BET & ELF Quantum Topological Analysis of Neutral 2-Aza-Cope Rearrangement of γ-Alkenyl Nitrones

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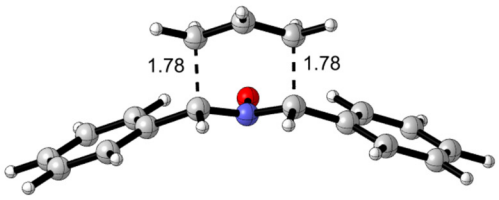
Electronic Supporting Information

Transition Structures



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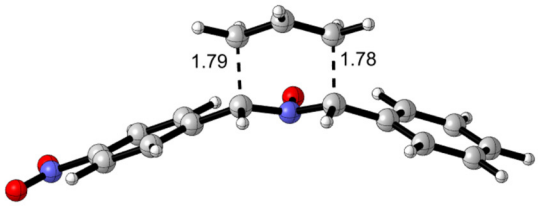

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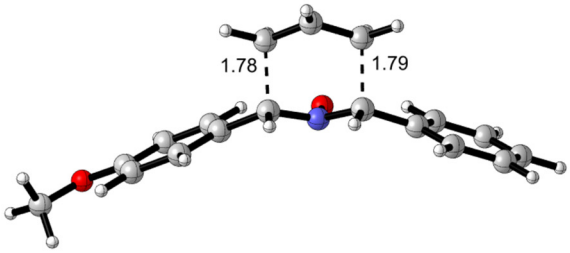

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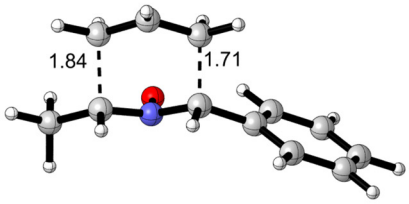

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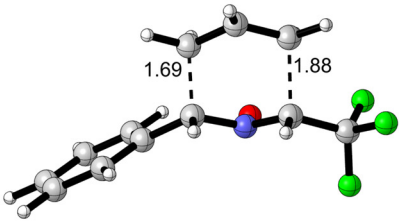

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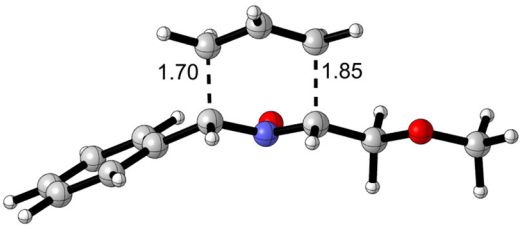

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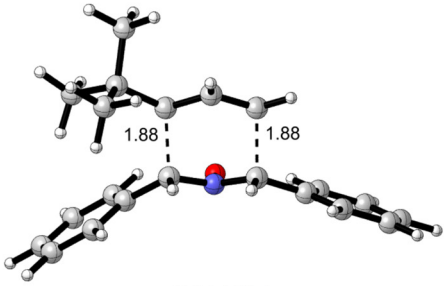
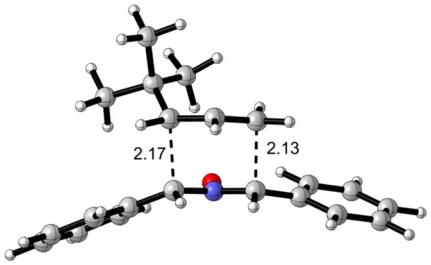


(*E*)-**TS07**



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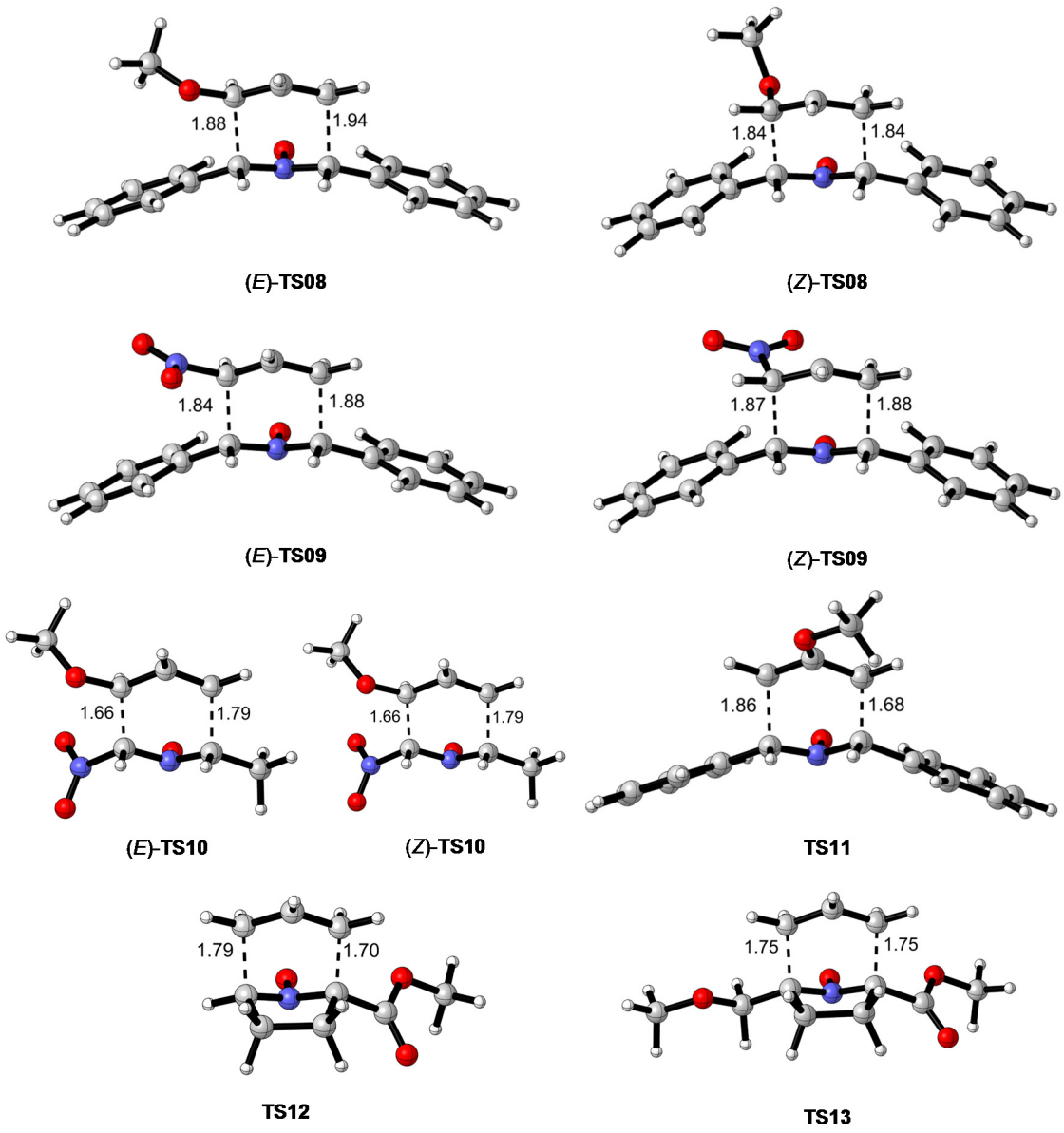

Figure S2. Transition structures for 2-aza-Cope rearrangements

Electronic populations (only 25 points before and 25 points after the TS are listed)

Table S1. Electronic population of basins for the rearrangement of nitrone **1**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.81	2.00	-	1.77	1.71	3.94	-	1.96	-	-	-	-	-	-	-
37	-	1.81	2.00	-	1.77	1.71	3.94	-	1.96	-	-	-	-	-	-	-
38	-	1.81	2.01	-	1.77	1.71	3.93	-	1.97	-	-	-	-	-	-	-
39	-	1.80	2.01	-	1.76	1.71	3.93	-	1.96	-	-	-	-	-	-	-
40	-	1.80	2.01	-	1.77	1.70	3.94	-	1.97	-	-	-	-	-	-	-
41	-	1.79	2.01	-	1.77	1.70	3.93	-	1.96	-	-	-	-	-	-	-
42	-	1.79	2.01	-	1.77	1.70	3.93	-	1.95	-	-	-	-	-	-	-
43	-	1.78	2.02	-	1.77	1.69	3.94	-	1.96	-	-	-	-	-	-	-
44	-	1.78	2.02	-	1.77	1.68	3.94	-	1.95	-	-	-	-	-	-	-
45	-	1.77	2.03	-	1.76	1.68	3.95	-	1.94	-	-	-	-	-	-	-
46	-	1.77	2.03	-	1.76	1.67	3.95	-	1.94	-	-	-	-	-	-	-
47	-	1.76	2.04	-	1.67	1.76	3.14	-	1.94	-	0.82	-	-	-	-	-
48	-	1.75	2.04	-	1.66	1.76	3.13	-	1.93	-	0.85	-	-	-	-	-
49	-	1.73	2.06	-	1.65	1.75	3.08	-	1.94	-	0.91	-	-	-	-	-
50	-	1.72	2.07	-	1.64	1.76	3.05	-	1.94	-	0.96	-	-	-	-	-
51	-	1.70	2.08	-	1.62	1.76	3.01	-	1.94	-	1.02	-	-	-	-	-
52	-	1.68	2.10	-	1.60	1.77	2.98	-	1.95	-	1.07	-	-	-	-	-
53	-	1.66	2.12	-	3.34	-	2.64	-	1.96	-	1.12	0.33	-	-	-	-
54	-	1.63	2.14	-	3.33	-	2.55	-	1.96	-	1.18	0.40	-	-	-	-
55	-	1.60	2.16	-	3.33	-	2.48	-	1.97	-	1.22	0.47	-	-	-	-
56	-	1.57	2.19	-	3.32	-	2.41	-	1.98	-	1.27	0.53	-	-	-	-
57	-	1.54	2.22	-	3.02	-	2.35	-	2.00	-	1.30	0.59	-	-	0.29	-
58	1.01	1.49	2.26	-	2.94	-	2.29	-	2.02	-	1.33	-	-	-	-	-
59	1.12	1.44	2.30	-	2.85	-	2.24	-	2.05	-	1.36	-	-	-	-	-
60	1.22	1.38	2.35	-	2.78	-	2.18	-	2.08	-	1.37	-	-	-	-	-
61	1.31	1.31	2.42	-	2.42	-	2.13	-	2.13	-	1.38	-	-	-	-	0.29
62	1.39	1.22	2.78	-	2.35	-	2.08	-	2.18	-	1.37	-	-	-	-	-
63	1.44	1.12	2.85	-	2.30	-	2.04	-	2.24	-	1.36	-	-	-	-	-
64	1.50	1.01	2.93	-	2.26	-	2.02	-	2.29	-	1.33	-	-	-	-	-
65	1.54	-	3.04	-	2.22	-	2.00	-	2.36	-	1.30	-	0.33	0.20	-	-
66	1.57	-	3.32	-	2.19	-	1.98	-	2.42	-	1.26	-	0.40	-	-	-
67	1.61	-	3.33	-	2.16	-	1.97	-	2.48	-	1.22	-	0.47	-	-	-
68	1.63	-	3.33	-	2.14	-	1.96	-	2.55	-	1.18	-	0.53	-	-	-
69	1.66	-	3.34	-	2.12	-	1.96	-	2.64	-	1.12	-	0.59	-	-	-
70	1.68	-	1.60	1.77	2.10	-	1.95	-	2.98	-	1.07	-	-	-	-	-
71	1.70	-	1.62	1.77	2.08	-	1.95	-	3.01	-	1.01	-	-	-	-	-
72	1.72	-	1.64	1.76	2.07	-	1.94	-	3.04	-	0.96	-	-	-	-	-
73	1.73	-	1.65	1.76	2.06	-	1.94	-	3.08	-	0.91	-	-	-	-	-
74	1.75	-	1.66	1.76	2.05	-	1.93	-	3.13	-	0.85	-	-	-	-	-
75	1.76	-	1.67	1.76	2.04	-	1.94	-	3.14	-	0.82	-	-	-	-	-
76	1.77	-	1.67	1.76	2.03	-	1.94	-	3.95	-	-	-	-	-	-	-
77	1.77	-	1.68	1.76	2.03	-	1.94	-	3.95	-	-	-	-	-	-	-

78	1.78	-	1.69	1.76	2.02	-	1.95	-	3.95	-	-	-	-	-	-	-
79	1.78	-	1.69	1.77	2.02	-	1.95	-	3.95	-	-	-	-	-	-	-
80	1.79	-	1.70	1.76	2.01	-	1.95	-	3.94	-	-	-	-	-	-	-
81	1.79	-	1.70	1.77	2.01	-	1.96	-	3.94	-	-	-	-	-	-	-
82	1.80	-	1.70	1.77	2.01	-	1.97	-	3.93	-	-	-	-	-	-	-
83	1.80	-	1.71	1.76	2.01	-	1.97	-	3.93	-	-	-	-	-	-	-
84	1.81	-	1.71	1.77	2.01	-	1.97	-	3.94	-	-	-	-	-	-	-
85	1.81	-	1.71	1.77	2.00	-	1.96	-	3.94	-	-	-	-	-	-	-
86	1.81	-	1.72	1.77	2.00	-	1.96	-	3.94	-	-	-	-	-	-	-

Table S2. Electronic population of basins for the rearrangement of nitrones **2**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	1.81	-	1.71	1.76	2.00	-	1.96	-	3.95	-	-	-	-	-	-	-
37	1.80	-	1.71	1.76	2.01	-	1.96	-	3.95	-	-	-	-	-	-	-
38	1.80	-	1.71	1.77	2.01	-	1.95	-	3.95	-	-	-	-	-	-	-
39	1.80	-	1.70	1.77	2.00	-	1.95	-	3.95	-	-	-	-	-	-	-
40	1.80	-	1.76	1.70	2.01	-	1.95	-	3.94	-	-	-	-	-	-	-
41	1.79	-	1.70	1.76	2.01	-	1.94	-	3.96	-	-	-	-	-	-	-
42	1.78	-	1.69	1.76	2.01	-	1.94	-	3.95	-	-	-	-	-	-	-
43	1.78	-	1.68	1.76	2.02	-	1.94	-	3.96	-	-	-	-	-	-	-
44	1.77	-	1.68	1.77	2.02	-	1.94	-	3.96	-	-	-	-	-	-	-
45	1.77	-	1.68	1.76	2.02	-	1.94	-	3.96	-	-	-	-	-	-	-
46	1.76	-	1.67	1.76	2.03	-	1.94	-	3.95	-	-	-	-	-	-	-
47	1.75	-	1.76	1.66	2.03	-	1.94	-	3.14	-	-	-	-	-	-	-
48	1.74	-	1.76	1.65	2.04	-	1.93	-	3.10	-	-	-	-	-	-	-
49	1.73	-	1.76	1.64	2.05	-	1.94	-	3.06	-	-	-	-	-	-	-
50	1.71	-	1.76	1.62	2.06	-	1.94	-	3.02	-	-	-	-	-	-	-
51	1.69	-	1.76	1.61	2.08	-	1.94	-	2.99	-	-	-	-	-	-	-
52	1.67	-	1.77	1.58	2.09	-	1.94	-	2.97	-	-	-	-	-	-	-
53	1.65	-	3.32	-	2.12	-	1.95	-	2.65	-	-	-	0.31	-	-	-
54	1.63	-	3.31	-	2.13	-	1.95	-	2.56	-	-	-	0.39	-	-	-
55	1.60	-	3.31	-	2.15	-	1.97	-	2.48	-	-	-	0.45	-	-	-
56	1.58	-	3.31	-	2.18	-	1.98	-	2.42	-	-	-	0.52	-	-	-
57	1.54	-	3.01	-	2.21	-	2.00	-	2.35	-	-	-	0.59	0.28	-	-
58	1.50	1.00	2.92	-	2.25	-	2.02	-	2.29	-	-	-	-	-	-	-
59	1.43	1.11	2.84	-	2.30	-	2.05	-	2.23	-	-	-	-	-	-	-
60	1.37	1.21	2.77	-	2.35	-	2.08	-	2.17	-	-	-	-	-	-	-
61	1.30	1.30	2.43	-	2.43	-	2.14	-	2.12	-	-	-	-	-	-	0.26
62	1.21	1.37	2.35	-	2.77	-	2.19	-	2.07	-	-	-	-	-	-	-
63	1.10	1.43	2.30	-	2.84	-	2.25	-	2.04	-	-	-	-	-	-	-
64	-	1.49	2.25	-	2.93	-	2.30	-	2.02	-	-	0.65	-	-	0.34	-
65	-	1.53	2.22	-	3.02	-	2.36	-	2.00	-	-	0.59	-	-	0.27	-
66	-	1.57	2.18	-	3.30	-	2.43	-	1.99	-	-	0.52	-	-	-	-
67	-	1.60	2.16	-	3.31	-	2.49	-	1.98	-	-	0.46	-	-	-	-
68	-	1.63	2.14	-	3.31	-	2.56	-	1.97	-	-	0.40	-	-	-	-
69	-	1.66	2.11	-	3.32	-	2.65	-	1.97	-	-	0.33	-	-	-	-
70	-	1.68	2.10	-	1.77	1.58	2.99	-	1.97	-	0.83	-	-	-	-	-

