C	0	-1.419028	1.772066	0.051025
H	0	2.315405	-2.204243	-0.288945
H	0	3.010110	0.111722	-0.255998
H	0	1.273552	1.798128	-0.833087
H	0	1.074551	1.492986	0.876245
H	0	-0.617481	0.447034	-1.440076
H	0	-0.630497	-0.569941	1.440076
H	0	-0.207111	-2.210214	-1.102721
H	0	0.038604	-2.707133	0.560272
H	0	-2.501796	-2.022476	0.887018
H	0	-1.113406	2.707133	-0.433587
H	0	-1.378570	1.936756	1.136274
H	0	-2.454588	1.567662	-0.228972

P-11+BU

B3LYP/6-31G(d) Geometry

C	0	1.938674	-0.389650	-0.117546
C	0	1.806348	0.936822	-0.183150
C	0	0.480144	1.649331	-0.160308
C	0	-0.709720	0.687888	-0.406635
C	0	-0.539460	-0.621016	0.399404
C	0	0.774452	-1.339564	-0.002950
C	0	-1.686574	-1.593505	0.192118
O	0	-2.491972	-1.516965	-0.707877
C	0	-1.968918	1.370521	-0.077731
N	0	-2.929616	1.953264	0.213857
H	0	2.929616	-0.838334	-0.156922
H	0	2.692628	1.564587	-0.254596
H	0	0.461305	2.440467	-0.920099
H	0	0.346098	2.161810	0.803063
H	0	-0.747613	0.423074	-1.470441
H	0	-0.483719	-0.380050	1.470441
H	0	0.631015	-1.864220	-0.960280
H	0	0.998823	-2.121831	0.734153
H	0	-1.714976	-2.440467	0.913845

P-12+BU

B3LYP/6-31G(d) Geometry

C 0	1.815516	-0.795933	1.163820
C 0	1.664542	1.205129	-1.078874
C 0	2.520062	-0.041650	-1.125123
C 0	2.583169	-0.926189	-0.124999
C 0	1.122507	0.575502	1.316189
C 0	0.563615	1.058304	-0.021610
C 0	-0.573856	0.216334	-0.547918
O 0	-1.107792	-0.657080	0.132517
Cl 0	-0.280867	2.692723	0.190738
H 0	1.072436	-1.601568	1.227929
H 0	2.491684	-0.946940	2.015598
H 0	2.269042	2.088331	-0.833898
H 0	1.218045	1.407968	-2.060433
H 0	3.103429	-0.195869	-2.030198
H 0	3.212689	-1.807600	-0.232408
H 0	0.324126	0.521296	2.060433
H 0	1.844194	1.325344	1.656864
H 0	-0.944485	0.412314	-1.562963
B 0	-2.349682	-1.575693	-0.391935
H 0	-1.899892	-2.692723	-0.299406
H 0	-3.212689	-1.331922	0.415472
H 0	-2.561605	-1.189349	-1.520977

P-13+BU

B3LYP/6-31G(d) Geometry

C 0	1.810599	-1.527104	1.048780
C 0	2.112675	0.631690	-1.024016
C 0	2.689526	-0.755745	-1.173919
C 0	2.544662	-1.714942	-0.253548
C 0	1.446489	-0.056288	1.317344
C 0	0.993031	0.684947	0.042656
C 0	-0.252044	0.076776	-0.542607
O 0	-1.028152	-0.622800	0.110980
C 0	0.622041	2.158618	0.355920
H 0	0.905232	-2.149463	1.049521
H 0	2.426470	-1.905714	1.875793
H 0	2.899669	1.347811	-0.743999
H 0	1.726307	0.987400	-1.990022
H 0	3.249477	-0.958723	-2.084926
H 0	2.970770	-2.699781	-0.438498
H 0	0.668136	0.005759	2.084926
H 0	2.324314	0.475991	1.704908
H 0	-0.515745	0.305904	-1.586767
H 0	0.307287	2.699781	-0.543999
H 0	1.500157	2.669378	0.765890
H 0	-0.185529	2.215310	1.093005
B 0	-2.416609	-1.222839	-0.485728
H 0	-2.272330	-2.415054	-0.357132
H 0	-3.249477	-0.752460	0.251874
H 0	-2.457936	-0.826293	-1.632148

P-14+BU

B3LYP/6-31G(d) Geometry

C 0	2.546711	-1.729748	0.121245
C 0	0.688413	0.640475	-0.270893
C 0	2.184862	0.670970	-0.495990
C 0	3.012022	-0.359845	-0.301162
C 0	1.033124	-1.895839	-0.064376
C 0	0.280928	-0.644947	0.476514
C 0	-1.181224	-0.943520	0.442909
O 0	-1.972442	-0.372324	-0.310924
C 0	0.225781	1.905388	0.477318
H 0	3.068630	-2.499684	-0.462324
H 0	2.823261	-1.915384	1.170893
H 0	0.184735	0.636214	-1.248861
H 0	2.590770	1.627899	-0.822344
H 0	4.081180	-0.227149	-0.458134
H 0	0.682416	-2.805391	0.438196
H 0	0.800570	-2.005666	-1.130744
H 0	0.549292	-0.550993	1.542103
H 0	-1.571710	-1.740757	1.093513
H 0	0.518316	2.805391	-0.074650
H 0	0.683357	1.962089	1.472569
H 0	-0.862354	1.925964	0.591366
B 0	-3.556351	-0.729665	-0.385984
H 0	-4.081180	0.318871	-0.096504
H 0	-3.705925	-1.044418	-1.542103
H 0	-3.709221	-1.625378	0.418907

P-15+BU

B3LYP/6-31G(d) Geometry

C 0	-1.079469	-0.522839	1.432469
C 0	-1.179289	0.473457	-1.419122
C 0	-1.369713	1.359713	-0.213316
C 0	-1.316333	0.913955	1.045667
C 0	-1.144122	-1.493150	0.222229
C 0	-0.495853	-0.857464	-1.037317
C 0	0.982913	-0.669209	-0.869548
O 0	1.627223	-1.221988	0.022089
C 0	-2.529827	-1.871438	-0.089221
N 0	-3.622708	-2.164675	-0.348741
H 0	-1.815396	-0.835623	2.182695
H 0	-0.097510	-0.626526	1.911320
H 0	-2.145863	0.255803	-1.892907
H 0	-0.582387	0.989694	-2.182695
H 0	-1.571519	2.411230	-0.405213
H 0	-1.449253	1.614499	1.867571
H 0	-0.602724	-2.411230	0.476332
H 0	-0.593905	-1.551761	-1.888447
H 0	1.521331	-0.038208	-1.591840
B 0	3.245973	-1.071582	0.192739
H 0	3.348102	-0.609613	1.303102
H 0	3.622708	-2.214292	0.102244
H 0	3.577402	-0.337342	-0.713219

P-16+BU

B3LYP/6-31G(d) Geometry

C 0	-1.459446	-1.019162	-1.138181
C 0	-2.139520	-0.575485	-0.077853
C 0	-1.490319	-0.173083	1.220930
C 0	-0.032421	-0.639918	1.313511
C 0	0.732341	-0.373017	-0.022045
C 0	0.041105	-1.160114	-1.180785
C 0	0.724814	1.075967	-0.318585
N 0	0.695136	2.214631	-0.538917
C 0	2.134228	-0.815791	0.109913
N 0	3.221794	-1.203641	0.224019
H 0	-1.988998	-1.299450	-2.046222
H 0	-3.221794	-0.479870	-0.138478
H 0	-2.049183	-0.595182	2.066199
H 0	-1.548632	0.918492	1.340176
H 0	0.011177	-1.720326	1.490166
H 0	0.488424	-0.147890	2.139921
H 0	0.336644	-2.214631	-1.094409

H 0 0.437429 -0.808379 -2.139921

P-17+BU

B3LYP/6-31G(d) Geometry

C 0 1.496453 -1.299855 -0.956896
C 0 2.172247 -0.549751 -0.082164
C 0 1.518882 0.374212 0.914767
C 0 0.023856 0.622747 0.596285
C 0 -0.650324 -0.735159 0.226606
C 0 -0.008093 -1.343008 -1.040085
C 0 -2.106679 -0.611191 0.097808
N 0 -3.259694 -0.521735 -0.000672
C 0 -0.129747 1.603173 -0.489471
N 0 -0.237128 2.376810 -1.347981
H 0 2.038893 -1.923279 -1.664562
H 0 3.259694 -0.582578 -0.071229
H 0 2.046484 1.334830 0.944200
H 0 1.593924 -0.042814 1.929678
H 0 -0.473268 1.036799 1.481120
H 0 -0.454704 -1.409937 1.070559
H 0 -0.358918 -0.802151 -1.929678
H 0 -0.355321 -2.376810 -1.154882

P-18+BU

B3LYP/6-31G(d) Geometry

C 0 -1.860107 -0.667059 0.024112
C 0 -1.860103 0.667067 -0.024119
C 0 -0.608682 1.504995 -0.041441
C 0 0.642453 0.689124 0.365260
C 0 0.642450 -0.689128 -0.365262
C 0 -0.608690 -1.504992 0.041440
C 0 1.861917 -1.460062 -0.093958
N 0 2.804289 -2.096967 0.136923
C 0 1.861922 1.460054 0.093956
N 0 2.804282 2.096977 -0.136931
H 0 -2.804289 -1.207140 0.053619
H 0 -2.804283 1.207153 -0.053630
H 0 -0.710823 2.355715 0.643210
H 0 -0.454596 1.941838 -1.038412
H 0 0.604342 0.493645 1.444825
H 0 0.604340 -0.493650 -1.444825
H 0 -0.454608 -1.941833 1.038412
H 0 -0.710833 -2.355715 -0.643209

P-19+BU

B3LYP/6-31G(d) Geometry

C 0 1.642537 -1.593459 -0.073207
C 0 2.142636 -0.358236 0.013001
C 0 1.289541 0.883388 0.054721
C 0 -0.178212 0.636271 -0.342301
C 0 -0.671570 -0.669933 0.340708
C 0 0.166268 -1.891164 -0.111630
C 0 -2.098212 -0.917621 0.092793
N 0 -3.221455 -1.123412 -0.119169
C 0 -1.055206 1.848488 -0.012351
H 0 2.313501 -2.449622 -0.117531
H 0 3.221455 -0.216882 0.057785
H 0 1.328730 1.325856 1.063713
H 0 1.713262 1.647311 -0.611881
H 0 -0.214059 0.461686 -1.426903
H 0 -0.547863 -0.548454 1.426903
H 0 -0.136938 -2.188136 -1.126192
H 0 -0.065943 -2.749561 0.531292
H 0 -0.660940 2.749561 -0.495999
H 0 -1.078316 2.034689 1.069125
H 0 -2.085778 1.705816 -0.352033

P-20+BU

B3LYP/6-31G(d) Geometry

C 0 1.260503 -0.574481 -1.163497
C 0 1.862023 0.240398 -0.292553
C 0 1.188513 0.773612 0.946037
C 0 -0.101696 0.009903 1.272089
C 0 -0.981258 -0.231093 0.016869
C 0 -0.165372 -1.046894 -1.023522
C 0 -1.348086 1.075129 -0.569381
N 0 -1.652258 2.103123 -1.016076
C 0 -2.280314 -0.974886 0.392497
H 0 1.804948 -0.931367 -2.036077
H 0 2.888015 0.556401 -0.474009
H 0 0.970844 1.843787 0.813429
H 0 1.874660 0.713454 1.801504
H 0 0.146565 -0.978118 1.681430
H 0 -0.681748 0.540181 2.036077
H 0 -0.673387 -1.012270 -1.995906
H 0 -0.183334 -2.103123 -0.713748
H 0 -2.883158 -0.386102 1.091216
H 0 -2.031823 -1.929444 0.869578
H 0 -2.888015 -1.180001 -0.494986

P-21+BU

B3LYP/6-31G(d) Geometry

C 0 -1.960486 -0.874702 -0.131737
C 0 -1.127707 -1.918280 -0.126738
C 0 0.371466 -1.782444 -0.076557
C 0 0.835794 -0.345440 -0.387179
C 0 -0.033393 0.683826 0.393995
C 0 -1.501745 0.555816 -0.044753
C 0 0.457329 2.122046 0.237737
O 0 -0.053972 2.931480 -0.504339
C 0 2.324159 -0.200373 -0.112513
F 0 3.034377 -1.199809 -0.678366
F 0 2.596552 -0.214994 1.215295
F 0 2.818277 0.960520 -0.606294
H 0 -3.034377 -1.042018 -0.195103
H 0 -1.522841 -2.931480 -0.169654
H 0 0.833723 -2.469392 -0.795270
H 0 0.748708 -2.086374 0.911567
H 0 0.708954 -0.153626 -1.459917
H 0 0.059654 0.431750 1.459917
H 0 -1.635750 1.069316 -1.006274
H 0 -2.133187 1.107081 0.664460
H 0 1.323996 2.404007 0.869448

P-22+BU

B3LYP/6-31G(d) Geometry

C 0 -1.927905 -1.886281 -0.029976
C 0 -2.678177 -0.793758 -0.192077
C 0 -2.101382 0.592466 -0.324441
C 0 -0.620333 0.672316 0.091553
C 0 0.175802 -0.516776 -0.501884
C 0 -0.419800 -1.861773 0.011525
B 0 1.731886 -0.538356 -0.176279
C 0 -0.020541 2.027232 -0.306662
C 0 2.756711 -0.852629 -1.337388

C 0	2.280447	-0.307040	1.289123
H 0	-2.405919	-2.859408	0.081725
H 0	-3.763120	-0.886372	-0.231921
H 0	-2.691869	1.298131	0.278429
H 0	-2.211848	0.938353	-1.366032
H 0	-0.581977	0.590044	1.188124
H 0	0.019786	-0.499834	-1.593133
H 0	-0.086895	-2.060711	1.043584
H 0	-0.025907	-2.696405	-0.586238
H 0	-0.617406	2.859408	0.086966
H 0	0.014980	2.133941	-1.398957
H 0	1.001310	2.146930	0.074197
H 0	2.863211	0.066802	-1.938105
H 0	2.383968	-1.610948	-2.039406
H 0	3.763120	-1.137723	-1.009198
H 0	2.749875	-1.238795	1.642249
H 0	1.543590	-0.000532	2.039406
H 0	3.095298	0.431595	1.285508

P-23+BU

B3LYP/6-31G(d) Geometry

C 0	-1.501955	-1.886839	-0.058443
C 0	-2.258363	-0.797167	-0.207541
C 0	-1.693975	0.597941	-0.278062
C 0	-0.222726	0.688634	0.168121
C 0	0.588685	-0.488706	-0.445870
C 0	0.002599	-1.850611	0.031641
B 0	2.126482	-0.438994	-0.131696
C 0	0.364883	2.060132	-0.189460
Cl 0	3.340101	-0.520507	-1.416244
Cl 0	2.721450	-0.359635	1.536768
H 0	-1.969971	-2.868512	0.003977
H 0	-3.340101	-0.898143	-0.285031
H 0	-2.299323	1.273979	0.342914
H 0	-1.792881	0.982828	-1.306686
H 0	-0.194041	0.573331	1.260808
H 0	0.461608	-0.441835	-1.536768
H 0	0.312864	-2.054301	1.067501
H 0	0.426044	-2.666625	-0.570151
H 0	-0.259466	2.868512	0.209416
H 0	0.423530	2.192580	-1.277379
H 0	1.373082	2.194628	0.220403

P-24+BU

B3LYP/6-31G(d) Geometry

C 0	-1.692842	0.663280	-0.071607
C 0	-1.692742	-0.664000	0.071588
C 0	-0.437321	-1.493781	0.155752
C 0	0.796062	-0.695749	-0.305698
C 0	0.795951	0.695402	0.305695
C 0	-0.437546	1.493251	-0.155762
N 0	2.027738	1.487421	-0.095195
N 0	2.027956	-1.487583	0.095222
O 0	2.288283	2.461758	0.598489
O 0	2.634911	1.137647	-1.103484
O 0	2.288786	-2.461758	-0.598575
O 0	2.634906	-1.137859	1.103668
H 0	-2.634911	1.203069	-0.136484
H 0	-2.634730	-1.203930	0.136459
H 0	-0.520942	-2.394414	-0.462119
H 0	-0.281926	-1.840465	1.188052
H 0	0.842031	-0.644531	-1.393321
H 0	0.841908	0.644179	1.393321
H 0	-0.282203	1.839963	-1.188061
H 0	-0.521304	2.393871	0.462108

P-25+BU

B3LYP/6-31G(d) Geometry

C 0	1.127710	-1.967833	1.094641
C 0	1.994627	-1.706335	0.110869
C 0	1.678091	-0.810248	-1.062908
C 0	-0.285971	-1.443792	1.129753
C 0	0.456266	0.094029	-0.767860
C 0	-0.685642	-0.804948	-0.219320
C 0	0.843600	1.247170	0.147984
C 0	-2.095549	-0.189914	-0.196091
O 0	-2.989121	-0.636891	-0.878773
O 0	-2.312621	0.839100	0.642270
O 0	0.228561	1.638500	1.128738
O 0	1.969087	1.866879	-0.247669
H 0	1.432614	-2.603566	1.924360
H 0	2.989121	-2.147935	0.136046
H 0	2.546188	-0.194813	-1.318069
H 0	1.459015	-1.412970	-1.955805
H 0	-0.399478	-0.729736	1.955805
H 0	-0.979620	-2.266318	1.348420
H 0	0.135488	0.562037	-1.709275
H 0	-0.781318	-1.614177	-0.948950
H 0	-1.463315	1.134947	1.042469
H 0	2.115476	2.603566	0.376736

P-26+BU

B3LYP/6-31G(d) Geometry

C 0	1.865306	0.668322	-0.711914
C 0	1.860886	-0.650514	-0.916279
C 0	0.610545	-1.483277	-1.022590
C 0	-0.650372	-0.731907	-0.485012
C 0	-0.636591	0.736227	-1.059661
C 0	0.617850	1.499316	-0.576686
C 0	-0.625354	-0.695802	0.992005
C 0	-1.861155	-1.448811	-0.929228
N 0	-2.785049	-2.028898	-1.323160
N 0	-0.576208	-0.658699	2.150128
C 0	-1.861353	1.475517	-0.735264
N 0	-2.811356	2.089806	-0.478029
H 0	2.811356	1.197416	-0.623268
H 0	2.800650	-1.189205	-1.012613
H 0	0.718680	-2.420105	-0.465214
H 0	0.415828	-1.767785	-2.065427
H 0	-0.589927	0.625860	-2.150128
H 0	0.479905	1.816902	0.465565
H 0	0.704716	2.420105	-1.165651

P-27+BU

B3LYP/6-31G(d) Geometry

C 0	-1.786852	-1.109061	-0.339652
C 0	-1.940979	0.126838	0.140554
C 0	-0.812424	1.117313	0.245465
C 0	0.435240	0.709124	-0.560792
C 0	0.757691	-0.808270	-0.355025
C 0	-0.464779	-1.654434	-0.811261
C 0	1.009498	-1.060474	1.079424
N 0	1.228003	-1.249734	2.204413

C 0	2.006329	-1.253163	-1.150177
C 0	1.610636	1.643447	-0.248606
H 0	-2.641600	-1.780401	-0.401643
H 0	-2.920296	0.452497	0.487729
H 0	-0.540269	1.255154	1.303682
H 0	-1.149386	2.103893	-0.102163
H 0	0.189148	0.801991	-1.628879
H 0	-0.335985	-2.688167	-0.465061
H 0	-0.446250	-1.704159	-1.910969
H 0	2.920296	-0.789862	-0.770791
H 0	1.887383	-0.977900	-2.204413
H 0	2.130262	-2.339565	-1.090987
H 0	1.955329	1.513159	0.784163
H 0	1.300426	2.688167	-0.365873
H 0	2.461994	1.477928	-0.916086

P-28+BU

B3LYP/6-31G(d) Geometry

C 0	1.604884	-1.597708	-0.606389
C 0	2.133399	-0.380453	-0.457021
C 0	1.301795	0.870024	-0.351400
C 0	-0.171937	0.659555	-0.747495
C 0	-0.719123	-0.671995	-0.125702
C 0	0.121930	-1.860413	-0.679346
C 0	-2.116454	-0.865090	-0.558706
N 0	-3.214831	-1.022972	-0.902161
C 0	-1.016395	1.897841	-0.424257
C 0	-0.688130	-0.670538	1.421967
H 0	2.256230	-2.466127	-0.690761
H 0	3.214831	-0.264310	-0.401696
H 0	1.363979	1.274297	0.671738
H 0	1.726865	1.653683	-0.994112
H 0	-0.200471	0.510314	-1.836008
H 0	-0.169556	-2.062210	-1.720111
H 0	-0.130178	-2.770503	-0.119574
H 0	-0.620270	2.770503	-0.956213
H 0	-1.000138	2.133548	0.646132
H 0	-2.059612	1.765223	-0.728403
H 0	-1.247900	0.172639	1.836008
H 0	0.344591	-0.618149	1.777100
H 0	-1.134586	-1.591643	1.809477

P-29+BU

B3LYP/6-31G(d) Geometry

C 0	0.021507	1.355998	1.114934
C 0	0.372699	1.874944	-0.064181
C 0	0.487762	1.067702	-1.331044
C 0	0.526861	-0.454831	-1.052031
C 0	-0.560066	-0.869702	0.004804
C 0	-0.309328	-0.098987	1.328062
C 0	-0.564357	-2.394540	0.244407
C 0	-1.873587	-0.484519	-0.548784
C 0	1.859237	-0.869253	-0.587734
N 0	-2.910766	-0.206293	-0.990362
N 0	2.910766	-1.199764	-0.222949
H 0	-0.030433	1.997022	1.992440
H 0	0.585608	2.938738	-0.144156
H 0	1.386792	1.355505	-1.888685
H 0	-0.364124	1.276770	-1.992440
H 0	0.327310	-0.998020	-1.984070
H 0	0.512821	-0.597136	1.861835
H 0	-1.193172	-0.198691	1.970034
H 0	0.411101	-2.714418	0.622859
H 0	-0.776658	-2.938738	-0.681379
H 0	-1.328598	-2.662120	0.980434

P-30+BU

B3LYP/6-31G(d) Geometry

C 0	-1.660901	-1.442492	0.135638
C 0	-2.145930	-0.305683	-0.369120
C 0	-1.284049	0.841585	-0.829894
C 0	0.191294	0.744963	-0.352290
C 0	0.659125	-0.739167	-0.548701
C 0	-0.189754	-1.724827	0.287090
C 0	2.090952	-0.917903	-0.277212
N 0	3.221607	-1.072691	-0.064711
C 0	0.258411	1.090439	1.081975
N 0	0.309964	1.375133	2.206222
C 0	1.078495	1.728081	-1.144581
H 0	-2.343187	-2.221055	0.470328
H 0	-3.221607	-0.170396	-0.461607
H 0	-1.704540	1.793389	-0.482400
H 0	-1.283282	0.898853	-1.928900
H 0	0.500633	-0.962392	-1.612686
H 0	0.105208	-1.661932	1.343460
H 0	0.038813	-2.748667	-0.032789
H 0	0.695819	2.748667	-1.047200
H 0	1.072954	1.456911	-2.206222
H 0	2.110997	1.710131	-0.786131

P-31+BU

B3LYP/6-31G(d) Geometry

C 0	-1.167301	-1.901954	-0.185560
C 0	-1.950318	-0.826200	-0.304142
C 0	-1.416378	0.570863	-0.496719
C 0	0.084052	0.729604	-0.146283
C 0	0.844592	-0.492078	-0.779053
C 0	0.334483	-1.839625	-0.244046
C 0	2.348954	-0.370207	-0.627519
O 0	3.033119	-1.075457	0.084307
C 0	0.265688	0.752921	1.385178
C 0	0.585347	2.062796	-0.734969
H 0	-1.614869	-2.883676	-0.036378
H 0	-3.033119	-0.938419	-0.267984
H 0	-1.995801	1.277111	0.115689
H 0	-1.584833	0.885206	-1.539640
H 0	0.647068	-0.437608	-1.862396
H 0	0.770449	-2.032630	0.745358
H 0	0.718600	-2.647223	-0.881883
H 0	2.824825	0.434144	-1.230874
H 0	-0.194827	-0.117279	1.862396
H 0	-0.205426	1.649666	1.805317
H 0	1.325180	0.770470	1.664997
H 0	-0.067929	2.883676	-0.415095
H 0	0.582519	2.045751	-1.832126
H 0	1.599937	2.308009	-0.402048

P-32+BU

B3LYP/6-31G(d) Geometry

C 0	1.882616	0.485659	-0.698971
C 0	1.853275	-0.839561	-0.856617
C 0	0.583789	-1.640740	-0.977620
C 0	-0.664831	-0.843122	-0.476463
C 0	-0.617973	0.613635	-1.067665
C 0	0.654244	1.351339	-0.632910
C 0	-1.880815	1.415830	-0.759232

O 0	-1.859408	2.573682	-0.412710
C 0	-0.668006	-0.784565	1.001277
C 0	-1.884663	-1.547623	-0.922695
N 0	-2.821760	-2.106868	-1.317481
N 0	-0.658751	-0.724601	2.159781
H 0	2.840339	0.991591	-0.595958
H 0	2.780556	-1.406349	-0.899415
H 0	0.654075	-2.573682	-0.407257
H 0	0.398949	-1.931041	-2.020881
H 0	-0.609099	0.470825	-2.159781
H 0	0.521442	1.749166	0.382302
H 0	0.774534	2.234597	-1.270985
H 0	-2.840339	0.876189	-0.901255

P-33+BU

B3LYP/6-31G(d) Geometry

C 0	1.858285	0.318582	0.586126
C 0	1.858284	-0.318583	-0.586130
C 0	0.612633	-0.722733	-1.327718
C 0	-0.654153	-0.682633	-0.415823
C 0	-0.654152	0.682635	0.415823
C 0	0.612637	0.722734	1.327716
C 0	-0.627845	1.812507	-0.534831
C 0	-0.627846	-1.812505	0.534831
C 0	-1.867879	-0.788630	-1.246588
N 0	-2.800383	-0.869947	-1.931042
N 0	-0.581104	-2.701244	1.278292
N 0	-0.581113	2.701244	-1.278297
C 0	-1.867875	0.788634	1.246591
N 0	-2.800375	0.869942	1.931051
H 0	2.800383	0.569164	1.067103
H 0	2.800380	-0.569169	-1.067108
H 0	0.707330	-1.738001	-1.727557
H 0	0.436617	-0.063284	-2.187012
H 0	0.436622	0.063287	2.187012
H 0	0.707336	1.738003	1.727553

P-34+BU

B3LYP/6-31G(d) Geometry

C 0	1.488537	-1.037928	-1.493301
C 0	2.064486	-0.813403	-0.310641
C 0	1.357783	-0.187760	0.862283
C 0	0.017069	0.500116	0.487587
C 0	-0.777862	-0.456023	-0.508072
C 0	0.055748	-0.699381	-1.805912
C 0	-1.025917	-1.744034	0.174097
C 0	0.301870	1.756355	-0.232023
C 0	-0.806466	0.823333	1.751627
N 0	0.534358	2.755075	-0.775727
N 0	-1.207436	-2.755075	0.713183
C 0	-2.084382	0.131327	-0.865282
N 0	-3.102335	0.600881	-1.163369
H 0	2.061245	-1.485932	-2.301763
H 0	3.102335	-1.098088	-0.153805
H 0	2.002368	0.560620	1.338823
H 0	1.153973	-0.946933	1.630242
H 0	-0.006674	0.205844	-2.423434
H 0	-0.420102	-1.502469	-2.379131
H 0	-0.218410	1.455358	2.423434
H 0	-1.060066	-0.101717	2.278495
H 0	-1.729560	1.352774	1.501166

P-35+BU

B3LYP/6-31G(d) Geometry

C 0	-1.629270	1.501921	-0.138493
C 0	-0.920562	1.604260	-1.264233
C 0	0.234260	0.700576	-1.604296
C 0	0.772939	-0.049436	-0.342860
C 0	-0.434064	-0.664825	0.481698
C 0	-1.375515	0.468355	0.926176
C 0	0.072161	-1.474722	1.695571
C 0	1.512287	0.896939	0.518857
C 0	1.720249	-1.099953	-0.772990
C 0	-1.177667	-1.666307	-0.417455
N 0	2.443013	-1.931602	-1.137497
N 0	2.077537	1.642899	1.204530
O 0	-2.381118	-1.755704	-0.479298
H 0	-2.443013	2.199308	0.048146
H 0	-1.163144	2.368661	-1.998626
H 0	1.056884	1.266869	-2.054824
H 0	-0.059769	-0.052584	-2.349203
H 0	-0.970417	0.952327	1.825597
H 0	-2.325397	0.008450	1.221019
H 0	0.682101	-0.842424	2.349203
H 0	0.676985	-2.335079	1.389786
H 0	-0.781420	-1.843280	2.273272
H 0	-0.524842	-2.368661	-0.979181

P-36+BU

B3LYP/6-31G(d) Geometry

C 0	1.656470	-1.208848	-0.639396
C 0	2.013354	-0.019200	-0.148124
C 0	1.023113	1.003200	0.342236
C 0	-0.438934	0.744261	-0.112585
C 0	-0.754471	-0.784092	0.084891
C 0	0.221938	-1.649062	-0.771143
C 0	-2.157736	-1.207727	-0.340433
O 0	-3.069557	-0.508923	-0.725052
C 0	-0.567362	1.147756	-1.600808
C 0	-1.372227	1.653327	0.713800
C 0	-0.625115	-1.240037	1.563277
H 0	2.417102	-1.908128	-0.983942
H 0	3.069557	0.238160	-0.077018
H 0	1.323104	2.002799	-0.003611
H 0	1.072571	1.056060	1.441320
H 0	-0.071988	-1.620738	-1.831621
H 0	0.127038	-2.702572	-0.472414
H 0	-2.307135	-2.312462	-0.262046
H 0	0.161861	0.630101	-2.231969
H 0	-0.379212	2.223197	-1.704720
H 0	-1.570844	0.945782	-1.981911
H 0	-1.093406	2.702572	0.556327
H 0	-1.294458	1.459342	1.789169
H 0	-2.414773	1.530472	0.413061
H 0	-1.264403	-0.657192	2.231969
H 0	0.409820	-1.152521	1.904568
H 0	-0.914044	-2.293453	1.664599

P-37+BU

B3LYP/6-31G(d) Geometry

C 0	-1.399089	-0.282695	-1.851208
C 0	-0.416543	-1.134951	0.864211
C 0	-0.528027	-2.062037	-0.317407
C 0	-0.960626	-1.684813	-1.521924
C 0	-1.684335	0.556227	-0.562700
C 0	-0.507160	0.356230	0.486670

C 0	0.773041	0.851952	-0.148331
O 0	1.833036	0.238773	-0.042467
C 0	-2.950735	0.110406	0.054340
C 0	-1.832485	1.979713	-0.929475
C 0	-0.718829	1.237760	1.743933
N 0	-3.937553	-0.249483	0.546605
N 0	-1.908826	3.096399	-1.235613
H 0	-0.632635	0.242171	-2.439903
H 0	-2.302197	-0.289137	-2.471270
H 0	0.537682	-1.299288	1.376390
H 0	-1.201576	-1.365533	1.597167
H 0	-0.237806	-3.096399	-0.149687
H 0	-1.006805	-2.402590	-2.337117
H 0	0.773569	1.821140	-0.668575
H 0	0.074754	1.042181	2.471270
H 0	-1.680177	0.992491	2.206481
H 0	-0.714612	2.305872	1.504717
B 0	3.255129	0.782552	-0.637790
H 0	3.575402	-0.107916	-1.386246
H 0	2.978486	1.839270	-1.162198
H 0	3.937553	0.854110	0.354854

P-38+BU

B3LYP/6-31G(d) Geometry

C 0	0.206484	1.878918	-0.634412
C 0	-0.206288	1.878939	0.634392
C 0	-0.466754	0.624528	1.423194
C 0	-0.576759	-0.653334	0.544906
C 0	0.576764	-0.653383	-0.544901
C 0	0.466850	0.624479	-1.423205
C 0	0.543780	-1.907171	-1.448147
C 0	-0.543870	-1.907117	1.448163
C 0	1.868014	-0.632424	0.171284
C 0	-1.868009	-0.632295	-0.171279
N 0	2.888277	-0.638401	0.725756
N 0	-2.888277	-0.638241	-0.725742
H 0	0.364507	2.821833	-1.153757
H 0	-0.364237	2.821871	1.153728
H 0	-1.390661	0.726934	2.006022
H 0	0.337685	0.465678	2.155657
H 0	-0.337605	0.465684	-2.155661
H 0	1.390760	0.726810	-2.006040
H 0	-0.438432	-1.997146	-1.922539
H 0	0.750645	-2.821871	-0.887252
H 0	1.300096	-1.817392	-2.234081
H 0	-1.300195	-1.817283	2.234081
H 0	0.438328	-1.997151	1.922573
H 0	-0.750782	-2.821809	0.887273

P-39+BU

B3LYP/6-31G(d) Geometry

C 0	1.606734	-1.002078	-1.112984
C 0	2.145231	-0.204841	-0.187186
C 0	1.332134	0.681595	0.718063
C 0	-0.142564	0.850252	0.257901
C 0	-0.716298	-0.563471	-0.176318
C 0	0.125252	-1.111368	-1.365534
C 0	-2.116378	-0.412665	-0.615731
N 0	-3.225289	-0.320655	-0.947360
C 0	-0.698755	-1.577975	0.994383
C 0	-0.158181	1.742097	-0.921713
N 0	-0.163922	2.462665	-1.831908
C 0	-0.978764	1.527623	1.366503
H 0	2.251869	-1.605376	-1.748497
H 0	3.225289	-0.174017	-0.058608
H 0	1.790449	1.676349	0.783018
H 0	1.335017	0.287433	1.744732
H 0	-0.135691	-0.569938	-2.284489
H 0	-0.155783	-2.157235	-1.540396
H 0	-1.264177	-1.217842	1.857184
H 0	0.327748	-1.792367	1.301205
H 0	-1.156328	-2.515986	0.666488
H 0	-0.566773	2.515986	1.591813
H 0	-0.952916	0.933624	2.284489
H 0	-2.019829	1.653577	1.056719

P-40+BU

B3LYP/6-31G(d) Geometry

C 0	1.603267	-1.557227	-0.530117
C 0	2.137043	-0.415102	-0.089202
C 0	1.315736	0.775530	0.330336
C 0	-0.158575	0.723776	-0.142447
C 0	-0.715036	-0.735729	0.128476
C 0	0.120623	-1.780854	-0.671493
C 0	-2.115564	-0.822567	-0.329442
N 0	-3.219129	-0.901098	-0.683725
C 0	-0.975837	1.789800	0.610817
C 0	-0.695889	-1.119190	1.631093
C 0	-0.221334	1.046453	-1.651704
H 0	2.250049	-2.383129	-0.821896
H 0	3.219129	-0.322271	-0.007626
H 0	1.358619	0.880659	1.425567
H 0	1.772150	1.695370	-0.062001
H 0	-0.161919	-1.758014	-1.732799
H 0	-0.144899	-2.786424	-0.320465
H 0	-0.576324	2.786424	0.389376
H 0	-0.934948	1.656921	1.696766
H 0	-2.027561	1.777454	0.304048
H 0	-1.281137	-0.424724	2.238131
H 0	0.331440	-1.138888	2.004337
H 0	-1.122365	-2.118348	1.764860
H 0	0.446711	0.408861	-2.238131
H 0	0.086438	2.085021	-1.818509
H 0	-1.238721	0.934399	-2.041546