71	-	1.70	2.08	-	1.76	1.62	3.01	-	1.97	-	0.88	-	-	-	-	-
72	-	1.72	2.07	-	1.75	1.63	3.06	-	1.96	-	0.93	-	-	-	-	-
73	-	1.73	2.06	-	1.75	1.64	3.09	-	1.97	-	0.99	-	-	-	-	-
74	-	1.74	2.05	-	1.76	1.65	3.12	-	1.97	-	1.04	-	-	-	-	-
75	-	1.75	2.04	-	1.66	1.76	3.89	-	1.98	-	1.09	-	-	-	-	-
76	-	1.76	2.03	-	1.67	1.76	3.89	-	1.97	-	1.14	-	-	-	-	-
77	-	1.77	2.03	-	1.67	1.76	3.89	-	1.98	-	1.19	-	-	-	-	-
78	-	1.78	2.02	-	1.68	1.76	3.89	-	1.98	-	1.23	-	-	-	-	-
79	-	1.79	2.02	-	1.69	1.76	3.88	-	1.98	-	1.27	-	-	-	-	-
80	-	1.79	2.01	-	1.69	1.76	3.88	-	1.99	-	1.30	-	-	-	-	-
81	-	1.79	2.01	-	1.69	1.76	3.87	-	1.99	-	1.33	-	-	-	-	-
82	-	1.80	2.01	-	1.70	1.76	3.88	-	1.98	-	1.36	-	-	-	-	-
83	-	1.80	2.02	-	1.70	1.77	3.87	-	1.99	-	1.37	-	-	-	-	-
84	-	1.81	2.01	-	1.71	1.76	3.88	-	1.99	-	1.37	-	-	-	-	-
85	-	1.81	2.00	-	1.71	1.76	3.88	-	1.99	-	1.36	-	-	-	-	-
86	-	1.81	2.01	-	1.71	1.77	3.88	-	2.00	-	1.34	-	-	-	-	-

Table S3. Electronic population of basins for the rearrangement of nitrones **3**

IRC	**V(C1,C6)**	**V(C3,C4)**	**V1(C4,C5)**	**V2(C4C5)**	**V1C5,C6)**	**V2(C5,C6)**	**V1(C1,N2)**	**V2(C1,N2)**	**V1(C3,N2)**	**V2(C3,N2)**	**V(N2)**	**V(C1)**	**V(C3)**	**V(C4)**	**V(C5)**	**V(C6)**
36	1.82	-	1.71	1.77	2.01	-	1.96		3.94		-	-	-	-	-	-
37	1.81	-	1.71	1.77	2.01	-	1.96		3.93		-	-	-	-	-	-
38	1.81	-	1.70	1.77	2.01	-	1.97		3.93		-	-	-	-	-	-
39	1.81	-	1.70	1.77	2.02	-	1.96		3.94		-	-	-	-	-	-
40	1.80	-	1.70	1.77	2.02	-	1.96		3.93		-	-	-	-	-	-
41	1.80	-	1.70	1.77	2.01	-	1.97		3.93		-	-	-	-	-	-
42	1.79	-	1.70	1.77	2.01	-	1.96		3.93		-	-	-	-	-	-
43	1.79	-	1.69	1.76	2.02	-	1.96		3.93		-	-	-	-	-	-
44	1.78	-	1.69	1.77	2.02	-	1.95		3.95		-	-	-	-	-	-
45	1.78	-	1.68	1.76	2.02	-	1.95		3.95		-	-	-	-	-	-
46	1.77	-	1.67	1.76	2.03	-	1.95		3.93		-	-	-	-	-	-
47	1.76	-	1.67	1.76	2.04	-	1.95		3.93		-	-	-	-	-	-
48	1.75	-	1.66	1.76	2.04	-	1.95		3.13		0.83	-	-	-	-	-
49	1.74	-	1.76	1.65	2.05	-	1.95		3.09		0.88	-	-	-	-	-
50	1.72	-	1.76	1.64	2.06	-	1.95		3.05		0.94	-	-	-	-	-
51	1.71	-	1.76	1.62	2.08	-	1.95		3.01		0.99	-	-	-	-	-
52	1.69	-	1.78	1.59	2.09	-	1.95		2.99		1.04	-	-	-	-	-
53	1.66	-	3.33	-	2.11	-	1.95		2.65		1.10	-	0.32	-	-	-
54	1.64	-	3.33	-	2.13	-	1.96		2.57		1.15	-	0.38	-	-	-
55	1.61	-	3.33	-	2.15	-	1.97		2.49		1.20	-	0.45	-	-	-
56	1.58	-	3.32	-	2.18	-	1.98		2.22		1.25	-	0.52	-	-	-
57	1.55	-	3.04	-	2.21	-	1.99		2.20		1.29	-	0.58	0.27	-	-
58	1.50	-	2.95	-	2.24	-	2.01		2.18		1.33	-	0.64	0.34	-	-
59	1.45	1.11	2.88	-	2.29	-	2.04		2.16		1.35	-	-	-	-	-
60	1.39	1.21	2.80	-	2.34	-	2.07		2.14		1.36	-	-	-	-	-
61	1.32	1.30	2.43	-	2.41	-	2.11		2.12		1.37	-	-	-	-	0.30

62	1.23	1.37	2.36	-	2.78	-	2.17	2.11	1.37	-	-	-	-	-
63	1.14	1.44	2.30	-	2.85	-	2.22	2.10	1.36	-	-	-	-	-
64	1.02	1.49	2.25	-	2.93	-	2.28	2.09	1.34	-	-	-	-	-
65	-	1.54	2.21	-	3.01	-	2.33	2.08	1.31	0.60	-	-	0.30	-
66	-	1.57	2.18	-	3.32	-	2.40	2.08	1.28	0.53	-	-	-	-
67	-	1.60	2.15	-	3.33	-	2.46	2.08	1.24	0.47	-	-	-	-
68	-	1.63	2.13	-	3.32	-	2.54	2.07	1.20	0.40	-	-	-	-
69	-	1.66	2.12	-	3.34	-	2.62	1.95	1.15	0.32	-	-	-	-
70	-	1.69	2.09	-	1.78	1.59	2.96	1.95	1.10	-	-	-	-	-
71	-	1.71	2.08	-	1.77	1.62	2.98	1.95	1.05	-	-	-	-	-
72	-	1.72	2.07	-	1.76	1.63	3.01	1.94	1.00	-	-	-	-	-
73	-	1.73	2.06	-	1.76	1.65	3.04	1.94	0.95	-	-	-	-	-
74	-	1.74	2.05	-	1.76	1.66	3.08	1.94	0.90	-	-	-	-	-
75	-	1.76	2.04	-	1.76	1.66	3.13	1.94	0.85	-	-	-	-	-
76	-	1.76	2.03	-	1.77	1.67	3.14	1.94	0.82	-	-	-	-	-
77	-	1.77	2.03	-	1.68	1.77	3.95	1.95	-	-	-	-	-	-
78	-	1.78	2.02	-	1.69	1.77	3.96	1.95	-	-	-	-	-	-
79	-	1.79	2.02	-	1.69	1.77	3.96	1.95	-	-	-	-	-	-
80	-	1.79	2.01	-	1.69	1.77	3.96	1.95	-	-	-	-	-	-
81	-	1.80	2.01	-	1.70	1.77	3.96	1.95	-	-	-	-	-	-
82	-	1.80	2.01	-	1.77	1.70	3.95	1.95	-	-	-	-	-	-
83	-	1.80	2.01	-	1.77	1.70	3.96	1.95	-	-	-	-	-	-
84	-	1.81	2.01	-	1.77	1.71	3.96	1.95	-	-	-	-	-	-
85	-	1.81	2.01	-	1.77	1.71	3.96	1.95	-	-	-	-	-	-
86	-	1.81	2.01	-	1.77	1.71	3.96	1.96	-	-	-	-	-	-

Table S4. Electronic population of basins for the rearrangement of nitrones **4**

IRC	**V(C1,C6)**	**V(C3,C4)**	**V1(C4,C5)**	**V2(C4C5)**	**V1C5,C6)**	**V2(C5,C6)**	**V1(C1,N2)**	**V2(C1,N2)**	**V1(C3,N2)**	**V2(C3,N2)**	**V(N2)**	**V(C1)**	**V(C3)**	**V(C4)**	**V(C5)**	**V(C6)**
36	-	1.82	2.01	-	1.72	1.77	3.98		1.98		-	-	-	-	-	-
37	-	1.81	2.01	-	1.72	1.76	3.98		1.98		-	-	-	-	-	-
38	-	1.81	2.01	-	1.72	1.76	3.98		1.98		-	-	-	-	-	-
39	-	1.81	2.01	-	1.77	1.71	3.98		1.98		-	-	-	-	-	-
40	-	1.80	2.01	-	1.71	1.76	3.98		1.97		-	-	-	-	-	-
41	-	1.80	2.01	-	1.71	1.76	3.98		1.97		-	-	-	-	-	-
42	-	1.80	2.02	-	1.70	1.76	3.98		1.98		-	-	-	-	-	-
43	-	1.79	2.02	-	1.70	1.76	3.98		1.97		-	-	-	-	-	-
44	-	1.79	2.02	-	1.70	1.76	3.98		1.97		-	-	-	-	-	-
45	-	1.78	2.03	-	1.69	1.76	3.99		1.97		-	-	-	-	-	-
46	-	1.78	2.03	-	1.69	1.76	4.00		1.97		-	-	-	-	-	-
47	-	1.77	2.04	-	1.68	1.75	3.99		1.96		-	-	-	-	-	-
48	-	1.76	2.05	-	1.67	1.75	4.00		1.96		-	-	-	-	-	-
49	-	1.75	2.05	-	1.67	1.75	4.01		1.96		-	-	-	-	-	-
50	-	1.74	2.06	-	1.66	1.75	4.03		1.96		-	-	-	-	-	-
51	-	1.72	2.07	-	1.65	1.75	4.02		1.96		-	-	-	-	-	-
52	-	1.71	2.08	-	1.63	1.75	3.18		1.97		0.88	-	-	-	-	-

53	-	1.69	2.09	-	1.62	1.76	3.13	1.97	0.95	-	-	-	-	-
54	-	1.67	2.11	-	3.35	-	2.72	1.97	1.01	0.38	-	-	-	-
55	-	1.65	2.13	-	3.35	-	2.63	1.97	1.07	0.44	-	-	-	-
56	-	1.63	2.14	-	3.35	-	2.55	1.97	1.13	0.49	-	-	-	-
57	-	1.61	2.16	-	3.35	-	2.48	1.98	1.18	0.54	-	-	-	-
58	-	1.57	2.19	-	3.05	-	2.41	2.00	1.22	0.60	1.57	-	0.30	-
59	-	1.55	2.21	-	2.97	-	2.36	2.00	1.27	0.66	1.55	-	0.36	-
60	1.13	1.51	2.25	-	2.90	-	2.30	2.02	1.30	-	-	-	-	-
61	1.22	1.47	2.29	-	2.84	-	2.24	2.04	1.33	-	-	-	-	-
62	1.31	1.42	2.36	-	2.49	-	2.19	2.07	1.36	-	-	-	-	0.24
63	1.39	1.36	2.41	-	2.42	-	2.14	2.10	1.37	-	-	-	-	0.25
64	1.46	1.28	2.51	-	2.35	-	2.08	2.15	1.37	-	-	-	-	0.22
65	1.51	1.20	2.84	-	2.27	-	2.05	2.20	1.36	-	-	-	-	-
66	1.56	1.10	2.91	-	2.23	-	2.02	2.25	1.34	-	-	-	-	-
67	1.59	-	2.98	-	2.20	-	2.00	2.31	1.31	-	0.64	0.34	-	-
68	1.62	-	3.07	-	2.18	-	1.99	2.38	1.26	-	0.58	0.27	-	-
69	1.65	-	3.34	-	2.15	-	1.99	2.44	1.22	-	0.52	-	-	-
70	1.67	-	3.34	-	2.13	-	1.98	2.51	1.17	-	0.46	-	-	-
71	1.69	-	3.34	-	2.11	-	1.97	2.58	1.12	-	0.40	-	-	-
72	1.71	-	3.35	-	2.10	-	1.97	2.67	1.07	-	0.33	-	-	-
73	1.73	-	1.60	1.78	2.08	-	1.97	3.01	1.03	-	-	-	-	-
74	1.74	-	1.62	1.76	2.07	-	1.97	3.04	0.97	-	-	-	-	-
75	1.75	-	1.64	1.76	2.06	-	1.96	3.06	0.92	-	-	-	-	-
76	1.77	-	1.65	1.77	2.05	-	1.97	3.10	0.87	-	-	-	-	-
77	1.78	-	1.66	1.76	2.04	-	1.96	3.15	0.82	-	-	-	-	-
78	1.79	-	1.67	1.77	2.03	-	1.97	3.93	-	-	-	-	-	-
79	1.80	-	1.67	1.77	2.03	-	1.97	3.94	-	-	-	-	-	-
80	1.81	-	1.68	1.76	2.02	-	1.97	3.93	-	-	-	-	-	-
81	1.81	-	1.69	1.77	2.02	-	1.97	3.93	-	-	-	-	-	-
82	1.81	-	1.69	1.77	2.01	-	1.97	3.93	-	-	-	-	-	-
83	1.82	-	1.69	1.77	2.01	-	1.97	3.94	-	-	-	-	-	-
84	1.82	-	1.70	1.76	2.01	-	1.97	3.93	-	-	-	-	-	-
85	1.83	-	1.70	1.76	2.01	-	1.97	3.93	-	-	-	-	-	-
86	1.83	-	1.71	1.77	2.01	-	1.97	3.93	-	-	-	-	-	-

Table S5. Electronic population of basins for the rearrangement of nitrones **5**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.81	2.02		3.46		4.00		2.03		-	-	-	-	-	-
37	-	1.81	2.02		3.46		4.00		2.03		-	-	-	-	-	-
38	-	1.81	2.02		3.45		4.00		2.03		-	-	-	-	-	-
39	-	1.81	2.02		3.45		3.99		2.03		-	-	-	-	-	-
40	-	1.80	2.02		3.45		3.99		2.03		-	-	-	-	-	-
41	-	1.80	2.02		3.45		3.99		2.03		-	-	-	-	-	-
42	-	1.80	2.02		3.44		3.99		2.03		-	-	-	-	-	-
43	-	1.79	2.02		3.44		4.00		2.02		-	-	-	-	-	-
44	-	1.78	2.02		3.44		4.00		2.02		-	-	-	-	-	-
45	-	1.78	2.03		3.42		4.00		2.02		-	-	-	-	-	-

46	-	1.77	2.03	3.42	4.00	2.02	-	-	-	-	-	-
47	-	1.77	2.03	3.41	4.01	2.02	-	-	-	-	-	-
48	-	1.76	2.04	3.40	4.01	2.01	-	-	-	-	-	-
49	-	1.75	2.05	3.40	4.03	2.01	-	-	-	-	-	-
50	-	1.74	2.05	3.38	4.04	2.00	-	-	-	-	-	-
51	-	1.73	2.06	3.38	3.63	2.00	-	0.42	-	-	-	-
52	-	1.72	2.07	3.36	3.63	2.00	-	0.44	-	-	-	-
53	-	1.70	2.08	3.35	2.85	2.00	0.77	0.48	-	-	-	-
54	-	1.69	2.10	3.33	2.78	1.99	0.84	0.51	-	-	-	-
55	-	1.67	2.11	3.31	2.69	1.99	0.91	0.55	-	-	-	-
56	-	1.64	2.13	3.28	2.61	1.99	0.98	0.60	-	-	-	-
57	-	1.62	2.15	3.29	2.54	2.00	1.05	0.64	-	-	-	-
58	-	1.59	2.17	3.28	2.48	2.00	1.11	0.69	1.59	-	-	-
59	-	1.57	2.20	3.02	2.41	2.00	1.18	0.74	1.57	-	0.23	-
60	1.08	1.53	2.23	2.94	2.35	2.01	1.23	-	-	-	-	-
61	1.18	1.50	2.26	2.87	2.29	2.02	1.27	-	-	-	-	-
62	1.28	1.46	2.30	2.50	2.24	2.05	1.31	-	-	-	-	0.30
63	1.36	1.41	2.35	2.42	2.18	2.07	1.35	-	-	-	-	0.32
64	1.43	1.35	2.40	2.35	2.11	2.14	1.37	-	-	-	-	0.32
65	1.50	1.28	2.78	2.29	2.06	2.17	1.38	-	-	-	-	-
66	1.55	1.19	2.84	2.25	2.03	2.21	1.38	-	-	-	-	-
67	1.59	1.07	2.92	2.22	2.01	2.26	1.37	-	-	-	-	-
68	1.62	-	2.98	2.18	1.99	2.32	1.34	-	0.63	0.32	-	-
69	1.64	-	3.07	2.16	1.98	2.38	1.30	-	0.57	0.25	-	-
70	1.67	-	3.33	2.13	1.97	2.44	1.25	-	0.50	-	-	-
71	1.69	-	3.34	2.11	1.96	2.52	1.21	-	0.43	-	-	-
72	1.71	-	3.33	2.09	1.95	2.60	1.16	-	0.36	-	-	-
73	1.73	-	3.36	2.08	1.95	2.98	1.10	-	-	-	-	-
74	1.74	-	3.38	2.06	1.94	3.00	1.05	-	-	-	-	-
75	1.76	-	3.39	2.05	1.94	3.03	1.00	-	-	-	-	-
76	1.77	-	3.40	2.04	1.94	3.06	0.95	-	-	-	-	-
77	1.78	-	3.41	2.03	1.94	3.10	0.89	-	-	-	-	-
78	1.79	-	3.42	2.03	1.94	3.13	0.85	-	-	-	-	-
79	1.80	-	3.43	2.02	1.95	3.95	-	-	-	-	-	-
80	1.80	-	3.44	2.02	1.95	3.96	-	-	-	-	-	-
81	1.81	-	3.45	2.01	1.95	3.96	-	-	-	-	-	-
82	1.82	-	3.45	2.01	1.95	3.96	-	-	-	-	-	-
83	1.82	-	3.46	2.00	1.95	3.97	-	-	-	-	-	-
84	1.83	-	3.46	2.00	1.95	3.97	-	-	-	-	-	-
85	1.83	-	3.47	2.00	1.95	3.97	-	-	-	-	-	-
86	1.83	-	3.47	2.00	1.95	3.96	-	-	-	-	-	-

Table S6. Electronic population of basins for the rearrangement of nitrones **6**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.81	2.01	-	1.72	1.76	3.97		1.99		-	-	-	-	-	-
37	-	1.81	2.01	-	1.72	1.77	3.98		1.99		-	-	-	-	-	-
38	-	1.81	2.01	-	1.72	1.77	3.98		1.99		-	-	-	-	-	-
39	-	1.81	2.01	-	1.71	1.77	3.98		1.99		-	-	-	-	-	-
40	-	1.80	2.01	-	1.76	1.70	3.97		1.99		-	-	-	-	-	-
41	-	1.80	2.02	-	1.76	1.70	3.98		1.99		-	-	-	-	-	-
42	-	1.80	2.01	-	1.76	1.70	3.98		1.98		-	-	-	-	-	-
43	-	1.79	2.02	-	1.76	1.70	3.98		1.98		-	-	-	-	-	-
44	-	1.79	2.02	-	1.76	1.69	3.98		1.98		-	-	-	-	-	-
45	-	1.78	2.03	-	1.76	1.69	3.99		1.97		-	-	-	-	-	-
46	-	1.78	2.03	-	1.76	1.68	3.99		1.97		-	-	-	-	-	-
47	-	1.77	2.03	-	1.76	1.68	4.00		1.97		-	-	-	-	-	-
48	-	1.76	2.04	-	1.75	1.67	4.00		1.96		-	-	-	-	-	-
49	-	1.75	2.05	-	1.75	1.66	4.01		1.96		-	-	-	-	-	-
50	-	1.74	2.05	-	1.75	1.66	4.02		1.96		-	-	-	-	-	-
51	-	1.72	2.06	-	1.65	1.75	4.03		1.97		-	-	-	-	-	-
52	-	1.71	2.08	-	1.64	1.75	3.21		1.96		0.85	-	-	-	-	-
53	-	1.70	2.09	-	1.75	1.62	3.17		1.96		0.91	-	-	-	-	-
54	-	1.68	2.10	-	1.65	1.72	2.78		1.97		0.97	0.36	-	-	-	-
55	-	1.66	2.12	-	3.33	-	2.68		1.97		1.03	0.43	-	-	-	-
56	-	1.64	2.14	-	3.34	-	2.61		1.97		1.09	0.48	-	-	-	-
57	-	1.61	2.16	-	3.33	-	2.53		1.98		1.15	0.54	-	-	-	-
58	-	1.58	2.19	-	3.07	-	2.45		1.99		1.20	0.60	-	-	0.25	-
59	-	1.55	2.21	-	2.99	-	2.39		2.00		1.24	0.66	-	-	0.32	-
60	1.09	1.51	2.24	-	2.92	-	2.33		2.02		1.28	-	-	-	-	-
61	1.19	1.48	2.27	-	2.85	-	2.27		2.03		1.32	-	-	-	-	-
62	1.29	1.43	2.32	-	2.47	-	2.22		2.06		1.34	-	-	-	-	0.32
63	1.37	1.37	2.37	-	2.39	-	2.16		2.10		1.36	-	-	-	-	0.33
64	1.44	1.31	2.44	-	2.33	-	2.10		2.15		1.37	-	-	-	-	0.32
65	1.50	1.22	2.82	-	2.28	-	2.06		2.20		1.36	-	-	-	-	-
66	1.54	1.12	2.88	-	2.24	-	2.04		2.26		1.34	-	-	-	-	-
67	1.58	1.00	2.96	-	2.21	-	2.02		2.32		1.31	-	-	-	-	-
68	1.61	-	3.04	-	2.18	-	2.01		2.37		1.27	-	0.59	0.28	-	-
69	1.64	-	3.32	-	2.16	-	2.00		2.44		1.22	-	0.53	-	-	-
70	1.66	-	3.33	-	2.14	-	1.99		2.51		1.18	-	0.47	-	-	-
71	1.68	-	3.33	-	2.12	-	1.98		2.59		1.13	-	0.40	-	-	-
72	1.70	-	3.34	-	2.10	-	1.97		2.67		1.09	-	0.33	-	-	-
73	1.72	-	1.78	1.58	2.08	-	1.97		3.02		1.03	-	-	-	-	-
74	1.74	-	1.77	1.61	2.07	-	1.97		3.04		0.98	-	-	-	-	-
75	1.75	-	1.76	1.63	2.06	-	1.97		3.06		0.93	-	-	-	-	-
76	1.76	-	1.76	1.64	2.05	-	1.97		3.11		0.87	-	-	-	-	-
77	1.78	-	1.76	1.65	2.04	-	1.97		3.14		0.82	-	-	-	-	-
78	1.79	-	1.66	1.76	2.04	-	1.98		3.92		-	-	-	-	-	-
79	1.79	-	1.67	1.76	2.03	-	1.98		3.94		-	-	-	-	-	-

80	1.80	-	1.76	1.67	2.03	-	1.97		3.94		-	-	-	-	-	-
81	1.81	-	1.76	1.68	2.02	-	1.97		3.94		-	-	-	-	-	-
82	1.81	-	1.76	1.68	2.02	-	1.97		3.94		-	-	-	-	-	-
83	1.82	-	1.77	1.69	2.01	-	1.97		3.93		-	-	-	-	-	-
84	1.82	-	1.77	1.70	2.01	-	1.97		3.94		-	-	-	-	-	-
85	1.82	-	1.76	1.70	2.01	-	1.98		3.93		-	-	-	-	-	-
86	1.83	-	1.76	1.70	2.01	-	1.98		3.93		-	-	-	-	-	-

Table S7. Electronic population of basins for the rearrangement of nitrones (*Z*)-**7**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.81	2.01	-	1.81	1.76	3.95	-	1.97	-	-	-	-	-	-	-
37	-	1.81	2.01	-	1.81	1.76	3.95	-	1.98	-	-	-	-	-	-	-
38	-	1.81	2.01	-	1.81	1.75	3.95	-	1.98	-	-	-	-	-	-	-
39	-	1.80	2.01	-	1.81	1.74	3.95	-	1.98	-	-	-	-	-	-	-
40	-	1.80	2.01	-	1.81	1.73	3.96	-	1.97	-	-	-	-	-	-	-
41	-	1.79	2.01	-	1.81	1.73	3.96	-	1.97	-	-	-	-	-	-	-
42	-	1.79	2.01	-	1.82	1.72	3.95	-	1.98	-	-	-	-	-	-	-
43	-	1.79	2.01	-	1.81	1.72	3.95	-	1.97	-	-	-	-	-	-	-
44	-	1.78	2.01	-	1.82	1.73	3.95	-	1.98	-	-	-	-	-	-	-
45	-	1.77	2.01	-	1.82	1.72	3.96	-	1.98	-	-	-	-	-	-	-
46	-	1.76	2.02	-	1.82	1.70	3.95	-	1.98	-	-	-	-	-	-	-
47	-	1.75	2.03	-	1.82	1.70	3.95	-	1.98	-	-	-	-	-	-	-
48	-	1.73	2.04	-	1.83	1.68	3.95	-	1.99	-	-	-	-	-	-	-
49	-	1.69	2.05	-	1.83	1.66	3.95	-	1.99	-	-	-	-	-	-	-
50	-	1.65	2.08	-	1.82	1.64	3.95	-	2.01	-	-	-	-	-	-	-
51	-	1.61	2.10	-	1.82	1.63	3.95	-	2.02	-	-	-	-	-	-	-
52	-	1.55	2.14	-	1.82	1.60	3.69	-	2.04	-	-	0.26	-	-	-	-
53	-	1.50	2.17	-	1.82	1.59	3.65	-	2.06	-	-	0.30	-	-	-	-
54	-	1.44	2.22	-	3.35	-	3.60	-	2.09	-	-	0.36	-	-	-	-
55	-	1.37	2.27	-	3.32	-	3.55	-	2.11	-	-	0.41	-	-	-	-
56	-	1.29	2.32	-	3.30	-	3.49	-	2.15	-	-	0.46	-	-	-	-
57	-	1.20	2.39	-	3.25	-	3.42	-	2.20	-	-	0.51	-	-	-	-
58	-	-	2.47	-	3.20	-	2.76	-	2.29	-	0.53	0.56	0.73	0.38	-	-
59	-	-	2.59	-	3.15	-	2.61	-	2.31	-	0.70	0.61	0.67	0.33	-	-
60	-	-	2.78	-	3.03	-	2.48	-	2.43	-	0.71	0.66	0.61	0.26	-	-
61	-	-	3.15	-	2.57	-	2.36	-	2.56	-	0.70	0.71	0.56	-	0.35	-
62	-	-	3.20	-	2.47	-	2.29	-	2.64	-	0.70	0.75	0.50	-	0.40	-
63	-	-	3.23	-	2.40	-	2.23	-	2.72	-	0.68	0.81	0.44	-	0.44	-
64	-	-	3.25	-	2.35	-	2.17	-	2.80	-	0.67	0.85	0.38	-	0.47	-
65	1.40	-	3.28	-	2.30	-	2.13	-	2.87	-	0.67	-	0.33	-	-	-
66	1.46	-	1.75	1.56	2.25	-	2.10	-	3.59	-	-	-	0.28	-	-	-
67	1.52	-	1.78	1.55	2.22	-	2.07	-	3.88	-	-	-	-	-	-	-
68	1.56	-	1.77	1.59	2.19	-	2.05	-	3.89	-	-	-	-	-	-	-
69	1.61	-	1.77	1.61	2.16	-	2.03	-	3.90	-	-	-	-	-	-	-
70	1.65	-	1.77	1.63	2.13	-	2.01	-	3.90	-	-	-	-	-	-	-

71	1.69	-	1.77	1.64	2.11	-	2.00	-	3.91	-	-	-	-	-	-	-
72	1.73	-	1.77	1.65	2.09	-	1.99	-	3.92	-	-	-	-	-	-	-
73	1.75	-	1.77	1.66	2.08	-	1.99	-	3.93	-	-	-	-	-	-	-
74	1.78	-	1.77	1.67	2.07	-	1.98	-	3.93	-	-	-	-	-	-	-
75	1.80	-	1.76	1.68	2.05	-	1.97	-	3.93	-	-	-	-	-	-	-
76	1.81	-	1.68	1.77	2.04	-	1.97	-	3.94	-	-	-	-	-	-	-
77	1.83	-	1.76	1.69	2.04	-	1.98	-	3.94	-	-	-	-	-	-	-
78	1.83	-	1.76	1.69	2.03	-	1.98	-	3.93	-	-	-	-	-	-	-
79	1.84	-	1.76	1.70	2.03	-	1.98	-	3.93	-	-	-	-	-	-	-
80	1.85	-	1.76	1.70	2.03	-	1.98	-	3.93	-	-	-	-	-	-	-
81	1.85	-	1.75	1.71	2.03	-	1.98	-	3.93	-	-	-	-	-	-	-
82	1.86	-	1.76	1.71	2.03	-	1.99	-	3.93	-	-	-	-	-	-	-
83	1.86	-	1.75	1.71	2.03	-	1.98	-	3.94	-	-	-	-	-	-	-
84	1.86	-	1.75	1.72	2.03	-	1.98	-	3.94	-	-	-	-	-	-	-
85	1.86	-	1.76	1.72	2.02	-	1.98	-	3.94	-	-	-	-	-	-	-
86	1.87	-	1.76	1.72	2.02	-	1.98	-	3.94	-	-	-	-	-	-	-

Table S8. Electronic population of basins for the rearrangement of nitrones (*E*)-**7**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.81	2.00		3.54		3.91	-	1.98	-	-	-	-	-	-	-
37	-	1.80	2.01		3.54		3.92	-	1.97	-	-	-	-	-	-	-
38	-	1.80	2.01		3.53		3.92	-	1.98	-	-	-	-	-	-	-
39	-	1.79	2.01		3.53		3.92	-	1.97	-	-	-	-	-	-	-
40	-	1.79	2.01		3.52		3.93	-	1.97	-	-	-	-	-	-	-
41	-	1.79	2.01		3.53		3.92	-	1.97	-	-	-	-	-	-	-
42	-	1.79	2.01		3.52		3.92	-	1.97	-	-	-	-	-	-	-
43	-	1.79	2.01		3.51		3.93	-	1.97	-	-	-	-	-	-	-
44	-	1.78	2.02		3.51		3.93	-	1.97	-	-	-	-	-	-	-
45	-	1.77	2.02		3.50		3.93	-	1.97	-	-	-	-	-	-	-
46	-	1.77	2.03		3.49		3.94	-	1.97	-	-	-	-	-	-	-
47	-	1.76	2.03		3.48		3.94	-	1.97	-	-	-	-	-	-	-
48	-	1.75	2.04		3.48		3.95	-	1.97	-	-	-	-	-	-	-
49	-	1.74	2.05		3.46		3.13	-	1.97	-	0.84	-	-	-	-	-
50	-	1.72	2.06		3.45		3.10	-	1.97	-	0.89	-	-	-	-	-
51	-	1.70	2.07		3.43		3.06	-	1.97	-	0.94	-	-	-	-	-
52	-	1.68	2.09		3.42		3.04	-	1.98	-	0.99	-	-	-	-	-
53	-	1.65	2.12		3.38		2.66	-	1.98	-	1.05	0.36	-	-	-	-
54	-	1.61	2.14		3.37		2.58	-	1.99	-	1.09	0.43	-	-	-	-
55	-	1.56	2.18		3.36		2.51	-	2.01	-	1.14	0.50	-	-	-	-
56	-	1.51	2.21		3.35		2.44	-	2.03	-	1.17	0.56	-	-	-	-
57	-	1.45	2.26		3.04		2.38	-	2.05	-	1.21	0.62	-	-	0.29	-
58	-	1.38	2.32		2.93		2.32	-	2.09	-	1.22	0.69	-	-	0.36	-
59	1.16	1.30	2.38		2.85		2.27	-	2.13	-	1.24	-	-	-	pop.	-
60	1.26	1.20	2.47		2.76		2.21	-	2.18	-	1.24	-	-	-	pop.	-
61	1.34	1.10	2.80		2.44		2.15	-	2.26	-	1.23	-	-	-	pop.	-
62	1.42	-	2.89		2.37		2.09	-	2.32	-	1.22	-	0.64	0.34	pop.	-
63	1.48	-	2.99		2.31		2.05	-	2.39	-	1.20	-	0.58	0.28	pop.	-