P-41+BU

B3LYP/6-31G(d) Geometry

C 0	-1.292349	-1.167619	-0.689336
C 0	-1.805290	0.044446	-0.924915
C 0	-1.486630	1.236294	-0.052154
C 0	-0.044946	1.216028	0.482437
C 0	0.548514	-0.214479	0.756996
C 0	-0.345123	-1.430652	0.456736
C 0	1.610719	0.078614	-0.318717
C 0	1.072712	1.488870	-0.577642
O 0	2.502256	-0.580486	-0.790900
H 0	-1.569353	-2.009776	-1.320511
H 0	-2.502256	0.188528	-1.748406
H 0	-2.185097	1.254276	0.799322
H 0	-1.662373	2.171974	-0.598286
H 0	0.038455	1.878654	1.348904
H 0	1.007684	-0.316585	1.748406
H 0	-0.918948	-1.697613	1.357361
H 0	0.299126	-2.291267	0.239035
H 0	1.777952	2.291267	-0.332229
H 0	0.723726	1.637693	-1.606774

P-42+BU

B3LYP/6-31G(d) Geometry

C 0	-1.059431	-1.158246	-1.140259
C 0	-1.759582	-0.131840	-0.648000
C 0	-1.326761	0.596972	0.602132
C 0	0.201529	0.693598	0.719678
C 0	1.021293	-0.561009	0.221664
C 0	0.195081	-1.667830	-0.473201
C 0	1.710404	0.376717	-0.793529
C 0	0.905718	1.596891	-0.344607
C 0	2.005152	-1.155580	1.234012
O 0	2.571419	0.191522	-1.617250
H 0	-1.404682	-1.679611	-2.030971
H 0	-2.678187	0.187253	-1.136646
H 0	-1.727124	0.074948	1.485702
H 0	-1.761067	1.604664	0.631518
H 0	0.478579	0.976225	1.740783
H 0	-0.077045	-2.428280	0.276594
H 0	0.841805	-2.177726	-1.198142
H 0	1.507436	2.428280	0.039658
H 0	0.246995	1.981669	-1.132853
H 0	1.467750	-1.684049	2.030971
H 0	2.623057	-0.379457	1.700673
H 0	2.678187	-1.867343	0.742563

P-43+BU

B3LYP/6-31G(d) Geometry

C 0	-1.305718	-1.899485	-0.039562
C 0	-1.776214	-0.885622	-0.772487
C 0	-1.425399	0.552232	-0.469828
C 0	0.017734	0.745112	0.041561
C 0	0.566439	-0.477156	0.878967
C 0	-0.368604	-1.674553	1.121962
C 0	0.175259	2.096323	0.739723
C 0	1.607852	-0.705783	-0.227706
C 0	1.110132	0.478302	-1.056085
O 0	2.465936	-1.538242	-0.384738
H 0	-1.606329	-2.921673	-0.260570
H 0	-2.465936	-1.079460	-1.591789
H 0	-2.124507	0.934910	0.291491
H 0	-1.581260	1.182721	-1.355055
H 0	1.043363	-0.171892	1.819890
H 0	-0.949331	-1.509782	2.042558
H 0	0.246747	-2.564185	1.303671
H 0	-0.475838	2.165090	1.620065
H 0	-0.086985	2.921673	0.065534
H 0	1.207552	2.256121	1.074626
H 0	1.847952	1.278196	-1.192320
H 0	0.731736	0.184336	-2.042558

P-44+BU

B3LYP/6-31G(d) Geometry

C 0	2.044668	-1.276316	0.173153
C 0	1.195111	-1.770412	-0.732283
C 0	-0.290319	-1.505066	-0.670140
C 0	-0.621004	-0.070471	-0.180908
C 0	0.425078	0.528964	0.853027
C 0	1.578686	-0.381781	1.296197
C 0	-2.004372	0.002442	0.284433
C 0	0.799848	1.569234	-0.216751
C 0	-0.255358	1.070345	-1.205259
O 0	1.645103	2.423679	-0.259721
N 0	-3.103046	0.060996	0.658342
H 0	3.103046	-1.521231	0.121783
H 0	1.554800	-2.423679	-1.523981
H 0	-0.760340	-2.226474	0.013372
H 0	-0.761394	-1.664238	-1.646787
H 0	-0.057660	0.998880	1.717411
H 0	1.263112	-0.988021	2.158181
H 0	2.396462	0.256850	1.650149
H 0	-1.057779	1.787598	-1.405347
H 0	0.152660	0.716495	-2.158181

P-45+BU

B3LYP/6-31G(d) Geometry

C 0	0.952026	-0.727407	1.213521
C 0	1.698850	-0.373875	0.162997
C 0	1.130835	-0.358434	-1.236871
C 0	-0.330386	0.115910	-1.259297
C 0	-1.202064	-0.367583	-0.046642
C 0	-0.488364	-1.160014	1.056315
C 0	-1.464344	1.124308	0.294590
C 0	-0.571733	1.605404	-0.849315
O 0	-2.110952	1.659628	1.152911
Cl 0	-2.743799	-1.215233	-0.523414
H 0	1.376569	-0.745850	2.214603
H 0	2.743799	-0.104229	0.299965
H 0	1.189750	-1.368996	-1.669369
H 0	1.729409	0.284807	-1.893514
H 0	-0.799109	-0.128423	-2.214603
H 0	-0.528302	-2.227749	0.798797
H 0	-1.048946	-1.040453	1.989649
H 0	-1.086897	2.227749	-1.588848
H 0	0.316113	2.141793	-0.495143

P-46+BU

B3LYP/6-31G(d) Geometry

C 0	-2.113801	0.896171	0.485332
C 0	-1.369764	1.768436	-0.199693
C 0	0.135173	1.669612	-0.223613
C 0	0.629572	0.199974	-0.282779
C 0	-0.257460	-0.848997	0.545721
C 0	-1.486774	-0.240978	1.252951
C 0	2.058616	0.153405	0.018883
C 0	-0.623259	-1.493799	-0.806728
C 0	0.262612	-0.550427	-1.617813
O 0	-1.353003	-2.406695	-1.094442
C 0	0.499396	-1.806763	1.471073
N 0	3.196013	0.126886	0.255823
H 0	-3.196013	0.999445	0.516571
H 0	-1.833711	2.594912	-0.733001
H 0	0.551227	2.145423	0.676130
H 0	0.554762	2.216016	-1.075978
H 0	-1.186496	0.103313	2.255082
H 0	-2.211410	-1.048681	1.410054
H 0	1.100919	-1.042827	-2.121018
H 0	-0.281422	0.058798	-2.347513
H 0	0.886399	-1.275276	2.347513
H 0	1.346271	-2.284578	0.969040
H 0	-0.179959	-2.594912	1.812916

P-47+BU

B3LYP/6-31G(d) Geometry

C 0	-1.168972	-1.864989	0.050904
C 0	-1.832115	-0.811054	-0.432498

C 0	-1.329033	0.593696	-0.213006
C 0	0.208981	0.711308	-0.272128
C 0	0.989038	-0.515226	0.391713
C 0	0.096371	-1.696096	0.852162
C 0	1.605686	-0.783036	-0.994594
C 0	0.807414	0.327323	-1.671384
C 0	2.039780	-0.215958	1.467040
O 0	2.436346	-1.571745	-1.374214
C 0	0.639033	2.103919	0.196069
H 0	-1.547453	-2.874162	-0.098899
H 0	-2.761040	-0.948049	-0.982647
H 0	-1.676126	0.956957	0.768334
H 0	-1.764261	1.279113	-0.952393
H 0	-0.164365	-1.540078	1.911656
H 0	0.701697	-2.610588	0.822231
H 0	1.414745	1.094873	-2.165768
H 0	0.080015	-0.060861	-2.394273
H 0	1.566610	0.128788	2.394273
H 0	2.761040	0.543418	1.150532
H 0	2.603440	-1.128375	1.691726
H 0	0.391714	2.269146	1.251562
H 0	0.121643	2.874162	-0.389724
H 0	1.714557	2.270363	0.073568

P-48+BU

B3LYP/6-31G(d) Geometry

C 0	-2.067281	-0.510842	-0.812725
C 0	-2.230189	0.698655	-0.270450
C 0	-1.196599	1.401707	0.568559
C 0	0.127022	0.635252	0.675189
C 0	0.071848	-0.901371	0.523850
C 0	-0.811137	-1.332047	-0.666453
C 0	1.559267	-1.279064	0.304074
C 0	1.203775	1.052186	-0.336691
C 0	2.123558	-0.151053	-0.584573
O 0	1.309581	2.143432	-0.852732
H 0	-2.865519	-0.938385	-1.417968
H 0	-3.164996	1.234780	-0.429688
H 0	-1.612274	1.584791	1.569960
H 0	-0.984421	2.394909	0.148058
H 0	0.588550	0.853755	1.653286
H 0	-0.324701	-1.362148	1.435392
H 0	-1.066222	-2.394909	-0.555990
H 0	-0.237770	-1.274292	-1.606042
H 0	1.673627	-2.271909	-0.143907
H 0	2.081986	-1.296369	1.268334
H 0	3.164996	0.113306	-0.372516
H 0	2.077783	-0.395054	-1.653286

P-49+BU

B3LYP/6-31G(d) Geometry

C 0	-1.408927	-0.995874	-1.255357
C 0	-2.062353	-0.184262	-0.420099
C 0	-1.391941	0.602536	0.674982
C 0	0.141218	0.604945	0.581284
C 0	0.759671	-0.731259	0.093422
C 0	0.083695	-1.199024	-1.234313
C 0	2.188818	-0.309651	-0.288385
C 0	0.751709	1.663639	-0.368495
C 0	2.209389	1.203828	-0.550355
O 0	3.143861	-1.051702	-0.371310
C 0	0.745162	-1.855660	1.130970
H 0	-1.960814	-1.536805	-2.023250
H 0	-3.143861	-0.085563	-0.504048
H 0	-1.703595	0.192233	1.647934
H 0	-1.762402	1.638342	0.670493
H 0	0.543654	0.802177	1.586272
H 0	0.330782	-2.256520	-1.392408
H 0	0.519939	-0.677308	-2.101173
H 0	0.671460	2.675247	0.042946
H 0	0.219289	1.662076	-1.327264
H 0	2.873584	1.655311	0.198965
H 0	2.648036	1.424548	-1.528969
H 0	-0.268312	-2.246646	1.273823
H 0	1.115593	-1.503956	2.101173
H 0	1.393254	-2.675247	0.803979

P-50+BU

B3LYP/6-31G(d) Geometry

C 0	-2.164579	-0.600056	1.155004
C 0	-2.149860	-1.564204	0.231231
C 0	-1.139647	-1.650486	-0.881120
C 0	-0.032974	-0.595161	-0.775179
C 0	-0.403139	0.762051	-0.120801
C 0	-1.155115	0.518977	1.215258
C 0	0.995869	1.378170	0.163627
C 0	1.213958	-1.045447	-0.003689
C 0	1.887925	0.197045	0.592439
O 0	1.603151	-2.186967	0.113965
C 0	-1.247956	1.645320	-1.046719
H 0	-2.925187	-0.615600	1.934469
H 0	-2.907148	-2.346584	0.259262
H 0	-1.658012	-1.563562	-1.847159
H 0	-0.666970	-2.642615	-0.882862
H 0	0.347640	-0.375672	-1.787959
H 0	-1.648379	1.452862	1.519390
H 0	-0.438186	0.301600	2.022649
H 0	0.945967	2.173234	0.916064
H 0	1.386394	1.830783	-0.756948
H 0	2.925187	0.269059	0.247899
H 0	1.932535	0.070611	1.681175
H 0	-2.240202	1.211622	-1.214626
H 0	-0.763124	1.771960	-2.022649
H 0	-1.390065	2.642615	-0.611686

P-51+BU

B3LYP/6-31G(d) Geometry

C 0	1.000814	1.231959	1.147732
C 0	0.629883	1.907937	0.058310
C 0	-0.049522	1.291087	-1.133905
C 0	-0.417282	-0.180966	-0.931770
C 0	0.500166	-1.011094	0.012527
C 0	0.770439	-0.244781	1.339207
C 0	-0.353628	-2.293599	0.276960
C 0	-1.818146	-0.440085	-0.356162
C 0	-1.800282	-1.777807	0.393909
O 0	-2.774251	0.289656	-0.484049
C 0	1.773537	-1.338995	-0.639588
N 0	2.774251	-1.611544	-1.162709
H 0	1.484925	1.755819	1.969549
H 0	0.830326	2.976129	-0.002020
H 0	0.598487	1.400175	-2.014381
H 0	-0.972879	1.839169	-1.366099
H 0	-0.427680	-0.688787	-1.909422
H 0	1.627907	-0.704002	1.845757
H 0	-0.084563	-0.398168	2.014381

H 0 -0.006880 -2.826281 1.167235
H 0 -0.255364 -2.976129 -0.573655
H 0 -2.543493 -2.459241 -0.032837
H 0 -2.105649 -1.595256 1.431045

P-52+BU
B3LYP/6-31G(d) Geometry
C 0 1.418235 -0.741148 1.171939
C 0 2.079280 -0.260540 0.116821
C 0 1.415253 0.149945 -1.170754
C 0 -0.110675 0.267725 -1.066703
C 0 -0.769290 -0.785494 -0.153543
C 0 -0.078821 -0.890115 1.227848
C 0 -2.192828 -0.226738 0.075001
C 0 -0.657192 1.596153 -0.488137
C 0 -2.132350 1.287417 -0.167520
O 0 -3.164357 -0.860987 0.404782
Cl 0 -0.813992 -2.419523 -0.947781
H 0 1.963035 -1.030809 2.068860
H 0 3.164357 -0.180031 0.155603
H 0 1.670528 -0.583475 -1.949467
H 0 1.830023 1.105988 -1.521138
H 0 -0.541577 0.145297 -2.068860
H 0 -0.370540 -1.841028 1.685664
H 0 -0.490723 -0.114462 1.894387
H 0 -0.540412 2.419523 -1.199625
H 0 -0.106140 1.870355 0.419094
H 0 -2.785796 1.503147 -1.023241
H 0 -2.544972 1.832346 0.687432

P-53+BU
B3LYP/6-31G(d) Geometry
C 0 -1.707242 -1.246755 -0.216545
C 0 -2.042963 0.043947 -0.248182
C 0 -1.056199 1.170353 -0.113455
C 0 0.419363 0.716910 -0.238175
C 0 0.725664 -0.673519 0.424733
C 0 -0.293177 -1.743014 -0.088068
C 0 2.065721 -1.060036 -0.231703
C 0 0.912157 0.509265 -1.706608
C 0 2.207494 -0.307635 -1.562674
O 0 2.858909 -1.853114 0.221760
C 0 1.270561 1.760534 0.366749
C 0 0.784428 -0.680369 1.952814
N 0 1.939164 2.595594 0.819880
H 0 -2.479688 -2.007739 -0.316036
H 0 -3.088008 0.329804 -0.353178
H 0 -1.204975 1.667526 0.855420
H 0 -1.252701 1.943212 -0.869315
H 0 -0.247054 -2.595594 0.600394
H 0 0.022644 -2.153427 -1.060082
H 0 1.058130 1.463567 -2.219731
H 0 0.144831 -0.048270 -2.253506
H 0 3.088008 0.341960 -1.483763
H 0 2.399487 -1.004459 -2.384361
H 0 -0.217113 -0.575860 2.384361
H 0 1.413542 0.128424 2.336490
H 0 1.214544 -1.627941 2.291428

P-54+BU
B3LYP/6-31G(d) Geometry
C 0 -1.443741 -1.542718 -0.768698
C 0 -2.066299 -0.417074 -0.414632
C 0 -1.358411 0.778996 0.160176
C 0 0.180232 0.731565 0.065913
C 0 0.770034 -0.708180 0.259154
C 0 0.045621 -1.734120 -0.677701
C 0 2.176413 -0.565060 -0.342851
C 0 0.712036 1.108723 -1.350485
C 0 2.144166 0.542651 -1.407344
O 0 3.148309 -1.223085 -0.039761
C 0 0.796042 -1.249723 1.690442
C 0 0.760387 1.728874 1.090298
H 0 -2.017030 -2.374819 -1.175723
H 0 -3.148309 -0.344007 -0.516802
H 0 -1.657801 0.889417 1.214537
H 0 -1.717275 1.695736 -0.332391
H 0 0.280664 -2.743677 -0.318025
H 0 0.462975 -1.697791 -1.696561
H 0 0.678018 2.191670 -1.512358
H 0 0.081911 0.648901 -2.119858
H 0 2.905472 1.287067 -1.146433
H 0 2.430913 0.139473 -2.384696
H 0 -0.218669 -1.448605 2.053432
H 0 1.281951 -0.558503 2.384696
H 0 1.363821 -2.185147 1.716887
H 0 0.438176 1.498113 2.110499
H 0 0.414880 2.743677 0.857665
H 0 1.856871 1.745393 1.086422

P-55+BU
B3LYP/6-31G(d) Geometry
C 0 1.638098 0.668352 -0.921962
C 0 1.637887 -0.668564 -0.921989
C 0 1.061562 -1.430085 0.246887
C 0 -0.243271 -0.771037 0.760708
C 0 -0.243033 0.771350 0.760721
C 0 1.062010 1.430006 0.246947
C 0 -1.414879 1.144729 -0.144041
C 0 -1.415253 -1.144039 -0.144033
O 0 -2.059054 0.000448 -0.590782
O 0 -1.784153 -2.236341 -0.467303
O 0 -1.783416 2.237148 -0.467330
H 0 2.059054 1.229364 -1.752639
H 0 2.058662 -1.229675 -1.752690
H 0 1.785695 -1.454697 1.074010
H 0 0.847030 -2.470877 -0.013261
H 0 -0.476648 -1.174240 1.752676
H 0 -0.476313 1.174606 1.752690
H 0 1.786144 1.454352 1.074075
H 0 0.847810 2.470877 -0.013160

P-56+BU
B3LYP/6-31G(d) Geometry
C 0 -1.249390 -1.486110 -0.898093
C 0 -1.933644 -0.337554 -0.892709
C 0 -1.711610 0.673074 0.206928
C 0 -0.212757 0.798706 0.557515
C 0 0.530131 -0.555058 0.661140
C 0 -0.272911 -1.802250 0.207460
C 0 1.781623 -0.378880 -0.204454
C 0 0.569945 1.558237 -0.544693
O 0 1.800165 0.852157 -0.776836
O 0 2.659636 -1.184993 -0.378575
H 0 -1.406044 -2.225993 -1.679932
H 0 -2.659636 -0.116457 -1.671962

H 0	-2.265972	0.374675	1.109592
H 0	-2.107286	1.656843	-0.075333
H 0	-0.112945	1.342954	1.502372
H 0	0.890774	-0.733451	1.679932
H 0	-0.824164	-2.197597	1.073410
H 0	0.436319	-2.582091	-0.087861
H 0	0.825523	2.582091	-0.258555
H 0	0.017099	1.582888	-1.489970

P-57+BU

B3LYP/6-31G(d) Geometry

C 0	-2.032049	-0.688333	-0.987885
C 0	-2.445619	0.352734	-0.261705
C 0	-1.590328	1.068952	0.750785
C 0	-0.111931	0.653830	0.703023
C 0	0.071704	-0.865639	0.422163
C 0	-0.650463	-1.280689	-0.875064
C 0	2.394569	-0.414422	-0.569590
C 0	0.714621	1.477251	-0.291202
C 0	2.190783	1.099854	-0.355839
O 0	0.246715	2.377816	-0.961935
C 0	1.565404	-1.244392	0.423140
H 0	-2.704302	-1.140299	-1.715854
H 0	-3.458648	0.730480	-0.393718
H 0	-1.661078	2.150562	0.584574
H 0	-1.990201	0.885473	1.759485
H 0	0.346667	0.851700	1.685531
H 0	-0.419003	-1.400254	1.247271
H 0	-0.062724	-0.989402	-1.759485
H 0	-0.708034	-2.377816	-0.914737
H 0	2.116814	-0.671040	-1.599431
H 0	3.458648	-0.660751	-0.470651
H 0	2.646142	1.388992	0.603857
H 0	2.667837	1.693217	-1.141357
H 0	1.966185	-1.096302	1.436378
H 0	1.676971	-2.313595	0.199243

P-58+BU

B3LYP/6-31G(d) Geometry

C 0	-2.444914	0.306076	0.221507
C 0	-1.877638	-0.393238	1.207964
C 0	-0.428550	-0.808919	1.214536
C 0	0.255506	-0.680220	-0.180817
C 0	-0.168566	0.665496	-0.860451
C 0	-1.701750	0.746039	-1.013089
C 0	1.928095	1.849373	-0.044659
C 0	1.785222	-0.688004	0.026094
C 0	2.414551	0.559572	0.639874
O 0	2.470451	-1.646465	-0.281603
C 0	0.398511	1.896485	-0.128228
C 0	-0.142698	-1.880963	-1.055194
H 0	-3.500914	0.565597	0.283848
H 0	-2.469238	-0.683166	2.075573
H 0	0.102051	-0.217297	1.974522
H 0	-0.340834	-1.851306	1.550155
H 0	0.267908	0.665484	-1.870787
H 0	-2.029399	0.137345	-1.869204
H 0	-1.984437	1.777065	-1.268673
H 0	2.314788	2.723735	0.492736
H 0	2.346988	1.896730	-1.059601
H 0	2.147715	0.595676	1.705928
H 0	3.500914	0.445308	0.582195
H 0	-0.034210	1.970601	0.878819
H 0	0.086550	2.803074	-0.662976
H 0	-1.230404	-1.987104	-1.100811
H 0	0.280752	-2.803074	-0.649323
H 0	0.240520	-1.769368	-2.075573

P-59+BU

B3LYP/6-31G(d) Geometry

C 0	2.054711	0.279280	1.212515
C 0	2.366495	1.136260	0.237303
C 0	1.532431	1.330150	-1.001744
C 0	0.146099	0.673426	-0.902633
C 0	0.184878	-0.731134	-0.210469
C 0	0.822132	-0.589767	1.195198
C 0	-2.268694	-0.370259	0.555732
C 0	-0.878546	1.594570	-0.225940
C 0	-2.283345	1.019528	-0.108116
O 0	-0.603809	2.712703	0.167561
C 0	-1.250308	-1.303377	-0.113849
C 0	1.035471	-1.700071	-1.055934
H 0	2.697061	0.200203	2.088542
H 0	3.269931	1.739001	0.318103
H 0	1.401444	2.402643	-1.185672
H 0	2.071592	0.932244	-1.873997
H 0	-0.246395	0.510132	-1.919939
H 0	0.093860	-0.179190	1.910893
H 0	1.065900	-1.592344	1.575985
H 0	-2.039347	-0.256452	1.622374
H 0	-3.269931	-0.815071	0.505900
H 0	-2.691620	0.926019	-1.126091
H 0	-2.908025	1.732218	0.437952
H 0	-1.597772	-1.533709	-1.132125
H 0	-1.217634	-2.261797	0.422094
H 0	2.087481	-1.401244	-1.080533
H 0	0.668309	-1.749724	-2.088542
H 0	0.987887	-2.712703	-0.636632

P-60+BU

B3LYP/6-31G(d) Geometry

C 0	2.053085	1.015583	1.178290
C 0	2.145135	1.785845	0.092523
C 0	1.447386	1.493537	-1.209254
C 0	0.387529	0.389058	-1.093625
C 0	0.850203	-0.790896	-0.167926
C 0	1.230934	-0.246126	1.236470
C 0	-1.611508	-1.336720	0.368994
C 0	-0.980108	0.913855	-0.624217
C 0	-2.067054	-0.143854	-0.493840
O 0	-1.188604	2.091382	-0.411087
C 0	-0.252644	-1.885123	-0.087115
C 0	2.046576	-1.406423	-0.774768
N 0	2.967787	-1.915081	-1.266291
H 0	2.579785	1.293090	2.089098
H 0	2.763235	2.681199	0.121021
H 0	0.960868	2.404470	-1.575485
H 0	2.191642	1.208897	-1.966104
H 0	0.205233	-0.043376	-2.089098
H 0	0.311747	-0.058997	1.809261
H 0	1.770086	-1.028724	1.785377
H 0	-1.566489	-1.028191	1.420202
H 0	-2.359173	-2.136547	0.318729
H 0	-2.299786	-0.503652	-1.507593
H 0	-2.967787	0.330152	-0.094192

H 0 -0.358273 -2.340909 -1.080051
H 0 0.082637 -2.681199 0.588095

P-61+BU

B3LYP/6-31G(d) Geometry
C 0 2.459007 -0.453544 0.090021
C 0 1.941003 0.127728 1.173895
C 0 0.559662 0.725892 1.222351
C 0 -0.091643 0.894179 -0.172252
C 0 0.212813 -0.316282 -1.099642
C 0 1.730602 -0.555536 -1.223833
C 0 -2.051734 -1.346855 -0.563735
C 0 -1.618211 1.101511 -0.004951
C 0 -2.409609 -0.157808 0.344620
O 0 -2.155992 2.179623 -0.120791
C 0 -0.537781 -1.575302 -0.616815
Cl 0 0.614275 2.397374 -0.948122
H 0 3.470213 -0.855232 0.127509
H 0 2.519586 0.182436 2.094354
H 0 -0.083630 0.090448 1.849278
H 0 0.576056 1.704486 1.715503
H 0 -0.178060 -0.064716 -2.094354
H 0 2.161859 0.166957 -1.930054
H 0 1.897803 -1.545834 -1.669336
H 0 -2.566566 -2.248147 -0.210593
H 0 -2.424793 -1.150392 -1.578114
H 0 -2.195447 -0.423224 1.389802
H 0 -3.470213 0.102616 0.287926
H 0 -0.162853 -1.886633 0.367366
H 0 -0.310688 -2.397374 -1.306815

P-62+BU

B3LYP/6-31G(d) Geometry
C 0 2.405996 0.143951 -0.365645
C 0 2.001155 -1.107155 -0.592107
C 0 0.589163 -1.580749 -0.373068
C 0 -0.277130 -0.614350 0.493602
C 0 -0.005956 0.877696 0.038260
C 0 1.505475 1.225273 0.165652
C 0 -2.001821 0.819305 -1.570648
C 0 -1.761986 -0.977186 0.242253
C 0 -2.361918 -0.604011 -1.111874
O 0 -2.410926 -1.585229 1.070407
C 0 -0.505455 1.111240 -1.416151
C 0 -0.749872 1.805627 0.914768
C 0 0.064127 -0.822971 1.977856
N 0 -1.330630 2.558064 1.582648
H 0 3.443347 0.420811 -0.544814
H 0 2.706189 -1.843476 -0.974601
H 0 0.125305 -1.764603 -1.352385
H 0 0.596951 -2.558064 0.127074
H 0 1.753179 1.428872 1.216346
H 0 1.689747 2.168401 -0.365135
H 0 -2.303152 0.959788 -2.615099
H 0 -2.572736 1.545659 -0.979888
H 0 -1.989772 -1.329541 -1.850132
H 0 -3.443347 -0.750244 -1.041863
H 0 0.087752 0.480138 -2.087822
H 0 -0.298445 2.150721 -1.695995
H 0 1.139199 -0.714420 2.149098
H 0 -0.237875 -1.825995 2.287325
H 0 -0.468618 -0.111364 2.615099

P-63+BU

B3LYP/6-31G(d) Geometry
C 0 2.428134 0.164533 -0.772015
C 0 1.875666 -0.741609 -1.581108
C 0 0.425984 -1.141795 -1.512658
C 0 -0.278050 -0.727441 -0.180272
C 0 0.128094 0.751206 0.213076
C 0 1.669898 0.862596 0.324504
C 0 -1.894594 1.684522 -1.093595
C 0 -1.802993 -0.775505 -0.414373
C 0 -2.394988 0.254620 -1.373849
O 0 -2.512542 -1.600941 0.131919
C 0 -0.375235 1.734230 -0.878237
C 0 0.098806 -1.752506 0.904111
C 0 -0.479450 1.155596 1.574418
H 0 3.484388 0.409624 -0.875718
H 0 2.476687 -1.217639 -2.354918
H 0 -0.091160 -0.722172 -2.386411
H 0 0.335203 -2.230624 -1.624781
H 0 2.002009 0.464583 1.295739
H 0 1.944513 1.927512 0.345173
H 0 -2.177727 2.343604 -1.923227
H 0 -2.407339 2.075256 -0.206408
H 0 -2.116026 -0.032800 -2.397447
H 0 -3.484388 0.180832 -1.307675
H 0 0.141883 1.529569 -1.823716
H 0 -0.085195 2.753022 -0.588673
H 0 1.180636 -1.769472 1.067265
H 0 -0.215924 -2.753022 0.594968
H 0 -0.399880 -1.546982 1.853877
H 0 -0.041741 0.583097 2.397447
H 0 -1.563647 1.005948 1.615550
H 0 -0.283106 2.216709 1.772562

P-64+BU

B3LYP/6-31G(d) Geometry
C 0 -1.535288 -1.209140 -0.204729
C 0 -0.091441 -0.897110 0.232154
O 0 -1.841844 -0.456817 -1.397463
C 0 -2.617714 -0.682147 0.752857
C 0 -2.064339 0.838463 -0.877390
C 0 0.053853 0.627304 0.538554
O 0 -2.834824 0.667722 0.308358
C 0 0.896833 -1.377103 -0.850312
C 0 -0.694537 1.445837 -0.519123
C 0 1.501277 1.091978 0.771228
C 0 2.270724 -0.776664 -0.719216
O 0 -0.293728 2.473786 -1.022682
C 0 2.533197 0.318396 -0.003461
H 0 -1.655955 -2.267640 -0.450763
H 0 0.118234 -1.445947 1.161118
H 0 -2.305073 -0.679427 1.802809
H 0 -3.552325 -1.246226 0.657677
H 0 -2.603844 1.449891 -1.603769
H 0 -0.516234 0.824359 1.457982
H 0 0.488659 -1.143257 -1.843689
H 0 0.962899 -2.473786 -0.807815
H 0 1.739242 1.034891 1.843689
H 0 1.563807 2.154730 0.505157
H 0 3.073641 -1.269666 -1.265073
H 0 3.552325 0.699780 0.040945

P-65+BU

B3LYP/6-31G(d) Geometry

C 0	-1.010536	-1.267939	-0.238878
C 0	0.265794	-0.768673	0.468929
O 0	-1.036195	-0.819163	-1.606028
C 0	-2.326395	-0.671340	0.284097
C 0	-1.439914	0.521782	-1.460596
C 0	0.503965	0.780968	0.276619
O 0	-2.464941	0.543674	-0.465259
C 0	1.495063	-1.632928	0.037910
C 0	-0.251635	1.342651	-0.953034
C 0	2.011558	1.097519	0.064146
C 0	2.302754	-1.037857	-1.086790
O 0	0.045027	2.398175	-1.475206
C 0	2.582209	0.266885	-1.055851
C 0	-0.003578	1.578255	1.504446
H 0	-1.034269	-2.360837	-0.256227
H 0	0.112576	-0.950570	1.541539
H 0	-2.313125	-0.447107	1.355091
H 0	-3.175342	-1.329825	0.064748
H 0	-1.817419	0.910720	-2.408815
H 0	1.161228	-2.646631	-0.210913
H 0	2.149460	-1.743640	0.915753
H 0	2.541979	0.894824	1.007661
H 0	2.112995	2.165779	-0.140497
H 0	2.664073	-1.685690	-1.881707
H 0	3.175342	0.746796	-1.830068
H 0	0.522925	1.251293	2.408815
H 0	-1.078398	1.452629	1.662991
H 0	0.188323	2.646631	1.361398

P-66+BU

B3LYP/6-31G(d) Geometry

C 0	1.477178	-0.965526	0.477605
C 0	0.025114	-0.738438	-0.016981
O 0	1.851926	0.087555	1.389886
C 0	2.574623	-0.806662	-0.590913
C 0	2.126475	1.156358	0.508257
C 0	-0.043712	0.643464	-0.756492
O 0	2.864162	0.601576	-0.575265
C 0	-0.904473	-0.728715	1.225424
C 0	0.780921	1.697645	-0.006479
C 0	-1.470569	1.116311	-1.081883
C 0	-2.241347	-0.078917	0.981368
O 0	0.446549	2.851589	0.161701
C 0	-2.488955	0.745462	-0.038595
C 0	-0.402514	-1.873160	-0.965907
H 0	1.551551	-1.908422	1.027177
H 0	2.265690	-1.102996	-1.597614
H 0	3.478585	-1.362636	-0.317323
H 0	2.707308	1.928103	1.017679
H 0	0.498145	0.524971	-1.706823
H 0	-0.400373	-0.216840	2.055636
H 0	-1.052279	-1.765025	1.562847
H 0	-1.783010	0.711221	-2.055636
H 0	-1.447753	2.206305	-1.202019
H 0	-3.025865	-0.292417	1.705791
H 0	-3.478585	1.186450	-0.148165
H 0	-0.269673	-2.851589	-0.487471
H 0	0.172275	-1.872749	-1.898897
H 0	-1.461011	-1.775276	-1.225513

P-67+BU

B3LYP/6-31G(d) Geometry

C 0	-1.408737	1.018240	0.655472
C 0	0.032105	0.672547	0.157012
O 0	-1.944606	-0.130902	1.322671
C 0	-2.438209	1.222924	-0.466982
C 0	-2.319833	-0.961780	0.236796
C 0	-0.037106	-0.535186	-0.850310
O 0	-2.908262	-0.110600	-0.734975
C 0	0.919641	0.335499	1.388473
C 0	-1.032876	-1.584685	-0.331852
C 0	1.336050	-1.112235	-1.225744
C 0	2.167006	-0.430896	1.041660
O 0	-0.859784	-2.781962	-0.387479
C 0	2.345771	-1.075672	-0.111979
C 0	0.580958	1.844300	-0.544842
N 0	0.976566	2.781962	-1.104832
H 0	-1.375582	1.839468	1.374650
H 0	-2.016209	1.659699	-1.377004
H 0	-3.277604	1.838659	-0.127380
H 0	-3.028158	-1.721439	0.572844
H 0	-0.512627	-0.160592	-1.766824
H 0	0.308457	-0.241410	2.094075
H 0	1.178547	1.270381	1.901896
H 0	1.735938	-0.570200	-2.094075
H 0	1.184937	-2.147790	-1.553272
H 0	2.943386	-0.454889	1.803562
H 0	3.277604	-1.609001	-0.289889

P-68+BU

B3LYP/6-31G(d) Geometry

C 0	1.380758	-1.150460	-0.770163
C 0	0.024178	-0.467545	-1.068933
O 0	1.460208	-1.370710	0.655810
C 0	2.668208	-0.346077	-1.002847
C 0	1.846209	-0.090100	1.118143
C 0	-0.134290	0.871799	-0.289924
O 0	2.843663	0.373259	0.230509
C 0	-1.076233	-1.517399	-0.712720
C 0	0.586652	0.800123	1.084135
C 0	-1.574927	1.383637	-0.168107
C 0	-2.358664	-0.983750	-0.145571
Cl 0	0.775466	2.230580	-1.196280
O 0	0.172124	1.360793	2.072876
C 0	-2.574779	0.301149	0.129738
H 0	1.411217	-2.130810	-1.252996
H 0	-0.045527	-0.232292	-2.136831
H 0	2.612195	0.357715	-1.834479
H 0	3.521922	-1.018906	-1.142670
H 0	2.234492	-0.157097	2.136831
H 0	-1.286626	-2.103547	-1.618951
H 0	-0.662812	-2.230580	0.011480
H 0	-1.850831	1.884432	-1.104531
H 0	-1.588718	2.150221	0.612718
H 0	-3.127375	-1.723653	0.071682
H 0	-3.521922	0.618169	0.561091

P-69+BU

B3LYP/6-31G(d) Geometry

C 0	1.366225	1.037452	-1.062512
C 0	-0.046716	0.700793	-0.466314
O 0	1.812572	-0.100896	-1.811695
C 0	2.523367	1.203025	-0.072880

C 0	2.260879	-0.964215	-0.783980
C 0	-0.007983	-0.591820	0.468090
O 0	2.977271	-0.147672	0.132448
C 0	-0.971536	0.521407	-1.719223
C 0	1.009042	-1.591603	-0.133347
C 0	-1.403283	-1.242627	0.658429
C 0	-2.228703	-0.260658	-1.488018
O 0	0.877193	-2.795575	-0.082593
C 0	-2.404527	-1.064595	-0.442284
C 0	-0.520778	1.860955	0.302687
C 0	0.514793	-0.313143	1.913935
N 0	-0.867378	2.795575	0.899449
H 0	1.273315	1.878095	-1.753581
H 0	2.233116	1.654432	0.878588
H 0	3.334612	1.788087	-0.518684
H 0	2.909447	-1.738404	-1.198569
H 0	-0.378317	0.028320	-2.498696
H 0	-1.211072	1.520070	-2.106538
H 0	-1.845332	-0.857187	1.588165
H 0	-1.229637	-2.311434	0.834240
H 0	-3.000780	-0.170670	-2.249417
H 0	-3.334612	-1.620027	-0.335388
H 0	-0.081265	0.474008	2.385098
H 0	1.568905	-0.043700	1.956790
H 0	0.390127	-1.230381	2.498696

P-70+BU

B3LYP/6-31G(d) Geometry

C 0	-1.454656	-1.110125	-0.783192
C 0	-0.035495	-0.755470	-0.248235
O 0	-1.778706	-0.249017	-1.896586
C 0	-2.660249	-0.827863	0.123244
C 0	-2.134975	0.943104	-1.234210
C 0	0.047935	0.770633	0.198476
O 0	-2.959198	0.554783	-0.138204
C 0	0.907703	-1.035594	-1.461469
C 0	-0.832185	1.617182	-0.752582
C 0	1.501715	1.326338	0.242517
C 0	2.269845	-0.412824	-1.377437
O 0	-0.565073	2.749358	-1.100155
C 0	2.521911	0.660399	-0.631105
C 0	0.347941	-1.707621	0.899112
C 0	-0.531489	1.069345	1.619259
H 0	-1.452733	-2.136475	-1.161634
H 0	-2.467501	-0.970351	1.189249
H 0	-3.520200	-1.440884	-0.169556
H 0	-2.683769	1.603419	-1.909093
H 0	0.420134	-0.691332	-2.382181
H 0	1.001888	-2.125540	-1.569338
H 0	1.865258	1.288928	1.279817
H 0	1.441688	2.393793	-0.005534
H 0	3.053847	-0.849445	-1.993982
H 0	3.520200	1.096029	-0.618915
H 0	0.307858	-2.749358	0.558433
H 0	-0.313188	-1.618293	1.766132
H 0	1.371754	-1.512891	1.235091
H 0	0.013608	0.506274	2.382181
H 0	-1.597725	0.870073	1.715987
H 0	-0.383014	2.134480	1.829223

TS-1+DMB

B3LYP/6-31G(d) Geometry

C 0	0.520539	-1.771156	0.210749
C 0	-0.501378	0.487789	1.540241
C 0	0.449878	0.645702	0.557466
C 0	0.990750	-0.495322	-0.107420
C 0	0.748789	2.033695	0.030471
C 0	1.856780	-0.306370	-1.330930
H 0	0.932655	-2.621708	-0.328543
H 0	0.246074	-2.004602	1.234083
H 0	-1.005546	1.354704	1.957862
H 0	-0.609162	-0.427324	2.106883
H 0	0.306884	2.800661	0.671842
H 0	0.343176	2.174642	-0.979413
H 0	1.828228	2.220664	-0.020678
H 0	1.352481	0.285234	-2.106883
H 0	2.140881	-1.267433	-1.768993
H 0	2.781522	0.230876	-1.082986
C 0	-1.464818	-1.813241	-0.380783
C 0	-2.201403	-0.750534	0.158989
C 0	-2.516700	0.392096	-0.628248
N 0	-2.768594	1.317290	-1.294000
H 0	-1.632279	-2.800661	0.040751
H 0	-1.269120	-1.808614	-1.448101
H 0	-2.781522	-0.884807	1.065946

TS-2+DMB

B3LYP/6-31G(d) Geometry

C 0	0.971486	-1.628792	0.500959
C 0	-0.356947	0.733414	1.290008
C 0	0.723160	0.804713	0.440445
C 0	1.422431	-0.381315	0.062104
C 0	1.047312	2.117900	-0.242917
C 0	2.466349	-0.315837	-1.028623
H 0	1.515608	-2.512716	0.174398
H 0	0.539719	-1.732741	1.490706
H 0	-0.978868	1.604983	1.470562
H 0	-0.503308	-0.088712	1.976907
H 0	0.382543	2.914005	0.102723
H 0	0.952855	2.052413	-1.334197
H 0	2.077827	2.431264	-0.032284
H 0	2.053668	0.056933	-1.976907
H 0	2.906084	-1.299041	-1.218168
H 0	3.281836	0.366703	-0.757634
C 0	-0.870300	-1.892028	-0.394596
C 0	-1.810744	-0.965316	0.064255
C 0	-2.282846	0.133911	-0.771128
O 0	-3.281836	0.806819	-0.563713
H 0	-0.935430	-2.914005	-0.030102
H 0	-0.544927	-1.814905	-1.429863
H 0	-2.400300	-1.173703	0.954035
H 0	-1.656022	0.312201	-1.678164

TS-3+DMB

B3LYP/6-31G(d) Geometry

C 0	2.419630	-1.282563	0.454882
C 0	0.591571	0.732828	1.347400
C 0	1.588564	1.044713	0.462453
C 0	2.539836	0.052316	0.046041
C 0	1.602183	2.412001	-0.190682
C 0	3.532891	0.393702	-1.036892
H 0	3.200673	-1.970890	0.139570
H 0	2.018132	-1.514645	1.435355
H 0	-0.209869	1.435793	1.554750
H 0	0.604253	-0.158352	1.960429
H 0	0.780775	3.029425	0.179952

H 0	1.504563	2.349214	-1.281208
H 0	2.541128	2.940483	0.016648
H 0	3.038424	0.724922	-1.960429
H 0	4.171073	-0.459874	-1.279818
H 0	4.183250	1.220876	-0.724721
C 0	0.830339	-1.997211	-0.542878
C 0	-0.372390	-1.559543	0.032204
C 0	-1.144863	-0.499438	-0.508466
O 0	-2.279079	-0.185583	-0.063412
B 0	-3.041797	1.106621	-0.574167
H 0	1.120689	-3.029425	-0.362002
H 0	1.070734	-1.651636	-1.545407
H 0	-0.781888	-2.072255	0.899373
H 0	-0.758606	0.056560	-1.372956
H 0	-2.947938	1.886711	0.358268
H 0	-2.450893	1.483457	-1.573421
H 0	-4.183250	0.758112	-0.772903

TS-4+DMB

B3LYP/6-31G(d) Geometry

C 0	-0.733747	-0.780115	0.523206
C 0	-1.333536	0.365112	-0.101682
C 0	-1.008309	1.653729	0.330519
C 0	0.136854	-0.622441	1.568200
C 0	-0.915694	-2.149006	-0.097112
C 0	-2.130785	0.187763	-1.369531
H 0	-1.502944	2.493488	-0.152788
H 0	-0.790298	1.828322	1.378837
H 0	0.695069	-1.470694	1.953781
H 0	0.194091	0.281009	2.160602
H 0	-0.488719	-2.179581	-1.105833
H 0	-1.976287	-2.417418	-0.174983
H 0	-0.420432	-2.917995	0.501647
H 0	-2.991723	-0.473000	-1.205180
H 0	-1.523477	-0.268141	-2.160602
H 0	-2.510828	1.144708	-1.737726
C 0	1.772930	0.946236	0.210661
C 0	0.925081	1.958058	-0.225990
N 0	2.054758	-0.147030	-0.656633
O 0	1.335551	-0.291824	-1.665536
O 0	2.991723	-0.901594	-0.362359
H 0	2.415749	0.984515	1.077290
H 0	1.018472	2.917995	0.274737
H 0	0.724791	2.000501	-1.290199

TS-5+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.056431	-0.786886	0.515265
C 0	-1.717194	0.294899	-0.136703
C 0	-1.512439	1.595900	0.300657
C 0	-0.201285	-0.531898	1.571339
C 0	-1.091729	-2.171544	-0.096074
C 0	-2.409573	0.056161	-1.460272
H 0	-1.963081	2.418756	-0.249597
H 0	-1.337089	1.808940	1.348324
H 0	0.384569	-1.338888	2.000817
H 0	-0.337699	0.323783	2.219962
H 0	-0.684957	-2.177957	-1.114277
H 0	-2.118114	-2.555291	-0.154382
H 0	-0.507000	-2.877631	0.499858
H 0	-3.207983	-0.690490	-1.366351
H 0	-1.711753	-0.321535	-2.219962
H 0	-2.860144	0.976089	-1.843974
C 0	0.646414	1.928800	-0.003741
C 0	1.369069	0.882660	0.553114
C 0	2.029571	-0.111608	-0.345000
F 0	1.261555	-0.412984	-1.423885
F 0	2.333593	-1.277978	0.273879
F 0	3.207983	0.359837	-0.837864
H 0	0.603087	2.877631	0.520836
H 0	0.541147	1.989568	-1.080778
H 0	1.870734	1.006537	1.507343

TS-6+DMB

B3LYP/6-31G(d) Geometry

C 0	1.208517	-0.931729	-0.880000
C 0	2.068297	0.107538	-0.423892
C 0	1.810560	1.440530	-0.756174
C 0	0.111086	-0.650977	-1.672539
C 0	1.404099	-2.342503	-0.363710
C 0	3.122771	-0.199628	0.616839
H 0	2.495441	2.199572	-0.384195
H 0	1.375807	1.687998	-1.718058
H 0	-0.567950	-1.446734	-1.963843
H 0	0.051520	0.242031	-2.278784
H 0	1.337714	-2.396429	0.729750
H 0	2.391523	-2.731738	-0.643284
H 0	0.652494	-3.020334	-0.777711
H 0	3.847408	-0.935783	0.245140
H 0	2.692252	-0.623629	1.534503
H 0	3.680271	0.699969	0.893196
C 0	0.060743	1.965746	0.245603
C 0	-1.007487	1.285363	-0.343087
B 0	-1.652367	-0.027469	0.135826
C 0	-2.976638	-0.559046	-0.578569
C 0	-1.207720	-0.738142	1.491637
H 0	0.209638	3.020334	0.016088
H 0	0.380390	1.687623	1.246663
H 0	-1.416924	1.760700	-1.240393
H 0	-3.162563	-0.126205	-1.570090
H 0	-3.847408	-0.303988	0.046338
H 0	-2.998619	-1.653205	-0.675954
H 0	-1.931691	-0.473614	2.278784
H 0	-0.217930	-0.453492	1.869042
H 0	-1.238209	-1.833530	1.420862

TS-7+DMB

B3LYP/6-31G(d) Geometry

C 0	0.938022	-0.911541	-0.655332
C 0	1.802400	0.015789	0.007406
C 0	1.643700	1.394238	-0.163648
C 0	-0.063780	-0.469244	-1.486358
C 0	1.023453	-2.384992	-0.316003
C 0	2.743351	-0.485059	1.077469
H 0	2.352026	2.048759	0.339417
H 0	1.296309	1.785923	-1.113513
H 0	-0.778957	-1.168340	-1.909028
H 0	-0.070151	0.518974	-1.924126
H 0	0.830720	-2.568868	0.747451
H 0	2.019112	-2.786864	-0.541746
H 0	0.294060	-2.961583	-0.890903
H 0	3.462414	-1.205690	0.666875
H 0	2.207123	-1.002907	1.883351
H 0	3.313123	0.335556	1.521920
C 0	-0.085253	1.900868	0.810603
C 0	-1.196859	1.386974	0.132492

B 0 -1.950980 0.132689 0.499397
Cl 0 -3.462414 -0.323683 -0.349359
Cl 0 -1.502180 -0.865728 1.924126
H 0 0.136260 2.961583 0.705668
H 0 0.159404 1.493475 1.787583
H 0 -1.569883 1.968418 -0.711154

TS-8+DMB

B3LYP/6-31G(d) Geometry
C 0 -0.222686 -1.723654 -0.403409
C 0 0.304296 0.920544 -1.327708
C 0 -0.880499 0.631050 -0.704229
C 0 -1.177525 -0.705386 -0.277154
C 0 -1.825575 1.758036 -0.337182
C 0 -2.418272 -0.962427 0.543207
H 0 -0.520152 -2.720975 -0.085178
H 0 0.451003 -1.736016 -1.255736
H 0 0.584504 1.948944 -1.535592
H 0 0.940716 0.168815 -1.772422
H 0 -1.434936 2.720975 -0.676410
H 0 -1.991362 1.824765 0.745236
H 0 -2.810278 1.617512 -0.800562
H 0 -2.425147 -0.382750 1.477499
H 0 -2.513087 -2.020152 0.803154
H 0 -3.323042 -0.670203 -0.004947
C 0 1.221211 -1.283533 0.893015
C 0 2.081263 -0.297250 0.399671
C 0 2.138043 1.067639 0.911028
O 0 2.988303 1.905941 0.663614
Cl 0 3.323042 -0.778099 -0.747847
H 0 1.592000 -2.304539 0.912862
H 0 0.643468 -1.008304 1.772422
H 0 1.309285 1.272940 1.626324

TS-9+DMB

B3LYP/6-31G(d) Geometry
C 0 1.534393 -0.672831 0.111602
C 0 1.075337 0.619848 0.513897
C 0 -0.097396 0.759720 1.214521
C 0 0.745018 -1.804835 0.348539
C 0 2.724728 -0.786777 -0.811595
C 0 1.800935 1.856569 0.022721
H 0 -0.514361 1.743767 1.406674
H 0 -0.548561 -0.050761 1.769242
H 0 1.139106 -2.766202 0.024468
H 0 0.157670 -1.875212 1.259445
H 0 3.620878 -0.337488 -0.364780
H 0 2.561726 -0.265003 -1.765839
H 0 2.954810 -1.831828 -1.037421
H 0 1.856376 1.897380 -1.072400
H 0 2.833546 1.884069 0.393389
H 0 1.301369 2.766202 0.366503
C 0 -1.781305 -0.644505 -0.316581
C 0 -0.887535 -1.600221 -0.821732
C 0 -1.914764 0.646891 -0.991029
O 0 -2.817637 1.453130 -0.803416
C 0 -2.802162 -0.999961 0.733109
H 0 -0.398854 -1.383358 -1.769242
H 0 -1.154435 -2.648970 -0.703049
H 0 -1.128384 0.844379 -1.755761
H 0 -3.245079 -0.094545 1.155667
H 0 -3.620878 -1.593338 0.303038
H 0 -2.365682 -1.600630 1.542275

TS-10+DMB

B3LYP/6-31G(d) Geometry
C 0 1.344055 -0.621432 0.023697
C 0 1.327982 0.725723 0.484640
C 0 0.323955 1.152309 1.329468
C 0 0.314479 -1.492764 0.385601
C 0 2.306805 -1.025821 -1.069460
C 0 2.279927 1.741310 -0.113940
H 0 0.213085 2.206155 1.567187
H 0 -0.205310 0.475409 1.986726
H 0 0.340940 -2.505401 -0.011063
H 0 -0.128580 -1.430659 1.373957
H 0 3.348007 -0.869633 -0.760074
H 0 2.164697 -0.436783 -1.986726
H 0 2.192903 -2.082200 -1.328618
H 0 2.198257 1.794863 -1.207004
H 0 3.323564 1.488400 0.113456
H 0 2.087912 2.741363 0.283981
C 0 -1.686349 0.560979 0.023616
C 0 -1.454328 -0.739826 -0.453057
C 0 -1.452328 1.740635 -0.803074
O 0 -1.928333 2.849858 -0.611320
C 0 -2.395967 -1.858062 -0.039088
H 0 -2.340675 0.710679 0.880779
H 0 -1.101260 -0.806232 -1.482000
H 0 -0.793757 1.552175 -1.685194
H 0 -3.348007 -1.767625 -0.577568
H 0 -1.987472 -2.849858 -0.257687
H 0 -2.622523 -1.811549 1.032245

TS-11+DMB

B3LYP/6-31G(d) Geometry
C 0 1.089559 -1.501797 -0.018825
C 0 1.562854 -0.281406 0.534135
C 0 0.714392 0.491359 1.322459
C 0 -0.211265 -1.918328 0.240084
C 0 1.904786 -2.217172 -1.073933
C 0 2.890587 0.289163 0.085979
H 0 1.035054 1.474349 1.655757
H 0 -0.043829 0.031009 1.944693
H 0 -0.605563 -2.796457 -0.264560
H 0 -0.696753 -1.695239 1.181609
H 0 2.880523 -2.523770 -0.677006
H 0 2.108304 -1.579345 -1.944693
H 0 1.393444 -3.116717 -1.426746
H 0 2.951502 0.400034 -1.004322
H 0 3.717751 -0.369368 0.380661
H 0 3.071713 1.269794 0.533509
C 0 -1.009165 0.977463 -0.020771
C 0 -1.452339 -0.228297 -0.601835
C 0 -0.236926 1.933673 -0.834240
O 0 -0.110706 3.116717 -0.583438
C 0 -2.707091 -0.790381 -0.208497
N 0 -3.717751 -1.262219 0.127494
H 0 -1.581021 1.413974 0.793239
H 0 -1.152725 -0.447391 -1.623480
H 0 0.244000 1.484083 -1.734338

TS-12+DMB

B3LYP/6-31G(d) Geometry
C 0 -1.152121 -1.981231 -0.327964
C 0 -0.129340 0.463197 -1.464773

C 0	-1.303609	0.455836	-0.767660
C 0	-1.844162	-0.770662	-0.231835
C 0	-1.990133	1.769444	-0.453047
C 0	-3.078694	-0.707366	0.631879
H 0	-1.653457	-2.871212	0.045164
H 0	-0.494112	-2.176772	-1.169115
H 0	0.337052	1.398293	-1.761284
H 0	0.351263	-0.435861	-1.827887
H 0	-1.439691	2.607919	-0.885623
H 0	-2.069425	1.945096	0.626661
H 0	-3.010072	1.791338	-0.856538
H 0	-2.937409	-0.051279	1.501623
H 0	-3.367152	-1.697273	0.994207
H 0	-3.926524	-0.292819	0.071832
C 0	0.380771	-1.819493	0.994050
C 0	1.450014	-1.130789	0.414126
C 0	1.705816	0.246509	0.658315
O 0	2.676859	0.885330	0.189746
B 0	2.769993	2.465481	0.373838
Cl 0	2.501314	-1.990378	-0.692441
H 0	0.469387	-2.896845	1.094305
H 0	-0.116300	-1.331908	1.827887
H 0	1.019121	0.759737	1.342375
H 0	2.433075	2.896845	-0.715419
H 0	1.983788	2.748822	1.262663
H 0	3.926524	2.697342	0.632903

TS-13+DMB

B3LYP/6-31G(d) Geometry

C 0	1.787430	-1.618347	0.262032
C 0	0.313316	0.580024	1.371044
C 0	1.424528	0.803317	0.604070
C 0	2.198444	-0.291517	0.085454
C 0	1.761366	2.219723	0.184254
C 0	3.332933	-0.003112	-0.866314
H 0	2.446115	-2.396006	-0.118219
H 0	1.261639	-1.910051	1.165761
H 0	-0.345601	1.397502	1.648691
H 0	0.095470	-0.375637	1.829357
H 0	1.046207	2.930368	0.604711
H 0	1.747541	2.340766	-0.905702
H 0	2.763848	2.506754	0.525622
H 0	2.994494	0.547524	-1.754964
H 0	3.818324	-0.923254	-1.201928
H 0	4.096296	0.624962	-0.389681
C 0	0.176075	-1.848316	-0.930719
C 0	-0.978198	-1.334372	-0.315066
C 0	-1.450148	-0.043919	-0.692112
O 0	-2.532361	0.444111	-0.269077
B 0	-2.915502	1.956976	-0.554728
C 0	-1.757698	-2.144182	0.689576
H 0	0.289428	-2.930368	-0.952152
H 0	0.540322	-1.357858	-1.829357
H 0	-0.872397	0.541355	-1.417288
H 0	-2.668900	2.522658	0.498354
H 0	-2.198551	2.327609	-1.470140
H 0	-4.096296	1.955635	-0.816074
H 0	-1.092402	-2.738486	1.328940
H 0	-2.432349	-2.849430	0.186189
H 0	-2.374834	-1.499050	1.319404

TS-14+DMB

B3LYP/6-31G(d) Geometry

C 0	-2.677821	0.393583	0.465505
C 0	-0.387234	-1.050929	1.356208
C 0	-1.251749	-1.620383	0.455371
C 0	-2.430055	-0.922414	0.040119
C 0	-0.870801	-2.923262	-0.217470
C 0	-3.277480	-1.501588	-1.065315
H 0	-3.622028	0.834110	0.154132
H 0	-2.380920	0.697269	1.463998
H 0	0.583403	-1.496467	1.553492
H 0	-0.663534	-0.224662	1.997496
H 0	0.098488	-3.278424	0.139893
H 0	-0.804289	-2.821021	-1.307205
H 0	-1.613989	-3.704345	-0.013197
H 0	-2.707437	-1.621830	-1.997496
H 0	-4.145627	-0.872501	-1.278170
H 0	-3.642093	-2.501502	-0.799151
C 0	-1.370327	1.582118	-0.464122
C 0	-0.083573	1.381599	0.085586
C 0	0.894260	0.546059	-0.504598
O 0	2.086869	0.487775	-0.100723
B 0	3.069085	-0.636331	-0.630187
C 0	-2.034699	2.933489	-0.235876
H 0	-1.507442	1.194007	-1.473215
H 0	0.223741	1.956849	0.957233
H 0	0.619204	-0.062397	-1.376287
H 0	3.068765	-1.466179	0.266539
H 0	2.582210	-1.064905	-1.664737
H 0	4.145627	-0.103699	-0.769444
H 0	-1.500964	3.704345	-0.804349
H 0	-2.002027	3.221082	0.820680
H 0	-3.078423	2.941658	-0.562983

TS-15+DMB

B3LYP/6-31G(d) Geometry

C 0	2.378179	0.101016	0.264591
C 0	-0.177008	-0.018541	1.449575
C 0	0.104359	0.976504	0.534185
C 0	1.403053	1.063564	-0.043950
C 0	-1.018444	1.850926	0.017397
C 0	1.652579	2.028421	-1.176798
H 0	3.350989	0.190060	-0.212616
H 0	2.432564	-0.314340	1.264963
H 0	-1.196911	-0.192310	1.779575
H 0	0.590848	-0.505153	2.036449
H 0	-1.970063	1.585407	0.483389
H 0	-1.144873	1.764082	-1.068315
H 0	-0.819313	2.908179	0.232842
H 0	0.997033	1.831138	-2.036449
H 0	2.688498	1.983276	-1.521840
H 0	1.445729	3.059229	-0.863913
C 0	1.681640	-1.668788	-0.524140
C 0	0.478847	-2.076601	0.106989
C 0	-0.788794	-1.870591	-0.511118
O 0	-1.846726	-2.388130	-0.087705
B 0	-3.270617	-1.991055	-0.691018
C 0	2.865683	-2.450557	-0.270253
N 0	3.832340	-3.059229	-0.052827
H 0	1.604940	-1.329750	-1.555168
H 0	0.515260	-2.733111	0.970764
H 0	-0.846801	-1.232647	-1.403710
H 0	-3.783149	-1.351514	0.208046

H	0	-3.036429	-1.328035	-1.686845
H	0	-3.832340	-3.039186	-0.901722

TS-16+DMB

B3LYP/6-31G(d) Geometry

C	0	0.538174	-1.685307	0.104205
C	0	0.099844	0.730024	1.577049
C	0	1.214638	0.588315	0.803518
C	0	1.471998	-0.641904	0.096533
C	0	2.114263	1.783210	0.565422
C	0	2.645289	-0.715997	-0.845074
H	0	0.829664	-2.616606	-0.377188
H	0	-0.086838	-1.835008	0.978997
H	0	-0.149416	1.692434	2.013994
H	0	-0.538935	-0.092501	1.869055
H	0	1.832401	2.616606	1.213465
H	0	2.041735	2.132106	-0.472040
H	0	3.166265	1.545585	0.761713
H	0	2.603439	0.071588	-1.609442
H	0	2.694018	-1.683648	-1.351225
H	0	3.590480	-0.570670	-0.305776
C	0	-0.949812	-1.130169	-1.076198
C	0	-1.613909	0.043379	-0.649823
C	0	-1.270925	1.299946	-1.227191
C	0	-2.706951	-0.032156	0.259134
N	0	-0.953492	2.296295	-1.745075
N	0	-3.590480	-0.136775	1.013886
H	0	-1.493657	-2.062436	-0.946210
H	0	-0.406869	-1.062972	-2.013994

TS-17+DMB

B3LYP/6-31G(d) Geometry

C	0	0.114806	-1.396137	1.045402
C	0	0.114806	1.396136	1.045403
C	0	0.818168	0.711054	0.060907
C	0	0.818170	-0.711054	0.060908
C	0	1.340712	1.465112	-1.140300
C	0	1.340719	-1.465112	-1.140297
H	0	0.031065	-2.478043	0.986767
H	0	0.002996	-0.990512	2.043848
H	0	0.031062	2.478041	0.986766
H	0	0.002998	0.990511	2.043849
H	0	1.286583	2.545223	-0.984079
H	0	0.763474	1.230314	-2.043849
H	0	2.385824	1.205428	-1.348110
H	0	0.763455	-1.230349	-2.043839
H	0	1.286632	-2.545223	-0.984058
H	0	2.385817	-1.205395	-1.348132
C	0	-1.997060	-0.706639	0.682149
C	0	-1.997062	0.706633	0.682150
C	0	-2.218395	-1.451961	-0.519509
C	0	-2.218396	1.451955	-0.519507
N	0	-2.385824	2.077275	-1.487442
N	0	-2.385823	-2.077279	-1.487444
H	0	-2.324294	-1.202861	1.590574
H	0	-2.324296	1.202852	1.590575

TS-18+DMB

B3LYP/6-31G(d) Geometry

C	0	-0.256313	-1.798720	-0.139285
C	0	0.664552	0.327576	1.433126
C	0	1.553384	-0.356874	0.606676
C	0	1.074910	-1.416097	-0.213644
C	0	2.939229	0.203426	0.384760
C	0	1.952014	-1.965961	-1.317181
H	0	-0.649547	-2.529848	-0.840739
H	0	-0.819991	-1.718387	0.781282
H	0	1.020131	1.190529	1.990585
H	0	-0.189029	-0.170702	1.877461
H	0	3.191785	0.948211	1.143605
H	0	3.021017	0.690373	-0.596180
H	0	3.698381	-0.586651	0.420699
H	0	2.311709	-1.177871	-1.990585
H	0	1.415963	-2.707509	-1.915844
H	0	2.841832	-2.457241	-0.903505
C	0	-1.368075	0.143549	-0.718463
C	0	-0.743973	1.202215	-0.022133
C	0	-2.658659	-0.299129	-0.298884
C	0	0.172667	2.043149	-0.732671
N	0	0.932014	2.707509	-1.314154
N	0	-3.698381	-0.679641	0.064348
H	0	-1.125843	-0.018220	-1.762170
H	0	-1.291254	1.687208	0.780403

TS-19+DMB

B3LYP/6-31G(d) Geometry

C	0	-0.186363	-1.803934	0.031640
C	0	0.714077	0.366733	1.552405
C	0	1.556531	-0.204441	0.619094
C	0	1.108229	-1.314732	-0.151063
C	0	2.843796	0.502011	0.249227
C	0	1.924930	-1.784037	-1.332947
H	0	-0.519142	-2.628296	-0.595901
H	0	-0.624318	-1.816585	1.024310
H	0	0.997916	1.290944	2.048541
H	0	-0.075811	-0.191456	2.037740
H	0	3.077140	1.293540	0.966282
H	0	2.774678	0.965605	-0.743030
H	0	3.692032	-0.192912	0.229404
H	0	2.119463	-0.974138	-2.048541
H	0	1.421550	-2.594943	-1.867374
H	0	2.906000	-2.158525	-1.012503
C	0	-1.536352	-0.277711	-0.508379
C	0	-1.126372	0.939580	0.066548
C	0	-2.831171	-0.906781	-0.031522
C	0	-0.369910	1.877661	-0.691083
N	0	0.252499	2.628296	-1.332458
H	0	-1.329438	-0.395577	-1.568788
H	0	-1.659142	1.337160	0.925577
H	0	-3.692032	-0.401040	-0.487608
H	0	-2.938856	-0.819040	1.056302
H	0	-2.896232	-1.967975	-0.292582

TS-20+DMB

B3LYP/6-31G(d) Geometry

C	0	0.818696	-1.786565	0.093338
C	0	0.084201	0.575125	1.436570
C	0	1.217435	0.557403	0.659424
C	0	1.622515	-0.645613	0.004412
C	0	1.912416	1.861469	0.327482
C	0	2.745374	-0.606584	-1.004993
H	0	1.146236	-2.682702	-0.430440
H	0	0.291668	-2.004015	1.017163
H	0	-0.297588	1.514163	1.827104
H	0	-0.337858	-0.317419	1.877872
H	0	1.513009	2.682702	0.928161

H 0	1.779801	2.129593	-0.728262
H 0	2.991286	1.801544	0.515891
H 0	2.547948	0.107215	-1.816924
H 0	2.911717	-1.590101	-1.453842
H 0	3.688179	-0.291076	-0.539404
C 0	-0.909752	-1.344011	-0.895154
C 0	-1.609871	-0.265982	-0.326025
C 0	-1.549846	1.002002	-0.979035
C 0	-2.738665	-0.493033	0.661611
N 0	-1.518029	2.028897	-1.534103
H 0	-1.324030	-2.336831	-0.730671
H 0	-0.470494	-1.206686	-1.877872
H 0	-2.530831	-1.370927	1.284276
H 0	-3.688179	-0.678342	0.140556
H 0	-2.889541	0.365977	1.321670

TS-21+DMB

B3LYP/6-31G(d) Geometry

C 0	0.936718	-1.534635	-0.007619
C 0	1.622593	-0.414525	0.544623
C 0	0.952727	0.461795	1.376574
C 0	-0.411864	-1.734524	0.275563
C 0	1.597389	-2.353038	-1.093479
C 0	3.013786	-0.064887	0.058876
H 0	1.424262	1.387392	1.693592
H 0	0.097725	0.155234	1.964538
H 0	-0.931890	-2.555416	-0.208260
H 0	-0.821017	-1.465729	1.242371
H 0	2.526602	-2.812143	-0.733097
H 0	1.870932	-1.741481	-1.964538
H 0	0.942348	-3.157405	-1.439013
H 0	3.051536	0.073037	-1.029095
H 0	3.727324	-0.862595	0.301253
H 0	3.373889	0.855686	0.525369
C 0	-0.853903	1.183416	-0.031979
C 0	-1.418684	0.008815	-0.538657
C 0	0.054611	1.995791	-0.847163
O 0	0.347855	3.157405	-0.624521
C 0	-2.816068	-0.335634	-0.103908
F 0	-2.954980	-0.255570	1.243313
F 0	-3.727324	0.507276	-0.642859
F 0	-3.186005	-1.583881	-0.474342
H 0	-1.316656	1.688031	0.811113
H 0	-1.224003	-0.251749	-1.575703
H 0	0.469849	1.463099	-1.735263

TS-22+DMB

B3LYP/6-31G(d) Geometry

C 0	1.203574	-1.352724	-0.869212
C 0	1.910895	-0.199813	-0.437415
C 0	1.467427	1.078610	-0.797387
C 0	0.070822	-1.231012	-1.658863
C 0	1.585444	-2.714990	-0.328692
C 0	3.001607	-0.335631	0.602459
H 0	2.048138	1.928145	-0.445003
H 0	1.021656	1.242053	-1.772645
H 0	-0.497153	-2.115166	-1.932382
H 0	-0.089338	-0.374630	-2.299028
H 0	1.543116	-2.753106	0.766593
H 0	2.610475	-2.980301	-0.618237
H 0	0.921243	-3.492398	-0.716351
H 0	3.825639	-0.962453	0.236926
H 0	2.640815	-0.805337	1.527876
H 0	3.422693	0.639402	0.864361
C 0	-0.341616	1.450193	0.161655
C 0	-1.274038	0.559906	-0.395177
B 0	-1.693466	-0.821313	0.130380
C 0	-2.935110	-1.570725	-0.539099
C 0	-1.134581	-1.402080	1.507473
C 0	-0.458163	2.941210	-0.118775
H 0	0.014500	1.216756	1.164172
H 0	-1.770780	0.935446	-1.297692
H 0	-3.196613	-1.206847	-1.541135
H 0	-3.825639	-1.425688	0.092884
H 0	-2.794246	-2.658700	-0.599595
H 0	-1.871308	-1.191145	2.299028
H 0	-0.183791	-0.971161	1.843934
H 0	-1.022977	-2.494305	1.492332
H 0	-1.288538	3.367780	0.458524
H 0	-0.665755	3.132372	-1.178233
H 0	0.447056	3.492398	0.157375

TS-23+DMB

B3LYP/6-31G(d) Geometry

C 0	0.844707	-1.604660	-0.592591
C 0	1.822419	-0.740305	-0.018592
C 0	1.822940	0.631237	-0.304904
C 0	-0.114163	-1.104099	-1.446627
C 0	0.757176	-3.047053	-0.140782
C 0	2.720790	-1.261162	1.078511
H 0	2.620601	1.226576	0.132941
H 0	1.529393	0.972980	-1.291918
H 0	-0.922279	-1.737809	-1.799006
H 0	0.010312	-0.175558	-1.985523
H 0	0.602132	-3.129375	0.941000
H 0	1.680451	-3.590425	-0.379340
H 0	-0.069331	-3.563152	-0.636393
H 0	3.336106	-2.097541	0.722428
H 0	2.145416	-1.638339	1.933966
H 0	3.397056	-0.482719	1.442344
C 0	0.202770	1.493475	0.590693
C 0	-0.959646	0.989792	-0.025531
B 0	-1.819859	-0.141703	0.470134
Cl 0	-3.397056	-0.517450	-0.301234
Cl 0	-1.443537	-1.034609	1.985523
C 0	0.564484	2.957588	0.384150
H 0	0.404999	1.124147	1.594577
H 0	-1.303849	1.526106	-0.912201
H 0	-0.127696	3.590425	0.953229
H 0	0.481654	3.246892	-0.669823
H 0	1.578016	3.189566	0.726060