64	1.54	-	3.29		2.26		2.02	-	2.45	-	1.18	-	0.51	-	pop.	-
65	1.59	-	3.31		2.22		2.00	-	2.52	-	1.14	-	0.44	-	pop.	-
66	1.63	-	3.31		2.19		1.98	-	2.60	-	1.10	-	0.38	-	pop.	-
67	1.66	-	3.35		2.16		1.97	-	2.69	-	1.05	-	0.29	-	pop.	-
68	1.69	-	3.36		2.13		1.96	-	3.00	-	1.00	-	-	-	pop.	-
69	1.72	-	3.38		2.11		1.95	-	3.03	-	0.95	-	-	-	pop.	-
70	1.74	-	3.40		2.09		1.95	-	3.07	-	0.90	-	-	-	pop.	-
71	1.76	-	3.40		2.08		1.94	-	3.12	-	0.84	-	-	-	pop.	-
72	1.78	-	3.42		2.07		1.94	-	3.13	-	0.81	-	-	-	-	-
73	1.79	-	3.44		2.06		1.95	-	3.94	-	-	-	-	-	-	-
74	1.81	-	3.44		2.05		1.95	-	3.93	-	-	-	-	-	-	-
75	1.82	-	3.45		2.05		1.95	-	3.93	-	-	-	-	-	-	-
76	1.82	-	3.46		2.04		1.95	-	3.93	-	-	-	-	-	-	-
77	1.83	-	3.46		2.04		1.95	-	3.93	-	-	-	-	-	-	-
78	1.84	-	3.47		2.04		1.95	-	3.93	-	-	-	-	-	-	-
79	1.84	-	3.47		2.03		1.95	-	3.93	-	-	-	-	-	-	-
80	1.85	-	3.47		2.03		1.95	-	3.93	-	-	-	-	-	-	-
81	1.85	-	3.47		2.03		1.95	-	3.94	-	-	-	-	-	-	-
82	1.85	-	3.47		2.03		1.95	-	3.94	-	-	-	-	-	-	-
83	1.86	-	3.48		2.03		1.95	-	3.94	-	-	-	-	-	-	-
84	1.86	-	3.48		2.03		1.96	-	3.94	-	-	-	-	-	-	-
85	1.86	-	3.48		2.02		1.96	-	3.94	-	-	-	-	-	-	-
86	1.86	-	3.49		2.02		1.96	-	3.95	-	-	-	-	-	-	-

Table S9. Electronic population of basins for the rearrangement of nitrones (*Z*)-**8**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1,82	2,00	-	1,83	1,86	3,96	-	1,97		-	-	-	-	-	-
37	-	1,81	1,99	-	1,83	1,85	3,95	-	1,97		-	-	-	-	-	-
38	-	1,81	2,00	-	1,82	1,85	3,96	-	1,96		-	-	-	-	-	-
39	-	1,81	2,00	-	1,82	1,86	3,96	-	1,95		-	-	-	-	-	-
40	-	1,80	2,01	-	1,81	1,87	3,96	-	1,96		-	-	-	-	-	-
41	-	1,80	2,01	-	1,81	1,87	3,96	-	1,96		-	-	-	-	-	-
42	-	1,80	2,01	-	1,81	1,87	3,96	-	1,96		-	-	-	-	-	-
43	-	1,80	2,01	-	1,80	1,87	3,95	-	1,96		-	-	-	-	-	-
44	-	1,79	2,01	-	1,80	1,87	3,95	-	1,96		-	-	-	-	-	-
45	-	1,79	2,02	-	1,87	1,79	3,95	-	1,97		-	-	-	-	-	-
46	-	1,78	2,02	-	1,88	1,79	3,94	-	1,97		-	-	-	-	-	-
47	-	1,77	2,02	-	1,88	1,78	3,95	-	1,97		-	-	-	-	-	-
48	-	1,76	2,02	-	1,88	1,77	3,95	-	1,97		-	-	-	-	-	-
49	-	1,75	2,02	-	1,89	1,76	3,95	-	1,98		-	-	-	-	-	-
50	-	1,73	2,03	-	1,90	1,76	3,96	-	1,98		-	-	-	-	-	-
51	-	1,72	2,04	-	1,91	1,74	3,96	-	1,98		-	-	-	-	-	-
52	-	1,70	2,05	-	1,92	1,73	3,97	-	1,99		-	-	-	-	-	-
53	-	1,68	2,06	-	1,70	1,95	3,64	-	1,99		-	0,35	-	-	-	-
54	-	1,65	2,08	-	3,64	-	3,58	-	2,01		-	0,41	-	-	-	-

55	-	1,61	2,10	-	3,64	-	2,76	-	2,01		0,80	0,48	-	-	-	-
56	-	1,57	2,12	-	3,64	-	2,66	-	2,03		0,85	0,54	-	-	-	-
57	-	1,52	2,15	-	3,11	-	2,58	-	2,05		0,90	0,60	-	-	-	0,53
58	-	1,46	2,19	-	2,67	-	2,51	-	2,08		0,94	0,66	-	-	0,39	0,56
59	-	1,40	2,24	-	2,55	-	2,44	-	2,12		0,96	0,72	-	-	0,48	0,58
60	-	1,32	2,29	-	2,46	-	2,36	-	2,17		0,98	0,77	-	-	0,54	0,59
61	1,40	1,23	2,35	-	2,39	-	2,24	-	2,29		0,99	-	-	-	-	0,58
62	1,48	1,13	2,43	-	2,33	-	2,15	-	2,38		0,99	-	-	-	-	0,57
63	1,55	1,01	2,53	-	2,29	-	2,09	-	2,45		0,99	-	-	-	-	0,53
64	1,61	-	2,67	-	2,24	-	2,06	-	2,51		0,97	-	0,63	0,24	-	0,49
65	1,66	-	3,40	-	2,21	-	2,03	-	2,58		0,94	-	0,56	-	-	-
66	1,69	-	3,40	-	2,19	-	2,01	-	2,65		0,91	-	0,50	-	-	-
67	1,73	-	3,38	-	2,17	-	1,99	-	2,74		0,87	-	0,43	-	-	-
68	1,76	-	1,78	1,62	2,15	-	1,98	-	2,83		0,82	-	0,35	-	-	-
69	1,78	-	1,77	1,64	2,13	-	1,98	-	3,20		0,78	-	-	-	-	-
70	1,80	-	1,77	1,65	2,12	-	1,97	-	3,95		-	-	-	-	-	-
71	1,82	-	1,77	1,66	2,11	-	1,96	-	3,96		-	-	-	-	-	-
72	1,83	-	1,77	1,67	2,10	-	1,96	-	3,95		-	-	-	-	-	-
73	1,84	-	1,76	1,68	2,10	-	1,96	-	3,95		-	-	-	-	-	-
74	1,85	-	1,75	1,68	2,09	-	1,96	-	3,95		-	-	-	-	-	-
75	1,86	-	1,76	1,69	2,09	-	1,96	-	3,95		-	-	-	-	-	-
76	1,87	-	1,75	1,69	2,08	-	1,96	-	3,95		-	-	-	-	-	-
77	1,87	-	1,70	1,76	2,08	-	1,96	-	3,95		-	-	-	-	-	-
78	1,88	-	1,75	1,70	2,08	-	1,95	-	3,96		-	-	-	-	-	-
79	1,88	-	1,71	1,75	2,08	-	1,95	-	3,96		-	-	-	-	-	-
80	1,89	-	1,71	1,75	2,07	-	1,96	-	3,96		-	-	-	-	-	-
81	1,89	-	1,74	1,72	2,07	-	1,96	-	3,96		-	-	-	-	-	-
82	1,89	-	1,72	1,74	2,07	-	1,96	-	3,97		-	-	-	-	-	-
83	1,89	-	1,72	1,74	2,07	-	1,96	-	3,96		-	-	-	-	-	-
84	1,90	-	1,72	1,74	2,07	-	1,96	-	3,97		-	-	-	-	-	-
85	1,90	-	1,73	1,74	2,07	-	1,96	-	3,96		-	-	-	-	-	-
86	1,90	-	1,74	1,73	2,07	-	1,97	-	3,97		-	-	-	-	-	-

Table S10. Electronic population of basins for the rearrangement of nitrones (*E*)-**8**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1,81	1,98	-	1,82	1,88	3,93	-	1,98	-	-	-	-	-	-	-
37	-	1,81	1,98	-	1,82	1,88	3,94	-	1,98	-	-	-	-	-	-	-
38	-	1,80	1,98	-	1,83	1,87	3,93	-	1,98	-	-	-	-	-	-	-
39	-	1,80	1,99	-	1,82	1,87	3,93	-	1,97	-	-	-	-	-	-	-
40	-	1,80	2,00	-	1,82	1,87	3,93	-	1,97	-	-	-	-	-	-	-
41	-	1,80	1,99	-	1,82	1,87	3,93	-	1,97	-	-	-	-	-	-	-
42	-	1,79	1,99	-	1,82	1,87	3,93	-	1,97	-	-	-	-	-	-	-
43	-	1,79	1,99	-	1,81	1,87	3,92	-	1,98	-	-	-	-	-	-	-
44	-	1,79	1,99	-	1,80	1,88	3,93	-	1,97	-	-	-	-	-	-	-
45	-	1,78	1,99	-	1,81	1,87	3,93	-	1,97	-	-	-	-	-	-	-
46	-	1,78	2,00	-	1,81	1,86	3,93	-	1,97	-	-	-	-	-	-	-
47	-	1,77	2,01	-	1,81	1,86	3,93	-	1,97	-	-	-	-	-	-	-

48	-	1,76	2,01	-	1,80	1,86	3,93	-	1,97	-	-	-	-	-	-	-
49	-	1,75	2,02	-	1,79	1,85	3,92	-	1,97	-	-	-	-	-	-	-
50	-	1,73	2,04	-	1,84	1,78	3,12	-	1,97	-	0,84	-	-	-	-	-
51	-	1,71	2,05	-	1,84	1,77	3,09	-	1,97	-	0,88	-	-	-	-	-
52	-	1,67	2,07	-	1,83	1,76	3,05	-	1,98	-	0,94	-	-	-	-	-
53	-	1,64	2,10	-	1,83	1,74	3,02	-	1,99	-	0,99	-	-	-	-	-
54	-	1,59	2,13	-	1,73	1,82	2,66	-	2,00	-	1,03	0,35	-	-	-	-
55	-	1,54	2,17	-	3,51	-	2,58	-	2,02	-	1,07	0,42	-	-	-	-
56	-	1,48	2,21	-	3,50	-	2,51	-	2,05	-	1,09	0,48	-	-	-	-
57	-	1,41	2,26	-	3,47	-	2,45	-	2,07	-	1,12	0,55	-	-	-	-
58	-	1,33	2,33	-	3,11	-	2,38	-	2,11	-	1,14	0,61	-	-	0,34	-
59	-	1,24	2,40	-	2,99	-	2,32	-	2,16	-	1,14	0,66	-	-	0,42	-
60	-	1,14	2,49	-	2,55	-	2,26	-	2,22	-	1,14	0,73	-	-	0,48	0,33
61	1,31	-	2,60	-	2,47	-	2,18	-	2,30	-	1,14	-	0,67	0,36	-	0,30
62	1,41	-	2,99	-	2,39	-	2,13	-	2,37	-	1,13	-	0,60	0,30	-	-
63	1,48	-	3,30	-	2,33	-	2,09	-	2,43	-	1,12	-	0,54	-	-	-
64	1,54	-	3,32	-	2,29	-	2,06	-	2,50	-	1,10	-	0,47	-	-	-
65	1,60	-	3,33	-	2,25	-	2,04	-	2,58	-	1,07	-	0,40	-	-	-
66	1,65	-	1,71	1,64	2,21	-	2,02	-	2,66	-	1,04	-	0,33	-	-	-
67	1,69	-	1,67	1,69	2,19	-	2,00	-	3,00	-	1,00	-	-	-	-	-
68	1,73	-	1,67	1,71	2,16	-	1,99	-	3,03	-	0,95	-	-	-	-	-
69	1,76	-	1,72	1,68	2,14	-	1,98	-	3,06	-	0,91	-	-	-	-	-
70	1,78	-	1,68	1,73	2,13	-	1,97	-	3,10	-	0,85	-	-	-	-	-
71	1,80	-	1,69	1,74	2,12	-	1,97	-	3,13	-	0,81	-	-	-	-	-
72	1,82	-	1,74	1,69	2,11	-	1,96	-	3,93	-	-	-	-	-	-	-
73	1,83	-	1,75	1,69	2,10	-	1,96	-	3,94	-	-	-	-	-	-	-
74	1,84	-	1,75	1,70	2,10	-	1,96	-	3,94	-	-	-	-	-	-	-
75	1,84	-	1,75	1,70	2,09	-	1,96	-	3,93	-	-	-	-	-	-	-
76	1,85	-	1,71	1,76	2,09	-	1,97	-	3,94	-	-	-	-	-	-	-
77	1,86	-	1,71	1,76	2,08	-	1,97	-	3,93	-	-	-	-	-	-	-
78	1,86	-	1,72	1,76	2,08	-	1,97	-	3,93	-	-	-	-	-	-	-
79	1,87	-	1,72	1,76	2,08	-	1,97	-	3,93	-	-	-	-	-	-	-
80	2,04	-	1,72	1,76	2,08	-	1,97	-	3,93	-	-	-	-	-	-	-
81	1,88	-	1,72	1,76	2,08	-	1,97	-	3,93	-	-	-	-	-	-	-
82	1,88	-	1,72	1,76	2,07	-	1,98	-	3,93	-	-	-	-	-	-	-
83	1,88	-	1,73	1,76	2,07	-	1,98	-	3,94	-	-	-	-	-	-	-
84	1,89	-	1,73	1,77	2,07	-	1,98	-	3,94	-	-	-	-	-	-	-
85	1,89	-	1,73	1,76	2,07	-	1,98	-	3,94	-	-	-	-	-	-	-
86	1,89	-	1,76	1,73	2,07	-	1,98	-	3,94	-	-	-	-	-	-	-

Table S11. Electronic population of basins for the rearrangement of nitrones (*Z*)-**9**

IRC	**V(C1,C6)**	**V(C3,C4)**	**V1(C4,C5)**	**V2(C4C5)**	**V1C5,C6)**	**V2(C5,C6)**	**V1(C1,N2)**	**V2(C1,N2)**	**V1(C3,N2)**	**V2(C3,N2)**	**V(N2)**	**V(C1)**	**V(C3)**	**V(C4)**	**V(C5)**	**V(C6)**
36	-	1,79	2,04	-	1,75	1,82	3,98	-	1,96	-	-	-	-	-	-	-
37	-	1,78	2,04	-	1,75	1,82	3,98	-	1,96	-	-	-	-	-	-	-
38	-	1,78	2,03	-	1,75	1,82	3,98	-	1,95	-	-	-	-	-	-	-