TS-24+DMB

B3LYP/6-31G(d) Geometry

C 0	-0.838693	-1.579813	-0.169778
C 0	-1.416379	-0.541433	0.629284
C 0	-0.607501	0.238605	1.440842
C 0	0.512991	-1.851546	-0.081126
C 0	-1.665399	-2.234733	-1.252537
C 0	-2.855395	-0.138523	0.407450
H 0	-1.036098	1.090248	1.962771
H 0	0.325122	-0.126326	1.855357
H 0	0.970377	-2.563587	-0.762525
H 0	1.079418	-1.653126	0.820506
H 0	-2.053945	-1.495835	-1.962771
H 0	-2.529915	-2.758204	-0.825511

H	0	-1.075924	-2.967600	-1.809653
H	0	-3.529885	-0.994012	0.532645
H	0	-3.005832	0.247924	-0.608524
H	0	-3.162342	0.637961	1.112516
C	0	0.732684	1.195227	-0.093321
C	0	1.432663	0.192934	-0.748110
N	0	-0.317112	1.863279	-0.837338
N	0	2.743975	-0.136436	-0.238033
O	0	-0.679216	2.967600	-0.431972
O	0	-0.802960	1.270161	-1.808921
O	0	2.981830	0.115438	0.952330
O	0	3.529885	-0.680396	-1.014200
H	0	1.175659	1.807821	0.677295
H	0	1.290209	-0.043664	-1.790200

TS-25+DMB

B3LYP/6-31G(d) Geometry

C	0	-0.379274	1.089386	0.096622
C	0	1.041147	0.985269	0.052598
C	0	1.707416	0.235132	0.999486
C	0	-1.095090	0.386726	1.076853
C	0	-1.124410	1.746296	-1.039903
C	0	1.797230	1.518189	-1.145616
H	0	2.771753	0.042755	0.899249
H	0	1.295987	0.033488	1.978954
H	0	-2.179057	0.460592	1.080480
H	0	-0.666143	0.264965	2.065854
H	0	-0.944802	1.235157	-1.993898
H	0	-0.804306	2.788213	-1.167642
H	0	-2.202229	1.742932	-0.861395
H	0	1.605924	2.587536	-1.294713
H	0	1.500632	1.000859	-2.065854
H	0	2.875621	1.388175	-1.019753
C	0	0.518418	-1.951842	0.654590
C	0	-0.852859	-1.602710	0.661028
C	0	1.375540	-2.128328	-0.499651
C	0	-1.870439	-1.688479	-0.466432
O	0	-3.044009	-1.825175	-0.186379
O	0	-1.467096	-1.552389	-1.731511
O	0	1.135121	-1.817500	-1.673917
O	0	2.562555	-2.705724	-0.190857
H	0	0.934793	-2.336144	1.579203
H	0	-1.359679	-1.893685	1.577308
H	0	-0.473060	-1.571823	-1.802329
H	0	3.044009	-2.788213	-1.034490

TS-26+DMB

B3LYP/6-31G(d) Geometry

C	0	0.591912	0.441501	-1.880830
C	0	-0.144481	-2.009253	-0.661633
C	0	1.072348	-1.445660	-0.375587
C	0	1.488927	-0.246804	-1.041195
C	0	1.906377	-1.996661	0.760787
C	0	2.774139	0.422976	-0.637953
H	0	0.968634	1.325871	-2.390322
H	0	-0.124035	-0.119166	-2.474143
H	0	-0.524917	-2.831166	-0.062419
H	0	-0.711857	-1.787824	-1.555276
H	0	1.431473	-2.875185	1.203715
H	0	2.043494	-1.253726	1.555040
H	0	2.904055	-2.293050	0.414819
H	0	2.702801	0.829151	0.381357
H	0	3.022142	1.251718	-1.304761
H	0	3.609198	-0.286982	-0.640336
C	0	-0.801810	1.220219	-0.698735
C	0	-1.587758	0.219570	-0.043340
C	0	-0.040278	2.137718	0.115385
C	0	-1.422729	-0.080321	1.339654
C	0	-2.714792	-0.310154	-0.733270
N	0	-1.279343	-0.307386	2.474143
N	0	0.605829	2.875185	0.739423
N	0	-3.609198	-0.737588	-1.347850
H	0	-1.303745	1.713710	-1.529216

TS-27+DMB

B3LYP/6-31G(d) Geometry

C	0	-0.734320	-1.570313	-0.975738
C	0	-0.073855	1.145350	-1.198093
C	0	-1.192809	0.775431	-0.486288
C	0	-1.571100	-0.597568	-0.415573
C	0	-1.904964	1.799115	0.373720
C	0	-2.717889	-1.016682	0.474037
H	0	-1.038059	-2.612198	-0.889200
H	0	-0.207724	-1.358973	-1.901427
H	0	0.297514	2.164775	-1.143465
H	0	0.312450	0.555055	-2.017520
H	0	-1.477899	2.795276	0.231951
H	0	-1.836831	1.558097	1.441859
H	0	-2.972333	1.854553	0.124596
H	0	-2.577067	-0.700097	1.516382
H	0	-2.850016	-2.102299	0.467584
H	0	-3.661515	-0.565765	0.138869
C	0	1.007947	-1.539235	0.113388
C	0	1.690910	-0.323363	-0.121050
C	0	0.567120	-1.918169	1.512892
C	0	1.822581	0.620378	0.942047
C	0	2.686598	-0.212018	-1.261207
N	0	1.961405	1.376192	1.821443
H	0	1.387633	-2.373905	-0.476570
H	0	0.036743	-1.096208	2.002567
H	0	1.439274	-2.154148	2.136169
H	0	-0.087317	-2.795276	1.502975
H	0	2.332380	-0.770631	-2.136169
H	0	3.661515	-0.633137	-0.979139
H	0	2.852461	0.825969	-1.563772

TS-28+DMB

B3LYP/6-31G(d) Geometry

C	0	0.195612	1.527697	-0.202003
C	0	0.401484	-1.022529	-1.340229
C	0	1.437491	-0.539464	-0.570462
C	0	1.351942	0.765519	-0.006143
C	0	2.543659	-1.477879	-0.136557
C	0	2.370332	1.207440	1.018690
H	0	0.153432	2.512856	0.258415
H	0	-0.324097	1.481304	-1.154019
H	0	0.397649	-2.060722	-1.660783
H	0	-0.282035	-0.373600	-1.871074
H	0	2.505388	-2.415784	-0.696948
H	0	2.460051	-1.726652	0.928970
H	0	3.533822	-1.033420	-0.294590
H	0	2.424749	0.516556	1.871074
H	0	2.138376	2.204021	1.405488
H	0	3.378913	1.246784	0.586597
C	0	-1.370613	0.569040	0.745366
C	0	-1.466216	-0.779497	0.319245

C 0	-2.490540	1.542407	0.421010
C 0	-0.864573	-1.765465	1.159035
C 0	-2.551671	-1.257730	-0.628046
N 0	-0.379596	-2.557688	1.866885
H 0	-0.944183	0.704523	1.735743
H 0	-3.414316	1.251844	0.938972
H 0	-2.716779	1.577973	-0.650037
H 0	-2.237451	2.557688	0.741135
H 0	-2.641383	-0.602412	-1.501228
H 0	-3.533822	-1.272959	-0.133723
H 0	-2.346895	-2.269565	-0.987278

TS-29+DMB

B3LYP/6-31G(d) Geometry

C 0	0.290105	-1.878179	-0.326949
C 0	-0.750365	0.320190	-1.689702
C 0	-1.559032	-0.375109	-0.789967
C 0	-1.017650	-1.484273	-0.084983
C 0	-2.890134	0.210862	-0.379019
C 0	-1.784702	-2.090573	1.070168
H 0	0.743637	-2.653679	0.284710
H 0	0.753689	-1.748804	-1.295686
H 0	-1.141219	1.217312	-2.163504
H 0	0.005485	-0.194322	-2.272136
H 0	-3.207170	0.997389	-1.068340
H 0	-2.844529	0.652863	0.625432
H 0	-3.673110	-0.556427	-0.359219
H 0	-2.089516	-1.337885	1.807977
H 0	-1.189144	-2.849708	1.584343
H 0	-2.704431	-2.575238	0.717923
C 0	1.486763	0.046879	0.264996
C 0	0.850187	1.102627	-0.444956
C 0	2.698564	-0.453139	-0.315125
C 0	1.358418	-0.068375	1.775307
C 0	0.089257	2.073108	0.286729
N 0	-0.541280	2.849708	0.883089
N 0	3.673110	-0.880154	-0.790916
H 0	1.355506	1.498266	-1.320971
H 0	0.316602	0.057509	2.081357
H 0	1.946508	0.713944	2.272136
H 0	1.714541	-1.037783	2.131597

TS-30+DMB

B3LYP/6-31G(d) Geometry

C 0	0.967913	0.913460	-1.475909
C 0	-0.122501	-1.547731	-0.757743
C 0	1.074436	-1.142023	-0.185639
C 0	1.645061	0.103176	-0.565080
C 0	1.626009	-1.891676	1.006044
C 0	2.808294	0.671555	0.213818
H 0	1.359256	1.904341	-1.692652
H 0	0.382087	0.482720	-2.280149
H 0	-0.617858	-2.440980	-0.387174
H 0	-0.391967	-1.266797	-1.768209
H 0	1.071517	-2.816459	1.183150
H 0	1.571543	-1.289345	1.921535
H 0	2.680308	-2.154509	0.854974
H 0	2.529205	0.881690	1.254717
H 0	3.162369	1.606451	-0.227636
H 0	3.650203	-0.030720	0.239558
C 0	-0.905193	1.354454	-0.439929
C 0	-1.594009	0.143610	-0.166824
C 0	-0.363563	2.156067	0.617726
C 0	-1.698932	-0.310593	1.190319
C 0	-2.731482	-0.266109	-1.090767
N 0	-1.813209	-0.706222	2.280149
N 0	0.097233	2.816459	1.458530
H 0	-1.260027	1.929126	-1.291924
H 0	-2.482578	-0.032814	-2.131866
H 0	-3.650203	0.277454	-0.836704
H 0	-2.947345	-1.335441	-1.019739

TS-31+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.365109	-0.589931	-0.323825
C 0	-1.350619	0.817341	-0.524603
C 0	-0.369321	1.383988	-1.317313
C 0	-0.345200	-1.374901	-0.868602
C 0	-2.326953	-1.196729	0.672800
C 0	-2.273670	1.710604	0.278977
H 0	-0.252493	2.462597	-1.365545
H 0	0.093571	0.839262	-2.129257
H 0	-0.362335	-2.444055	-0.667656
H 0	0.072430	-1.126615	-1.837772
H 0	-3.368145	-1.023546	0.370329
H 0	-2.220489	-0.763883	1.676919
H 0	-2.183049	-2.277581	0.756745
H 0	-2.163230	1.564365	1.361140
H 0	-3.325658	1.507369	0.039999
H 0	-2.084969	2.765803	0.063343
C 0	1.675538	0.583219	-0.305183
C 0	1.471105	-0.768560	0.061334
C 0	1.615612	1.729258	0.599250
O 0	2.161790	2.804276	0.387728
C 0	1.177347	-1.121521	1.513747
C 0	2.370787	-1.783444	-0.637303
H 0	2.250531	0.780147	-1.208840
H 0	1.037978	1.575212	1.536674
H 0	0.388262	-0.502156	1.947275
H 0	0.870552	-2.168896	1.605775
H 0	2.077845	-0.988257	2.129257
H 0	3.368145	-1.776503	-0.176595
H 0	1.982025	-2.804276	-0.554614
H 0	2.499907	-1.548870	-1.699329

TS-32+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.155348	-1.421975	-0.592950
C 0	-1.494591	-0.071977	-0.918014
C 0	-0.579772	0.732975	-1.627729
C 0	0.020450	-1.967845	-1.047736
C 0	-1.999742	-2.190890	0.401115
C 0	-2.718833	0.562027	-0.309549
H 0	-0.890752	1.744042	-1.880197
H 0	0.030164	0.270350	-2.398257
H 0	0.353715	-2.936182	-0.686034
H 0	0.580768	-1.569329	-1.882108
H 0	-3.054965	-2.203657	0.105442
H 0	-1.942190	-1.743407	1.401282
H 0	-1.661419	-3.226498	0.483151
H 0	-2.747117	0.443075	0.781033
H 0	-3.630598	0.085339	-0.694745
H 0	-2.775686	1.628371	-0.540629
C 0	0.960034	1.108916	-0.466452
C 0	1.593298	-0.075468	0.026644
C 0	0.327445	2.060867	0.506226

O 0	0.123948	3.226498	0.242074
C 0	2.723391	-0.603772	-0.661470
C 0	1.298073	-0.580107	1.328887
N 0	3.630598	-1.018703	-1.265590
N 0	1.024255	-0.957630	2.398257
H 0	1.513597	1.630789	-1.244712
H 0	0.042484	1.630143	1.486575

TS-33+DMB

B3LYP/6-31G(d) Geometry

C 0	0.094975	1.388902	-1.392788
C 0	0.095038	-1.388989	-1.392786
C 0	1.259580	-0.708710	-1.026305
C 0	1.259555	0.708670	-1.026319
C 0	2.402325	-1.469306	-0.399389
C 0	2.402270	1.469319	-0.399412
H 0	0.051378	2.469069	-1.284916
H 0	-0.584915	0.988418	-2.134890
H 0	0.051461	-2.469153	-1.284874
H 0	-0.584875	-0.988535	-2.134882
H 0	2.269194	-2.547944	-0.506915
H 0	2.487433	-1.247281	0.672283
H 0	3.357310	-1.195913	-0.863243
H 0	2.487204	1.247506	0.672320
H 0	2.269223	2.547944	-0.507170
H 0	3.357299	1.195764	-0.863072
C 0	-1.361623	0.725446	0.169417
C 0	-1.361649	-0.725482	0.169432
C 0	-2.481522	1.412118	-0.416624
C 0	-0.728430	1.407990	1.267097
C 0	-0.728478	-1.408041	1.267110
N 0	-3.357310	1.987236	-0.921260
C 0	-2.481529	-1.412134	-0.416656
N 0	-0.190634	1.965156	2.134868
N 0	-0.190709	-1.965222	2.134890
N 0	-3.357309	-1.987234	-0.921331

TS-34+DMB

B3LYP/6-31G(d) Geometry

C 0	0.226232	1.043353	-1.647182
C 0	0.224360	-1.738217	-1.204525
C 0	1.323553	-0.999000	-0.837280
C 0	1.363067	0.401578	-1.112208
C 0	2.398246	-1.629802	0.021190
C 0	2.499662	1.235915	-0.587526
H 0	0.326405	2.101910	-1.874990
H 0	-0.390184	0.512533	-2.366611
H 0	0.109941	-2.762666	-0.862550
H 0	-0.477817	-1.424956	-1.964828
H 0	2.219083	-2.699947	0.148353
H 0	2.428609	-1.175396	1.018552
H 0	3.390958	-1.506235	-0.427741
H 0	2.471324	1.292080	0.509970
H 0	2.458181	2.258348	-0.969471
H 0	3.468949	0.802546	-0.859811
C 0	-1.201810	1.067543	-0.261054
C 0	-1.516237	-0.277350	0.163668
C 0	-0.551751	1.895026	0.738764
C 0	-0.986138	-0.812348	1.374079
C 0	-2.596167	-0.973083	-0.450808
N 0	-0.541247	-1.232676	2.366611
N 0	-0.020628	2.597463	1.497453
N 0	-3.468949	-1.527589	-0.990938
C 0	-2.289981	1.824220	-1.034678
H 0	-3.124168	2.055372	-0.364377
H 0	-2.674486	1.213267	-1.854864
H 0	-1.903086	2.762666	-1.438176

TS-35+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.468841	-0.825211	-0.842509
C 0	-1.269920	0.576198	-0.964749
C 0	-0.052205	1.062728	-1.488753
C 0	-0.487107	-1.693299	-1.280347
C 0	-2.640421	-1.360839	-0.048377
C 0	-2.253248	1.536435	-0.343217
H 0	0.056499	2.140719	-1.582855
H 0	0.407182	0.520278	-2.309416
H 0	-0.546207	-2.752368	-1.046347
H 0	0.231269	-1.434402	-2.046217
H 0	-3.589044	-0.947313	-0.409441
H 0	-2.548963	-1.104327	1.014471
H 0	-2.699577	-2.449464	-0.121776
H 0	-2.450983	1.301698	0.710075
H 0	-3.221620	1.483912	-0.859064
H 0	-1.899417	2.568727	-0.404550
C 0	1.482661	0.603387	-0.284288
C 0	1.390323	-0.777896	0.128113
C 0	1.145974	1.634676	0.761155
O 0	1.615775	2.752368	0.764679
C 0	2.310902	-1.740439	-0.387189
C 0	0.704820	-1.136051	1.332247
C 0	2.656513	0.987713	-1.171977
N 0	3.056875	-2.514544	-0.838163
N 0	0.124300	-1.396771	2.309416
H 0	0.416623	1.314031	1.529971
H 0	2.547719	2.016155	-1.521284
H 0	3.589044	0.930563	-0.600123
H 0	2.751283	0.317742	-2.030565

TS-36+DMB

B3LYP/6-31G(d) Geometry

C 0	1.515004	0.287333	-0.667196
C 0	1.336187	-1.124184	-0.688296
C 0	0.214143	-1.669385	-1.276374
C 0	0.485866	1.124556	-1.128649
C 0	2.692534	0.884563	0.067993
C 0	2.290971	-2.020932	0.074764
H 0	-0.004257	-2.728407	-1.176384
H 0	-0.335260	-1.158483	-2.053949
H 0	0.668768	2.196629	-1.086529
H 0	-0.089875	0.834090	-2.002963
H 0	3.641002	0.567727	-0.386175
H 0	2.735663	0.573684	1.120834
H 0	2.664226	1.977532	0.042731
H 0	2.372261	-1.742823	1.133149
H 0	3.304212	-1.965607	-0.343845
H 0	1.970764	-3.065297	0.026566
C 0	-1.718410	-0.345033	-0.205963
C 0	-1.117080	0.908610	0.118091
C 0	-1.692962	-1.492220	0.706646
O 0	-2.440597	-2.462902	0.624873
C 0	-2.708647	-0.448277	-1.340317
C 0	-0.492077	1.096826	1.497852
C 0	-1.872761	2.159777	-0.338180
H 0	-0.961476	-1.433833	1.536245

H	0	-2.966495	-1.496023	-1.508292
H	0	-3.641002	0.086294	-1.110978
H	0	-2.322400	-0.017275	-2.274286
H	0	0.212042	0.303410	1.757213
H	0	0.046841	2.049201	1.544862
H	0	-1.268438	1.118319	2.274286
H	0	-2.817853	2.247245	0.214920
H	0	-1.290925	3.065297	-0.137549
H	0	-2.117158	2.143784	-1.403570

TS-37+DMB

B3LYP/6-31G(d) Geometry

C	0	-2.709866	-0.173228	-1.036329
C	0	-0.118478	0.548184	-1.735580
C	0	-0.923372	1.472700	-1.063856
C	0	-2.253609	1.124387	-0.740104
C	0	-0.308475	2.743702	-0.523424
C	0	-3.087064	2.021755	0.141654
H	0	-3.698268	-0.468212	-0.693659
H	0	-2.397779	-0.678818	-1.943831
H	0	0.934312	0.765786	-1.892321
H	0	-0.544838	-0.149486	-2.445640
H	0	0.767055	2.776573	-0.713521
H	0	-0.466680	2.850650	0.555782
H	0	-0.760909	3.622907	-1.000119
H	0	-2.688959	2.055686	1.164662
H	0	-4.120953	1.673241	0.200316
H	0	-3.094888	3.049209	-0.239053
C	0	-1.430796	-1.449713	0.104968
C	0	-0.095401	-1.368356	-0.447608
C	0	0.939108	-0.689038	0.301344
O	0	2.146768	-0.835676	0.028371
C	0	-2.173189	-2.661931	-0.152952
C	0	0.333720	-2.379306	-1.484994
C	0	-1.679716	-0.884798	1.412732
N	0	-2.782518	-3.622907	-0.391950
N	0	-1.885779	-0.392217	2.445640
H	0	0.664423	-0.013801	1.119331
H	0	-0.442414	-2.542845	-2.239382
H	0	0.532970	-3.348090	-1.010935
H	0	1.253783	-2.055463	-1.974765
B	0	3.291543	0.073606	0.704041
H	0	3.671814	0.751341	-0.229673
H	0	2.729198	0.704317	1.577825
H	0	4.120953	-0.713524	1.088656

TS-38+DMB

B3LYP/6-31G(d) Geometry

C	0	0.074159	-1.645075	-0.892460
C	0	-0.450912	0.963882	-1.687396
C	0	-1.433046	0.251360	-1.003868
C	0	-1.166694	-1.084996	-0.606117
C	0	-2.656889	0.971490	-0.484476
C	0	-2.125963	-1.806142	0.314527
H	0	0.324281	-2.627181	-0.499648
H	0	0.619490	-1.379093	-1.789132
H	0	-0.618540	2.014712	-1.908420
H	0	0.221997	0.464985	-2.374209
H	0	-2.723857	1.982713	-0.893136
H	0	-2.647359	1.057417	0.609960
H	0	-3.575553	0.436963	-0.756449
H	0	-2.320217	-1.244060	1.237107
H	0	-1.743830	-2.792094	0.592557
H	0	-3.098649	-1.953338	-0.172236
C	0	1.496460	-0.271295	0.228149
C	0	1.297635	1.043537	-0.303611
C	0	2.650432	-0.986576	-0.239523
C	0	1.074853	-0.592962	1.655246
C	0	0.691984	2.003423	0.580409
C	0	2.293559	1.633056	-1.296472
N	0	0.207888	2.792094	1.288336
N	0	3.575553	-1.588483	-0.613526
H	0	0.056843	-0.242292	1.842367
H	0	1.733766	-0.090031	2.374209
H	0	1.117676	-1.667778	1.847188
H	0	2.558057	0.898855	-2.062664
H	0	3.219681	1.923081	-0.785818
H	0	1.885463	2.520629	-1.786676

TS-39+DMB

B3LYP/6-31G(d) Geometry

C	0	0.351254	1.387200	-1.255455
C	0	0.351257	-1.387205	-1.255454
C	0	1.430649	-0.709533	-0.695689
C	0	1.430648	0.709531	-0.695689
C	0	2.438886	-1.467770	0.136537
C	0	2.438882	1.467770	0.136537
H	0	0.301210	2.469090	-1.164976
H	0	-0.183897	0.984926	-2.107391
H	0	0.301214	-2.469095	-1.164974
H	0	-0.183896	-0.984932	-2.107388
H	0	2.329904	-2.547138	0.004588
H	0	2.319259	-1.250387	1.205706
H	0	3.465468	-1.195612	-0.137203
H	0	2.319249	1.250394	1.205707
H	0	2.329904	2.547138	0.004582
H	0	3.465465	1.195607	-0.137196
C	0	-1.408924	0.716312	-0.031943
C	0	-1.408925	-0.716314	-0.031942
C	0	-2.476882	1.473616	-0.813174
C	0	-0.969306	1.389758	1.160883
C	0	-0.969308	-1.389759	1.160884
C	0	-2.476883	-1.473619	-0.813173
N	0	-0.625816	-1.975282	2.107391
N	0	-0.625814	1.975282	2.107387
H	0	-3.465468	1.333306	-0.357067
H	0	-2.538132	1.131367	-1.850326
H	0	-2.263593	2.545222	-0.822037
H	0	-2.538130	-1.131371	-1.850327
H	0	-3.465468	-1.333308	-0.357068
H	0	-2.263594	-2.545225	-0.822035

TS-40+DMB

B3LYP/6-31G(d) Geometry

C	0	-0.228696	-1.359008	-0.951420
C	0	-0.485450	1.358614	-1.523382
C	0	-1.478032	0.726152	-0.803203
C	0	-1.379382	-0.670234	-0.549721
C	0	-2.543867	1.549614	-0.111247
C	0	-2.381356	-1.342848	0.359560
H	0	-0.172182	-2.422232	-0.726486
H	0	0.253953	-1.097150	-1.887668
H	0	-0.475596	2.442102	-1.604040
H	0	0.115960	0.836739	-2.255099
H	0	-2.478325	2.600974	-0.402940
H	0	-2.450498	1.503606	0.981118

H	0	-3.550394	1.193554	-0.364846
H	0	-2.443933	-0.859630	1.343726
H	0	-2.132086	-2.396084	0.516634
H	0	-3.391378	-1.302003	-0.069916
C	0	1.382361	-0.607222	0.138110
C	0	1.519463	0.775324	-0.192687
C	0	2.439530	-1.557773	-0.415661
C	0	0.960053	-0.952693	1.559805
C	0	1.146918	1.749433	0.784665
C	0	2.514232	1.254741	-1.237027
N	0	0.870980	2.547010	1.591929
H	0	3.403074	-1.379093	0.082054
H	0	2.600866	-1.440581	-1.490981
H	0	2.165413	-2.600974	-0.229295
H	0	0.119600	-0.342203	1.898525
H	0	1.791395	-0.771923	2.255099
H	0	0.680070	-2.007976	1.643892
H	0	2.412070	0.704239	-2.179202
H	0	3.550394	1.119496	-0.895590
H	0	2.373475	2.316826	-1.454037

TS-41+DMB

B3LYP/6-31G(d) Geometry

C	0	1.116491	-0.671519	-0.056209
C	0	0.723980	0.654881	0.313346
C	0	-0.152561	0.856095	1.353040
C	0	0.523052	-1.774427	0.556717
C	0	2.019964	-0.881115	-1.251291
C	0	1.143009	1.830976	-0.546427
H	0	-0.552035	1.845648	1.554709
H	0	-0.282885	0.131885	2.145840
H	0	0.820958	-2.766137	0.222371
H	0	0.240089	-1.738769	1.602982
H	0	3.032491	-0.510510	-1.039403
H	0	1.676213	-0.347553	-2.145840
H	0	2.104856	-1.942349	-1.501461
H	0	0.803575	1.729960	-1.584544
H	0	2.235474	1.931285	-0.575473
H	0	0.734599	2.766137	-0.154383
C	0	-2.129546	-0.560094	0.688270
C	0	-1.514763	-1.654178	0.047873
C	0	-2.412422	0.114331	-0.592385
C	0	-1.696466	-1.043916	-1.351764
O	0	-3.032491	1.090119	-0.955378
H	0	-2.542805	-0.430803	1.683835
H	0	-1.616787	-2.703653	0.304416
H	0	-0.774748	-0.771718	-1.878876
H	0	-2.356507	-1.587496	-2.037717

TS-42+DMB

B3LYP/6-31G(d) Geometry

C	0	-1.551040	-0.688318	-0.483984
C	0	-1.197095	0.604462	-0.994223
C	0	-0.100671	0.758068	-1.803230
C	0	-0.705954	-1.783052	-0.695017
C	0	-2.730281	-0.830367	0.451240
C	0	-1.957112	1.830291	-0.526440
H	0	0.244272	1.748117	-2.086446
H	0	0.334190	-0.063695	-2.353355
H	0	-1.017083	-2.739003	-0.277966
H	0	-0.171779	-1.887826	-1.634822
H	0	-3.673366	-0.658731	-0.086710
H	0	-2.710666	-0.109619	1.277692
H	0	-2.776323	-1.835441	0.879956
H	0	-1.927009	1.949350	0.563484
H	0	-3.015278	1.773008	-0.811918
H	0	-1.542420	2.739003	-0.970723
C	0	1.846149	-0.468165	-0.434062
C	0	1.022923	-1.356922	0.297632
C	0	1.750435	0.571333	0.606000
C	0	0.810315	-0.346880	1.438206
O	0	2.288554	1.639182	0.819744
C	0	2.789019	-0.650011	-1.578695
H	0	1.207851	-2.419429	0.435543
H	0	-0.217283	0.012311	1.570399
H	0	1.221814	-0.626318	2.414924
H	0	2.329273	-1.193806	-2.414924
H	0	3.673366	-1.227806	-1.274696
H	0	3.139299	0.318930	-1.948549

TS-43+DMB

B3LYP/6-31G(d) Geometry

C	0	1.294099	-0.989344	-0.087293
C	0	1.563239	0.300080	0.462496
C	0	0.786388	0.780006	1.496517
C	0	0.187530	-1.713853	0.351627
C	0	2.080112	-1.474566	-1.285942
C	0	2.557263	1.221163	-0.215333
H	0	0.890840	1.808676	1.829503
H	0	0.293868	0.116427	2.195308
H	0	-0.016146	-2.673295	-0.118372
H	0	-0.129264	-1.661910	1.387151
H	0	3.123146	-1.678950	-1.007552
H	0	2.115057	-0.738906	-2.098842
H	0	1.660443	-2.401971	-1.686284
H	0	2.274672	1.444560	-1.251798
H	0	3.558470	0.772886	-0.245287
H	0	2.635183	2.172569	0.317386
C	0	-1.451678	0.687826	0.610264
C	0	-1.545513	-0.518673	-0.128338
C	0	-1.226678	1.493547	-0.602932
C	0	-1.255056	0.200230	-1.464189
O	0	-1.154089	2.673295	-0.873323
C	0	-2.561357	-1.618833	0.062447
H	0	-1.835792	0.960750	1.589487
H	0	-0.321768	-0.070882	-1.969917
H	0	-2.073984	0.194331	-2.195308
H	0	-3.558470	-1.251764	-0.217891
H	0	-2.614594	-1.944175	1.107514
H	0	-2.350000	-2.495609	-0.557831

TS-44+DMB

B3LYP/6-31G(d) Geometry

C	0	1.041028	-1.458606	-0.101198
C	0	1.620789	-0.343799	0.573673
C	0	0.906543	0.304726	1.575859
C	0	-0.239441	-1.875616	0.223667
C	0	1.743750	-2.064127	-1.298490
C	0	2.899796	0.274300	0.053286
H	0	1.315316	1.207851	2.020842
H	0	0.223435	-0.243482	2.214739
H	0	-0.721859	-2.652881	-0.362425
H	0	-0.647255	-1.747591	1.217702
H	0	2.666010	-2.573488	-0.989479

H 0	2.035951	-1.312669	-2.041898
H 0	1.109526	-2.804437	-1.793557
H 0	2.786903	0.657110	-0.969239
H 0	3.712468	-0.462217	0.030345
H 0	3.220546	1.107639	0.683299
C 0	-0.923083	1.071036	0.617486
C 0	-1.488714	0.060420	-0.202685
C 0	-0.367565	1.770916	-0.579440
C 0	-0.924845	0.656284	-1.507222
O 0	0.221775	2.804437	-0.777864
C 0	-2.709571	-0.640597	-0.027159
N 0	-3.712468	-1.219617	0.111160
H 0	-1.274466	1.474094	1.562177
H 0	-0.189326	0.048396	-2.044748
H 0	-1.672619	1.032887	-2.214739

TS-45+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.220900	-0.642638	-0.449316
C 0	-0.973513	0.514556	-1.270106
C 0	0.174077	0.618621	-2.005066
C 0	-0.240842	-1.629071	-0.292093
C 0	-2.475646	-0.708195	0.388905
C 0	-1.943503	1.679199	-1.228074
H 0	0.416906	1.540321	-2.525627
H 0	0.816044	-0.222566	-2.222300
H 0	-0.502517	-2.488894	0.321360
H 0	0.413609	-1.885193	-1.120075
H 0	-3.361103	-0.815448	-0.253460
H 0	-2.637548	0.196206	0.987707
H 0	-2.456148	-1.565815	1.066865
H 0	-2.056084	2.090442	-0.217470
H 0	-2.943462	1.375553	-1.562438
H 0	-1.606691	2.488894	-1.880425
C 0	2.126912	-0.036917	-0.101870
C 0	1.262420	-0.771496	0.731825
C 0	1.853858	1.258345	0.531864
C 0	0.850514	0.514915	1.470798
O 0	2.287519	2.385737	0.482129
Cl 0	3.361103	-0.583353	-1.199895
H 0	1.506901	-1.713112	1.213576
H 0	-0.200456	0.803412	1.359235
H 0	1.140273	0.565118	2.525627

TS-46+DMB

B3LYP/6-31G(d) Geometry

C 0	1.382427	-0.371080	-0.794912
C 0	1.142695	0.995473	-0.469444
C 0	-0.060498	1.591707	-0.840042
C 0	0.454191	-1.070488	-1.549645
C 0	2.544374	-1.110582	-0.165715
C 0	2.095107	1.737521	0.443140
H 0	-0.274001	2.604065	-0.507716
H 0	-0.563947	1.318688	-1.760051
H 0	0.573903	-2.139767	-1.699064
H 0	-0.157675	-0.569615	-2.288792
H 0	2.505196	-1.095424	0.930586
H 0	3.500606	-0.657190	-0.456033
H 0	2.562154	-2.156348	-0.482736
H 0	3.056925	1.905817	-0.059782
H 0	2.318788	1.187244	1.365097
H 0	1.694315	2.716125	0.720826
C 0	-1.567794	0.336402	0.186592
C 0	-1.590919	-0.955697	-0.421398
C 0	-2.584161	1.328366	0.079213
C 0	-0.947591	-0.190825	1.496471
C 0	-1.055811	-1.581607	0.818131
C 0	-2.466415	-1.519429	-1.498304
O 0	-0.880731	-2.716125	1.198143
N 0	-3.419551	2.136383	-0.010744
H 0	-1.575451	-0.099800	2.389331
H 0	0.062336	0.169643	1.719961
H 0	-2.131100	-2.518968	-1.790556
H 0	-2.486335	-0.881549	-2.389331
H 0	-3.500606	-1.605064	-1.140081

TS-47+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.544517	0.530147	0.416543
C 0	-1.501427	-0.874161	0.680906
C 0	-0.490702	-1.398244	1.451486
C 0	-0.486444	1.349183	0.825356
C 0	-2.624525	1.098016	-0.476701
C 0	-2.471845	-1.806066	-0.017303
H 0	-0.364741	-2.473242	1.541612
H 0	0.047927	-0.803106	2.174903
H 0	-0.559098	2.408768	0.590160
H 0	0.015916	1.159825	1.769240
H 0	-3.603917	1.045520	0.019424
H 0	-2.728179	0.553581	-1.423268
H 0	-2.432270	2.149002	-0.710646
H 0	-2.411675	-1.729307	-1.109900
H 0	-3.508720	-1.579271	0.262254
H 0	-2.275968	-2.847156	0.252766
C 0	1.663953	-0.496065	0.355584
C 0	1.194985	0.723192	-0.214839
C 0	1.358305	-1.260375	-0.863056
C 0	0.766297	0.015122	-1.518335
O 0	1.600672	-2.379618	-1.271245
C 0	2.590115	-0.777671	1.495111
C 0	1.941296	2.040429	-0.177592
H 0	-0.310632	0.001116	-1.722881
H 0	1.300010	0.323896	-2.426042
H 0	2.270109	-0.290306	2.426042
H 0	3.603917	-0.409959	1.279502
H 0	2.661872	-1.854411	1.678110
H 0	2.896939	1.937419	-0.710327
H 0	2.169154	2.351401	0.848326
H 0	1.381211	2.847156	-0.660819

TS-48+DMB

B3LYP/6-31G(d) Geometry

C 0	1.283574	-0.618233	0.187041
C 0	0.858239	0.737126	0.301506
C 0	-0.029301	1.099875	1.293571
C 0	0.743422	-1.589352	1.036789
C 0	2.136256	-1.043090	-0.988437
C 0	1.232614	1.741740	-0.769414
H 0	-0.477376	2.089238	1.298906
H 0	-0.093403	0.559946	2.228398
H 0	1.064964	-2.620564	0.901471
H 0	0.528152	-1.341054	2.070782
H 0	3.115408	-0.546234	-0.960635
H 0	1.686593	-0.784708	-1.956021
H 0	2.316043	-2.121926	-0.978044
H 0	0.937134	1.417045	-1.775255

H 0	2.318550	1.900897	-0.796785
H 0	0.761702	2.709990	-0.579858
C 0	-1.896295	-0.458757	0.954939
C 0	-1.298304	-1.689805	0.643508
C 0	-2.398735	0.203749	-0.259158
O 0	-3.115408	1.189692	-0.331439
C 0	-1.886191	-0.617590	-1.456231
C 0	-1.469000	-1.972596	-0.853808
H 0	-2.258460	-0.172936	1.935687
H 0	-1.370963	-2.525178	1.335522
H 0	-1.032657	-0.089699	-1.900417
H 0	-2.657545	-0.688204	-2.228398
H 0	-0.573185	-2.396239	-1.318192
H 0	-2.272475	-2.709990	-0.983834

TS-49+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.488023	-0.681450	-0.594531
C 0	-1.071611	0.679054	-0.698143
C 0	0.045942	1.007714	-1.430578
C 0	-0.696176	-1.699219	-1.152899
C 0	-2.653341	-1.045182	0.297495
C 0	-1.769336	1.746688	0.121142
H 0	0.456242	2.012714	-1.395628
H 0	0.409918	0.385911	-2.234830
H 0	-1.057179	-2.720472	-1.040366
H 0	-0.213094	-1.532880	-2.112319
H 0	-3.587197	-0.607293	-0.081588
H 0	-2.536165	-0.675921	1.324906
H 0	-2.795223	-2.128738	0.343242
H 0	-1.767714	1.521149	1.195258
H 0	-2.820841	1.847862	-0.177196
H 0	-1.291667	2.720472	-0.016754
C 0	1.856322	-0.643178	-0.553959
C 0	1.059412	-1.744933	-0.181124
C 0	2.056425	0.256607	0.593568
O 0	2.825270	1.207251	0.653590
C 0	2.728326	-0.561019	-1.771372
C 0	1.184727	-0.262796	1.747915
C 0	0.799573	-1.695576	1.329707
H 0	1.277259	-2.718214	-0.619610
H 0	3.123368	0.452952	-1.884302
H 0	2.196118	-0.841113	-2.690342
H 0	3.587197	-1.241584	-1.685469
H 0	0.307154	0.386113	1.854754
H 0	1.737953	-0.210774	2.690342
H 0	-0.227718	-1.961871	1.596453
H 0	1.454963	-2.424539	1.824072

TS-50+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.329031	-0.971415	-0.110945
C 0	-1.525156	0.320640	-0.671654
C 0	-0.689711	0.756188	-1.685789
C 0	-0.266173	-1.761003	-0.557587
C 0	-2.126749	-1.399798	1.101988
C 0	-2.494580	1.292984	-0.031742
H 0	-0.719965	1.790991	-2.014944
H 0	-0.248412	0.063775	-2.390932
H 0	-0.111745	-2.726945	-0.081164
H 0	0.009509	-1.748638	-1.606237
H 0	-3.192339	-1.495025	0.852966
H 0	-2.066027	-0.681270	1.929257
H 0	-1.790072	-2.371613	1.474600
H 0	-2.290802	1.453540	1.034924
H 0	-3.526286	0.924115	-0.102721
H 0	-2.456681	2.267036	-0.526693
C 0	1.480089	0.522423	-0.767460
C 0	1.566269	-0.740809	-0.145164
C 0	1.327378	1.596431	0.228164
O 0	1.427652	2.800063	0.050765
C 0	2.479597	-1.820449	-0.695509
C 0	1.052903	0.911327	1.576935
C 0	1.542595	-0.533491	1.379116
H 0	1.881517	0.740800	-1.751599
H 0	3.526286	-1.568368	-0.476561
H 0	2.386770	-1.919157	-1.782524
H 0	2.280585	-2.800063	-0.246988
H 0	-0.026546	0.949277	1.770335
H 0	1.547158	1.449112	2.390932
H 0	0.937252	-1.277893	1.905833
H 0	2.569946	-0.638504	1.757495

TS-51+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.034712	-1.617777	-0.014280
C 0	-1.559422	-0.522276	-0.752609
C 0	-0.765372	0.091144	-1.722936
C 0	0.250975	-2.070621	-0.277681
C 0	-1.792338	-2.159964	1.179905
C 0	-2.864018	0.121526	-0.339537
H 0	-1.124957	0.993907	-2.209615
H 0	-0.085255	-0.500818	-2.325030
H 0	0.697033	-2.833502	0.355117
H 0	0.678024	-2.012895	-1.269992
H 0	-2.742253	-2.611264	0.865284
H 0	-2.044251	-1.381806	1.911353
H 0	-1.216199	-2.934220	1.693988
H 0	-2.868304	0.430517	0.714103
H 0	-3.700363	-0.579322	-0.461379
H 0	-3.078913	1.004645	-0.946371
C 0	0.987818	0.823535	-0.705276
C 0	1.568271	-0.184231	0.099005
C 0	0.353590	1.845041	0.175131
O 0	-0.065627	2.934220	-0.163884
C 0	2.744475	-0.881073	-0.312395
C 0	0.333413	1.274600	1.599995
C 0	1.352986	0.121838	1.592291
N 0	3.700363	-1.461835	-0.640923
H 0	1.412965	1.130756	-1.654304
H 0	-0.682466	0.920044	1.814188
H 0	0.557509	2.061762	2.325030
H 0	1.024130	-0.751079	2.161456
H 0	2.306581	0.446330	2.027255

TS-52+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.154768	-0.618088	-0.563683
C 0	-0.839378	0.470476	-1.435872
C 0	0.348541	0.487694	-2.123346
C 0	-0.205187	-1.628474	-0.318056
C 0	-2.425908	-0.580796	0.251259
C 0	-1.758939	1.674193	-1.498837
H 0	0.660854	1.373320	-2.669258
H 0	0.931213	-0.401201	-2.312469
H 0	-0.524758	-2.439790	0.334486

H 0	0.419370	-1.978803	-1.136290
H 0	-3.307649	-0.644545	-0.401776
H 0	-2.537368	0.348243	0.825296
H 0	-2.474503	-1.419917	0.950709
H 0	-1.914926	2.134974	-0.515051
H 0	-2.750631	1.394404	-1.876473
H 0	-1.355235	2.439790	-2.166669
C 0	2.141731	-0.122236	-0.201093
C 0	1.309232	-0.858653	0.662880
C 0	2.192581	1.309175	0.111645
O 0	2.934901	2.158457	-0.350522
Cl 0	3.307649	-0.880061	-1.254609
C 0	1.150319	1.521010	1.224021
C 0	0.829781	0.107072	1.756350
H 0	1.641080	-1.846747	0.974860
H 0	0.267836	2.012239	0.799264
H 0	1.557801	2.191402	1.986293
H 0	-0.226168	-0.027590	2.007532
H 0	1.404337	-0.092411	2.669258

TS-53+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.194435	-1.224438	-0.641250
C 0	-1.386799	0.107399	-1.091247
C 0	-0.382704	0.728657	-1.826511
C 0	0.011681	-1.872738	-0.917754
C 0	-2.189234	-1.860289	0.305929
C 0	-2.578822	0.911601	-0.619181
H 0	-0.460976	1.786431	-2.061654
H 0	0.235213	0.157971	-2.507440
H 0	0.188877	-2.859157	-0.496170
H 0	0.527920	-1.705267	-1.856032
H 0	-3.170432	-1.967687	-0.174647
H 0	-2.351512	-1.264633	1.213438
H 0	-1.862388	-2.858009	0.611538
H 0	-2.694454	0.900876	0.472166
H 0	-3.510193	0.504799	-1.034871
H 0	-2.502344	1.954122	-0.939100
C 0	1.542536	0.633854	-0.593317
C 0	1.549528	-0.639980	0.041845
C 0	1.058267	1.650526	0.380069
O 0	1.118596	2.859157	0.239895
C 0	2.484138	1.042914	-1.695129
C 0	2.588004	-1.581193	-0.261276
C 0	0.519356	0.913892	1.610978
C 0	1.102553	-0.506579	1.512069
N 0	3.426534	-2.352603	-0.504105
H 0	2.209067	2.028851	-2.078823
H 0	3.510193	1.109903	-1.311318
H 0	2.498024	0.323784	-2.521047
H 0	-0.576165	0.913511	1.573448
H 0	0.808935	1.446443	2.521047
H 0	1.983130	-0.606048	2.158117
H 0	0.398039	-1.287362	1.809148

TS-54+DMB

B3LYP/6-31G(d) Geometry

C 0	1.519827	0.453929	-0.625696
C 0	1.451557	-0.930908	-0.944959
C 0	0.398425	-1.407567	-1.697613
C 0	0.472312	1.306354	-1.013584
C 0	2.599944	0.964502	0.301528
C 0	2.433148	-1.905516	-0.325939
H 0	0.241242	-2.475867	-1.814912
H 0	-0.126344	-0.782192	-2.404678
H 0	0.569866	2.357217	-0.747183
H 0	0.011120	1.163904	-1.987145
H 0	3.593311	0.846485	-0.153110
H 0	2.633190	0.424906	1.257029
H 0	2.464809	2.027665	0.520068
H 0	2.450626	-1.850378	0.770098
H 0	3.456543	-1.701090	-0.666751
H 0	2.191787	-2.934925	-0.604366
C 0	-1.657981	-0.489059	-0.541195
C 0	-1.250189	0.784279	-0.059003
C 0	-1.482865	-1.518016	0.497464
O 0	-1.919320	-2.661555	0.477461
C 0	-2.588612	-0.724347	-1.694815
C 0	-0.720867	-0.873000	1.663226
C 0	-0.884601	0.638318	1.429661
C 0	-2.049738	2.023497	-0.436540
H 0	-2.685832	-1.798231	-1.878367
H 0	-2.257600	-0.233689	-2.619671
H 0	-3.593311	-0.333684	-1.476159
H 0	0.330318	-1.181288	1.617543
H 0	-1.119651	-1.223257	2.619671
H 0	-0.003658	1.223886	1.711207
H 0	-1.723163	1.021506	2.028341
H 0	-3.064002	1.951768	-0.020685
H 0	-2.146870	2.143212	-1.520462
H 0	-1.594275	2.934925	-0.034485

TS-55+DMB

B3LYP/6-31G(d) Geometry

C 0	-0.784635	-0.711809	0.048326
C 0	-0.784773	0.711845	0.048350
C 0	-0.134048	1.401290	1.065373
C 0	-0.133781	-1.401162	1.065329
C 0	-1.266161	-1.465375	-1.171941
C 0	-1.266440	1.465362	-1.171892
H 0	-0.034409	2.481197	1.000642
H 0	-0.072581	0.998646	2.069347
H 0	-0.033924	-2.481046	1.000557
H 0	-0.072398	-0.998544	2.069319
H 0	-0.698029	-1.191596	-2.069347
H 0	-2.320501	-1.243630	-1.379222
H 0	-1.171071	-2.544905	-1.032446
H 0	-2.320728	1.243401	-1.379200
H 0	-0.698236	1.191747	-2.069304
H 0	-1.171574	2.544905	-1.032350
C 0	1.998786	0.698002	0.878334
C 0	1.998929	-0.697437	0.878342
C 0	2.175632	-1.142485	-0.521514
C 0	2.175386	1.143065	-0.521533
O 0	2.134342	0.000279	-1.332037
O 0	2.320728	-2.239797	-0.988939
O 0	2.320235	2.240401	-0.988977
H 0	2.300097	1.341006	1.694533
H 0	2.300359	-1.340369	1.694553

TS-56+DMB

B3LYP/6-31G(d) Geometry

C 0	0.685806	0.680295	0.208936
C 0	1.178059	-0.639185	-0.009024
C 0	0.724633	-1.688227	0.792004
C 0	-0.165849	0.930019	1.266063

C 0	0.900971	1.747800	-0.843276
C 0	1.984455	-0.942074	-1.252811
H 0	1.074734	-2.695673	0.573508
H 0	0.508219	-1.524419	1.842012
H 0	-0.661911	1.891995	1.354749
H 0	-0.141012	0.337027	2.171604
H 0	0.455966	1.461883	-1.804751
H 0	1.969333	1.925219	-1.019552
H 0	0.450547	2.695673	-0.538207
H 0	2.934717	-0.391900	-1.247135
H 0	1.460919	-0.648299	-2.171604
H 0	2.223618	-2.007363	-1.322112
C 0	-1.367418	-1.799048	0.432449
C 0	-1.955646	-0.582146	0.779620
C 0	-2.360008	0.127590	-0.446208
O 0	-2.934717	1.178967	-0.597349
C 0	-1.524098	-1.927891	-1.073914
O 0	-1.937280	-0.631446	-1.526123
H 0	-1.448511	-2.685532	1.053011
H 0	-2.390170	-0.324579	1.735389
H 0	-2.308202	-2.656273	-1.325333
H 0	-0.614250	-2.201533	-1.613131

TS-57+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.006159	1.116073	-0.125363
C 0	-1.533100	-0.187473	-0.349044
C 0	-1.042894	-0.959683	-1.409866
C 0	-0.083238	1.647313	-1.003840
C 0	-1.304967	1.840863	1.171512
C 0	-2.447163	-0.820583	0.676662
H 0	-1.444453	-1.963903	-1.535192
H 0	-0.797959	-0.480089	-2.351890
H 0	0.446880	2.564564	-0.765363
H 0	-0.065759	1.368034	-2.048106
H 0	-1.015116	1.258890	2.056611
H 0	-2.378468	2.047646	1.269662
H 0	-0.779388	2.798672	1.214568
H 0	-3.386253	-0.257251	0.761245
H 0	-2.010253	-0.844833	1.683617
H 0	-2.704578	-1.846420	0.397899
C 0	0.979079	-1.317756	-1.066250
C 0	1.654685	-0.084554	-1.148034
C 0	2.461955	0.470931	-0.051920
O 0	3.197605	1.441020	-0.209056
C 0	1.071136	-2.122691	0.223294
C 0	2.446038	-0.279024	1.281940
C 0	1.253300	-1.226407	1.454643
H 0	0.981677	-1.921833	-1.972914
H 0	1.901228	0.324879	-2.123816
H 0	1.937140	-2.798672	0.140177
H 0	0.193108	-2.768026	0.343071
H 0	2.507364	0.457734	2.090288
H 0	3.386253	-0.850086	1.319704
H 0	1.386788	-1.843240	2.351890
H 0	0.341837	-0.640000	1.612264

TS-58+DMB

B3LYP/6-31G(d) Geometry

C 0	-0.974538	-1.321310	-0.178616
C 0	-1.417760	-0.234721	0.630974
C 0	-0.646856	0.177142	1.734380
C 0	0.152655	-2.032227	0.165986
C 0	-1.656362	-1.599931	-1.503432
C 0	-2.592606	0.606716	0.187874
H 0	-1.041862	1.006267	2.320129
H 0	-0.179427	-0.581064	2.357798
H 0	0.582024	-2.758193	-0.518328
H 0	0.512242	-2.088871	1.181947
H 0	-1.654193	-0.727981	-2.170772
H 0	-2.707477	-1.878040	-1.353704
H 0	-1.168705	-2.425302	-2.029383
H 0	-3.514218	0.009051	0.161316
H 0	-2.466204	1.020795	-0.821494
H 0	-2.762815	1.440951	0.874312
C 0	1.102106	0.901509	1.116640
C 0	1.937974	-0.175156	0.729325
C 0	2.448600	-0.311511	-0.645191
O 0	3.302573	-1.146298	-0.944363
C 0	0.821056	2.020141	0.120643
C 0	2.005437	0.714822	-1.690999
C 0	0.751883	1.514373	-1.324262
C 0	2.641097	-0.986864	1.788880
H 0	1.292463	1.266963	2.128206
H 0	1.634135	2.758193	0.204600
H 0	-0.100228	2.551809	0.387492
H 0	1.893643	0.194376	-2.648506
H 0	2.860782	1.395585	-1.818250
H 0	0.628400	2.360226	-2.012195
H 0	-0.133548	0.883399	-1.445469
H 0	1.988601	-1.191386	2.648506
H 0	3.514218	-0.443613	2.177879
H 0	3.007028	-1.929905	1.377381

TS-59+DMB

B3LYP/6-31G(d) Geometry

C 0	1.059988	-1.020244	-0.972008
C 0	1.292181	0.299693	-0.500945
C 0	0.517115	1.351965	-0.998682
C 0	0.123364	-1.231268	-1.970284
C 0	1.662234	-2.205422	-0.246117
C 0	2.217931	0.537673	0.672378
H 0	0.679753	2.346153	-0.586927
H 0	0.237823	1.361488	-2.046016
H 0	-0.189844	-2.237813	-2.231210
H 0	-0.055814	-0.487998	-2.736273
H 0	1.391509	-2.229580	0.818269
H 0	2.758786	-2.179651	-0.289922
H 0	1.336181	-3.147736	-0.694811
H 0	3.256916	0.311443	0.396394
H 0	1.984662	-0.092258	1.540053
H 0	2.185809	1.582084	0.996058
C 0	-1.554294	0.986551	-0.550482
C 0	-1.864106	-0.252246	-1.161790
C 0	-2.302637	-1.445312	-0.415982
O 0	-2.794721	-2.418225	-0.978953
C 0	-1.609609	1.053171	0.974967
C 0	-2.225872	-1.394211	1.110488
C 0	-1.311611	-0.290033	1.649720
C 0	-2.068433	2.242726	-1.242793
H 0	-2.217692	-0.245409	-2.190450
H 0	-2.626113	1.375502	1.257973
H 0	-0.935957	1.832843	1.350369
H 0	-1.935927	-2.386556	1.472994
H 0	-3.256916	-1.233192	1.460415
H 0	-1.429912	-0.196794	2.736273

H 0	-0.266483	-0.561452	1.472371
H 0	-1.956555	2.182402	-2.330664
H 0	-1.557529	3.147736	-0.895280
H 0	-3.139062	2.371566	-1.031440

TS-60+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.408980	-0.188968	-1.169615
C 0	-1.141105	-1.373328	-0.435078
C 0	0.031907	-2.077671	-0.678771
C 0	-0.491071	0.236574	-2.133822
C 0	-2.536029	0.727561	-0.750964
C 0	-2.023714	-1.765395	0.731730
H 0	0.300580	-2.917733	-0.043200
H 0	0.474154	-2.110853	-1.665220
H 0	-0.637740	1.193556	-2.626255
H 0	0.027233	-0.497992	-2.740228
H 0	-2.431253	1.073698	0.287063
H 0	-3.503317	0.212437	-0.809713
H 0	-2.589185	1.610138	-1.393602
H 0	-3.025702	-2.044530	0.380412
H 0	-2.162646	-0.953052	1.455758
H 0	-1.611702	-2.626868	1.264504
C 0	1.722606	-0.500872	-0.296244
C 0	1.373464	0.586457	-1.144121
C 0	1.093326	1.943173	-0.584378
O 0	1.000207	2.917733	-1.314713
C 0	1.681901	-0.333744	1.224447
C 0	1.006012	2.082641	0.931691
C 0	0.706256	0.766004	1.655494
C 0	2.708649	-1.419919	-0.786107
N 0	3.503317	-2.179079	-1.174792
H 0	1.855642	0.636391	-2.116210
H 0	2.694583	-0.067358	1.565034
H 0	1.438461	-1.283722	1.710033
H 0	0.274047	2.863831	1.162047
H 0	1.982692	2.472025	1.257820
H 0	0.770717	0.909661	2.740228
H 0	-0.320617	0.451802	1.442390

TS-61+DMB

B3LYP/6-31G(d) Geometry

C 0	0.847885	-1.002208	0.913576
C 0	1.169993	-1.265034	-0.454132
C 0	0.217036	-1.858840	-1.309702
C 0	-0.357427	-1.402233	1.435100
C 0	1.785588	-0.160847	1.757258
C 0	2.456009	-0.727843	-1.034647
H 0	0.558018	-2.070076	-2.322671
H 0	-0.411353	-2.654754	-0.915638
H 0	-0.667821	-1.079747	2.424942
H 0	-0.962443	-2.177923	0.992039
H 0	1.969657	0.829459	1.320727
H 0	2.764401	-0.645628	1.862111
H 0	1.380582	-0.013829	2.762024
H 0	3.326128	-1.168457	-0.528890
H 0	2.552828	0.360068	-0.917310
H 0	2.540793	-0.961073	-2.099489
C 0	-1.267406	-0.653620	-1.627634
C 0	-2.135351	-0.664946	-0.510451
C 0	-2.469279	0.490536	0.327623
O 0	-3.326128	0.472065	1.202808
C 0	-0.738797	0.707421	-2.074865
C 0	-1.774924	1.807812	-0.043321
C 0	-0.515084	1.671189	-0.904621
Cl 0	-3.168006	-2.085191	-0.328276
H 0	-1.611742	-1.272648	-2.456026
H 0	-1.481153	1.140129	-2.762024
H 0	0.182208	0.582495	-2.656152
H 0	-1.575311	2.349472	0.887190
H 0	-2.534484	2.395577	-0.579806
H 0	-0.214981	2.654754	-1.286747
H 0	0.313849	1.311393	-0.287711

TS-62+DMB

B3LYP/6-31G(d) Geometry

C 0	1.460735	-0.285219	-1.398823
C 0	1.434350	1.035725	-0.887902
C 0	0.289365	1.818806	-1.081830
C 0	0.370596	-0.752995	-2.126587
C 0	2.561936	-1.241345	-0.994495
C 0	2.533324	1.524576	0.029887
H 0	0.243926	2.802431	-0.620280
H 0	-0.259068	1.758523	-2.015148
H 0	0.312919	-1.800953	-2.406319
H 0	-0.180679	-0.084340	-2.773519
H 0	2.658972	-1.339274	0.095091
H 0	3.535315	-0.893761	-1.364075
H 0	2.388869	-2.238666	-1.407554
H 0	3.492153	1.566990	-0.503348
H 0	2.688851	0.868939	0.896376
H 0	2.320240	2.530426	0.402027
C 0	-1.351595	0.764847	-0.131309
C 0	-1.543930	-0.444671	-0.876629
C 0	-1.392289	-1.768889	-0.202782
O 0	-1.758333	-2.802431	-0.748963
C 0	-0.959307	0.698332	1.351737
C 0	-0.869128	-1.816570	1.230267
C 0	-0.144633	-0.551406	1.691644
C 0	-2.495929	-0.444484	-2.056622
C 0	-2.269710	1.843456	-0.409511
N 0	-2.998735	2.730104	-0.605584
H 0	-1.886431	0.692712	1.944199
H 0	-0.419907	1.606915	1.638293
H 0	-0.248131	-2.712824	1.333183
H 0	-1.754801	-1.990325	1.860021
H 0	0.029713	-0.589636	2.773519
H 0	0.839455	-0.492949	1.220157
H 0	-2.350033	0.428466	-2.701595
H 0	-3.535315	-0.411793	-1.705679
H 0	-2.375309	-1.357637	-2.641364

TS-63+DMB

B3LYP/6-31G(d) Geometry

C 0	1.251305	-1.043863	-1.215602
C 0	1.470027	0.313713	-0.853578
C 0	0.500540	1.283248	-1.175196
C 0	0.140631	-1.387134	-1.958911
C 0	2.138122	-2.133230	-0.646561
C 0	2.623559	0.678726	0.052854
H 0	0.725594	2.307758	-0.883773
H 0	0.014771	1.227728	-2.146157
H 0	-0.129988	-2.429122	-2.103059
H 0	-0.326266	-0.693339	-2.640893
H 0	2.160012	-2.129851	0.451241
H 0	3.176055	-2.009390	-0.981305

H 0	1.802425	-3.121783	-0.971642
H 0	3.585223	0.450436	-0.426692
H 0	2.613910	0.124112	1.000970
H 0	2.620273	1.746593	0.289569
C 0	-1.234671	0.947823	-0.200064
C 0	-1.825098	-0.205362	-0.806186
C 0	-2.058272	-1.457332	-0.057763
O 0	-2.745928	-2.371257	-0.513822
C 0	-0.871364	0.860092	1.285686
C 0	-1.547889	-1.563685	1.379606
C 0	-0.475645	-0.540911	1.755882
C 0	-1.871508	2.302072	-0.532372
C 0	-2.635802	-0.060273	-2.072237
H 0	-1.754125	1.188024	1.858807
H 0	-0.080045	1.583790	1.517415
H 0	-1.212862	-2.593783	1.542714
H 0	-2.433774	-1.431558	2.019153
H 0	-0.318845	-0.537028	2.841957
H 0	0.479041	-0.824278	1.306315
H 0	-2.895376	2.337359	-0.136664
H 0	-1.927797	2.497236	-1.606304
H 0	-1.312117	3.121783	-0.068710
H 0	-2.114874	0.524663	-2.841957
H 0	-3.585223	0.458525	-1.876014
H 0	-2.879091	-1.046484	-2.471226

TS-64+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.214666	-1.438097	-0.031398
C 0	-0.755984	-0.713107	1.225285
O 0	-0.894085	-0.638561	-1.181425
C 0	-2.756898	-1.496110	-0.146877
C 0	-1.862590	0.390195	-1.097140
C 0	-0.944035	0.681166	1.226320
O 0	-3.096376	-0.262271	-0.786762
C 0	-1.526092	1.351163	0.059362
O 0	-1.832417	2.535042	-0.000202
H 0	-0.742394	-2.414486	-0.155198
H 0	-0.924851	-1.250101	2.158063
H 0	-3.260135	-1.567117	0.823035
H 0	-3.073300	-2.332367	-0.782650
H 0	-1.945932	0.909084	-2.053948
H 0	-0.956554	1.241946	2.155925
C 0	1.279456	-1.139689	1.344154
C 0	1.844149	-0.660455	0.158929
C 0	1.818485	0.739286	-0.121715
C 0	2.240153	-1.633605	-0.926468
C 0	1.337595	1.624167	0.815011
C 0	2.114373	1.223161	-1.524821
H 0	1.295144	-2.214110	1.520774
H 0	1.353568	-0.556518	2.255858
H 0	1.578903	-1.557962	-1.798689
H 0	2.211532	-2.665742	-0.564567
H 0	3.260135	-1.436352	-1.280444
H 0	1.167462	2.665742	0.559831
H 0	1.343833	1.404011	1.874125
H 0	1.437853	0.763718	-2.255858
H 0	3.137930	0.969599	-1.828581
H 0	2.007028	2.308903	-1.597046

TS-65+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.210433	-1.560786	0.545663
C 0	-1.034536	-0.282551	1.352918
O 0	-0.837105	-1.314005	-0.818138
C 0	-2.698670	-1.947021	0.368261
C 0	-1.932958	-0.547931	-1.277775
C 0	-1.458590	0.914350	0.729239
O 0	-3.100809	-1.222854	-0.798599
C 0	-1.923594	0.863520	-0.662035
O 0	-2.409780	1.807483	-1.277913
C 0	-1.789480	2.142345	1.537092
H 0	-0.599131	-2.383625	0.921860
H 0	-1.279287	-0.385774	2.412091
H 0	-3.322596	-1.663502	1.222623
H 0	-2.808068	-3.022374	0.180852
H 0	-1.943175	-0.519492	-2.368723
H 0	-1.053837	2.322507	2.332003
H 0	-2.768214	2.036844	2.026474
H 0	-1.843454	3.022374	0.891782
C 0	0.932015	-0.193856	1.768545
C 0	1.631994	-0.323293	0.558917
C 0	1.526800	0.695383	-0.437956
C 0	2.285020	-1.639123	0.211564
C 0	0.840838	1.854351	-0.176732
C 0	2.014096	0.413329	-1.843017
H 0	1.053721	-0.992049	2.499837
H 0	0.842301	0.784644	2.232609
H 0	1.763924	-2.145202	-0.611587
H 0	2.303593	-2.315387	1.071562
H 0	3.322596	-1.490942	-0.114680
H 0	0.629764	2.566548	-0.968876
H 0	0.663826	2.211595	0.827172
H 0	1.507251	-0.459471	-2.271913
H 0	3.090916	0.202970	-1.858579
H 0	1.834572	1.268930	-2.499837

TS-66+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.300164	-0.732522	-0.881387
C 0	-0.909858	-0.742957	0.597775
O 0	-0.718006	0.410807	-1.526638
C 0	-2.804516	-0.443927	-1.113685
C 0	-1.535642	1.461847	-1.050532
C 0	-0.871098	0.538649	1.196450
O 0	-2.879068	0.984630	-1.144425
C 0	-1.227638	1.740190	0.431703
O 0	-1.369579	2.861006	0.902816
C 0	-1.445866	-1.907956	1.418044
H 0	-0.960933	-1.628820	-1.405209
H 0	-3.454459	-0.832938	-0.324093
H 0	-3.133460	-0.844756	-2.080440
H 0	-1.411445	2.349892	-1.673192
H 0	-0.960411	0.633233	2.275692
H 0	-1.215184	-2.878125	0.963134
H 0	-2.536403	-1.844769	1.525851
H 0	-1.024843	-1.899938	2.428816
C 0	1.097509	-1.444596	0.479558
C 0	1.823164	-0.520620	-0.276594
C 0	1.953302	0.816439	0.192426
C 0	2.243739	-0.867136	-1.685790
C 0	1.436262	1.162567	1.424719
C 0	2.429981	1.899456	-0.750375
H 0	0.984747	-2.452356	0.083585
H 0	1.144751	-1.413650	1.562339
H 0	1.684040	-0.285998	-2.428816

H 0	2.087769	-1.929408	-1.896580
H 0	3.308372	-0.652089	-1.843134
H 0	1.378909	2.203647	1.728041
H 0	1.356656	0.444719	2.231039
H 0	1.798086	1.958929	-1.645603
H 0	3.454459	1.707795	-1.093910
H 0	2.421086	2.878125	-0.262897

TS-67+DMB

B3LYP/6-31G(d) Geometry

C 0	1.440576	0.278418	-1.085190
C 0	1.130675	0.702988	0.353511
O 0	0.668330	-0.888831	-1.396810
C 0	2.872645	-0.278835	-1.233654
C 0	1.343904	-1.895671	-0.666144
C 0	0.850834	-0.338379	1.276522
O 0	2.737397	-1.647920	-0.829519
C 0	1.004536	-1.749954	0.825526
O 0	0.928273	-2.714793	1.565041
C 0	1.766918	1.897120	0.814496
N 0	2.282074	2.882578	1.165185
H 0	1.204892	1.056180	-1.811913
H 0	3.605444	0.225406	-0.597753
H 0	3.201613	-0.237211	-2.279018
H 0	1.082868	-2.882578	-1.053707
H 0	1.070006	-0.176967	2.327592
C 0	-0.912099	1.797355	0.037541
C 0	-1.731919	0.752770	-0.362252
C 0	-1.910191	-0.365896	0.497486
C 0	-2.240536	0.698750	-1.785403
C 0	-1.268980	-0.390225	1.734514
C 0	-2.562845	-1.622187	-0.028989
H 0	-0.684200	2.603682	-0.655223
H 0	-0.790575	2.061190	1.079645
H 0	-1.779293	-0.122682	-2.346534
H 0	-2.032386	1.632708	-2.315200
H 0	-3.325621	0.540173	-1.810161
H 0	-1.319880	-1.286172	2.346534
H 0	-1.123220	0.526888	2.294061
H 0	-2.050374	-1.996851	-0.924546
H 0	-3.605444	-1.435604	-0.316477
H 0	-2.560603	-2.415673	0.722630

TS-68+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.174812	1.076683	-0.915814
C 0	-1.336127	-0.386715	-1.316242
O 0	-0.718804	1.147625	0.440397
C 0	-2.535074	1.809011	-0.808928
C 0	-1.895896	0.819017	1.153747
C 0	-1.952638	-1.187406	-0.331621
O 0	-2.934960	1.585163	0.547714
C 0	-2.261544	-0.677971	1.001590
O 0	-2.866061	-1.263050	1.887983
Cl 0	-2.653629	-2.724593	-0.818174
H 0	-0.454541	1.599327	-1.547975
H 0	-1.682711	-0.538403	-2.338391
H 0	-3.290612	1.415648	-1.496965
H 0	-2.418791	2.886700	-0.973859
H 0	-1.792177	1.096389	2.203748
C 0	0.466452	-1.057251	-1.733503
C 0	1.332119	-0.695861	-0.686087
C 0	1.199677	-1.295696	0.610305
C 0	2.256369	0.482972	-0.861553
C 0	0.303887	-2.307071	0.821129
C 0	1.942887	-0.693697	1.783678
H 0	0.662220	-0.601412	-2.703368
H 0	0.134268	-2.088708	-1.818864
H 0	1.980676	1.314130	-0.199625
H 0	2.250582	0.847504	-1.892825
H 0	3.290612	0.212512	-0.611073
H 0	0.099910	-2.668382	1.824852
H 0	-0.134455	-2.886700	0.022163
H 0	1.653938	0.352284	1.941988
H 0	3.028019	-0.710512	1.623922
H 0	1.734546	-1.246882	2.703368

TS-69+DMB

B3LYP/6-31G(d) Geometry

C 0	1.316727	0.302980	-1.472135
C 0	1.302804	0.717496	0.007040
O 0	0.495559	-0.857089	-1.636675
C 0	2.688970	-0.247124	-1.919093
C 0	1.305938	-1.868968	-1.071883
C 0	1.294040	-0.339473	0.972114
O 0	2.629340	-1.630400	-1.546757
C 0	1.331900	-1.736195	0.458216
O 0	1.473937	-2.720225	1.167597
C 0	2.082237	1.891160	0.291709
C 0	1.882874	-0.127385	2.350100
N 0	2.709513	2.853416	0.485984
H 0	0.938948	1.092603	-2.122562
H 0	3.535583	0.238442	-1.425332
H 0	2.805559	-0.168898	-3.006523
H 0	0.960048	-2.853416	-1.392201
H 0	1.547640	0.813119	2.799463
H 0	2.978171	-0.085777	2.293150
H 0	1.618596	-0.958759	3.006523
C 0	-0.602929	1.772522	0.157732
C 0	-1.555002	0.823565	-0.222299
C 0	-1.682220	-0.370238	0.533799
C 0	-2.255797	0.956100	-1.554512
C 0	-0.896230	-0.546399	1.664732
C 0	-2.478530	-1.530312	-0.017454
H 0	-0.452193	2.648853	-0.468773
H 0	-0.381570	1.949194	1.203998
H 0	-1.938492	0.175940	-2.257537
H 0	-2.058126	1.929859	-2.011735
H 0	-3.342588	0.860627	-1.438345
H 0	-0.885530	-1.504805	2.175450
H 0	-0.611785	0.297188	2.279774
H 0	-2.109904	-1.835974	-1.004675
H 0	-3.535583	-1.262214	-0.139677
H 0	-2.430937	-2.395550	0.649160