39	-	1,78	2,03	-	1,76	1,81	3,98	-	1,95	-	-	-	-	-	-	-
40	-	1,77	2,04	-	1,76	1,81	3,96	-	1,95	-	-	-	-	-	-	-
41	-	1,77	2,04	-	1,76	1,80	3,96	-	1,95	-	-	-	-	-	-	-
42	-	1,76	2,04	-	1,76	1,80	3,96	-	1,96	-	-	-	-	-	-	-
43	-	1,76	2,05	-	1,76	1,79	3,95	-	1,96	-	-	-	-	-	-	-
44	-	1,75	2,05	-	1,77	1,78	3,94	-	1,97	-	-	-	-	-	-	-
45	-	1,75	2,05	-	1,77	1,78	3,94	-	1,97	-	-	-	-	-	-	-
46	-	1,74	2,06	-	1,77	1,78	3,93	-	1,98	-	-	-	-	-	-	-
47	-	1,73	2,07	-	1,77	1,78	3,93	-	1,98	-	-	-	-	-	-	-
48	-	1,72	2,07	-	1,77	1,77	3,92	-	1,98	-	-	-	-	-	-	-
49	-	1,70	2,08	-	1,77	1,78	3,92	-	1,99	-	-	-	-	-	-	-
50	-	1,69	2,09	-	1,78	1,77	3,92	-	1,99	-	-	-	-	-	-	-
51	-	1,67	2,10	-	1,77	1,79	3,92	-	2,00	-	-	-	-	-	-	-
52	-	1,65	2,12	-	1,76	1,80	3,61	-	2,01	-	-	0,32	-	-	-	-
53	-	1,62	2,13	-	3,55	-	3,59	-	2,02	-	-	0,36	-	-	-	-
54	-	1,59	2,15	-	3,57	-	3,54	-	2,04	-	-	0,41	-	-	-	-
55	-	1,54	2,17	-	3,59	-	2,75	-	2,04	-	0,76	0,47	-	-	-	-
56	-	1,49	2,20	-	3,60	-	2,67	-	2,06	-	0,80	0,51	-	-	-	-
57	-	1,44	2,24	-	3,16	-	2,60	-	2,09	-	0,84	0,56	-	-	0,45	-
58	-	1,38	2,28	-	2,66	-	2,53	-	2,12	-	0,87	0,61	-	-	0,53	-
59	-	1,30	2,32	-	2,56	-	2,46	-	2,15	-	0,90	0,65	-	-	0,59	-
60	-	1,22	2,39	-	2,48	-	2,39	-	2,21	-	0,92	0,69	-	-	0,65	-
61	-	1,12	2,47	-	2,41	-	2,23	-	2,37	-	0,93	0,72	-	-	0,69	-
62	-	1,01	2,57	-	2,35	-	2,15	-	2,46	-	0,92	0,71	-	-	0,77	-
63	1,54	-	3,09	-	2,30	-	2,10	-	2,53	-	0,92	-	0,64	0,25	-	-
64	1,59	-	3,33	-	2,27	-	2,07	-	2,59	-	0,90	-	0,57	-	-	-
65	1,63	-	3,36	-	2,22	-	2,04	-	2,67	-	0,87	-	0,51	-	-	-
66	1,68	-	3,36	-	2,20	-	2,01	-	2,75	-	0,84	-	0,44	-	-	-
67	1,71	-	3,36	-	2,17	-	1,99	-	2,85	-	0,80	-	0,37	-	-	-
68	1,74	-	1,79	1,60	2,15	-	1,98	-	2,91	-	0,78	-	0,31	-	-	-
69	1,76	-	1,77	1,62	2,13	-	1,97	-	3,97	-	-	-	-	-	-	-
70	1,78	-	1,77	1,64	2,12	-	1,97	-	3,96	-	pop.	-	-	-	-	-
71	1,80	-	1,77	1,65	2,10	-	1,96	-	3,96	-	pop.	-	-	-	-	-
72	1,82	-	1,77	1,67	2,10	-	1,95	-	3,96	-	pop.	-	-	-	-	-
73	1,83	-	1,76	1,67	2,09	-	1,95	-	3,96	-	pop.	-	-	-	-	-
74	1,84	-	1,76	1,68	2,08	-	1,95	-	3,96	-	pop.	-	-	-	-	-
75	1,84	-	1,76	1,69	2,08	-	1,95	-	3,96	-	pop.	-	-	-	-	-
76	1,86	-	1,75	1,70	2,07	-	1,95	-	3,96	-	pop.	-	-	-	-	-
77	1,86	-	1,75	1,70	2,07	-	1,94	-	3,97	-	pop.	-	-	-	-	-
78	1,87	-	1,75	1,71	2,07	-	1,95	-	3,97	-	pop.	-	-	-	-	-
79	1,87	-	1,75	1,71	2,07	-	1,95	-	3,97	-	pop.	-	-	-	-	-
80	1,88	-	1,75	1,72	2,07	-	1,95	-	3,97	-	pop.	-	-	-	-	-
81	1,88	-	1,75	1,72	2,07	-	1,95	-	3,97	-	pop.	-	-	-	-	-
82	1,88	-	1,75	1,72	2,07	-	1,95	-	3,97	-	pop.	-	-	-	-	-
83	1,88	-	1,74	1,73	2,06	-	1,96	-	3,98	-	pop.	-	-	-	-	-
84	1,89	-	1,75	1,73	2,06	-	1,96	-	3,98	-	pop.	-	-	-	-	-
85	1,89	-	1,75	1,73	2,06	-	1,96	-	3,97	-	pop.	-	-	-	-	-
86	1,89	-	1,75	1,73	2,06	-	1,96	-	3,98	-	pop.	-	-	-	-	-

Table S12. Electronic population of basins for the rearrangement of nitrones (*E*)-**9**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.78	2.03	-	1.75	1.78	3.94	-	1.96	-	-	-	-	-	-	-
37	-	1.78	2.03	-	1.74	1.78	3.94	-	1.96	-	-	-	-	-	-	-
38	-	1.78	2.03	-	1.79	1.74	3.94	-	1.96	-	-	-	-	-	-	-
39	-	1.77	2.03	-	1.73	1.79	3.93	-	1.96	-	-	-	-	-	-	-
40	-	1.77	2.03	-	1.73	1.80	3.94	-	1.96	-	-	-	-	-	-	-
41	-	1.77	2.04	-	1.73	1.79	3.93	-	1.96	-	-	-	-	-	-	-
42	-	1.77	2.04	-	1.72	1.80	3.92	-	1.96	-	-	-	-	-	-	-
43	-	1.77	2.04	-	1.72	1.80	3.93	-	1.95	-	-	-	-	-	-	-
44	-	1.76	2.04	-	1.71	1.80	3.93	-	1.96	-	-	-	-	-	-	-
45	-	1.76	2.05	-	1.70	1.80	3.92	-	1.95	-	-	-	-	-	-	-
46	-	1.75	2.05	-	1.70	1.80	3.92	-	1.95	-	-	-	-	-	-	-
47	-	1.74	2.05	-	1.69	1.80	3.91	-	1.95	-	-	-	-	-	-	-
48	-	1.73	2.06	-	1.69	1.81	3.92	-	1.95	-	-	-	-	-	-	-
49	-	1.72	2.07	-	1.68	1.81	3.90	-	1.96	-	-	-	-	-	-	-
50	-	1.71	2.08	-	1.82	1.67	3.09	-	1.95	-	0.84	-	-	-	-	-
51	-	1.69	2.09	-	1.83	1.65	3.05	-	1.96	-	0.88	-	-	-	-	-
52	-	1.67	2.11	-	1.84	1.64	3.00	-	1.97	-	0.94	-	-	-	-	-
53	-	1.64	2.13	-	1.78	1.69	2.97	-	1.98	-	0.99	-	-	-	-	-
54	-	1.60	2.16	-	3.45	-	2.68	-	1.99	-	1.04	0.28	-	-	-	-
55	-	1.56	2.19	-	3.46	-	2.59	-	2.00	-	1.08	0.35	-	-	-	-
56	-	1.51	2.22	-	3.46	-	2.51	-	2.02	-	1.12	0.41	-	-	-	-
57	-	1.45	2.27	-	3.05	-	2.44	-	2.04	-	1.15	0.47	-	-	0.42	-
58	-	1.38	2.32	-	2.94	-	2.38	-	2.07	-	1.18	0.52	-	-	0.52	-
59	-	1.31	2.40	-	2.61	-	2.32	-	2.11	-	1.20	0.56	-	-	0.60	-
60	-	1.22	2.72	-	2.56	-	2.26	-	2.16	-	1.21	0.60	-	-	0.66	-
61	1.35	1.11	2.81	-	2.43	-	2.17	-	2.24	-	1.21	-	-	-	-	-
62	1.43	1.00	2.89	-	2.37	-	2.12	-	2.30	-	1.21	-	-	-	-	-
63	1.49	-	2.98	-	2.32	-	2.08	-	2.36	-	1.19	-	0.58	0.30	-	-
64	1.55	-	3.29	-	2.27	-	2.05	-	2.43	-	1.17	-	0.52	-	-	-
65	1.60	-	3.31	-	2.23	-	2.02	-	2.50	-	1.15	-	0.45	-	-	-
66	1.64	-	3.32	-	2.20	-	2.00	-	2.57	-	1.12	-	0.38	-	-	-
67	1.67	-	3.32	-	2.17	-	1.98	-	2.65	-	1.08	-	0.30	-	-	-
68	1.70	-	1.78	1.58	2.15	-	1.97	-	2.98	-	1.03	-	-	-	-	-
69	1.73	-	1.77	1.60	2.13	-	1.96	-	3.00	-	0.99	-	-	-	-	-
70	1.75	-	1.76	1.63	2.11	-	1.95	-	3.03	-	0.94	-	-	-	-	-
71	1.77	-	1.77	1.64	2.10	-	1.95	-	3.08	-	0.89	-	-	-	-	-
72	1.79	-	1.77	1.65	2.09	-	1.94	-	3.11	-	0.84	-	-	-	-	-
73	1.80	-	1.65	1.77	2.08	-	1.95	-	3.92	-	-	-	-	-	-	-
74	1.81	-	1.66	1.77	2.08	-	1.94	-	3.94	-	-	-	-	-	-	-
75	1.82	-	1.67	1.77	2.07	-	1.94	-	3.95	-	-	-	-	-	-	-
76	1.82	-	1.67	1.77	2.07	-	1.94	-	3.95	-	-	-	-	-	-	-
77	1.83	-	1.68	1.78	2.06	-	1.94	-	3.95	-	-	-	-	-	-	-
78	1.84	-	1.68	1.78	2.06	-	1.94	-	3.95	-	-	-	-	-	-	-
79	1.84	-	1.69	1.78	2.06	-	1.94	-	3.95	-	-	-	-	-	-	-
80	1.84	-	1.69	1.77	2.06	-	1.94	-	3.95	-	-	-	-	-	-	-

81	1.85	-	1.69	1.78	2.06	-	1.94	-	3.96	-	-	-	-	-	-	-
82	1.85	-	1.69	1.78	2.05	-	1.94	-	3.96	-	-	-	-	-	-	-
83	1.85	-	1.70	1.78	2.05	-	1.94	-	3.96	-	-	-	-	-	-	-
84	1.85	-	1.78	1.70	2.05	-	1.94	-	3.95	-	-	-	-	-	-	-
85	1.85	-	1.70	1.77	2.05	-	1.94	-	3.95	-	-	-	-	-	-	-
86			1.70	1.77	2.05	-	1.95	-	3.95	-			-	-	-	-

Table S13. Electronic population of basins for the rearrangement of nitrones **10**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	1.80	-	1.82	1.86	2.10	-	1.95	-	3.96	-	-	-	-	-	-	-
37	1.80	-	1.81	1.86	2.10	-	1.94	-	3.96	-	-	-	-	-	-	-
38	1.80	-	1.81	1.86	2.10	-	1.94	-	3.96	-	-	-	-	-	-	-
39	1.79	-	1.81	1.86	2.10	-	1.94	-	3.95	-	-	-	-	-	-	-
40	1.78	-	1.80	1.86	2.10	-	1.93	-	3.14	-	0.84	-	-	-	-	-
41	1.78	-	1.80	1.85	2.11	-	1.93	-	3.09	-	0.90	-	-	-	-	-
42	1.77	-	1.79	1.84	2.12	-	1.92	-	3.04	-	0.96	-	-	-	-	-
43	1.77	-	1.78	1.83	2.12	-	1.91	-	3.00	-	1.03	-	-	-	-	-
44	1.76	-	1.77	1.82	2.13	-	1.91	-	2.96	-	1.09	-	-	-	-	-
45	1.75	-	1.77	1.81	2.14	-	1.90	-	2.93	-	1.15	-	-	-	-	-
46	1.74	-	1.75	1.81	2.15	-	1.90	-	2.89	-	1.21	-	-	-	-	-
47	1.73	-	1.73	1.82	2.16	-	1.90	-	2.87	-	1.27	-	-	-	-	-
48	1.71	-	3.51	-	2.18	-	1.90	-	2.84	-	1.34	-	-	-	-	-
49	1.70	-	3.50	-	2.20	-	1.90	-	2.52	-	1.40	-	0.31	-	-	-
50	1.68	-	3.50	-	2.21	-	1.90	-	2.44	-	1.45	-	0.38	-	-	-
51	1.67	-	3.17	-	2.23	-	1.91	-	2.37	-	1.51	-	0.44	0.32	-	-
52	1.65	-	3.07	-	2.26	-	1.91	-	2.31	-	1.56	-	0.49	0.41	-	-
53	1.63	-	2.99	-	2.28	-	1.92	-	2.25	-	1.61	-	0.55	0.48	-	-
54	1.61	-	2.93	-	2.31	-	1.93	-	2.20	-	1.65	-	0.60	0.54	-	-
55	1.58	1.23	2.87	-	2.34	-	1.94	-	2.16	-	1.69	-	-	-	-	-
56	1.55	1.31	2.80	-	2.37	-	1.96	-	2.11	-	1.71	-	-	-	-	-
57	1.51	1.38	2.74	-	2.42	-	1.98	-	2.08	-	1.73	-	-	-	-	-
58	1.45	1.44	2.67	-	2.49	-	2.02	-	2.04	-	1.72	-	-	-	-	-
59	1.38	1.48	2.55	-	2.63	-	2.06	-	2.01	-	1.70	-	-	-	-	-
60	1.30	1.52	2.45	-	2.75	-	2.12	-	1.99	-	1.67	-	-	-	-	-
61	1.20	1.55	2.40	-	2.83	-	2.17	-	1.97	-	1.64	-	-	-	-	-
62	-	1.57	2.35	-	2.90	-	2.22	-	1.95	-	1.60	0.60	-	-	0.51	-
63	-	1.60	2.32	-	2.98	-	2.27	-	1.94	-	1.56	0.54	-	-	0.46	-
64	-	1.62	2.29	-	3.06	-	2.33	-	1.93	-	1.52	0.49	-	-	0.38	-
65	-	1.64	2.27	-	3.14	-	2.39	-	1.92	-	1.47	0.44	-	-	0.32	-
66	-	1.66	2.24	-	3.46	-	2.46	-	1.92	-	1.41	0.38	-	-	-	-
67	-	1.68	2.22	-	3.46	-	2.54	-	1.92	-	1.35	0.31	-	-	-	-
68	-	1.70	2.20	-	1.71	1.79	2.86	-	1.92	-	1.29	-	-	-	-	-
69	-	1.71	2.19	-	1.79	1.73	2.88	-	1.91	-	1.24	-	-	-	-	-
70	-	1.73	2.17	-	1.79	1.75	2.92	-	1.91	-	1.17	-	-	-	-	-
71	-	1.74	2.16	-	1.79	1.76	2.95	-	1.92	-	1.11	-	-	-	-	-
72	-	1.75	2.15	-	1.80	1.76	2.98	-	1.92	-	1.06	-	-	-	-	-

73	-	1.76	2.14	-	1.81	1.77	3.02	-	1.92	-	0.99	-	-	-	-	-
74	-	1.77	2.13	-	1.82	1.78	3.06	-	1.93	-	0.94	-	-	-	-	-
75	-	1.78	2.13	-	1.83	1.78	3.11	-	1.93	-	0.87	-	-	-	-	-
76	-	1.78	2.12	-	1.83	1.79	3.14	-	1.93	-	0.84	-	-	-	-	-
77	-	1.79	2.12	-	1.84	1.79	3.96	-	1.94	-	-	-	-	-	-	-
78	-	1.79	2.11	-	1.84	1.80	3.96	-	1.94	-	-	-	-	-	-	-
79	-	1.80	2.11	-	1.84	1.80	3.95	-	1.94	-	-	-	-	-	-	-
80	-	1.80	2.10	-	1.85	1.80	3.96	-	1.95	-	-	-	-	-	-	-
81	-	1.80	2.10	-	1.85	1.81	3.95	-	1.95	-	-	-	-	-	-	-
82	-	1.81	2.10	-	1.85	1.81	3.95	-	1.95	-	-	-	-	-	-	-
83	-	1.81	2.10	-	1.85	1.81	3.95	-	1.96	-	-	-	-	-	-	-
84	-	1.81	2.10	-	1.86	1.82	3.95	-	1.96	-	-	-	-	-	-	-
85	-	1.81	2.10	-	1.86	1.82	3.95	-	1.96	-	-	-	-	-	-	-
86	-	1.81	2.10	-	1.86	1.82	3.96	-	1.95	-	-	-	-	-	-	-