TS-70+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.210740	-1.322178	-0.888873
C 0	-1.138807	-0.759716	0.535100
O 0	-0.582377	-0.418157	-1.806191
C 0	-2.647520	-1.352354	-1.467172
C 0	-1.549731	0.607540	-1.900301
C 0	-1.376770	0.646312	0.628410
O 0	-2.803956	-0.060194	-2.061766
C 0	-1.613398	1.422029	-0.597709
O 0	-1.968979	2.597092	-0.629294

C 0	-1.787552	-1.665924	1.581815
C 0	-1.811898	1.285274	1.922796
H 0	-0.708770	-2.289609	-0.965658
H 0	-3.422853	-1.513941	-0.712114
H 0	-2.738583	-2.120569	-2.244918
H 0	-1.351241	1.237459	-2.769032
H 0	-1.522047	-2.716646	1.418047
H 0	-2.881485	-1.589266	1.545142
H 0	-1.480986	-1.400255	2.597247
H 0	-1.170662	1.005956	2.769032
H 0	-2.835229	0.984114	2.190581
H 0	-1.808250	2.372231	1.816496
C 0	0.780660	-1.108071	1.054621
C 0	1.642702	-0.592344	0.070617
C 0	1.695423	0.813453	-0.150653
C 0	2.310872	-1.529577	-0.905605
C 0	0.992140	1.664615	0.669867
C 0	2.354175	1.350530	-1.402886
H 0	0.791384	-2.187732	1.197858
H 0	0.669703	-0.568472	1.991522
H 0	1.894004	-1.424074	-1.915490
H 0	2.198609	-2.573334	-0.597195
H 0	3.385855	-1.321017	-0.981914
H 0	0.888101	2.716646	0.421504
H 0	0.728473	1.400700	1.683584
H 0	1.901726	0.924938	-2.306923
H 0	3.422853	1.102583	-1.429564
H 0	2.266091	2.439188	-1.457242

P-1+DMB

B3LYP/6-31G(d) Geometry

C 0	1.146466	0.670393	0.039098
C 0	1.634505	-0.583438	-0.014674
C 0	0.727528	-1.801843	-0.022771
C 0	-0.725527	-1.514155	0.364201
C 0	-1.207837	-0.245155	-0.364707
C 0	-0.344852	0.959077	0.063922
C 0	-2.633419	0.014117	-0.127612
N 0	-3.758763	0.219454	0.072941
C 0	1.980228	1.928630	0.091343
C 0	3.100109	-0.940233	-0.084735
H 0	1.139134	-2.558960	0.659685
H 0	0.762008	-2.267174	-1.021267
H 0	-1.366587	-2.367554	0.118923
H 0	-0.806639	-1.349631	1.445836
H 0	-1.080783	-0.398392	-1.445836
H 0	-0.644430	1.279929	1.073006
H 0	-0.562317	1.812901	-0.591654
H 0	1.835484	2.532788	-0.815449
H 0	3.049684	1.742516	0.202838
H 0	1.665993	2.558960	0.934956
H 0	3.417434	-1.470148	0.824550
H 0	3.758763	-0.080276	-0.217777
H 0	3.283361	-1.628430	-0.921718

P-2+DMB

B3LYP/6-31G(d) Geometry

C 0	-0.826524	0.645359	-0.032769
C 0	-1.425178	-0.561337	-0.033226
C 0	-0.625524	-1.853741	-0.023774
C 0	0.851604	-1.675974	-0.383498
C 0	1.434338	-0.474642	0.385552
C 0	0.683554	0.803520	0.013465
C 0	2.927673	-0.375074	0.159745
O 0	3.504410	0.576241	-0.320638
C 0	-1.548933	1.970945	-0.083921
C 0	-2.917881	-0.790981	-0.031582
H 0	-1.087844	-2.566372	-0.722136
H 0	-0.712528	-2.325343	0.968968
H 0	0.951940	-1.487585	-1.460808
H 0	1.411543	-2.594366	-0.164479
H 0	1.304019	-0.686400	1.460808
H 0	1.051012	1.167215	-0.957532
H 0	0.941979	1.600816	0.724218
H 0	3.498079	-1.283839	0.465862
H 0	-1.397960	2.535692	0.847164
H 0	-2.623909	1.882890	-0.251634
H 0	-1.138709	2.594366	-0.890521
H 0	-3.242335	-1.275275	-0.963795
H 0	-3.504410	0.121024	0.092687
H 0	-3.196477	-1.474877	0.782746

P-3+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.774239	-1.793216	0.069447
C 0	-0.263194	0.755385	-0.056941
C 0	-1.779595	0.714945	0.034907
C 0	-2.468141	-0.441742	0.076312
C 0	-0.274267	-1.732228	0.368683
C 0	0.362887	-0.583855	-0.450045
C 0	1.847554	-0.627938	-0.317708
O 0	2.510228	0.296601	0.157954
C 0	-2.393281	2.093826	0.083063
C 0	-3.973168	-0.555372	0.124514
H 0	-2.259094	-2.449439	0.805920
H 0	-1.939162	-2.281238	-0.904895
H 0	0.158859	1.088237	0.902384
H 0	0.035803	1.526020	-0.780434
H 0	0.201250	-2.694043	0.141007
H 0	-0.110905	-1.533313	1.435263
H 0	0.155023	-0.799997	-1.512154
H 0	2.380866	-1.533492	-0.644663
H 0	-2.223348	2.632059	-0.860139
H 0	-1.916295	2.694043	0.870124
H 0	-3.466806	2.090598	0.278296
H 0	-4.302545	-0.990964	1.078494
H 0	-4.328415	-1.234578	-0.663116
H 0	-4.491894	0.395820	-0.005532
B 0	4.125579	0.246800	0.322948
H 0	4.278646	0.391449	1.512154
H 0	4.447861	-0.839846	-0.112072
H 0	4.491894	1.193015	-0.331863

P-4+DMB

B3LYP/6-31G(d) Geometry

C 0	0.986616	0.644490	-0.023365
C 0	1.484840	-0.606362	-0.039979
C 0	0.585046	-1.829383	-0.007987
C 0	-0.867819	-1.536394	0.382229
C 0	-1.342737	-0.299622	-0.378409
C 0	-0.508351	0.919815	0.009333
N 0	-2.805795	-0.044437	-0.072880
O 0	-3.603926	-0.150243	-0.999903
O 0	-3.100661	0.235382	1.087592
C 0	1.807672	1.911486	-0.022856
C 0	2.952238	-0.955066	-0.106229

H 0	1.001031	-2.564441	0.695115
H 0	0.616447	-2.323267	-0.992288
H 0	-1.507674	-2.397359	0.157654
H 0	-0.946275	-1.335042	1.456088
H 0	-1.322457	-0.471368	-1.456088
H 0	-0.810392	1.246854	1.013558
H 0	-0.739670	1.754139	-0.667239
H 0	1.643391	2.485045	-0.945993
H 0	2.880355	1.738339	0.077455
H 0	1.499572	2.564441	0.805492
H 0	3.276720	-1.456580	0.816437
H 0	3.603926	-0.094367	-0.265715
H 0	3.137387	-1.664994	-0.924374

P-5+DMB

B3LYP/6-31G(d) Geometry

C 0	0.977566	0.674912	0.013170
C 0	1.489192	-0.568659	-0.055157
C 0	0.601953	-1.801195	-0.068006
C 0	-0.846659	-1.537738	0.352008
C 0	-1.367576	-0.279039	-0.350955
C 0	-0.518520	0.935396	0.048509
C 0	-2.838504	-0.039917	-0.070266
F 0	-3.291176	1.076525	-0.688553
F 0	-3.088237	0.110817	1.253024
F 0	-3.602928	-1.070368	-0.502538
C 0	1.788615	1.947573	0.070008
C 0	2.960518	-0.898003	-0.138295
H 0	1.038806	-2.563977	0.592179
H 0	0.623160	-2.247702	-1.075600
H 0	-0.900957	-1.385394	1.437151
H 0	-1.477394	-2.401212	0.114988
H 0	-1.296187	-0.424631	-1.437151
H 0	-0.807499	1.264541	1.058413
H 0	-0.753711	1.779797	-0.612615
H 0	1.623803	2.557771	-0.829423
H 0	2.862661	1.781529	0.169750
H 0	1.469927	2.563977	0.922345
H 0	3.293770	-1.432708	0.762580
H 0	3.602928	-0.024818	-0.265580
H 0	3.150894	-1.573186	-0.984401

P-6+DMB

B3LYP/6-31G(d) Geometry

C 0	1.475118	0.621398	-0.018655
C 0	2.060184	-0.559365	-0.293385
C 0	1.245605	-1.817128	-0.540434
C 0	-0.219158	-1.708109	-0.106159
C 0	-0.837522	-0.390359	-0.596357
C 0	-0.036855	0.787108	0.023150
B 0	-2.375045	-0.139786	-0.290560
C 0	-3.176008	0.918754	-1.147529
C 0	-3.108784	-0.928232	0.867402
C 0	2.209099	1.906354	0.286662
C 0	3.549833	-0.785193	-0.399322
H 0	1.728974	-2.660330	-0.024314
H 0	1.297764	-2.070347	-1.612604
H 0	-0.781237	-2.573087	-0.482308
H 0	-0.277457	-1.754210	0.990639
H 0	-0.681943	-0.325163	-1.687046
H 0	-0.336891	0.942589	1.074594
H 0	-0.300367	1.724100	-0.488530
H 0	-2.566883	1.540560	-1.813762
H 0	-3.800578	1.573193	-0.524363
H 0	-3.887917	0.364785	-1.782601
H 0	-2.554180	-0.843756	1.813762
H 0	-3.116550	-2.005786	0.642305
H 0	-4.143097	-0.616693	1.051206
H 0	2.021904	2.660330	-0.491584
H 0	3.290118	1.786740	0.382001
H 0	1.842050	2.339815	1.227977
H 0	3.900131	-1.465664	0.390143
H 0	4.143097	0.129340	-0.339828
H 0	3.792435	-1.273209	-1.354092

P-7+DMB

B3LYP/6-31G(d) Geometry

C 0	1.076809	0.545137	0.277853
C 0	1.676806	-0.533430	-0.259003
C 0	0.880880	-1.719499	-0.774272
C 0	-0.583378	-1.736679	-0.327444
C 0	-1.210597	-0.343788	-0.515238
C 0	-0.436111	0.672767	0.369662
B 0	-2.741379	-0.232344	-0.197248
Cl 0	-3.745142	0.981098	-1.008312
Cl 0	-3.526574	-1.247746	1.021082
C 0	1.792582	1.741710	0.859365
C 0	3.168537	-0.702591	-0.423377
H 0	1.374730	-2.646989	-0.449338
H 0	0.935920	-1.736198	-1.875242
H 0	-1.137116	-2.498641	-0.889225
H 0	-0.645478	-2.020937	0.730444
H 0	-1.061731	-0.033170	-1.559998
H 0	-0.737338	0.562940	1.424432
H 0	-0.722842	1.696011	0.089726
H 0	1.589402	2.646989	0.269615
H 0	2.875294	1.618288	0.921173
H 0	1.426808	1.947487	1.875242
H 0	3.541305	-1.522967	0.206433
H 0	3.745142	0.192492	-0.182694
H 0	3.406307	-0.978944	-1.460241

P-8+DMB

B3LYP/6-31G(d) Geometry

C 0	-0.791957	0.537214	0.044358
C 0	-1.210829	-0.702163	-0.275546
C 0	-0.257236	-1.782307	-0.750469
C 0	1.161936	-1.297407	-1.095036
C 0	1.618027	-0.257120	-0.084537
C 0	0.672691	0.941375	-0.060005
Cl 0	3.319261	0.348065	-0.515509
C 0	1.832161	-0.828896	1.320534
O 0	1.773422	-2.003964	1.595416
C 0	-1.675516	1.671918	0.503872
C 0	-2.640263	-1.180300	-0.187125
H 0	-0.685960	-2.273601	-1.635441
H 0	-0.195188	-2.561359	0.020738
H 0	1.176096	-0.835296	-2.088214
H 0	1.856653	-2.141446	-1.108360
H 0	0.835870	1.540299	-0.966670
H 0	0.937066	1.599685	0.779508
H 0	2.069785	-0.061873	2.088214
H 0	-1.431322	1.967858	1.533929
H 0	-2.740894	1.438760	0.467159
H 0	-1.510736	2.561359	-0.120377
H 0	-3.032489	-1.417909	-1.186006

H	0	-3.319261	-0.462948	0.276970
H	0	-2.692858	-2.110734	0.394432

P-9+DMB

B3LYP/6-31G(d) Geometry

C	0	-1.026309	0.687481	-0.259738
C	0	-1.444455	-0.560296	0.022053
C	0	-0.487467	-1.737814	0.036432
C	0	0.851197	-1.467418	-0.656471
C	0	1.434603	-0.099273	-0.250160
C	0	0.424537	1.008963	-0.576242
C	0	2.780123	0.145142	-0.969416
C	0	1.754760	-0.128463	1.242368
O	0	1.443266	0.713259	2.054282
C	0	-1.911563	1.910278	-0.301048
C	0	-2.859449	-0.944714	0.382738
H	0	-0.972361	-2.604872	-0.434885
H	0	-0.314912	-2.043623	1.082069
H	0	0.713665	-1.466610	-1.745858
H	0	1.565859	-2.271037	-0.430760
H	0	0.507316	1.264998	-1.644509
H	0	0.710550	1.916326	-0.028372
H	0	2.644909	0.067336	-2.054282
H	0	3.535746	-0.593131	-0.673229
H	0	3.173499	1.142923	-0.744245
H	0	2.360360	-1.014440	1.552861
H	0	-1.647716	2.604872	0.508615
H	0	-2.976843	1.687233	-0.217699
H	0	-1.761864	2.459163	-1.241509
H	0	-3.285293	-1.623653	-0.370119
H	0	-3.535746	-0.094404	0.486452
H	0	-2.873790	-1.493446	1.335164

P-10+DMB

B3LYP/6-31G(d) Geometry

C	0	1.130792	-0.963437	-0.132785
C	0	1.309964	0.369688	-0.132215
C	0	0.140387	1.334368	-0.084515
C	0	-1.244143	0.732851	-0.376824
C	0	-1.369907	-0.602919	0.369668
C	0	-0.253897	-1.581269	-0.072619
C	0	-2.686695	-1.328612	0.179622
O	0	-3.502165	-1.099454	-0.687720
C	0	-2.350020	1.736247	-0.021818
C	0	2.229528	-1.995904	-0.218243
C	0	2.650917	1.063624	-0.163401
H	0	0.327123	2.155144	-0.793090
H	0	0.122450	1.817687	0.907479
H	0	-1.309318	0.513731	-1.451574
H	0	-1.249370	-0.428583	1.451574
H	0	-0.505901	-1.993408	-1.063295
H	0	-0.232936	-2.447109	0.605509
H	0	-2.850655	-2.171374	0.892416
H	0	-2.175064	2.694193	-0.526160
H	0	-2.368792	1.932938	1.058672
H	0	-3.333434	1.368756	-0.322938
H	0	2.269847	-2.604420	0.696589
H	0	3.220931	-1.568852	-0.379496
H	0	2.033665	-2.694193	-1.044222
H	0	2.774714	1.631659	-1.096357
H	0	3.502165	0.386725	-0.068830
H	0	2.718749	1.795894	0.653343

P-11+DMB

B3LYP/6-31G(d) Geometry

C	0	1.293282	-0.597947	-0.079921
C	0	1.242787	0.745379	-0.126936
C	0	-0.069028	1.507071	-0.117031
C	0	-1.314475	0.639996	-0.404376
C	0	-1.237405	-0.672930	0.397156
C	0	0.037411	-1.447439	-0.004259
C	0	-2.432303	-1.580929	0.170152
O	0	-3.216729	-1.459972	-0.743665
C	0	-2.531111	1.406108	-0.098908
N	0	-3.457293	2.050847	0.173401
C	0	2.554414	-1.427115	-0.122173
C	0	2.443645	1.659617	-0.177019
H	0	-0.025728	2.317987	-0.856094
H	0	-0.192403	2.007430	0.854938
H	0	-1.347323	0.382986	-1.470346
H	0	-1.181377	-0.441121	1.470346
H	0	-0.125472	-1.936003	-0.978278
H	0	0.198149	-2.266988	0.710159
H	0	-2.521154	-2.424514	0.891065
H	0	2.693875	-1.975889	0.819897
H	0	3.457293	-0.842723	-0.305963
H	0	2.485863	-2.185291	-0.914659
H	0	2.483206	2.200711	-1.132716
H	0	3.395179	1.141946	-0.045341
H	0	2.372342	2.424514	0.608399

P-12+DMB

B3LYP/6-31G(d) Geometry

C	0	-0.516004	0.011667	1.542503
C	0	0.058193	-2.051888	-0.503668
C	0	-1.273077	-1.312938	-0.453602
C	0	-1.527805	-0.374158	0.479033
C	0	0.730908	-0.888081	1.619066
C	0	1.168611	-1.292188	0.218883
C	0	1.675534	-0.147896	-0.624216
O	0	1.907813	0.962102	-0.149105
Cl	0	2.680228	-2.363807	0.293277
C	0	-2.233073	-1.777162	-1.521889
C	0	-2.811684	0.412960	0.581382
H	0	-0.208720	1.052967	1.376443
H	0	-1.010226	0.007016	2.523939
H	0	-0.034826	-3.048141	-0.050036
H	0	0.348611	-2.227732	-1.548104
H	0	1.541590	-0.375304	2.143054
H	0	0.506212	-1.807110	2.170455
H	0	1.862366	-0.327552	-1.691431
H	0	-2.335751	-2.870981	-1.492714
H	0	-1.857067	-1.527741	-2.523939
H	0	-3.232723	-1.351514	-1.424661
H	0	-2.594645	1.489337	0.598950
H	0	-3.331614	0.185661	1.522413
H	0	-3.507795	0.230581	-0.238571
B	0	2.469996	2.215994	-1.025970
H	0	1.608835	3.048141	-0.867584
H	0	3.507795	2.480362	-0.469877
H	0	2.573968	1.781043	-2.152716

P-13+DMB

B3LYP/6-31G(d) Geometry

C	0	0.825886	-0.733997	1.498809
C	0	0.724869	1.560331	-0.370101

C 0	1.853859	0.542802	-0.404597
C 0	1.889851	-0.506502	0.440589
C 0	-0.161349	0.425762	1.682536
C 0	-0.550243	1.061875	0.338236
C 0	-1.248907	0.082465	-0.564311
O 0	-1.834608	-0.917520	-0.143957
C 0	-1.552965	2.229711	0.532606
C 0	2.901186	0.863664	-1.444140
C 0	2.957210	-1.574492	0.445425
H 0	0.277485	-1.655191	1.255971
H 0	1.320492	-0.939818	2.458808
H 0	1.064214	2.482101	0.127046
H 0	0.479491	1.864986	-1.399054
H 0	-1.053499	0.079675	2.214949
H 0	0.293954	1.214290	2.295221
H 0	-1.290051	0.290338	-1.644792
H 0	-1.825831	2.697225	-0.420620
H 0	-1.091469	2.996576	1.164183
H 0	-2.469356	1.884728	1.022525
H 0	3.250135	1.899344	-1.325493
H 0	2.484237	0.793145	-2.458808
H 0	3.778561	0.216584	-1.398017
H 0	2.494687	-2.569817	0.403036
H 0	3.535752	-1.541872	1.379392
H 0	3.659707	-1.502838	-0.386578
B 0	-2.662279	-1.940504	-1.096971
H 0	-2.107358	-2.996576	-0.907433
H 0	-3.778561	-1.890205	-0.638036
H 0	-2.543526	-1.486711	-2.216637

P-14+DMB

B3LYP/6-31G(d) Geometry

C 0	1.792258	-1.893849	0.146987
C 0	0.276790	0.680332	-0.045774
C 0	1.787306	0.579744	-0.266841
C 0	2.476349	-0.570696	-0.136676
C 0	0.302655	-1.878726	-0.189899
C 0	-0.347598	-0.632972	0.461586
C 0	-1.824722	-0.729376	0.265295
O 0	-2.470248	0.043144	-0.446857
C 0	-0.085670	1.830851	0.919938
C 0	2.433199	1.890409	-0.667744
C 0	3.976345	-0.696332	-0.268480
H 0	2.284934	-2.683341	-0.437573
H 0	1.936656	-2.178084	1.201814
H 0	-0.187595	0.916355	-1.014992
H 0	-0.182823	-2.799786	0.155501
H 0	0.164433	-1.824762	-1.276832
H 0	-0.181950	-0.727755	1.547983
H 0	-2.364483	-1.558300	0.747989
H 0	0.244936	2.799786	0.537067
H 0	0.382135	1.678260	1.900529
H 0	-1.169565	1.891638	1.059907
H 0	2.594914	2.555139	0.191133
H 0	1.785539	2.434832	-1.366969
H 0	3.395913	1.749884	-1.162513
H 0	4.249040	-1.254112	-1.175996
H 0	4.380453	-1.269385	0.577538
H 0	4.499064	0.261302	-0.290781
B 0	-4.069206	-0.097114	-0.701455
H 0	-4.499064	0.956241	-0.296119
H 0	-4.140402	-0.221552	-1.900529
H 0	-4.399758	-1.072998	-0.059426

P-15+DMB

B3LYP/6-31G(d) Geometry

C 0	1.272025	-0.047194	1.378635
C 0	1.524302	-0.286388	-1.576405
C 0	2.246128	-1.223409	-0.623399
C 0	2.119238	-1.117418	0.713844
C 0	0.763705	1.067093	0.433571
C 0	0.346257	0.460133	-0.926927
C 0	-0.853213	-0.431028	-0.800448
O 0	-1.587081	-0.424983	0.188448
C 0	1.786033	2.099977	0.212913
N 0	2.593748	2.912855	0.026734
C 0	3.122251	-2.222758	-1.339158
C 0	2.781136	-2.027346	1.720642
H 0	1.845586	0.413147	2.193093
H 0	0.401301	-0.514387	1.856927
H 0	2.228790	0.451770	-1.984196
H 0	1.161258	-0.854481	-2.444700
H 0	-0.101989	1.555371	0.895202
H 0	0.026729	1.263427	-1.612019
H 0	-1.109372	-1.094928	-1.639186
H 0	3.794575	-1.703763	-2.036309
H 0	2.518581	-2.912855	-1.945142
H 0	3.743065	-2.819346	-0.669699
H 0	2.041052	-2.393675	2.444700
H 0	3.539364	-1.481284	2.298878
H 0	3.262273	-2.898802	1.274462
B 0	-2.921683	-1.355685	0.329072
H 0	-2.680214	-2.008593	1.315436
H 0	-3.794575	-0.537717	0.487057
H 0	-2.968634	-1.977243	-0.710962

P-16+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.140647	0.523534	-0.161290
C 0	-1.591440	-0.719242	-0.413543
C 0	-0.660032	-1.849876	-0.809850
C 0	0.744797	-1.404011	-1.217393
C 0	1.287043	-0.340893	-0.219077
C 0	0.331636	0.887285	-0.240613
C 0	1.351351	-0.914658	1.142793
N 0	1.381117	-1.378074	2.206038
C 0	2.645992	0.079225	-0.614160
N 0	3.697965	0.421347	-0.964472
C 0	-1.998469	1.707251	0.217102
C 0	-3.033097	-1.154046	-0.311130
H 0	-1.104048	-2.406648	-1.646463
H 0	-0.597077	-2.569685	0.019780
H 0	0.730687	-0.931713	-2.206038
H 0	1.429657	-2.255665	-1.267343
H 0	0.535928	1.451037	-1.161831
H 0	0.596131	1.556615	0.586879
H 0	-1.795809	2.022187	1.250200
H 0	-3.068524	1.514197	0.129000
H 0	-1.765597	2.569685	-0.422717
H 0	-3.419566	-1.457072	-1.294301
H 0	-3.697965	-0.387290	0.089260
H 0	-3.116123	-2.035131	0.339732

P-17+DMB

B3LYP/6-31G(d) Geometry

C 0	1.173740	0.611368	0.258043

C 0	1.566178	-0.551054	-0.296410
C 0	0.578410	-1.546332	-0.880368
C 0	-0.890585	-1.299562	-0.477236
C 0	-1.186430	0.218041	-0.632263
C 0	-0.284129	1.032420	0.313529
C 0	-2.606950	0.535373	-0.444634
N 0	-3.729633	0.794065	-0.303406
C 0	-1.151639	-1.759528	0.895513
N 0	-1.343100	-2.128656	1.979153
C 0	2.092095	1.621848	0.901886
C 0	2.996864	-1.017362	-0.418549
H 0	0.864537	-2.562805	-0.581920
H 0	0.639859	-1.532320	-1.979153
H 0	-1.551972	-1.867613	-1.141875
H 0	-0.930726	0.474053	-1.669103
H 0	-0.659409	0.943767	1.342761
H 0	-0.370160	2.095463	0.054298
H 0	2.099859	2.562805	0.334089
H 0	3.123069	1.278250	0.997827
H 0	1.732645	1.870385	1.909658
H 0	3.173951	-1.900881	0.210388
H 0	3.729633	-0.257370	-0.143704
H 0	3.211618	-1.323415	-1.451893

P-18+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.265000	0.672457	-0.018416
C 0	-1.265000	-0.672457	0.018416
C 0	0.018756	-1.481003	0.028130
C 0	1.273166	-0.679144	-0.376749
C 0	1.273166	0.679144	0.376750
C 0	0.018756	1.481002	-0.028130
C 0	2.486438	1.465166	0.119899
N 0	3.424092	2.113346	-0.098798
C 0	2.486438	-1.465166	-0.119899
N 0	3.424093	-2.113345	0.098798
C 0	-2.497351	1.543425	-0.068202
C 0	-2.497351	-1.543425	0.068202
H 0	-0.081840	-2.335951	-0.652921
H 0	0.175475	-1.918723	1.025101
H 0	1.235229	-0.466086	-1.453048
H 0	1.235229	0.466086	1.453048
H 0	0.175474	1.918723	-1.025101
H 0	-0.081840	2.335951	0.652922
H 0	-2.592226	2.139430	0.850159
H 0	-3.424092	0.983608	-0.202199
H 0	-2.422944	2.261261	-0.896554
H 0	-2.592225	-2.139430	-0.850160
H 0	-3.424093	-0.983608	0.202199
H 0	-2.422944	-2.261261	0.896553

P-19+DMB

B3LYP/6-31G(d) Geometry

C 0	1.234059	-1.008946	-0.047898
C 0	1.464630	0.315474	0.013799
C 0	0.332880	1.327133	0.031317
C 0	-1.048600	0.785461	-0.363031
C 0	-1.255253	-0.567580	0.360209
C 0	-0.172343	-1.577498	-0.073980
C 0	-2.594066	-1.127003	0.128919
N 0	-3.646734	-1.576068	-0.069347
C 0	-2.155134	1.803243	-0.068931
C 0	2.296922	-2.079649	-0.113358
C 0	2.830696	0.955133	0.083479
H 0	0.272088	1.780946	1.035105
H 0	0.588471	2.159609	-0.640617
H 0	-1.043211	0.574613	-1.441878
H 0	-1.160348	-0.391639	1.441878
H 0	-0.405841	-1.945216	-1.084550
H 0	-0.222171	-2.461156	0.576411
H 0	-1.954137	2.748966	-0.585142
H 0	-2.217849	2.017784	1.005641
H 0	-3.133706	1.439448	-0.397823
H 0	2.274422	-2.711494	0.785863
H 0	3.309164	-1.686382	-0.221445
H 0	2.110822	-2.748966	-0.964868
H 0	3.032031	1.547079	-0.820600
H 0	3.646734	0.240417	0.203942
H 0	2.879213	1.656773	0.927923

P-20+DMB

B3LYP/6-31G(d) Geometry

C 0	1.078370	0.575653	-0.127042
C 0	1.435078	-0.720212	-0.199898
C 0	0.434389	-1.808843	-0.541894
C 0	-0.879804	-1.290331	-1.128905
C 0	-1.420639	-0.078359	-0.335335
C 0	-0.348271	1.037408	-0.370241
C 0	-1.661096	-0.483559	1.065646
N 0	-1.869527	-0.807081	2.161569
C 0	-2.753230	0.426112	-0.928370
C 0	2.011327	1.721343	0.185202
C 0	2.821331	-1.255353	0.066360
H 0	0.229754	-2.401572	0.362701
H 0	0.893950	-2.510793	-1.252157
H 0	-0.722524	-0.952148	-2.161569
H 0	-1.629958	-2.089072	-1.160027
H 0	-0.609776	1.812996	0.362601
H 0	-0.410784	1.530095	-1.353430
H 0	-3.524934	-0.348544	-0.876198
H 0	-2.607422	0.698547	-1.979510
H 0	-3.116331	1.307805	-0.390168
H 0	3.062935	1.432554	0.225662
H 0	1.752203	2.184337	1.147846
H 0	1.915901	2.510793	-0.573787
H 0	3.524934	-0.503354	0.427618
H 0	3.246469	-1.706669	-0.841432
H 0	2.779462	-2.055354	0.818464

P-21+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.485592	0.254412	-0.089489
C 0	-1.164890	-1.052162	-0.090258
C 0	0.276404	-1.523009	-0.063894
C 0	1.304805	-0.430138	-0.393876
C 0	0.963232	0.858513	0.399368
C 0	-0.430439	1.340037	-0.020538
C 0	2.001410	1.964724	0.220866
O 0	1.868228	2.899599	-0.537959
C 0	2.716130	-0.936523	-0.142013
F 0	2.933026	-2.125624	-0.744555
F 0	2.965183	-1.103766	1.179699
F 0	3.653009	-0.079042	-0.615810
C 0	-2.889923	0.804492	-0.160244
C 0	-2.150871	-2.195489	-0.109027
H 0	0.398747	-2.348915	-0.776108

H 0	0.506803	-1.951666	0.923791
H 0	1.257271	-0.196088	-1.464812
H 0	0.964801	0.588206	1.464812
H 0	-0.350409	1.855545	-0.987685
H 0	-0.760549	2.115872	0.684377
H 0	2.910073	1.874147	0.850361
H 0	-3.148430	1.336799	0.766023
H 0	-3.653009	0.043783	-0.333817
H 0	-2.967350	1.541986	-0.970979
H 0	-2.069917	-2.769935	-1.042664
H 0	-3.189727	-1.879997	0.000873
H 0	-1.932427	-2.899599	0.706078

P-22+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.550012	-1.206129	-0.049591
C 0	-2.025186	0.047092	-0.163255
C 0	-1.100013	1.247741	-0.231651
C 0	0.354981	0.978501	0.179702
C 0	0.848131	-0.329143	-0.475797
C 0	-0.058812	-1.499067	-0.009413
B 0	2.350278	-0.748092	-0.168239
C 0	1.245078	2.180295	-0.163114
C 0	3.255509	-1.283373	-1.348096
C 0	2.949061	-0.701299	1.295199
C 0	-2.396330	-2.452205	0.063767
C 0	-3.487022	0.417453	-0.248360
H 0	-1.513897	2.051613	0.396989
H 0	-1.118109	1.653009	-1.258213
H 0	0.374822	0.838726	1.271055
H 0	0.701507	-0.225862	-1.563979
H 0	0.207400	-1.800527	1.018056
H 0	0.137745	-2.388651	-0.626997
H 0	0.856996	3.105208	0.281428
H 0	1.295953	2.332072	-1.249493
H 0	2.269668	2.042944	0.204025
H 0	3.589538	-0.407805	-1.930536
H 0	2.698103	-1.905986	-2.061091
H 0	4.157893	-1.822529	-1.036833
H 0	3.159970	-1.731971	1.621794
H 0	2.322511	-0.231753	2.061091
H 0	3.928933	-0.201896	1.298340
H 0	-2.252066	-3.105208	-0.809085
H 0	-3.465572	-2.252721	0.158242
H 0	-2.092978	-3.041310	0.941058
H 0	-3.793803	1.007278	0.627451
H 0	-4.157893	-0.440567	-0.324728
H 0	-3.666604	1.055372	-1.125457

P-23+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.180399	-1.258618	-0.024994
C 0	-1.725998	-0.035420	-0.147056
C 0	-0.872588	1.217914	-0.197545
C 0	0.592324	1.042989	0.227216
C 0	1.156914	-0.244422	-0.425572
C 0	0.322691	-1.465021	0.046643
B 0	2.678108	-0.508022	-0.141751
C 0	1.408377	2.295032	-0.120434
Cl 0	3.820690	-0.844049	-1.450637
Cl 0	3.314887	-0.544521	1.512933
C 0	-1.951387	-2.553873	0.070990
C 0	-3.204776	0.248652	-0.260939
H 0	-1.336350	1.989790	0.435400
H 0	-0.906702	1.631350	-1.220102
H 0	0.620502	0.902028	1.316991
H 0	1.023182	-0.151310	-1.512933
H 0	0.596587	-1.729314	1.079906
H 0	0.586085	-2.345141	-0.557986
H 0	0.953128	3.192795	0.314466
H 0	1.458994	2.442138	-1.206953
H 0	2.435275	2.232703	0.259080
H 0	-1.755458	-3.192795	-0.801958
H 0	-3.031539	-2.417924	0.150308
H 0	-1.626441	-3.126867	0.950873
H 0	-3.564230	0.811519	0.612302
H 0	-3.820690	-0.647422	-0.357292
H 0	-3.403528	0.881300	-1.137485

P-24+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.100689	0.670107	-0.060125
C 0	-1.100685	-0.670134	0.060131
C 0	0.186860	-1.471966	0.128443
C 0	1.422895	-0.683589	-0.324837
C 0	1.422891	0.683573	0.324837
C 0	0.186852	1.471946	-0.128441
N 0	2.649863	1.494579	-0.051529
N 0	2.649870	-1.494590	0.051533
O 0	2.906666	2.448567	0.671622
O 0	3.259080	1.178575	-1.069904
O 0	2.906692	-2.448567	-0.671623
O 0	3.259047	-1.178616	1.069941
C 0	-2.330266	1.539731	-0.157932
C 0	-2.330257	-1.539764	0.157940
H 0	0.104789	-2.371371	-0.493005
H 0	0.345415	-1.827626	1.157892
H 0	1.465891	-0.604577	-1.410914
H 0	1.465888	0.604562	1.410914
H 0	0.345403	1.827605	-1.157890
H 0	0.104780	2.371352	0.493006
H 0	-2.413833	2.196208	0.719124
H 0	-3.259080	0.974102	-0.243946
H 0	-2.262395	2.199158	-1.033868
H 0	-2.413832	-2.196228	-0.719126
H 0	-3.259073	-0.974142	0.243972
H 0	-2.262373	-2.199205	1.033864

P-25+DMB

B3LYP/6-31G(d) Geometry

C 0	0.930004	-1.265212	0.401169
C 0	1.449667	-0.363147	-0.454550
C 0	0.569592	0.524799	-1.320025
C 0	-0.566210	-1.498595	0.525007
C 0	-0.879335	0.633736	-0.802244
C 0	-1.393810	-0.808535	-0.575790
C 0	-0.953773	1.535633	0.421757
C 0	-2.909816	-0.992769	-0.388680
O 0	-3.567691	-1.631567	-1.178599
O 0	-3.474610	-0.454084	0.706416
O 0	-1.568511	1.317357	1.455254
O 0	-0.277011	2.686327	0.258973
C 0	1.735793	-2.150030	1.322298
C 0	2.923561	-0.126169	-0.680745
H 0	1.013603	1.523486	-1.390229
H 0	0.541463	0.136355	-2.348797

H 0	-0.901360	-1.180633	1.521536
H 0	-0.762447	-2.579060	0.482021
H 0	-1.487338	1.132031	-1.570971
H 0	-1.197535	-1.329939	-1.517112
H 0	-2.820505	0.104981	1.184759
H 0	-0.412909	3.205548	1.075027
H 0	2.798379	-1.902817	1.351865
H 0	1.642638	-3.205548	1.030672
H 0	1.350981	-2.078427	2.348797
H 0	3.567691	-0.842629	-0.168318
H 0	3.213317	0.883115	-0.355774
H 0	3.156604	-0.183444	-1.753314

P-26+DMB

B3LYP/6-31G(d) Geometry

C 0	1.270685	0.661614	-0.602910
C 0	1.249859	-0.677719	-0.726131
C 0	-0.041787	-1.461744	-0.862291
C 0	-1.317522	-0.675553	-0.438467
C 0	-1.241955	0.740556	-1.110762
C 0	0.003638	1.494354	-0.605931
C 0	-1.368578	-0.542586	1.032518
C 0	-2.512141	-1.410775	-0.896988
N 0	-3.421046	-2.008208	-1.299921
N 0	-1.378536	-0.433993	2.187183
C 0	-2.459644	1.532852	-0.904586
N 0	-3.403477	2.187882	-0.742509
C 0	2.512663	1.499402	-0.421402
C 0	2.464637	-1.573694	-0.756069
H 0	0.010599	-2.377010	-0.261075
H 0	-0.183000	-1.791818	-1.900984
H 0	-1.142589	0.553726	-2.187183
H 0	-0.189820	1.882966	0.403373
H 0	0.143858	2.377010	-1.242668
H 0	2.663684	2.165650	-1.281928
H 0	3.421046	0.910736	-0.287832
H 0	2.406720	2.146929	0.459312
H 0	2.508179	-2.201141	0.144748
H 0	3.405335	-1.026717	-0.830473
H 0	2.413709	-2.259748	-1.612504

P-27+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.287820	-0.872120	-0.515523
C 0	-1.337865	0.452611	-0.287669
C 0	-0.091732	1.314896	-0.328001
C 0	1.141510	0.664245	-0.971975
C 0	1.306086	-0.796171	-0.453490
C 0	0.019255	-1.583441	-0.807794
C 0	1.476446	-0.779776	1.014790
N 0	1.631738	-0.763373	2.165916
C 0	2.530023	-1.508522	-1.072908
C 0	2.384123	1.542986	-0.782135
C 0	-2.474819	-1.805307	-0.523017
C 0	-2.586583	1.229739	0.051800
H 0	0.156811	1.632534	0.697423
H 0	-0.317582	2.244686	-0.870561
H 0	0.948716	0.561727	-2.050140
H 0	0.034893	-2.546702	-0.279596
H 0	0.069447	-1.836611	-1.878789
H 0	3.471516	-1.058654	-0.747908
H 0	2.474731	-1.449415	-2.165916
H 0	2.544563	-2.565289	-0.786628
H 0	2.675304	1.592720	0.273808
H 0	2.177032	2.565289	-1.118524
H 0	3.241578	1.176339	-1.355252
H 0	-3.435516	-1.293336	-0.444873
H 0	-2.409695	-2.526607	0.303836
H 0	-2.491549	-2.397049	-1.449338
H 0	-3.471516	0.605640	0.187526
H 0	-2.811761	1.969134	-0.729858
H 0	-2.437854	1.797518	0.980721

P-28+DMB

B3LYP/6-31G(d) Geometry

C 0	1.208055	-1.011910	-0.469321
C 0	1.459593	0.307629	-0.388550
C 0	0.341523	1.331681	-0.394055
C 0	-1.040690	0.802791	-0.804742
C 0	-1.308501	-0.566243	-0.102478
C 0	-0.206295	-1.557379	-0.562131
C 0	-2.611934	-1.094362	-0.549873
N 0	-3.635460	-1.513845	-0.904969
C 0	-2.132159	1.856023	-0.580537
C 0	-1.334869	-0.462753	1.441555
C 0	2.254694	-2.099908	-0.509556
C 0	2.832415	0.925789	-0.271736
H 0	0.279914	1.804909	0.599722
H 0	0.612572	2.151102	-1.076291
H 0	-1.006015	0.581879	-1.880840
H 0	-0.407524	-1.867912	-1.598151
H 0	-0.282802	-2.475343	0.036750
H 0	-1.912272	2.755458	-1.167017
H 0	-2.195462	2.159580	0.470828
H 0	-3.115746	1.487007	-0.888825
H 0	-2.084766	0.255180	1.784996
H 0	-0.354495	-0.155475	1.815512
H 0	-1.576587	-1.435662	1.880840
H 0	2.187761	-2.742353	0.379808
H 0	3.276801	-1.722800	-0.574437
H 0	2.089705	-2.755458	-1.376026
H 0	3.063743	1.533831	-1.157726
H 0	3.635460	0.197004	-0.147983
H 0	2.871056	1.608617	0.588548

P-29+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.123021	-0.497031	0.507721
C 0	-1.403201	-0.038188	-0.725955
C 0	-0.315114	0.361605	-1.704819
C 0	1.075447	0.555698	-1.064819
C 0	1.395320	-0.620105	-0.082021
C 0	0.300936	-0.656448	1.010009
C 0	2.800676	-0.482689	0.541444
C 0	1.357382	-1.872125	-0.864143
C 0	1.157118	1.841860	-0.356281
N 0	1.353771	-2.859016	-1.475944
N 0	1.224185	2.859016	0.199631
C 0	-2.148133	-0.884264	1.545800
C 0	-2.788447	0.117838	-1.304564
H 0	-0.603392	1.288186	-2.217259
H 0	-0.226406	-0.401363	-2.491013
H 0	1.837664	0.574211	-1.853899
H 0	0.524598	0.138311	1.737062
H 0	0.390102	-1.600381	1.563524
H 0	2.870369	0.455882	1.099414

H 0	3.576466	-0.489175	-0.230935
H 0	2.996072	-1.311801	1.228308
H 0	-2.092025	-1.959225	1.767121
H 0	-3.174227	-0.654772	1.254757
H 0	-1.949092	-0.360474	2.491013
H 0	-3.017192	1.176950	-1.487996
H 0	-3.576466	-0.290868	-0.670510
H 0	-2.852753	-0.388330	-2.277594

P-30+DMB

B3LYP/6-31G(d) Geometry

C 0	1.240337	0.923692	-0.283320
C 0	1.416796	-0.378175	-0.574102
C 0	0.251973	-1.307756	-0.863409
C 0	-1.144857	-0.782177	-0.450931
C 0	-1.224247	0.704238	-0.923104
C 0	-0.136192	1.559011	-0.244807
C 0	-2.555979	1.292266	-0.729520
N 0	-3.604789	1.767502	-0.581985
C 0	-1.271807	-0.841105	1.019447
N 0	-1.372421	-0.905024	2.174245
C 0	-2.257537	-1.645281	-1.081932
C 0	2.340513	1.898364	0.059903
C 0	2.751462	-1.078609	-0.658806
H 0	0.422797	-2.270416	-0.363708
H 0	0.220271	-1.537795	-1.939858
H 0	-1.033471	0.684664	-2.004831
H 0	-0.426055	1.757591	0.796523
H 0	-0.103546	2.539333	-0.737639
H 0	-2.138654	-2.693333	-0.790464
H 0	-2.199353	-1.581890	-2.174245
H 0	-3.248558	-1.308596	-0.766186
H 0	2.409676	2.693333	-0.695781
H 0	3.323995	1.434917	0.150940
H 0	2.121090	2.395726	1.014505
H 0	2.856497	-1.815639	0.149526
H 0	3.604789	-0.400807	-0.607234
H 0	2.831203	-1.637573	-1.601557

P-31+DMB

B3LYP/6-31G(d) Geometry

C 0	1.097064	1.082037	-0.234874
C 0	1.361955	-0.235390	-0.310786
C 0	0.257165	-1.265845	-0.464852
C 0	-1.169248	-0.792773	-0.110819
C 0	-1.358377	0.602415	-0.795814
C 0	-0.318138	1.616638	-0.310040
C 0	-2.770477	1.134859	-0.642957
O 0	-3.083028	2.092343	0.033613
C 0	-1.327535	-0.683613	1.419559
C 0	-2.178654	-1.825563	-0.649128
C 0	2.129878	2.169892	-0.058392
C 0	2.741486	-0.849508	-0.281352
H 0	0.496235	-2.141442	0.158236
H 0	0.267118	-1.643050	-1.501248
H 0	-1.220772	0.427664	-1.875757
H 0	-0.623393	2.013141	0.668094
H 0	-0.337759	2.490281	-0.977382
H 0	-3.550523	0.580206	-1.210294
H 0	-0.545328	-0.062418	1.865753
H 0	-1.260868	-1.678643	1.875757
H 0	-2.297756	-0.254765	1.695258
H 0	-1.919221	-2.828686	-0.289508
H 0	-2.177979	-1.856635	-1.745999
H 0	-3.201590	-1.616834	-0.316542
H 0	2.158036	2.828686	-0.938016
H 0	3.141188	1.795796	0.111486
H 0	1.866001	2.809492	0.795356
H 0	2.876320	-1.469807	0.616247
H 0	3.550523	-0.117146	-0.305702
H 0	2.878850	-1.520065	-1.141579

P-32+DMB

B3LYP/6-31G(d) Geometry

C 0	1.284742	0.545777	-0.598595
C 0	1.300577	-0.795042	-0.708166
C 0	0.029709	-1.608329	-0.864564
C 0	-1.265783	-0.851108	-0.445469
C 0	-1.233311	0.572029	-1.098594
C 0	-0.001120	1.347223	-0.631947
C 0	-2.526642	1.355598	-0.885142
O 0	-2.550852	2.529620	-0.597903
C 0	-1.333869	-0.732712	1.027307
C 0	-2.438630	-1.620267	-0.910821
N 0	-3.336803	-2.230870	-1.319811
N 0	-1.375491	-0.627851	2.181913
C 0	2.505376	1.411852	-0.404746
C 0	2.535511	-1.663908	-0.705033
H 0	0.097443	-2.529620	-0.273572
H 0	-0.096970	-1.928041	-1.908594
H 0	-1.171423	0.382539	-2.181913
H 0	-0.196984	1.775324	0.361074
H 0	0.122866	2.215803	-1.290488
H 0	-3.465185	0.783013	-1.040331
H 0	2.651860	2.076315	-1.267508
H 0	3.426464	0.846863	-0.254961
H 0	2.370775	2.063200	0.469186
H 0	2.571134	-2.289409	0.197720
H 0	3.465185	-1.095683	-0.756365
H 0	2.522947	-2.352505	-1.561183

P-33+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.265072	0.604370	-0.294889
C 0	-1.265072	-0.604370	0.294889
C 0	0.013020	-1.338389	0.650275
C 0	1.283309	-0.793008	-0.063687
C 0	1.283309	0.793008	0.063687
C 0	0.013020	1.338389	-0.650275
C 0	1.257433	1.157097	1.494937
C 0	1.257433	-1.157097	-1.494937
C 0	2.490953	-1.374930	0.551457
N 0	3.418460	-1.848460	1.061618
N 0	1.210243	-1.450620	-2.615864
N 0	1.210243	1.450621	2.615864
C 0	2.490953	1.374930	-0.551457
N 0	3.418459	1.848460	-1.061618
C 0	-2.495613	1.378513	-0.700074
C 0	-2.495613	-1.378513	0.700074
H 0	-0.079483	-2.400490	0.395541
H 0	0.190161	-1.297591	1.732904
H 0	0.190161	1.297591	-1.732904
H 0	-0.079483	2.400490	-0.395540
H 0	-2.597363	2.290668	-0.096554
H 0	-3.418460	0.805642	-0.603792
H 0	-2.415399	1.700858	-1.746769

H	0	-2.597361	-2.290669	0.096556
H	0	-3.418460	-0.805642	0.603790
H	0	-2.415400	-1.700856	1.746769

P-34+DMB

B3LYP/6-31G(d) Geometry

C	0	1.240042	-0.629286	-0.508846
C	0	1.440766	0.256769	0.483133
C	0	0.294277	0.922733	1.219605
C	0	-1.093147	0.812298	0.543538
C	0	-1.271273	-0.685917	0.056195
C	0	-0.148198	-1.037030	-0.961939
C	0	-1.183817	-1.582515	1.228748
C	0	-1.125681	1.683148	-0.647433
C	0	-2.215832	1.246214	1.508758
N	0	-1.150789	2.392503	-1.565806
N	0	-1.103529	-2.282277	2.150586
C	0	-2.591822	-0.885915	-0.573481
N	0	-3.621124	-1.039051	-1.086094
C	0	2.323973	-1.310871	-1.307923
C	0	2.789966	0.687013	1.004662
H	0	0.516960	1.989053	1.353849
H	0	0.213930	0.504964	2.233429
H	0	-0.397147	-0.552564	-1.915319
H	0	-0.180625	-2.116807	-1.149049
H	0	-2.037380	2.270879	1.847534
H	0	-2.230768	0.588859	2.383580
H	0	-3.194200	1.210101	1.022003
H	0	2.329486	-2.392503	-1.115071
H	0	3.323054	-0.926412	-1.099174
H	0	2.140556	-1.185044	-2.383580
H	0	2.968501	1.749702	0.790067
H	0	3.621124	0.115882	0.589108
H	0	2.828045	0.577451	2.097002

P-35+DMB

B3LYP/6-31G(d) Geometry

C	0	1.452197	0.198564	0.475101
C	0	1.235010	-0.743042	-0.460182
C	0	-0.161343	-1.102026	-0.928440
C	0	-1.287611	-0.645593	0.045441
C	0	-1.047639	0.862786	0.445587
C	0	0.322566	0.974467	1.125283
C	0	-2.171522	1.391360	1.364083
C	0	-1.266900	-1.483906	1.262831
C	0	-2.601870	-0.832399	-0.606342
C	0	-1.099101	1.721363	-0.827985
N	0	-3.620229	-0.966500	-1.146668
N	0	-1.239759	-2.132490	2.224505
O	0	-0.312975	2.603585	-1.082004
C	0	2.808080	0.595236	1.004891
C	0	2.300854	-1.537199	-1.175872
H	0	-0.244529	-2.185978	-1.071971
H	0	-0.364643	-0.655081	-1.912945
H	0	0.231498	0.666399	2.176688
H	0	0.590310	2.037724	1.140925
H	0	-2.250842	0.772886	2.264201
H	0	-3.144721	1.390039	0.861326
H	0	-1.945822	2.417440	1.671308
H	0	-1.963851	1.518792	-1.496010
H	0	3.044733	1.629380	0.720000
H	0	3.620229	-0.044708	0.656841
H	0	2.809920	0.564454	2.102811
H	0	2.233043	-2.603585	-0.919444
H	0	3.314180	-1.201700	-0.951445
H	0	2.165624	-1.468128	-2.264201

P-36+DMB

B3LYP/6-31G(d) Geometry

C	0	1.222919	-0.935453	-0.290725
C	0	1.376267	0.376307	-0.030317
C	0	0.186973	1.288726	0.199610
C	0	-1.188706	0.749928	-0.259933
C	0	-1.303605	-0.733041	0.232886
C	0	-0.150298	-1.573617	-0.382167
C	0	-2.594508	-1.444096	-0.164643
O	0	-3.567533	-0.978073	-0.716013
C	0	-1.261169	0.833385	-1.803077
C	0	-2.290558	1.660650	0.321097
C	0	-1.229920	-0.869961	1.777416
C	0	2.343501	-1.913817	-0.553447
C	0	2.703827	1.086631	0.089975
H	0	0.369974	2.244346	-0.314779
H	0	0.147689	1.551199	1.269112
H	0	-0.366554	-1.797997	-1.438534
H	0	-0.121196	-2.554505	0.115357
H	0	-2.588173	-2.525139	0.119062
H	0	-0.424738	0.314805	-2.282112
H	0	-1.210938	1.884188	-2.112689
H	0	-2.197627	0.417424	-2.181448
H	0	-2.135180	2.689853	-0.025420
H	0	-2.274513	1.685357	1.416243
H	0	-3.282441	1.338853	-0.003769
H	0	-1.991197	-0.268948	2.282112
H	0	-0.245574	-0.569950	2.147145
H	0	-1.383361	-1.915055	2.073780
H	0	2.377238	-2.689853	0.224455
H	0	3.329832	-1.449068	-0.603854
H	0	2.178421	-2.438834	-1.504971
H	0	2.819950	1.832455	-0.709036
H	0	3.567533	0.420045	0.052936
H	0	2.755273	1.641163	1.037458

P-37+DMB

B3LYP/6-31G(d) Geometry

C	0	0.169498	-1.731780	1.216192
C	0	-0.345375	-0.712243	-1.517767
C	0	-1.462734	-1.177293	-0.602179
C	0	-1.230052	-1.636745	0.640291
C	0	1.299852	-1.667915	0.146473
C	0	1.010359	-0.464909	-0.839664
C	0	1.011464	0.814184	-0.033266
O	0	0.162551	1.688121	-0.197867
C	0	1.336120	-2.926788	-0.626637
C	0	2.606111	-1.509065	0.818985
C	0	2.140484	-0.300711	-1.887648
N	0	1.356082	-3.911202	-1.240026
N	0	3.616991	-1.346677	1.365229
C	0	-2.821848	-1.074151	-1.248672
C	0	-2.283368	-2.085050	1.624080
H	0	0.343115	-0.923067	1.942182
H	0	0.282450	-2.663991	1.782154
H	0	-0.650239	0.219413	-2.008481
H	0	-0.206005	-1.444541	-2.325225
H	0	1.827998	0.999234	0.680214
H	0	1.886751	0.504121	-2.583970

H 0	2.250152	-1.229072	-2.457173
H 0	3.103175	-0.066629	-1.422057
H 0	-2.806401	-1.543963	-2.241233
H 0	-3.096252	-0.021802	-1.402478
H 0	-3.616991	-1.549297	-0.672751
H 0	-2.156375	-1.566167	2.583970
H 0	-2.191326	-3.159768	1.833182
H 0	-3.301407	-1.894106	1.282926
B 0	0.173595	3.118889	0.589751
H 0	-0.898899	3.115069	1.142983
H 0	1.141505	3.057923	1.316163
H 0	0.250490	3.911202	-0.317360

P-38+DMB

B3LYP/6-31G(d) Geometry

C 0	1.286598	-0.368510	-0.562477
C 0	1.286598	0.368507	0.562478
C 0	0.001058	0.813712	1.230294
C 0	-1.278911	0.700377	0.365020
C 0	-1.278912	-0.700379	-0.365020
C 0	0.001058	-0.813714	-1.230294
C 0	-2.528678	-0.920156	-1.247728
C 0	-2.528678	0.920155	1.247728
C 0	-1.255396	-1.752091	0.671378
C 0	-1.255395	1.752090	-0.671379
N 0	-1.259640	-2.588934	1.476612
N 0	-1.259638	2.588934	-1.476612
C 0	2.517856	-0.824544	-1.306789
C 0	2.517856	0.824541	1.306789
H 0	0.102592	1.856540	1.558878
H 0	-0.159933	0.227586	2.146957
H 0	-0.159932	-0.227589	-2.146957
H 0	0.102591	-1.856543	-1.558877
H 0	-2.621243	-0.102803	-1.969690
H 0	-3.444399	-0.971854	-0.653498
H 0	-2.433105	-1.860007	-1.800076
H 0	-2.433105	1.860007	1.800076
H 0	-2.621243	0.102802	1.969690
H 0	-3.444399	0.971854	0.653497
H 0	2.611997	-1.918976	-1.272720
H 0	3.444399	-0.395640	-0.922183
H 0	2.444040	-0.550749	-2.368287
H 0	2.611999	1.918974	1.272717
H 0	3.444399	0.395635	0.922185
H 0	2.444039	0.550750	2.368287

P-39+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.232238	-0.876819	0.280525
C 0	-1.440992	0.356763	-0.214942
C 0	-0.294972	1.261874	-0.622262
C 0	1.106704	0.831686	-0.123596
C 0	1.261988	-0.724015	-0.352368
C 0	0.161561	-1.448992	0.465390
C 0	2.584566	-1.168392	0.127274
N 0	3.628220	-1.535551	0.479744
C 0	1.152523	-1.106896	-1.849091
C 0	1.185597	1.106208	1.327797
N 0	1.245382	1.353187	2.460614
C 0	2.209281	1.664191	-0.815053
C 0	-2.313190	-1.821204	0.748100
C 0	-2.792688	0.992293	-0.436581
H 0	-0.489241	2.279311	-0.257672
H 0	-0.260547	1.350034	-1.718474
H 0	0.423431	-1.428323	1.531959
H 0	0.162710	-2.509315	0.180546
H 0	1.899976	-0.595583	-2.460614
H 0	0.155426	-0.874874	-2.230614
H 0	1.314627	-2.183318	-1.958322
H 0	2.075369	2.725461	-0.584730
H 0	2.157214	1.545392	-1.900951
H 0	3.203818	1.363017	-0.474354
H 0	-2.340446	-2.725461	0.124167
H 0	-3.310996	-1.379941	0.744745
H 0	-2.104763	-2.157264	1.772946
H 0	-2.935046	1.848504	0.237328
H 0	-3.628220	0.306612	-0.287532
H 0	-2.868030	1.386374	-1.459641

P-40+DMB

B3LYP/6-31G(d) Geometry

C 0	1.222648	-0.984976	-0.227601
C 0	1.434935	0.322938	0.009462
C 0	0.288474	1.298611	0.198441
C 0	-1.100297	0.814608	-0.270256
C 0	-1.292023	-0.661110	0.257237
C 0	-0.175386	-1.564523	-0.333889
C 0	-2.596316	-1.185832	-0.193800
N 0	-3.622610	-1.606076	-0.540236
C 0	-2.186904	1.760860	0.273658
C 0	-1.265365	-0.764616	1.804440
C 0	-1.160739	0.849534	-1.813584
C 0	2.299906	-2.021651	-0.444164
C 0	2.792408	0.971502	0.142803
H 0	0.244654	1.592136	1.259264
H 0	0.523369	2.229545	-0.338828
H 0	-0.396153	-1.791455	-1.386176
H 0	-0.205781	-2.534998	0.180092
H 0	-2.032971	2.770447	-0.124566
H 0	-2.166330	1.835998	1.365547
H 0	-3.187958	1.433046	-0.027856
H 0	-2.041074	-0.152458	2.270358
H 0	-0.290042	-0.455642	2.189602
H 0	-1.434046	-1.802571	2.108444
H 0	-0.326050	0.309892	-2.270358
H 0	-1.107813	1.888367	-2.158728
H 0	-2.096642	0.421338	-2.188166
H 0	2.289266	-2.770447	0.360348
H 0	3.306756	-1.604125	-0.499059
H 0	2.119482	-2.571098	-1.378620
H 0	2.960355	1.694467	-0.667868
H 0	3.622610	0.263044	0.135643
H 0	2.853135	1.541210	1.080641

P-41+DMB

B3LYP/6-31G(d) Geometry

C 0	0.861200	0.739362	0.004109
C 0	1.111743	-0.556003	-0.268413
C 0	0.236671	-1.638215	0.350016
C 0	-1.256556	-1.288498	0.379952
C 0	-1.536826	0.223306	0.679133
C 0	-0.303576	1.104153	0.913103
C 0	-2.149909	0.335847	-0.729433
C 0	-1.954146	-1.157941	-1.013931
O 0	-2.577709	1.263591	-1.368917
C 0	1.661338	1.918199	-0.489523

C 0	2.248652	-1.072393	-1.114837
H 0	0.575303	-1.830839	1.380821
H 0	0.376662	-2.585043	-0.188204
H 0	-1.786346	-1.969667	1.052584
H 0	-2.288203	0.394223	1.460618
H 0	0.005523	1.026467	1.967489
H 0	-0.590236	2.151377	0.755753
H 0	-2.894887	-1.711040	-1.119512
H 0	-1.330780	-1.366282	-1.891687
H 0	1.029286	2.585043	-1.092179
H 0	2.527094	1.640388	-1.093911
H 0	2.025392	2.518135	0.356725
H 0	2.879716	-1.760922	-0.534682
H 0	2.894887	-0.286214	-1.510055
H 0	1.866451	-1.651360	-1.967489

P-42+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.043247	0.715071	0.068867
C 0	-1.474110	-0.558982	0.134922
C 0	-0.587172	-1.672581	-0.403095
C 0	0.896147	-1.483563	-0.069007
C 0	1.411832	-0.004444	-0.210871
C 0	0.311023	1.015934	-0.555498
C 0	1.735149	-0.039126	1.298947
C 0	1.256735	-1.485462	1.452292
C 0	2.656681	0.191631	-1.080825
O 0	2.194450	0.780400	2.055147
C 0	-1.807968	1.933363	0.521563
C 0	-2.809675	-1.011833	0.669064
H 0	-0.702210	-1.736100	-1.497404
H 0	-0.925994	-2.642018	-0.013897
H 0	1.502861	-2.193907	-0.640586
H 0	0.207091	1.061464	-1.652326
H 0	0.656345	2.009949	-0.243445
H 0	2.041161	-2.187189	1.758547
H 0	0.410401	-1.591695	2.141402
H 0	2.412510	0.053690	-2.141402
H 0	3.447087	-0.522613	-0.821537
H 0	3.062879	1.201177	-0.950481
H 0	-2.801928	1.708507	0.914031
H 0	-1.931627	2.642018	-0.309718
H 0	-1.250591	2.468279	1.303044
H 0	-3.447087	-0.193158	1.009100
H 0	-2.677867	-1.705243	1.511769
H 0	-3.364502	-1.566935	-0.100970

P-43+DMB

B3LYP/6-31G(d) Geometry

C 0	1.407210	0.431665	0.298897
C 0	1.219196	-0.776934	-0.264642
C 0	-0.070016	-1.538839	0.008512
C 0	-1.342492	-0.672924	0.007683
C 0	-1.094468	0.747406	0.636675
C 0	0.314176	1.022826	1.176827
C 0	-2.528791	-1.431568	0.602149
C 0	-1.374523	1.358812	-0.745429
C 0	-1.652005	-0.005375	-1.380419
O 0	-1.343767	2.488779	-1.165765
C 0	2.642638	1.286318	0.172949
C 0	2.216674	-1.511435	-1.125252
H 0	0.010582	-2.039396	0.987676
H 0	-0.189448	-2.347518	-0.725474
H 0	-1.853700	1.040606	1.374070
H 0	0.398274	0.623624	2.200125
H 0	0.445424	2.108802	1.261769
H 0	-2.334272	-1.717144	1.643488
H 0	-2.734284	-2.349908	0.037376
H 0	-3.440858	-0.822140	0.588170
H 0	-2.680975	-0.129728	-1.739399
H 0	-0.967379	-0.252953	-2.200125
H 0	2.397913	2.248525	-0.297791
H 0	3.440858	0.821542	-0.409292
H 0	3.050113	1.522504	1.166280
H 0	2.461059	-2.488779	-0.684916
H 0	3.154234	-0.970784	-1.270053
H 0	1.794138	-1.719535	-2.118479

P-44+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.562001	0.122540	-0.462758
C 0	-1.143321	-0.944071	0.244742
C 0	0.305245	-1.397242	0.132284
C 0	1.321300	-0.229902	0.138639
C 0	0.793591	1.042356	-0.637800
C 0	-0.563538	0.878799	-1.327040
C 0	2.636757	-0.691208	-0.298553
C 0	0.749365	1.779162	0.712584
C 0	1.365152	0.602663	1.474940
O 0	0.335352	2.859905	1.040741
N 0	3.682301	-1.057622	-0.649356
C 0	-2.968383	0.661887	-0.505019
C 0	-2.004258	-1.815344	1.124419
H 0	0.441607	-1.968546	-0.797472
H 0	0.556046	-2.085250	0.948223
H 0	1.537466	1.474720	-1.316721
H 0	-0.425257	0.368291	-2.292367
H 0	-0.947136	1.879299	-1.559807
H 0	2.373043	0.803670	1.852796
H 0	0.750321	0.211730	2.292367
H 0	-2.994061	1.692483	-0.125291
H 0	-3.682301	0.072689	0.073608
H 0	-3.332357	0.702808	-1.541121
H 0	-1.972346	-2.859905	0.784024
H 0	-3.051209	-1.507944	1.150486
H 0	-1.630038	-1.816243	2.157764

P-45+DMB

B3LYP/6-31G(d) Geometry

C 0	-0.744134	0.674575	-0.346611
C 0	-1.230032	-0.577419	-0.447809
C 0	-0.322178	-1.683898	-0.967153
C 0	1.102780	-1.602281	-0.407995
C 0	1.656061	-0.141853	-0.341246
C 0	0.689318	0.954976	-0.783671
C 0	1.797508	-0.314307	1.195250
C 0	1.241122	-1.739104	1.143421
O 0	2.173786	0.421049	2.066839
C 0	-1.502170	1.889571	0.123458
C 0	-2.639177	-1.005164	-0.125149
Cl 0	3.281070	0.088025	-1.136581
H 0	-0.278260	-1.641515	-2.066839
H 0	-0.746056	-2.666249	-0.722831
H 0	1.771043	-2.275305	-0.948862
H 0	0.739443	1.040936	-1.878908
H 0	1.040143	1.909560	-0.376436

H 0	1.947987	-2.501689	1.488265
H 0	0.302359	-1.853459	1.696762
H 0	-2.539940	1.680174	0.390143
H 0	-1.507664	2.666249	-0.654083
H 0	-1.011677	2.332869	1.000874
H 0	-3.111697	-1.463177	-1.005636
H 0	-3.281070	-0.186419	0.205585
H 0	-2.643725	-1.773686	0.660505

P-46+DMB

B3LYP/6-31G(d) Geometry

C 0	1.434100	-0.402079	-0.570630
C 0	1.254917	0.846545	-0.101442
C 0	-0.116715	1.488295	-0.230686
C 0	-1.276023	0.528022	0.130870
C 0	-1.064853	-0.953773	-0.424883
C 0	0.253772	-1.125488	-1.199355
C 0	-2.554606	1.140671	-0.221155
C 0	-0.945927	-1.409620	1.043948
C 0	-1.236216	-0.017494	1.606355
O 0	-0.699047	-2.476488	1.544180
C 0	-2.244836	-1.595085	-1.159835
N 0	-3.567143	1.637242	-0.501999
C 0	2.725138	-1.178689	-0.559626
C 0	2.313023	1.725754	0.515325
H 0	-0.268895	1.844044	-1.260392
H 0	-0.186973	2.376416	0.408509
H 0	0.101369	-0.778800	-2.234028
H 0	0.462345	-2.200242	-1.262997
H 0	-2.186033	0.050677	2.146949
H 0	-0.440458	0.396840	2.234028
H 0	-2.383878	-1.137465	-2.145690
H 0	-3.183206	-1.486982	-0.606883
H 0	-2.052874	-2.664691	-1.296087
H 0	2.609888	-2.102650	0.023433
H 0	3.567143	-0.621906	-0.143736
H 0	2.998966	-1.485820	-1.578641
H 0	2.411161	2.664691	-0.047445
H 0	3.298818	1.258313	0.552742
H 0	2.037530	2.008805	1.540971

P-47+DMB

B3LYP/6-31G(d) Geometry

C 0	1.282684	-0.850744	-0.398518
C 0	1.396910	0.444421	-0.051622
C 0	0.221023	1.373273	-0.302944
C 0	-1.155127	0.777766	0.055220
C 0	-1.288285	-0.746897	-0.380474
C 0	-0.014499	-1.326443	-1.029838
C 0	-1.379234	-1.100565	1.116747
C 0	-1.273322	0.357177	1.562402
C 0	-2.530477	-1.170133	-1.171966
O 0	-1.493391	-2.150505	1.700612
C 0	2.345896	-1.909323	-0.253459
C 0	2.619788	1.097799	0.540944
C 0	-2.267469	1.721915	-0.405681
H 0	0.208484	1.667992	-1.365633
H 0	0.354816	2.307150	0.260098
H 0	-0.022865	-1.070197	-2.102388
H 0	-0.077679	-2.420706	-0.978479
H 0	-2.166770	0.725759	2.081533
H 0	-0.399386	0.561793	2.191690
H 0	-2.504175	-0.767346	-2.191690
H 0	-3.461021	-0.838058	-0.700900
H 0	-2.569527	-2.263070	-1.238759
H 0	3.286876	-1.532578	0.153097
H 0	2.565463	-2.372828	-1.225759
H 0	1.994531	-2.717557	0.402785
H 0	3.461021	0.413877	0.671535
H 0	2.391364	1.537637	1.522182
H 0	2.961355	1.927135	-0.094950
H 0	-2.270110	1.839429	-1.496162
H 0	-2.124173	2.717557	0.032893
H 0	-3.260838	1.373027	-0.104179

P-48+DMB

B3LYP/6-31G(d) Geometry

C 0	1.505300	0.609809	-0.280022
C 0	1.619976	-0.681395	0.081210
C 0	0.458387	-1.485421	0.634116
C 0	-0.889173	-0.765998	0.671997
C 0	-0.844410	0.767116	0.791382
C 0	0.189702	1.361870	-0.179068
C 0	-2.290399	1.189995	0.424181
C 0	-1.796885	-1.000005	-0.543370
C 0	-2.705399	0.226764	-0.708173
O 0	-1.797077	-1.982488	-1.252752
C 0	2.615406	1.451855	-0.863664
C 0	2.888552	-1.496894	-0.006760
H 0	0.726830	-1.826655	1.645212
H 0	0.338067	-2.402832	0.039225
H 0	-1.479275	-1.155607	1.519251
H 0	-0.587827	1.070886	1.812577
H 0	0.389600	2.402832	0.113579
H 0	-0.242349	1.435955	-1.191225
H 0	-2.353985	2.243561	0.131794
H 0	-2.945507	1.054685	1.293556
H 0	-3.758675	-0.072579	-0.681492
H 0	-2.528854	0.646908	-1.706008
H 0	3.535392	0.898996	-1.061446
H 0	2.863564	2.288026	-0.194169
H 0	2.292751	1.903673	-1.812577
H 0	3.758675	-0.927873	-0.338256
H 0	2.756840	-2.342250	-0.696643
H 0	3.132427	-1.933658	0.972076

P-49+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.078206	-0.761246	-0.624826
C 0	-1.507120	0.422304	-0.149638
C 0	-0.553213	1.459331	0.413229
C 0	0.935978	1.200680	0.168126
C 0	1.327753	-0.291777	0.247142
C 0	0.393521	-1.129870	-0.671124
C 0	2.708809	-0.308637	-0.428640
C 0	1.487611	1.660528	-1.203527
C 0	2.839745	0.934321	-1.322306
O 0	3.556636	-1.162659	-0.281520
C 0	1.365516	-0.869992	1.662812
C 0	-1.962425	-1.841062	-1.203664
C 0	-2.951984	0.856807	-0.077977
H 0	-0.736654	1.539052	1.496703
H 0	-0.821340	2.448719	0.011078
H 0	1.506833	1.736352	0.941763
H 0	0.518371	-2.188604	-0.406429
H 0	0.724707	-1.069435	-1.720865