Table S14. Electronic population of basins for the rearrangement of nitrones (*Z*)-**11**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.84	1.99	-	1.87	1.80	3.57	0.50	2.06	-	-	-	-	-	-	-
37	-	1.84	1.99	-	1.87	1.80	3.60	0.48	2.05	-	-	-	-	-	-	-
38	-	1.84	1.99	-	1.87	1.80	3.62	0.45	2.05	-	-	-	-	-	-	-
39	-	1.83	1.99	-	1.88	1.79	3.64	0.43	2.05	-	-	-	-	-	-	-
40	-	1.82	2.00	-	1.88	1.78	3.67	0.40	2.05	-	-	-	-	-	-	-
41	-	1.82	2.00	-	1.87	1.78	3.71	0.36	2.06	-	-	-	-	-	-	-
42	-	1.81	2.00	-	1.88	1.77	3.34	0.34	2.05	-	-	0.39	-	-	-	-
43	-	1.81	2.00	-	1.77	1.88	3.66	-	2.05	-	-	0.42	-	-	-	-
44	-	1.80	2.00	-	1.76	1.89	3.63	-	2.05	-	-	0.45	-	-	-	-
45	-	1.79	2.01	-	1.75	1.89	3.59	-	2.05	-	-	0.49	-	-	-	-
46	-	1.78	2.01	-	1.89	1.74	3.55	-	2.05	-	-	0.53	-	-	-	-
47	-	1.77	2.02	-	1.73	1.90	3.51	-	2.05	-	-	0.56	-	-	-	-
48	-	1.76	2.02	-	1.91	1.72	3.47	-	2.05	-	-	0.61	-	-	-	-
49	-	1.75	2.03	-	1.70	1.92	3.43	-	2.05	-	-	0.66	-	-	-	-
50	-	1.73	2.04	-	1.67	1.94	3.41	-	2.05	-	-	0.70	-	-	-	-
51	-	1.71	2.05	-	3.59	-	3.39	-	2.05	-	-	0.74	-	-	-	-
52	-	1.69	2.07	-	3.59	-	2.70	-	2.05	-	0.70	0.79	-	-	-	-
53	-	1.67	2.08	-	3.59	-	2.63	-	2.06	-	0.76	0.83	-	-	-	-
54	-	1.65	2.10	-	3.59	-	2.56	-	2.06	-	0.82	0.87	-	-	-	-
55	-	1.62	2.12	-	3.05	-	2.50	-	2.08	-	0.87	0.92	-	-	-	0.53
56	-	1.59	2.14	-	2.70	-	2.43	-	2.10	-	0.93	1.05	-	-	0.20	0.57
57	1.40	1.56	2.16	-	2.56	-	2.34	-	2.15	-	0.98	-	-	-	-	0.60
58	1.48	1.52	2.18	-	2.48	-	2.24	-	2.22	-	1.03	-	-	-	-	0.62
59	1.55	1.49	2.21	-	2.42	-	2.18	-	2.25	-	1.06	-	-	-	-	0.64
60	1.61	1.44	2.24	-	2.36	-	2.13	-	2.28	-	1.09	-	-	-	-	0.64
61	1.66	1.38	2.28	-	2.32	-	2.10	-	2.31	-	1.11	-	-	-	-	0.64
62	1.70	1.32	2.33	-	2.28	-	2.07	-	2.34	-	1.12	-	-	-	-	0.63
63	1.73	1.24	2.39	-	2.25	-	2.05	-	2.37	-	1.12	-	-	-	-	0.60

64	1.76	1.15	2.46	-	2.23	-	2.03	-	2.41	-	1.11	-	-	-	-	0.58
65	1.78	1.05	2.55	-	2.21	-	2.02	-	2.46	-	1.09	-	-	-	-	0.54
66	1.81	-	2.67	-	2.19	-	2.02	-	2.51	-	1.06	-	0.68	0.26	-	0.48
67	1.82	-	3.21	-	2.17	-	2.01	-	2.57	-	1.02	-	0.62	0.21	-	-
68	1.84	-	3.41	-	2.16	-	2.00	-	2.63	-	0.98	-	0.57	-	-	-
69	1.85	-	3.41	-	2.15	-	1.99	-	2.71	-	0.94	-	0.51	-	-	-
70	1.87	-	3.40	-	2.13	-	1.98	-	2.78	-	0.89	-	0.46	-	-	-
71	1.88	-	1.78	1.64	2.12	-	1.98	-	2.84	-	0.87	-	0.41	-	-	-
72	1.89	-	1.76	1.65	2.11	-	1.98	-	3.73	-	-	-	0.36	-	-	-
73	1.90	-	1.75	1.66	2.10	-	1.98	-	4.07	-	-	-	-	-	-	-
74	1.91	-	1.75	1.67	2.10	-	1.98	-	4.07	-	-	-	-	-	-	-
75	1.91	-	1.75	1.67	2.10	-	1.98	-	4.06	-	-	-	-	-	-	-
76	1.92	-	1.76	1.68	2.09	-	1.97	-	4.06	-	-	-	-	-	-	-
77	1.93	-	1.74	1.68	2.09	-	1.98	-	4.06	-	-	-	-	-	-	-
78	1.93	-	1.74	1.69	2.08	-	1.98	-	4.06	-	-	-	-	-	-	-
79	1.94	-	1.75	1.69	2.08	-	1.97	-	4.06	-	-	-	-	-	-	-
80	1.94	-	1.75	1.70	2.07	-	1.98	-	4.05	-	-	-	-	-	-	-
81	1.95	-	1.74	1.70	2.07	-	1.98	-	4.06	-	-	-	-	-	-	-
82	1.95	-	1.74	1.70	2.06	-	1.98	-	4.06	-	-	-	-	-	-	-
83	1.96	-	1.74	1.70	2.07	-	1.98	-	4.06	-	-	-	-	-	-	-
84	1.96	-	1.74	1.71	2.07	-	1.98	-	4.07	-	-	-	-	-	-	-
85	1.96	-	1.71	1.74	2.06	-	1.98	-	4.07	-	-	-	-	-	-	-
86	1.96	-	1.72	1.74	2.06	-	1.98	-	4.08	-	-	-	-	-	-	-

Table S15. Electronic population of basins for the rearrangement of nitrones (*E*)-**11**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.83	1.96		3.66		3.91	-	2.12	-	-	-	-	-	-	-
37	-	1.82	1.97		3.65		3.91	-	2.12	-	-	-	-	-	-	-
38	-	1.82	1.97		3.64		3.91	-	2.12	-	-	-	-	-	-	-
39	-	1.81	1.97		3.64		3.92	-	2.11	-	-	-	-	-	-	-
40	-	1.80	1.98		3.64		3.92	-	2.11	-	-	-	-	-	-	-
41	-	1.79	1.99		3.63		3.93	-	2.12	-	-	-	-	-	-	-
42	-	1.80	1.98		3.62		3.94	-	2.11	-	-	-	-	-	-	-
43	-	1.78	1.99		3.62		3.94	-	2.12	-	-	-	-	-	-	-
44	-	1.79	2.00		3.60		3.95	-	2.11	-	-	-	-	-	-	-
45	-	1.78	2.00		3.60		3.96	-	2.11	-	-	-	-	-	-	-
46	-	1.76	2.01		3.59		3.98	-	2.11	-	-	-	-	-	-	-
47	-	1.75	2.02		3.58		4.00	-	2.10	-	-	-	-	-	-	-
48	-	1.74	2.03		3.56		4.02	-	2.10	-	-	-	-	-	-	-
49	-	1.72	2.04		3.55		4.05	-	2.09	-	-	-	-	-	-	-
50	-	1.72	2.05		3.53		3.54	-	2.08	-	-	0.55	-	-	-	-
51	-	1.70	2.07		3.52		3.52	-	2.08	-	-	0.58	-	-	-	-
52	-	1.68	2.09		3.50		2.83	-	2.06	-	0.70	0.62	-	-	-	-
53	-	1.65	2.11		3.46		2.73	-	2.06	-	0.80	0.67	-	-	-	-
54	-	1.63	2.13		3.45		2.65	-	2.05	-	0.88	0.72	-	-	-	-
55	-	1.61	2.15		3.43		2.57	-	2.05	-	0.96	0.77	-	-	-	-
56	-	1.57	2.18		3.18		2.49	-	2.05	-	1.04	0.82	-	-	0.22	-

57	1.17	1.54	2.21	3.09	2.42	-	2.05	-	1.11	-	-	-	-	-
58	1.28	1.50	2.25	3.00	2.35	-	2.06	-	1.18	-	-	-	-	-
59	1.37	1.45	2.30	2.92	2.30	-	2.07	-	1.23	-	-	-	-	-
60	1.46	1.39	2.36	2.83	2.24	-	2.09	-	1.27	-	-	-	-	-
61	1.54	1.33	2.42	2.76	2.19	-	2.13	-	1.30	-	-	-	-	-
62	1.60	1.24	2.72	2.45	2.14	-	2.18	-	1.31	-	-	-	-	-
63	1.65	1.15	2.79	2.39	2.10	-	2.22	-	1.31	-	-	-	-	-
64	1.69	1.05	2.86	2.35	2.08	-	2.28	-	1.29	-	-	-	-	-
65	1.73	0.93	2.93	2.31	2.06	-	2.34	-	1.26	-	-	-	-	-
66	1.77	-	3.03	2.28	2.04	-	2.41	-	1.21	-	0.58	0.18	-	-
67	1.79	-	3.09	2.25	2.03	-	2.50	-	1.16	-	0.47	0.19	-	-
68	1.82	-	3.28	2.23	2.03	-	2.58	-	1.10	-	0.40	-	-	-
69	1.84	-	3.28	2.21	2.02	-	2.69	-	1.03	-	0.34	-	-	-
70	1.86	-	3.29	2.18	2.01	-	3.07	-	0.97	-	-	-	-	-
71	1.88	-	3.32	2.16	2.01	-	4.01	-	-	-	-	-	-	-
72	1.89	-	3.33	2.15	2.01	-	3.99	-	-	-	-	-	-	-
73	1.90	-	3.35	2.14	2.01	-	3.98	-	-	-	-	-	-	-
74	1.91	-	3.36	2.13	2.01	-	3.96	-	-	-	-	-	-	-
75	1.92	-	3.37	2.12	2.01	-	3.95	-	-	-	-	-	-	-
76	1.93	-	3.38	2.11	2.00	-	3.93	-	-	-	-	-	-	-
77	1.94	-	3.38	2.10	2.01	-	3.92	-	-	-	-	-	-	-
78	1.95	-	3.40	2.10	2.01	-	3.90	-	-	-	-	-	-	-
79	1.96	-	3.48	2.09	2.01	-	3.89	-	-	-	-	-	-	-
80	1.96	-	3.41	2.09	2.01	-	3.89	-	-	-	-	-	-	-
81	1.97	-	3.41	2.08	2.01	-	3.90	-	-	-	-	-	-	-
82	1.97	-	3.41	2.08	2.01	-	3.90	-	-	-	-	-	-	-
83	1.97	-	3.42	2.08	2.01	-	3.89	-	-	-	-	-	-	-
84	1.97	-	3.43	2.07	2.02	-	3.89	-	-	-	-	-	-	-
85	1.98	-	3.43	2.07	2.02	-	3.89	-	-	-	-	-	-	-
86	1.99	-	3.42	2.07	2.02	-	3.89	-	-	-	-	-	-	-

Table S16. Electronic population of basins for the rearrangement of nitrones **12**

IRC	**V(C1,C6)**	**V(C3,C4)**	**V1(C4,C5)**	**V2(C4C5)**	**V1C5,C6)**	**V2(C5,C6)**	**V1(C1,N2)**	**V2(C1,N2)**	**V1(C3,N2)**	**V2(C3,N2)**	**V(N2)**	**V(C1)**	**V(C3)**	**V(C4)**	**V(C5)**	**V(C6)**
36	1.82	-	1.76	1.69	2.01	-	2.00		3.99		-	-	-	-	-	-
37	1.82	-	1.76	1.69	2.01	-	2.01		4.00		-	-	-	-	-	-
38	1.82	-	1.76	1.69	2.01	-	2.00		4.00		-	-	-	-	-	-
39	1.81	-	1.76	1.68	2.01	-	2.00		3.99		-	-	-	-	-	-
40	1.81	-	1.76	1.68	2.02	-	2.00		4.00		-	-	-	-	-	-
41	1.80	-	1.75	1.68	2.02	-	2.00		4.01		-	-	-	-	-	-
42	1.79	-	1.75	1.67	2.03	-	1.99		4.02		-	-	-	-	-	-
43	1.79	-	1.75	1.67	2.04	-	1.99		4.03		-	-	-	-	-	-
44	1.77	-	1.75	1.66	2.04	-	1.99		4.03		-	-	-	-	-	-
45	1.76	-	1.65	1.75	2.05	-	1.98		2.92		0.74	-	0.40	-	-	-
46	1.75	-	1.64	1.74	2.06	-	1.98		2.89		0.77	-	0.43	-	-	-
47	1.74	-	1.63	1.74	2.07	-	1.98		2.81		0.83	-	0.47	-	-	-

48	1.72	-	1.61	1.76	2.08	-	1.98	2.73	0.90	-	0.51	-	-	-
49	1.70	-	3.34	-	2.10	-	1.98	2.65	0.96	-	0.55	-	-	-
50	1.69	-	3.33	-	2.11	-	1.98	2.59	1.01	-	0.59	-	-	-
51	1.67	-	3.34	-	2.12	-	1.98	2.52	1.07	-	0.64	-	-	-
52	1.65	-	3.33	-	2.14	-	1.98	2.46	1.12	-	0.68	-	-	-
53	1.63	-	3.06	-	2.16	-	1.99	2.40	1.17	-	0.73	0.26	-	-
54	1.61	-	2.98	-	2.19	-	2.00	2.35	1.22	-	0.77	0.32	-	-
55	1.58	1.19	2.92	-	2.21	-	2.00	2.29	1.27	-	-	-	-	-
56	1.55	1.27	2.86	-	2.24	-	2.01	2.24	1.30	-	-	-	-	-
57	1.52	1.35	2.80	-	2.27	-	2.03	2.18	1.34	-	-	-	-	-
58	1.49	1.42	2.43	-	2.31	-	2.05	2.14	1.36	-	-	-	-	0.32
59	1.44	1.47	2.37	-	2.35	-	2.09	2.10	1.37	-	-	-	-	0.33
60	1.38	1.52	2.32	-	2.41	-	2.14	2.05	1.37	-	-	-	-	0.33
61	1.30	1.56	2.29	-	2.78	-	2.19	2.02	1.36	-	-	-	-	-
62	1.21	1.59	2.25	-	2.85	-	2.24	2.01	1.33	-	-	-	-	-
63	1.12	1.63	2.21	-	2.91	-	2.29	1.98	1.30	-	-	-	-	-
64	1.02	1.65	2.19	-	2.97	-	2.35	1.97	1.26	-	-	-	-	-
65	-	1.67	2.17	-	3.05	-	2.41	1.96	1.22	0.66	-	-	0.22	-
66	-	1.69	2.15	-	3.11	-	2.48	1.95	1.17	0.56	-	-	0.24	-
67	-	1.71	2.13	-	3.35	-	2.54	1.95	1.12	0.51	-	-	-	-
68	-	1.73	2.12	-	3.34	-	2.61	1.95	1.07	0.46	-	-	-	-
69	-	1.75	2.10	-	3.35	-	2.70	1.94	1.01	0.40	-	-	-	-
70	-	1.76	2.08	-	1.63	1.74	2.78	1.94	0.94	0.36	-	-	-	-
71	-	1.77	2.07	-	1.76	1.62	3.18	1.93	0.88	-	-	-	-	-
72	-	1.78	2.06	-	1.64	1.75	4.01	1.94	-	-	-	-	-	-
73	-	1.80	2.05	-	1.65	1.75	4.02	1.93	-	-	-	-	-	-
74	-	1.81	2.05	-	1.66	1.75	4.00	1.94	-	-	-	-	-	-
75	-	1.81	2.04	-	1.67	1.75	4.00	1.94	-	-	-	-	-	-
76	-	1.82	2.04	-	1.68	1.75	3.99	1.94	-	-	-	-	-	-
77	-	1.83	2.03	-	1.68	1.75	3.97	1.95	-	-	-	-	-	-
78	-	1.84	2.03	-	1.69	1.75	3.97	1.95	-	-	-	-	-	-
79	-	1.85	2.02	-	1.69	1.76	3.98	1.95	-	-	-	-	-	-
80	-	1.85	2.02	-	1.69	1.76	3.98	1.95	-	-	-	-	-	-
81	-	1.85	2.01	-	1.70	1.75	3.97	1.95	-	-	-	-	-	-
82	-	1.86	2.01	-	1.70	1.76	3.97	1.95	-	-	-	-	-	-
83	-	1.86	2.01	-	1.70	1.76	3.97	1.95	-	-	-	-	-	-
84	-	1.86	2.01	-	1.70	1.76	3.97	1.96	-	-	-	-	-	-
85	-	1.87	2.00	-	1.71	1.76	3.97	1.96	-	-	-	-	-	-
86	-	1.88	2.00	-	1.71	1.76	3.97	1.96	-	-	-	-	-	-

Table S17. Electronic population of basins for the rearrangement of nitrones **13**

IRC	V(C1,C6)	V(C3,C4)	V1(C4,C5)	V2(C4C5)	V1C5,C6)	V2(C5,C6)	V1(C1,N2)	V2(C1,N2)	V1(C3,N2)	V2(C3,N2)	V(N2)	V(C1)	V(C3)	V(C4)	V(C5)	V(C6)
36	-	1.86	2.00	-	1.76	1.71	4.08	-	1.94	-	-	-	-	-	-	-
37	-	1.85	2.00	-	1.76	1.70	4.08	-	1.94	-	-	-	-	-	-	-
38	-	1.85	2.01	-	1.76	1.69	4.08	-	1.93	-	-	-	-	-	-	-
39	-	1.84	2.01	-	1.76	1.69	4.08	-	1.93	-	-	-	-	-	-	-
40	-	1.84	2.01	-	1.76	1.68	4.09	-	1.93	-	-	-	-	-	-	-

41	-	1.83	2.02	-	1.76	1.68	4.08	-	1.93	-	-	-	-	-	-	-
42	-	1.83	2.02	-	1.76	1.68	4.09	-	1.93	-	-	-	-	-	-	-
43	-	1.82	2.02	-	1.76	1.67	4.09	-	1.93	-	-	-	-	-	-	-
44	-	1.82	2.03	-	1.75	1.67	4.10	-	1.93	-	-	-	-	-	-	-
45	-	1.81	2.04	-	1.76	1.66	4.10	-	1.93	-	-	-	-	-	-	-
46	-	1.80	2.05	-	1.66	1.75	4.11	-	1.93	-	-	-	-	-	-	-
47	-	1.79	2.05	-	1.75	1.65	4.07	-	1.93	-	-	-	-	-	-	-
48	-	1.77	2.06	-	1.64	1.75	3.26	-	1.93	-	0.88	-	-	-	-	-
49	-	1.76	2.07	-	1.63	1.75	3.23	-	1.94	-	0.91	-	-	-	-	-
50	-	1.75	2.08	-	1.77	1.60	2.81	-	1.94	-	0.97	0.38	-	-	-	-
51	-	1.74	2.10	-	3.34	-	2.73	-	1.94	-	1.03	0.43	-	-	-	-
52	-	1.72	2.11	-	3.34	-	2.65	-	1.94	-	1.08	0.48	-	-	-	-
53	-	1.71	2.13	-	3.34	-	2.57	-	1.96	-	1.13	0.53	-	-	-	-
54	-	1.68	2.15	-	3.34	-	2.51	-	1.96	-	1.16	0.58	-	-	-	-
55	-	1.66	2.17	-	3.06	-	2.44	-	1.98	-	1.21	0.63	-	-	0.27	-
56	-	1.63	2.19	-	2.99	-	2.38	-	2.00	-	1.25	0.68	-	-	0.33	-
57	1.10	1.61	2.22	-	2.93	-	2.32	-	2.01	-	1.29	-	-	-	-	-
58	1.20	1.57	2.25	-	2.87	-	2.27	-	2.03	-	1.32	-	-	-	-	-
59	1.28	1.54	2.28	-	2.81	-	2.22	-	2.05	-	1.33	-	-	-	-	-
60	1.35	1.50	2.33	-	2.46	-	2.17	-	2.09	-	1.35	-	-	-	-	0.30
61	1.42	1.45	2.38	-	2.38	-	2.10	-	2.15	-	1.34	-	-	-	-	0.31
62	1.47	1.38	2.44	-	2.34	-	2.07	-	2.20	-	1.33	-	-	-	-	0.30
63	1.52	1.31	2.79	-	2.29	-	2.05	-	2.24	-	1.31	-	-	-	-	-
64	1.56	1.23	2.86	-	2.26	-	2.04	-	2.28	-	1.28	-	-	-	-	-
65	1.59	1.14	2.91	-	2.23	-	2.02	-	2.34	-	1.24	-	-	-	-	-
66	1.62	-	2.98	-	2.20	-	2.02	-	2.39	-	1.19	-	0.74	0.30	-	-
67	1.64	-	3.09	-	2.18	-	2.01	-	2.44	-	1.15	-	0.71	0.18	-	-
68	1.67	-	3.32	-	2.16	-	2.01	-	2.50	-	1.09	-	0.64	-	-	-
69	1.68	-	3.32	-	2.14	-	2.00	-	2.57	-	1.05	-	0.59	-	-	-
70	1.70	-	3.32	-	2.12	-	2.00	-	2.63	-	0.99	-	0.55	-	-	-
71	1.72	-	3.33	-	2.11	-	2.00	-	2.70	-	0.93	-	0.51	-	-	-
72	1.73	-	1.59	1.76	2.09	-	2.01	-	2.77	-	0.88	-	0.47	-	-	-
73	1.76	-	1.62	1.75	2.08	-	2.01	-	2.85	-	0.82	-	0.42	-	-	-
74	1.77	-	1.64	1.75	2.07	-	2.01	-	2.93	-	0.74	-	0.38	-	-	-
75	1.78	-	1.75	1.64	2.06	-	2.01	-	3.31	-	0.73	-	-	-	-	-
76	1.79	-	1.65	1.75	2.05	-	2.01	-	4.00	-	-	-	-	-	-	-
77	1.80	-	1.66	1.75	2.04	-	2.02	-	3.99	-	-	-	-	-	-	-
78	1.81	-	1.67	1.75	2.04	-	2.02	-	3.99	-	-	-	-	-	-	-
79	1.82	-	1.67	1.75	2.03	-	2.02	-	3.98	-	-	-	-	-	-	-
80	1.83	-	1.68	1.76	2.03	-	2.02	-	3.97	-	-	-	-	-	-	-
81	1.83	-	1.68	1.76	2.03	-	2.03	-	3.96	-	-	-	-	-	-	-
82	1.83	-	1.68	1.76	2.02	-	2.03	-	3.97	-	-	-	-	-	-	-
83	1.84	-	1.68	1.76	2.01	-	2.03	-	3.96	-	-	-	-	-	-	-
84	1.85	-	1.69	1.76	2.01	-	2.03	-	3.96	-	-	-	-	-	-	-
85	1.85	-	1.69	1.76	2.01	-	2.04	-	3.95	-	-	-	-	-	-	-
86	1.85	-	1.70	1.76	2.01	-	2.04	-	3.95	-	-	-	-	-	-	-

Graphical Representations of ELF Analyses

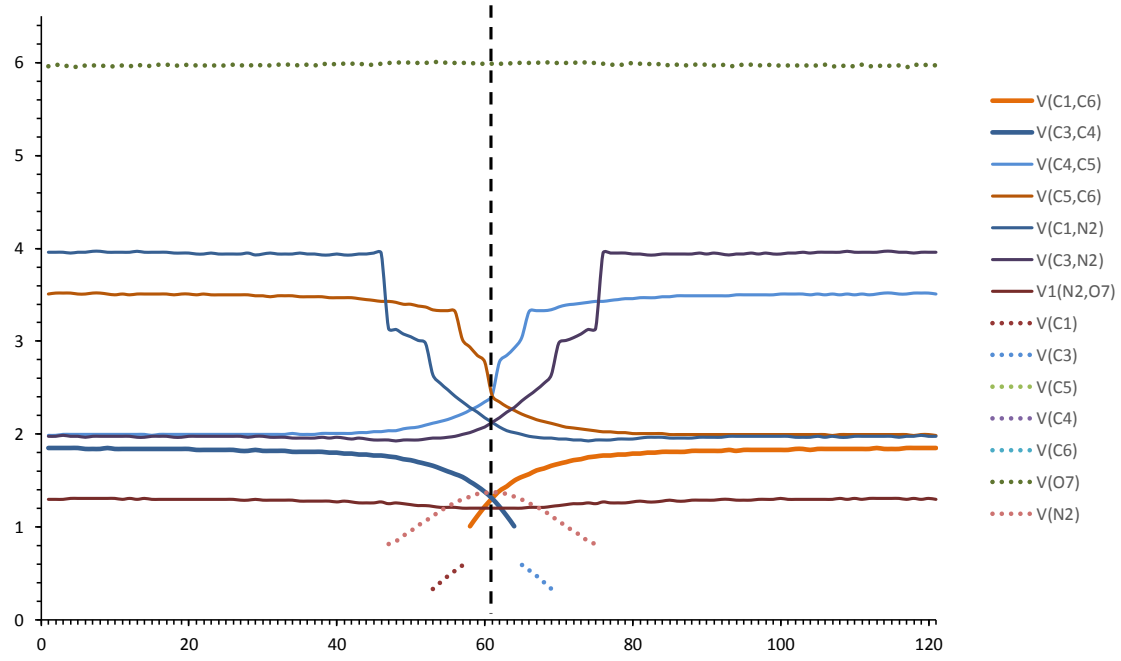

Figura S3. Graphical representation of ELF analysis for the rearrangement of nitrone **1**.

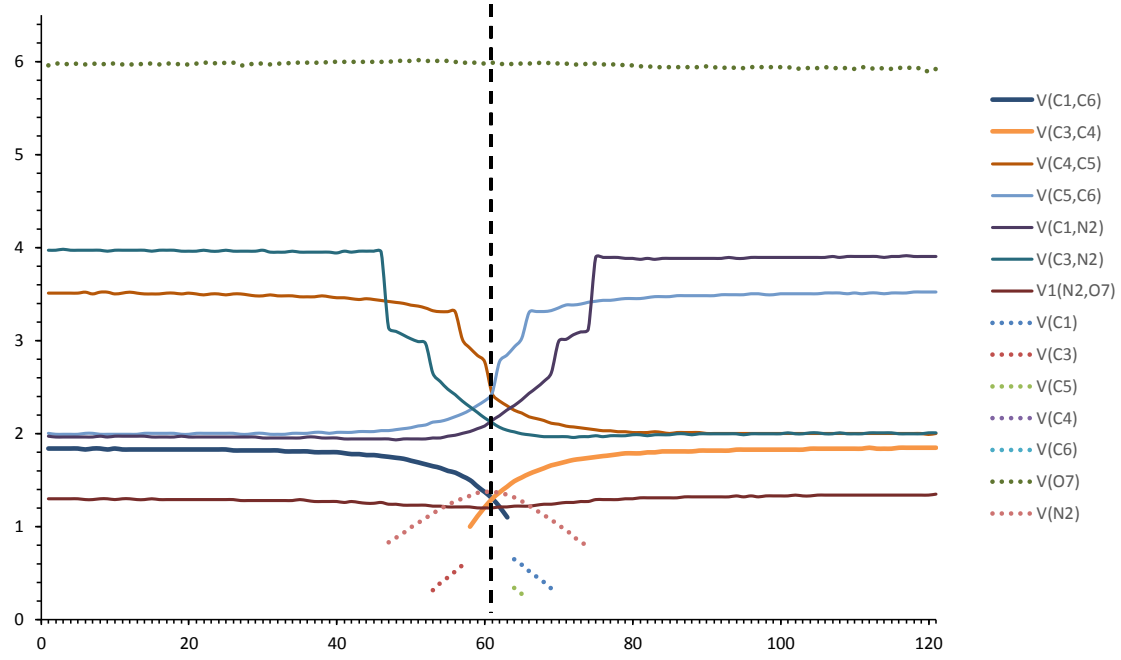

Figura S4. Graphical representation of ELF analysis for the rearrangement of nitrones **2**.

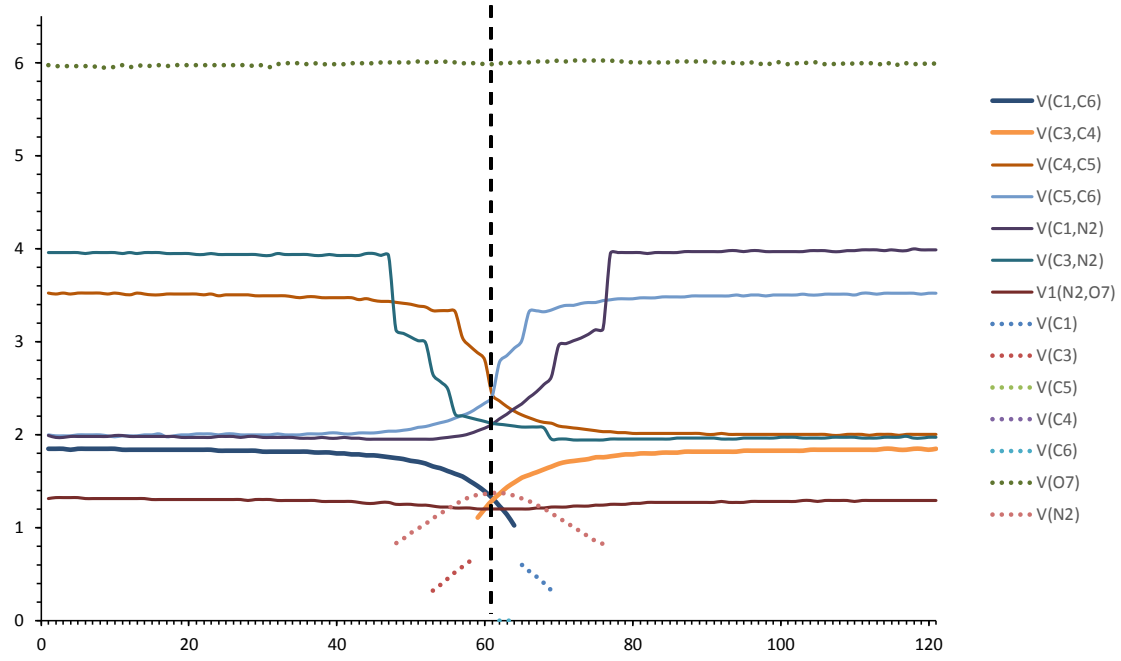

Figura S5. Graphical representation of ELF analysis for the rearrangement of nitrones **3**.