H 0	1.582056	2.750010	-1.259989
H 0	0.806697	1.354119	-2.006777
H 0	3.662300	1.540103	-0.918690
H 0	3.129943	0.654361	-2.340286
H 0	0.353837	-0.984016	2.067651
H 0	1.933504	-0.221330	2.340286
H 0	1.851917	-1.850820	1.654802
H 0	-3.010082	-1.550577	-1.300549
H 0	-1.921215	-2.750010	-0.586979
H 0	-1.607100	-2.131557	-2.202484
H 0	-3.662300	0.082798	-0.373408
H 0	-3.126737	1.734429	-0.716561
H 0	-3.207497	1.166044	0.945355

P-50+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.418495	-0.282445	-0.553303
C 0	-1.585060	0.804730	0.222030
C 0	-0.444169	1.431456	1.000282
C 0	0.935222	0.824178	0.750558
C 0	0.970268	-0.677851	0.391557
C 0	-0.064033	-0.950017	-0.725252
C 0	2.412209	-0.852258	-0.164261
C 0	1.748100	1.486559	-0.368392
C 0	2.712485	0.441930	-0.946215
O 0	1.648838	2.637427	-0.734755
C 0	0.700630	-1.581462	1.599917
C 0	-2.501994	-0.938821	-1.376047
C 0	-2.892273	1.532858	0.428567
H 0	-0.686394	1.379701	2.072473
H 0	-0.390626	2.504157	0.763392
H 0	1.557131	0.968409	1.651500
H 0	-0.206994	-2.037303	-0.811755
H 0	0.344620	-0.644610	-1.702122
H 0	2.507799	-1.755636	-0.777165
H 0	3.111808	-0.956989	0.675039
H 0	3.746998	0.790548	-0.854652
H 0	2.512548	0.349028	-2.020507
H 0	-0.326197	-1.461993	1.963621
H 0	1.383218	-1.350442	2.427134
H 0	0.839774	-2.637427	1.335910
H 0	-3.455522	-0.408175	-1.357793
H 0	-2.683045	-1.967409	-1.032519
H 0	-2.189068	-1.016702	-2.427134
H 0	-3.746998	1.052513	-0.050781
H 0	-2.826650	2.561033	0.046016
H 0	-3.118875	1.617260	1.500822

P-51+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.404960	0.100953	0.501226
C 0	-1.577988	-0.686748	-0.575201
C 0	-0.439750	-1.071945	-1.500029
C 0	0.951381	-0.616293	-1.068168
C 0	1.011068	0.693615	-0.242907
C 0	-0.044505	0.649855	0.890704
C 0	2.459967	0.672135	0.343716
C 0	1.739646	-1.603359	-0.194407
C 0	2.720813	-0.809412	0.677593
O 0	1.609920	-2.806051	-0.202255
C 0	0.790339	1.872689	-1.088787
N 0	0.630707	2.806051	-1.761688
C 0	-2.488112	0.506812	1.471861
C 0	-2.897337	-1.273416	-1.016455
H 0	-0.660682	-0.680224	-2.503037
H 0	-0.412844	-2.165820	-1.606795
H 0	1.581813	-0.481788	-1.961900
H 0	-0.158697	1.661666	1.300814
H 0	0.358261	0.048099	1.719974
H 0	2.550100	1.335949	1.208502
H 0	3.163520	1.026301	-0.416925
H 0	3.748116	-1.128393	0.472588
H 0	2.524482	-1.052435	1.728342
H 0	-3.445255	0.014307	1.294164
H 0	-2.656168	1.592362	1.434523
H 0	-2.185710	0.275081	2.503037
H 0	-3.748116	-0.946711	-0.416793
H 0	-2.862299	-2.371172	-0.982455
H 0	-3.105036	-1.002014	-2.060657

P-52+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.040909	-0.863817	-0.433799
C 0	-1.472517	0.025085	0.478530
C 0	-0.517802	0.787830	1.376967
C 0	0.957303	0.737307	0.978897
C 0	1.396486	-0.625481	0.422567
C 0	0.433418	-1.132110	-0.669106
C 0	2.757282	-0.327378	-0.248040
C 0	1.408828	1.713723	-0.135000
C 0	2.784255	1.173003	-0.571043
O 0	3.626432	-1.127941	-0.490434
C 0	-1.921668	-1.672165	-1.356556
C 0	-2.921434	0.339511	0.763956
Cl 0	1.559801	-1.867896	1.739731
H 0	-0.625130	0.396991	2.400037
H 0	-0.837369	1.839231	1.436076
H 0	1.567832	0.947977	1.866755
H 0	0.612611	-2.204334	-0.808107
H 0	0.717854	-0.675371	-1.632202
H 0	1.453762	2.744127	0.231050
H 0	0.695963	1.695118	-0.967600
H 0	3.596850	1.614529	0.021119
H 0	3.036745	1.338201	-1.623178
H 0	-1.596861	-1.554066	-2.400037
H 0	-2.976575	-1.397222	-1.308996
H 0	-1.842139	-2.744127	-1.127835
H 0	-3.138912	0.195867	1.831543
H 0	-3.626432	-0.273910	0.200571
H 0	-3.141481	1.393665	0.543486

P-53+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.320375	-0.756566	-0.070273
C 0	-1.446235	0.581425	-0.102361
C 0	-0.250015	1.508284	-0.032948
C 0	1.127335	0.842287	-0.231283
C 0	1.238168	-0.565851	0.440157
C 0	0.031724	-1.439898	-0.013750
C 0	2.459386	-1.178823	-0.272713
C 0	1.506773	0.546262	-1.718137
C 0	2.654911	-0.473227	-1.623172
O 0	3.133107	-2.087935	0.155711
C 0	2.159310	1.748103	0.311887
C 0	1.369770	-0.570455	1.963422
N 0	2.972243	2.472899	0.716290

C 0	-2.463888	-1.741365	-0.133312
C 0	-2.753334	1.335255	-0.169519
H 0	-0.263528	2.023451	0.938547
H 0	-0.361042	2.307800	-0.779781
H 0	-0.017656	-2.299276	0.667411
H 0	0.225207	-1.886456	-1.002494
H 0	1.783694	1.459978	-2.250880
H 0	0.632703	0.120860	-2.221649
H 0	3.633696	0.021651	-1.599254
H 0	2.686395	-1.200393	-2.440362
H 0	0.422096	-0.297033	2.440362
H 0	2.142720	0.125054	2.304195
H 0	1.651958	-1.573832	2.296826
H 0	-3.435253	-1.277062	-0.310887
H 0	-2.531706	-2.317719	0.799792
H 0	-2.295705	-2.472899	-0.935948
H 0	-3.633696	0.694122	-0.104475
H 0	-2.823899	1.909775	-1.103814
H 0	-2.816199	2.066847	0.647868

P-54+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.170153	-1.062126	-0.189746
C 0	-1.470547	0.241204	-0.054577
C 0	-0.402583	1.289756	0.180045
C 0	1.058934	0.860400	-0.025170
C 0	1.324153	-0.603155	0.449467
C 0	0.260025	-1.563585	-0.167423
C 0	2.629965	-0.954722	-0.280170
C 0	1.473217	0.797113	-1.527332
C 0	2.715228	-0.114474	-1.564161
O 0	3.452655	-1.765947	0.086856
C 0	1.418414	-0.829107	1.960170
C 0	-2.170412	-2.169845	-0.424064
C 0	-2.865614	0.819769	-0.075339
C 0	1.973200	1.875743	0.691865
H 0	-0.525658	1.672144	1.206547
H 0	-0.607538	2.159478	-0.464726
H 0	0.308234	-2.511461	0.385107
H 0	0.534240	-1.836924	-1.199482
H 0	1.670305	1.797663	-1.927419
H 0	0.658990	0.368526	-2.121791
H 0	3.655500	0.448880	-1.538446
H 0	2.771432	-0.766082	-2.442912
H 0	0.446714	-0.674450	2.442912
H 0	2.147616	-0.164137	2.431628
H 0	1.743633	-1.855616	2.156740
H 0	-3.192696	-1.817053	-0.571821
H 0	-2.176287	-2.873898	0.419940
H 0	-1.892512	-2.756400	-1.311240
H 0	-3.655500	0.068400	-0.126837
H 0	-2.992707	1.499464	-0.929960
H 0	-3.042599	1.423478	0.825926
H 0	1.745628	1.946105	1.760161
H 0	1.832878	2.873898	0.259218
H 0	3.036037	1.622307	0.596870

P-55+DMB

B3LYP/6-31G(d) Geometry

C 0	0.992831	0.673465	-0.237189
C 0	0.992619	-0.673754	-0.237262
C 0	0.053911	-1.389566	0.721070
C 0	-1.360844	-0.768801	0.717350
C 0	-1.360585	0.769264	0.717322
C 0	0.054397	1.389480	0.721266
C 0	-2.103412	1.145251	-0.561076
C 0	-2.103968	-1.144563	-0.560966
O 0	-2.532667	0.000419	-1.218001
O 0	-2.319459	-2.236689	-1.002970
O 0	-2.318371	2.237446	-1.003172
C 0	1.855644	1.568039	-1.088396
C 0	1.855092	-1.568515	-1.088615
H 0	0.447012	-1.344376	1.747480
H 0	-0.033025	-2.450642	0.466095
H 0	-1.938653	-1.180263	1.552904
H 0	-1.938401	1.180924	1.552777
H 0	0.447393	1.343897	1.747696
H 0	-0.032057	2.450642	0.466495
H 0	2.532356	1.020611	-1.747696
H 0	2.466742	2.228949	-0.457716
H 0	1.232980	2.223440	-1.712410
H 0	2.465235	-2.230395	-0.458040
H 0	2.532667	-1.021246	-1.747156
H 0	1.232192	-2.222956	-1.713414

P-56+DMB

B3LYP/6-31G(d) Geometry

C 0	0.643406	0.736444	-0.057413
C 0	0.964287	-0.553048	-0.277695
C 0	0.205573	-1.613331	0.504700
C 0	-1.321310	-1.377014	0.512681
C 0	-1.682374	0.110285	0.714525
C 0	-0.464488	1.028389	0.940449
C 0	-2.410569	0.522406	-0.566240
C 0	-1.990841	-1.738774	-0.841580
O 0	-2.603526	-0.551540	-1.372838
O 0	-2.781804	1.629114	-0.866290
C 0	1.274810	1.941677	-0.703257
C 0	2.042161	-1.056773	-1.202640
H 0	0.558849	-1.628572	1.547411
H 0	0.415970	-2.613644	0.105014
H 0	-1.763956	-1.988931	1.305059
H 0	-2.393509	0.244210	1.538553
H 0	-0.100044	0.890581	1.969619
H 0	-0.799751	2.067396	0.858863
H 0	-2.774180	-2.495619	-0.734646
H 0	-1.265795	-2.091823	-1.582129
H 0	2.075191	1.692948	-1.403601
H 0	1.694288	2.613644	0.058681
H 0	0.516608	2.521770	-1.246396
H 0	2.781804	-1.652137	-0.648532
H 0	2.580025	-0.257441	-1.716765
H 0	1.622258	-1.722954	-1.969619

P-57+DMB

B3LYP/6-31G(d) Geometry

C 0	1.560438	0.637066	-0.269596
C 0	1.820230	-0.586542	0.225288
C 0	0.763523	-1.425017	0.920908
C 0	-0.673455	-0.910226	0.799918
C 0	-0.735629	0.634817	0.893570
C 0	0.182833	1.265843	-0.164014
C 0	-2.915135	0.645474	-0.460269
C 0	-1.391695	-1.392728	-0.464363
C 0	-2.823283	-0.887345	-0.611185

O 0	-0.878867	-2.135569	-1.280175
C 0	-2.190276	1.136187	0.803260
C 0	2.550088	1.508700	-1.005337
C 0	3.160052	-1.280273	0.163847
H 0	0.807131	-2.445625	0.519876
H 0	1.028056	-1.508351	1.986744
H 0	-1.268690	-1.311722	1.636407
H 0	-0.336968	0.911020	1.879682
H 0	-0.291314	1.229793	-1.158019
H 0	0.292078	2.337805	0.059329
H 0	-2.482645	1.118884	-1.350332
H 0	-3.968270	0.950320	-0.433805
H 0	-3.422230	-1.360728	0.181980
H 0	-3.216981	-1.229331	-1.572910
H 0	-2.738387	0.785182	1.689719
H 0	-2.209335	2.233383	0.841394
H 0	3.516797	1.032064	-1.177284
H 0	2.729658	2.445625	-0.458383
H 0	2.147607	1.797976	-1.986744
H 0	3.968270	-0.649352	-0.210552
H 0	3.103808	-2.171753	-0.476330
H 0	3.453179	-1.634580	1.162308

P-58+DMB

B3LYP/6-31G(d) Geometry

C 0	1.839953	0.166478	0.177884
C 0	1.438985	-0.841391	-0.618796
C 0	-0.014534	-1.272229	-0.707966
C 0	-0.931743	-0.760016	0.436871
C 0	-0.621103	0.745724	0.703522
C 0	0.864619	0.927310	1.056391
C 0	-2.548375	1.508101	-0.766931
C 0	-2.400973	-0.916213	-0.010670
C 0	-2.915828	0.046295	-1.077661
O 0	-3.128453	-1.772428	0.459270
C 0	-1.053441	1.653797	-0.462964
C 0	-0.698332	-1.604136	1.701020
C 0	3.266372	0.638616	0.331430
C 0	2.339448	-1.644258	-1.528138
H 0	-0.400668	-0.962282	-1.690554
H 0	-0.062624	-2.370684	-0.720804
H 0	-1.211905	1.051419	1.580634
H 0	1.037879	0.638096	2.104303
H 0	1.110499	1.999095	1.015986
H 0	-2.839609	2.151153	-1.606346
H 0	-3.128822	1.847711	0.102357
H 0	-2.473691	-0.237315	-2.043544
H 0	-3.996628	-0.100237	-1.161600
H 0	-0.461382	1.426084	-1.359773
H 0	-0.828628	2.696416	-0.203299
H 0	0.363964	-1.637803	1.959330
H 0	-1.050998	-2.626482	1.543973
H 0	-1.252153	-1.196974	2.554387
H 0	3.376722	1.671533	-0.028392
H 0	3.996628	0.021897	-0.195582
H 0	3.550954	0.651553	1.393033
H 0	2.375407	-2.696416	-1.212027
H 0	3.365026	-1.273311	-1.571731
H 0	1.945612	-1.645042	-2.554387

P-59+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.540620	-0.301620	-0.581053
C 0	-1.817782	0.675909	0.300531
C 0	-0.773443	1.219058	1.256746
C 0	0.668428	0.795232	0.958708
C 0	0.765976	-0.702073	0.531592
C 0	-0.156068	-0.918023	-0.688601
C 0	2.901590	-0.131365	-0.830715
C 0	1.339767	1.708210	-0.075934
C 0	2.779099	1.347138	-0.415558
O 0	0.777742	2.663729	-0.578184
C 0	2.234211	-1.059798	0.193632
C 0	0.302603	-1.608562	1.689183
C 0	-2.514537	-0.870847	-1.585330
C 0	-3.160684	1.346814	0.462320
H 0	-0.823349	2.314779	1.241741
H 0	-1.040687	0.920736	2.281907
H 0	1.272484	0.908737	1.874243
H 0	0.319133	-0.527775	-1.602030
H 0	-0.258041	-2.000068	-0.863022
H 0	2.448454	-0.265613	-1.820684
H 0	3.959499	-0.398494	-0.941632
H 0	3.388517	1.517365	0.485143
H 0	3.136316	2.026674	-1.194695
H 0	2.816207	-1.032652	1.127062
H 0	2.277337	-2.097585	-0.163954
H 0	-0.758428	-1.467605	1.914902
H 0	0.877466	-1.409788	2.602327
H 0	0.448914	-2.663729	1.426992
H 0	-3.486785	-0.374798	-1.587723
H 0	-2.683924	-1.941868	-1.403075
H 0	-2.104086	-0.793003	-2.602327
H 0	-3.959499	0.885110	-0.121028
H 0	-3.099079	2.404712	0.171401
H 0	-3.471329	1.333307	1.516682

P-60+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.550237	-0.049765	0.510617
C 0	-1.822733	-0.682179	-0.644428
C 0	-0.787183	-0.856422	-1.738929
C 0	0.653862	-0.543386	-1.332019
C 0	0.735193	0.727647	-0.426992
C 0	-0.178811	0.528955	0.807143
C 0	2.899252	-0.173734	0.647842
C 0	1.359651	-1.722721	-0.642793
C 0	2.792864	-1.451051	-0.207951
O 0	0.825071	-2.802833	-0.488877
C 0	2.208198	1.022381	-0.021872
C 0	0.243325	1.883570	-1.201824
N 0	-0.112767	2.802833	-1.815994
C 0	-2.516981	0.141849	1.654276
C 0	-3.160807	-1.274258	-1.013326
H 0	-0.825075	-1.891609	-2.098463
H 0	-1.066443	-0.223773	-2.593915
H 0	1.248578	-0.337047	-2.235107
H 0	0.334622	-0.125320	1.526826
H 0	-0.290663	1.494627	1.318787
H 0	2.464829	-0.362416	1.636542
H 0	3.954073	0.069150	0.820303
H 0	3.396130	-1.322361	-1.119465
H 0	3.170394	-2.331013	0.320158
H 0	2.762819	1.303166	-0.926613
H 0	2.230471	1.894552	0.642035
H 0	-3.465274	-0.379979	1.517119

H 0 -2.737908 1.207993 1.805333
H 0 -2.076081 -0.220425 2.593915
H 0 -3.954073 -1.051635 -0.297887
H 0 -3.085476 -2.366416 -1.106950
H 0 -3.485278 -0.898829 -1.993692

P-61+DMB

B3LYP/6-31G(d) Geometry
C 0 -1.831430 -0.126459 -0.636599
C 0 -1.428008 -0.750279 0.484289
C 0 0.027444 -1.096452 0.736942
C 0 0.961924 -0.993035 -0.485269
C 0 0.623517 0.256419 -1.336031
C 0 -0.859303 0.248684 -1.738379
C 0 2.517875 1.561723 -0.249275
C 0 2.435942 -0.975096 -0.007950
C 0 2.905576 0.343164 0.605792
O 0 3.169615 -1.934361 -0.090012
C 0 1.025576 1.549313 -0.595042
Cl 0 0.712163 -2.483944 -1.524568
C 0 -3.262234 0.224530 -0.966577
C 0 -2.322800 -1.169735 1.626097
H 0 0.406432 -0.439160 1.534780
H 0 0.105296 -2.113088 1.141415
H 0 1.228823 0.204419 -2.250806
H 0 -1.005696 -0.440757 -2.581436
H 0 -1.120255 1.244567 -2.125210
H 0 2.785703 2.483944 0.279811
H 0 3.104884 1.551399 -1.177782
H 0 2.453239 0.441796 1.603126
H 0 3.986960 0.263734 0.748501
H 0 0.420694 1.668777 0.313498
H 0 0.785617 2.403792 -1.239889
H 0 -3.388307 1.313356 -1.048916
H 0 -3.986960 -0.142021 -0.237591
H 0 -3.538151 -0.193145 -1.944827
H 0 -2.349502 -2.264650 1.717051
H 0 -3.350917 -0.817338 1.528030
H 0 -1.934083 -0.789228 2.581436

P-62+DMB

B3LYP/6-31G(d) Geometry
C 0 -1.668030 0.492386 -0.155397
C 0 -1.486585 -0.837930 -0.082038
C 0 -0.113009 -1.470997 -0.197376
C 0 1.007848 -0.569255 -0.786984
C 0 0.895321 0.858994 -0.130388
C 0 -0.515546 1.448344 -0.389301
C 0 2.603471 0.239340 1.678562
C 0 2.366190 -1.215495 -0.418109
C 0 2.808462 -1.145811 1.041608
O 0 3.032942 -1.801668 -1.248122
C 0 1.206153 0.801878 1.392793
C 0 1.880233 1.773302 -0.745124
C 0 0.863049 -0.509403 -2.316473
N 0 2.651114 2.510992 -1.204603
C 0 -2.999325 1.199819 -0.065047
C 0 -2.578347 -1.855767 0.148750
H 0 0.167920 -1.856030 0.793421
H 0 -0.182558 -2.363610 -0.834314
H 0 -0.570882 1.829755 -1.418525
H 0 -0.639092 2.332641 0.250979
H 0 2.767409 0.178675 2.760654
H 0 3.356763 0.933174 1.286331
H 0 2.227210 -1.893522 1.600766
H 0 3.854252 -1.462907 1.082056
H 0 0.433396 0.194980 1.878544
H 0 1.119066 1.813356 1.806072
H 0 -0.148288 -0.204443 -2.600824
H 0 1.062139 -1.495696 -2.741362
H 0 1.580093 0.187056 -2.760654
H 0 -3.039235 1.846071 0.822986
H 0 -3.854252 0.522873 -0.025092
H 0 -3.141053 1.858875 -0.932820
H 0 -2.691452 -2.509974 -0.726899
H 0 -3.552522 -1.413855 0.364126
H 0 -2.319288 -2.510992 0.992085

P-63+DMB

B3LYP/6-31G(d) Geometry
C 0 1.750605 0.298628 0.068155
C 0 1.439937 -0.960002 -0.289169
C 0 0.012853 -1.474149 -0.258017
C 0 -0.996082 -0.631317 0.575927
C 0 -0.774217 0.900142 0.271696
C 0 0.696458 1.267934 0.563900
C 0 -2.519306 0.810811 -1.627676
C 0 -2.424762 -1.025205 0.144505
C 0 -2.856235 -0.649607 -1.271122
O 0 -3.183336 -1.615936 0.892289
C 0 -1.087806 1.187805 -1.221880
C 0 -0.807558 -0.975878 2.064251
C 0 3.142012 0.886164 0.067092
C 0 2.421628 -1.993177 -0.790021
C 0 -1.678750 1.788190 1.154749
H 0 -0.324695 -1.582994 -1.298461
H 0 0.011365 -2.497521 0.143832
H 0 0.834635 1.401464 1.648512
H 0 0.895959 2.261599 0.133556
H 0 -2.659837 0.969444 -2.703780
H 0 -3.233038 1.475465 -1.126235
H 0 -2.343462 -1.321649 -1.973431
H 0 -3.927104 -0.856297 -1.356096
H 0 -0.368496 0.656316 -1.856967
H 0 -0.927417 2.257540 -1.410439
H 0 0.212819 -0.753938 2.391115
H 0 -0.993451 -2.041477 2.223695
H 0 -1.509218 -0.435398 2.703780
H 0 3.216916 1.708767 -0.658336
H 0 3.927104 0.164108 -0.165082
H 0 3.374124 1.321114 1.049470
H 0 2.493390 -2.835908 -0.087902
H 0 3.428863 -1.602926 -0.946986
H 0 2.079691 -2.416880 -1.744891
H 0 -1.383977 1.743244 2.207185
H 0 -2.734492 1.500913 1.100844
H 0 -1.602911 2.835908 0.838307

P-64+DMB

B3LYP/6-31G(d) Geometry
C 0 -2.060409 -1.188109 0.120107
C 0 -0.664131 -0.692260 0.541635
O 0 -2.337442 -0.740044 -1.224098
C 0 -3.222743 -0.531119 0.884193
C 0 -2.652667 0.622531 -1.018696
C 0 -0.613833 0.861038 0.502541

O 0	-3.479181	0.672009	0.140151
C 0	0.408602	-1.312597	-0.367632
C 0	-1.335557	1.374843	-0.747505
C 0	0.796638	1.429695	0.692461
C 0	1.769864	-0.647077	-0.328114
O 0	-0.952380	2.281784	-1.455834
C 0	1.941762	0.598289	0.148604
C 0	2.858868	-1.513888	-0.914121
C 0	3.262492	1.327669	0.217256
H 0	-2.111090	-2.280263	0.112617
H 0	-0.478664	-1.011960	1.576960
H 0	-2.973602	-0.277735	1.920476
H 0	-4.121040	-1.158690	0.873428
H 0	-3.180051	1.023492	-1.886919
H 0	-1.241246	1.231955	1.326289
H 0	0.043420	-1.312677	-1.404948
H 0	0.521542	-2.374186	-0.100283
H 0	0.974202	1.603633	1.764971
H 0	0.826236	2.422623	0.224429
H 0	2.575253	-1.853022	-1.920476
H 0	3.002062	-2.422623	-0.311929
H 0	3.824706	-1.013032	-0.998066
H 0	3.440751	1.700945	1.235690
H 0	3.252305	2.210501	-0.437138
H 0	4.121040	0.714420	-0.061878

P-65+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.476464	-1.537727	0.065920
C 0	-0.526035	-0.771528	1.006629
O 0	-1.132804	-1.284515	-1.309917
C 0	-2.938615	-1.065713	0.086960
C 0	-1.684285	-0.004474	-1.511759
C 0	-0.394175	0.753766	0.637938
O 0	-2.959363	0.005102	-0.867643
C 0	0.864557	-1.471940	1.067717
C 0	-0.787262	1.034436	-0.831899
C 0	1.076325	1.218226	0.808415
C 0	1.878267	-0.958123	0.061848
O 0	-0.441683	2.039267	-1.421753
C 0	2.015363	0.376103	-0.034365
C 0	2.651786	-1.999446	-0.701524
C 0	2.970849	1.124314	-0.924864
C 0	-1.313499	1.631558	1.522547
H 0	-1.389116	-2.615436	0.228091
H 0	-0.965006	-0.838904	2.011872
H 0	-3.267336	-0.698071	1.063712
H 0	-3.617961	-1.859374	-0.246220
H 0	-1.792337	0.199360	-2.579357
H 0	0.729626	-2.554986	0.958455
H 0	1.268403	-1.326597	2.081193
H 0	1.336682	1.156961	1.876779
H 0	1.140662	2.271563	0.522845
H 0	1.969433	-2.612005	-1.307094
H 0	3.169427	-2.687191	-0.017627
H 0	3.401172	-1.572830	-1.372050
H 0	2.416007	1.770709	-1.617814
H 0	3.617846	0.469093	-1.513017
H 0	3.617961	1.785458	-0.331041
H 0	-1.050603	1.504688	2.579357
H 0	-2.370982	1.382229	1.395522
H 0	-1.187739	2.687191	1.260789

P-66+DMB

B3LYP/6-31G(d) Geometry

C 0	-2.050293	-1.038433	-0.227895
C 0	-0.647264	-0.745322	0.365568
O 0	-2.273491	-0.211606	-1.389242
C 0	-3.239256	-0.604724	0.649823
C 0	-2.574096	1.039165	-0.805378
C 0	-0.577312	0.760384	0.775810
O 0	-3.446495	0.770962	0.286691
C 0	0.406112	-1.026412	-0.730675
C 0	-1.256811	1.638740	-0.281713
C 0	0.836246	1.229690	1.136425
C 0	1.774853	-0.409222	-0.510524
O 0	-0.835965	2.706993	-0.673908
C 0	1.966612	0.622988	0.329851
C 0	2.844279	-1.046129	-1.365972
C 0	3.291649	1.298600	0.591464
C 0	-0.382012	-1.650520	1.582323
H 0	-2.119580	-2.079497	-0.556228
H 0	-3.048464	-0.671336	1.724879
H 0	-4.141167	-1.179693	0.410855
H 0	-3.056896	1.691700	-1.535911
H 0	-1.215411	0.888077	1.663433
H 0	0.019897	-0.684119	-1.700292
H 0	0.519697	-2.116707	-0.832150
H 0	1.024601	1.037227	2.203692
H 0	0.867023	2.321214	1.024088
H 0	2.535978	-1.050601	-2.421004
H 0	2.994921	-2.098301	-1.084710
H 0	3.811350	-0.543505	-1.310050
H 0	3.493939	1.340176	1.671080
H 0	3.270230	2.339994	0.241319
H 0	4.141167	0.803816	0.117404
H 0	-0.514020	-2.706993	1.317078
H 0	-1.051048	-1.426891	2.421004
H 0	0.646739	-1.526720	1.933953

P-67+DMB

B3LYP/6-31G(d) Geometry

C 0	-2.065297	0.869025	0.439339
C 0	-0.649271	0.746556	-0.212701
O 0	-2.281500	-0.275052	1.274525
C 0	-3.229491	0.739454	-0.556133
C 0	-2.592392	-1.284317	0.328126
C 0	-0.582109	-0.555069	-1.082209
O 0	-3.444122	-0.681486	-0.634343
C 0	0.421942	0.707209	0.905994
C 0	-1.271606	-1.708389	-0.338724
C 0	0.831743	-0.876536	-1.570699
C 0	1.780922	0.171691	0.500800
O 0	-0.855480	-2.844946	-0.294209
C 0	1.962853	-0.554677	-0.615236
C 0	2.853820	0.516923	1.505575
C 0	3.284290	-1.118414	-1.078374
C 0	-0.428015	1.916082	-1.078987
N 0	-0.292017	2.844946	-1.763162
H 0	-2.121919	1.759948	1.068384
H 0	-3.003254	1.137348	-1.549856
H 0	-4.135840	1.219761	-0.172844
H 0	-3.089695	-2.121341	0.821977
H 0	-1.221925	-0.395792	-1.961004
H 0	0.021622	0.099044	1.727670
H 0	0.536372	1.721261	1.313023

H 0	1.013238	-0.347552	-2.517672
H 0	0.862918	-1.946251	-1.813454
H 0	2.538540	0.226739	2.517672
H 0	3.027714	1.601897	1.533267
H 0	3.810104	0.029898	1.309237
H 0	3.481608	-0.820917	-2.117496
H 0	3.260126	-2.216872	-1.068899
H 0	4.135840	-0.795804	-0.477432

P-68+DMB

B3LYP/6-31G(d) Geometry

C 0	1.477735	-1.536958	-0.543459
C 0	0.621223	-0.482254	-1.268217
O 0	1.026704	-1.671008	0.818560
C 0	2.957663	-1.162687	-0.339115
C 0	1.644733	-0.560573	1.434353
C 0	0.565408	0.864166	-0.482332
O 0	2.966349	-0.491874	0.930677
C 0	-0.817348	-1.022442	-1.533878
C 0	0.868073	0.701148	1.035886
C 0	-0.784838	1.569275	-0.648419
C 0	-1.858856	-0.621750	-0.503090
Cl 0	1.895363	1.999032	-1.113692
O 0	0.493064	1.507626	1.857588
C 0	-1.875201	0.661638	-0.100473
C 0	-2.806544	-1.707141	-0.068933
C 0	-2.825867	1.291605	0.880959
H 0	1.360753	-2.511920	-1.023516
H 0	1.088553	-0.285130	-2.238968
H 0	3.349972	-0.496194	-1.111170
H 0	3.586720	-2.057247	-0.269178
H 0	1.651805	-0.682501	2.519593
H 0	-1.140589	-0.656255	-2.519593
H 0	-0.775312	-2.113913	-1.624435
H 0	-0.935435	1.798629	-1.712279
H 0	-0.753759	2.516053	-0.105778
H 0	-2.253323	-2.516053	0.427731
H 0	-3.311443	-2.156381	-0.935717
H 0	-3.578098	-1.356214	0.619586
H 0	-3.343909	2.146112	0.423633
H 0	-2.271213	1.684604	1.742953
H 0	-3.586720	0.600401	1.250635

P-69+DMB

B3LYP/6-31G(d) Geometry

C 0	1.998449	1.141014	-0.800555
C 0	0.666033	0.865884	-0.015897
O 0	2.122662	0.145602	-1.826028
C 0	3.312005	0.934031	-0.039327
C 0	2.577453	-0.972574	-1.087561
C 0	0.638547	-0.585226	0.626013
O 0	3.559913	-0.476576	-0.188175
C 0	-0.468005	1.060271	-1.070278
C 0	1.357096	-1.555330	-0.341359
C 0	-0.800389	-1.051543	0.948697
C 0	-1.816766	0.453542	-0.769440
O 0	1.028417	-2.711130	-0.502022
C 0	-1.957977	-0.531580	0.129265
C 0	-2.916694	1.032841	-1.625527
C 0	-3.258425	-1.216652	0.473949
C 0	0.519925	1.887516	1.032038
C 0	1.424467	-0.707842	1.969872
N 0	0.432442	2.711130	1.846791
H 0	1.935859	2.116826	-1.287026
H 0	3.259893	1.198989	1.019320
H 0	4.127149	1.491524	-0.512525
H 0	3.011052	-1.716255	-1.759092
H 0	-0.103728	0.650529	-2.020650
H 0	-0.582656	2.140050	-1.237632
H 0	-1.010167	-0.811235	2.001514
H 0	-0.789376	-2.148076	0.898714
H 0	-2.639212	0.992682	-2.688350
H 0	-3.078180	2.093357	-1.386223
H 0	-3.871617	0.516459	-1.516819
H 0	-3.442559	-1.167603	1.556154
H 0	-3.213577	-2.283473	0.214875
H 0	-4.127149	-0.786530	-0.027048
H 0	1.060958	0.032909	2.688350
H 0	2.502696	-0.605008	1.858165
H 0	1.233691	-1.704014	2.382243

P-70+DMB

B3LYP/6-31G(d) Geometry

C 0	-1.995273	-1.374472	-0.369152
C 0	-0.666838	-0.825975	0.232115
O 0	-2.157472	-0.876210	-1.715328
C 0	-3.316353	-0.892373	0.246178
C 0	-2.597704	0.440793	-1.474876
C 0	-0.645369	0.758162	0.236130
O 0	-3.571610	0.347077	-0.438454
C 0	0.438596	-1.373300	-0.716695
C 0	-1.372889	1.269434	-1.030146
C 0	0.791809	1.334668	0.326188
C 0	1.803496	-0.729586	-0.647649
O 0	-1.049799	2.263959	-1.647025
C 0	1.954944	0.524478	-0.196456
C 0	2.902503	-1.604616	-1.200231
C 0	3.261783	1.277961	-0.126435
C 0	-0.446876	-1.409987	1.639554
C 0	-1.418858	1.428046	1.417705
H 0	-1.941590	-2.465008	-0.435382
H 0	-3.276053	-0.717844	1.324126
H 0	-4.128325	-1.595105	0.027394
H 0	-3.042078	0.863827	-2.378391
H 0	0.083957	-1.307590	-1.753483
H 0	0.541781	-2.450541	-0.516764
H 0	1.005607	1.571666	1.379639
H 0	0.774304	2.306217	-0.185660
H 0	2.647706	-1.945763	-2.213738
H 0	3.022196	-2.511898	-0.591000
H 0	3.873474	-1.109171	-1.255713
H 0	3.441889	1.646136	0.893603
H 0	3.231537	2.165872	-0.773320
H 0	4.128325	0.682030	-0.418729
H 0	-0.415171	-2.505383	1.594520
H 0	-1.234971	-1.131858	2.345959
H 0	0.509354	-1.072320	2.052673
H 0	-1.008036	1.104300	2.378391
H 0	-2.492643	1.246590	1.403845
H 0	-1.274952	2.511898	1.347525