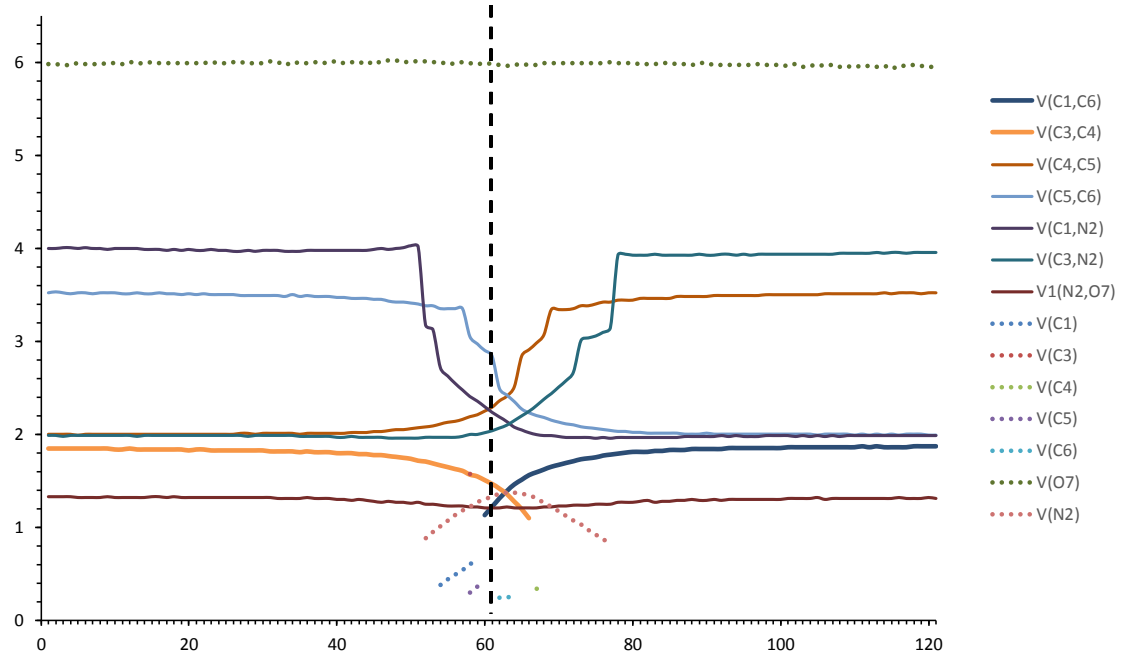

Figura S6. Graphical representation of ELF analysis for the rearrangement of nitrones **4**.

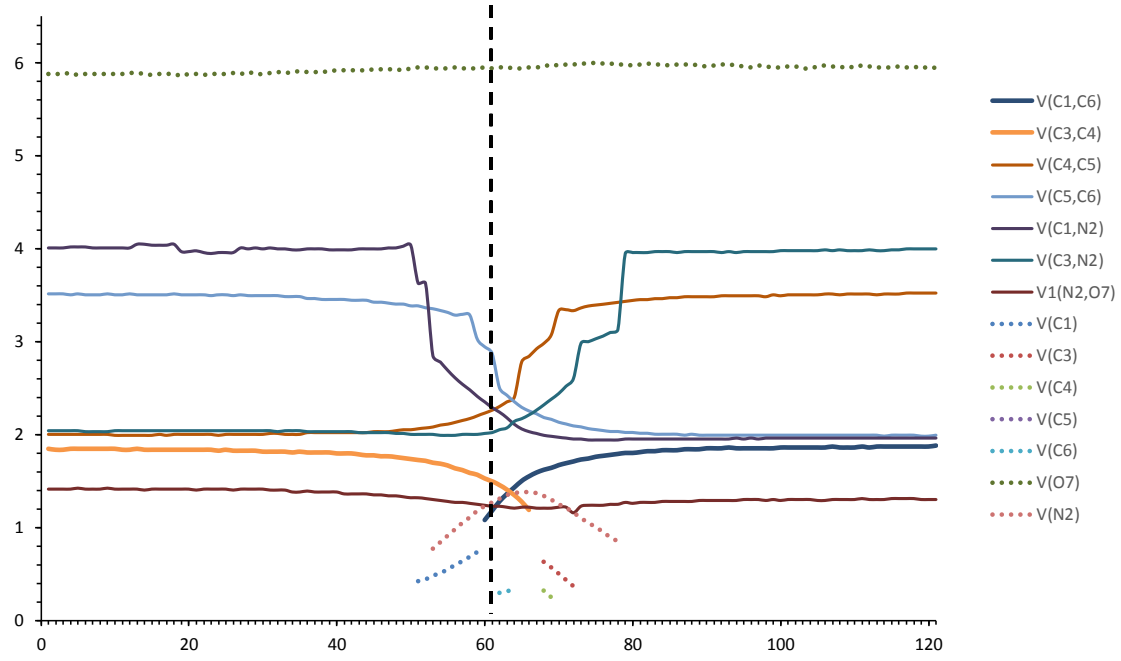

Figura S7. Graphical representation of ELF analysis for the rearrangement of nitrones **5**.

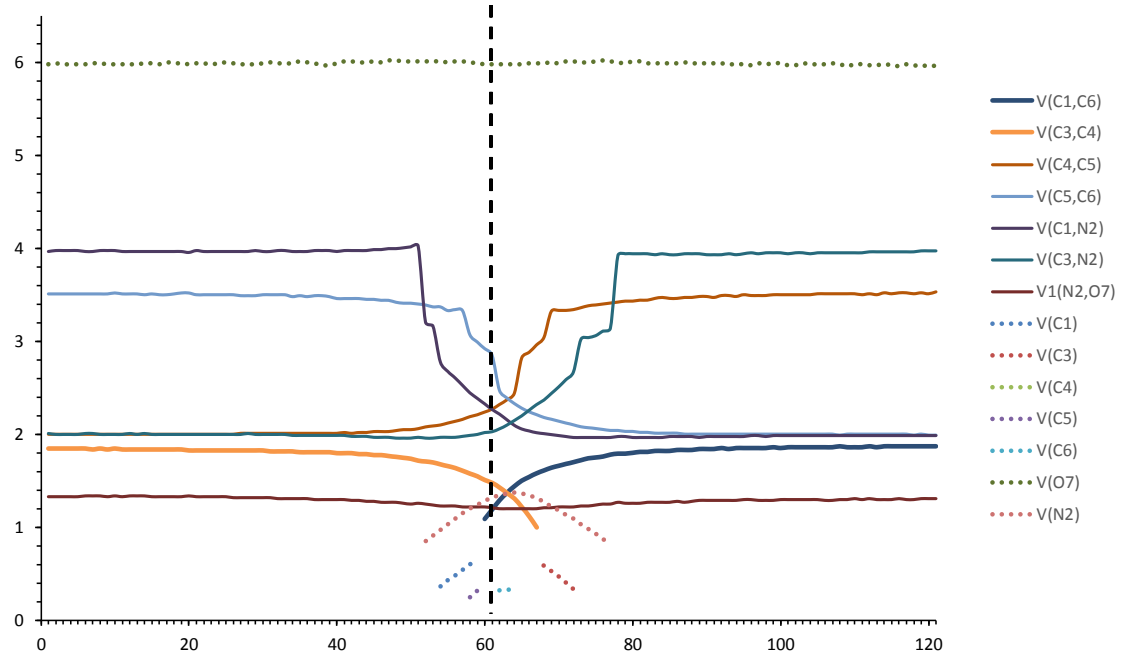

Figura S8. Graphical representation of ELF analysis for the rearrangement of nitrones **6**.

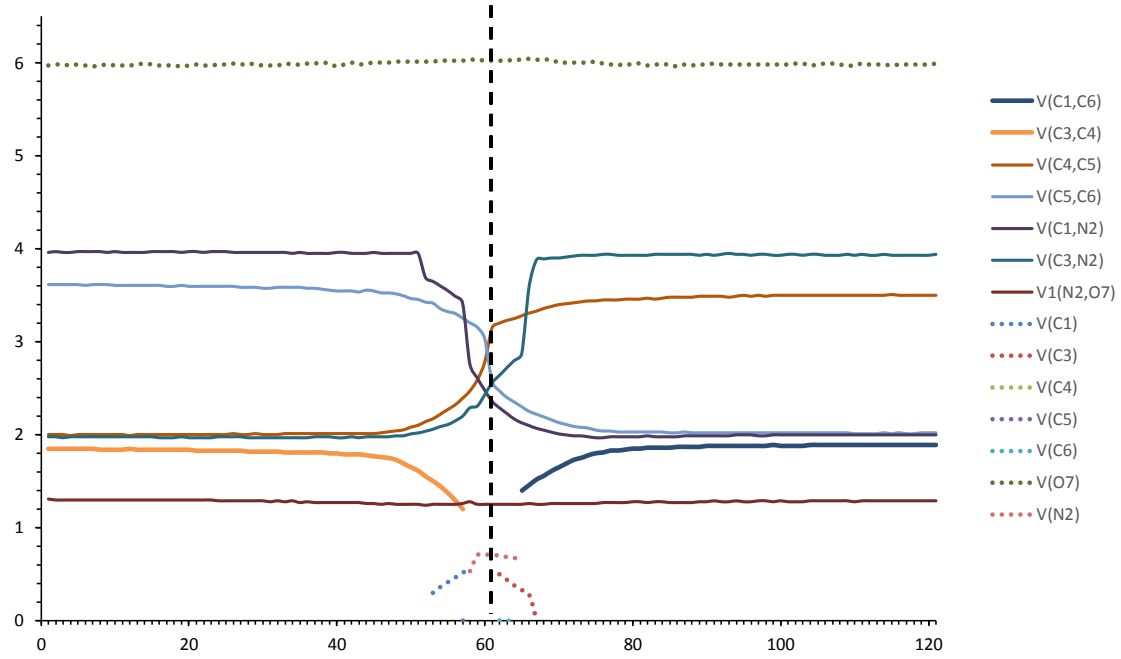

Figura S9. Graphical representation of ELF analysis for the rearrangement of nitrones (*Z*)-**7**.

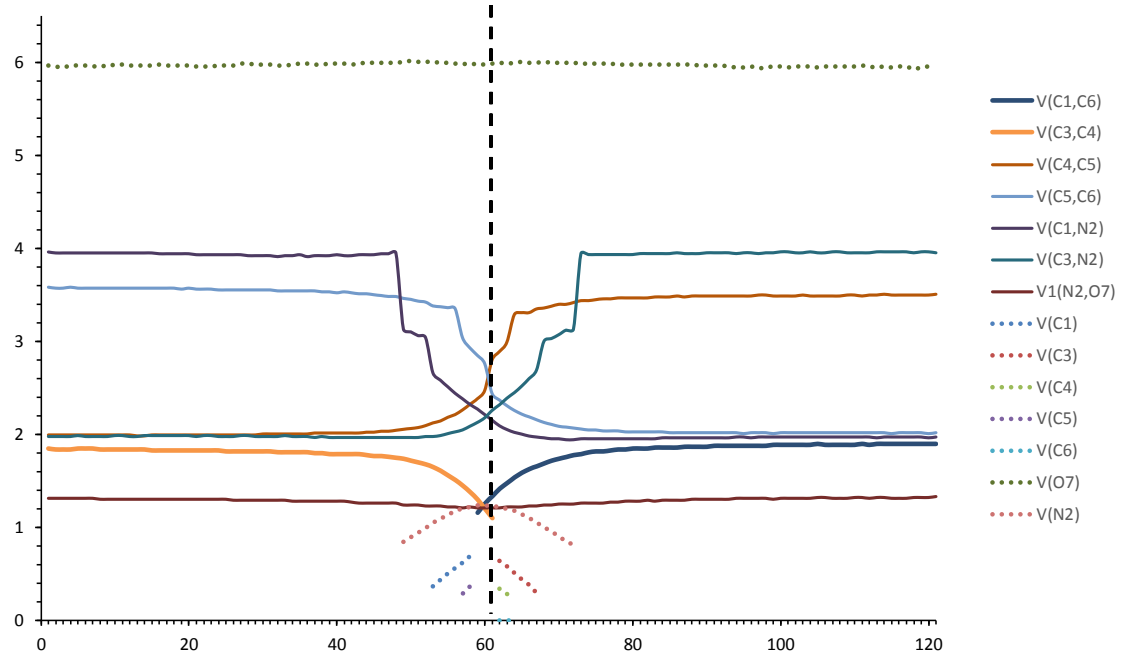

Figura S10. Graphical representation of ELF analysis for the rearrangement of nitrones (*E*)-**7**.

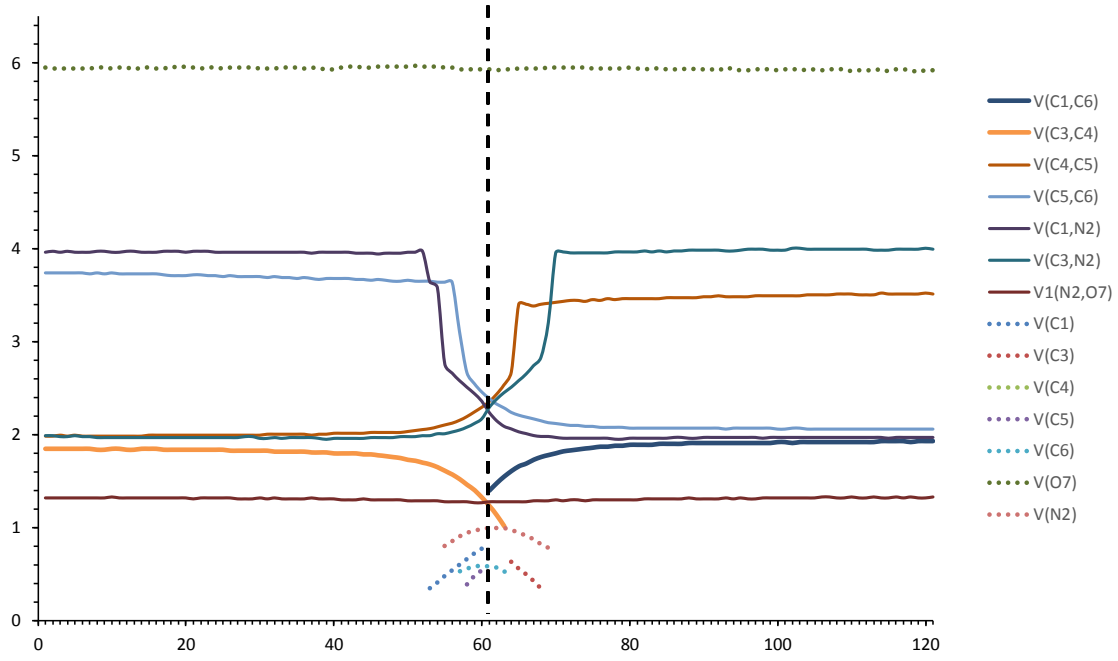

Figura S11. Graphical representation of ELF analysis for the rearrangement of nitrones (*Z*)-**8**.

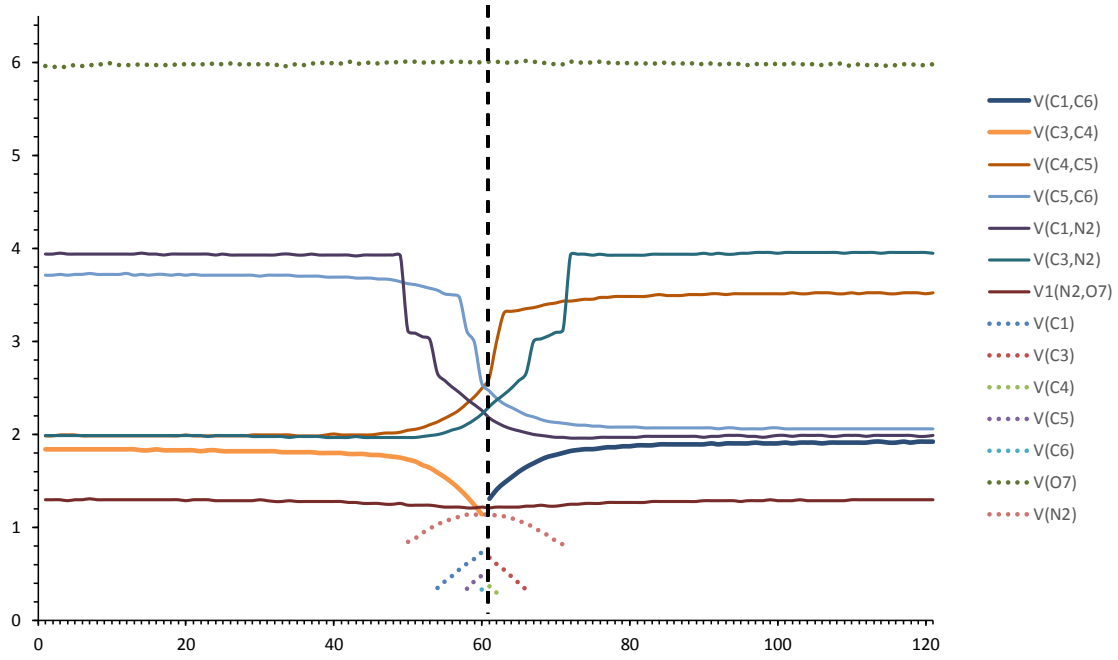

Figura S12. Graphical representation of ELF analysis for the rearrangement of nitrones (*E*)-**8**.

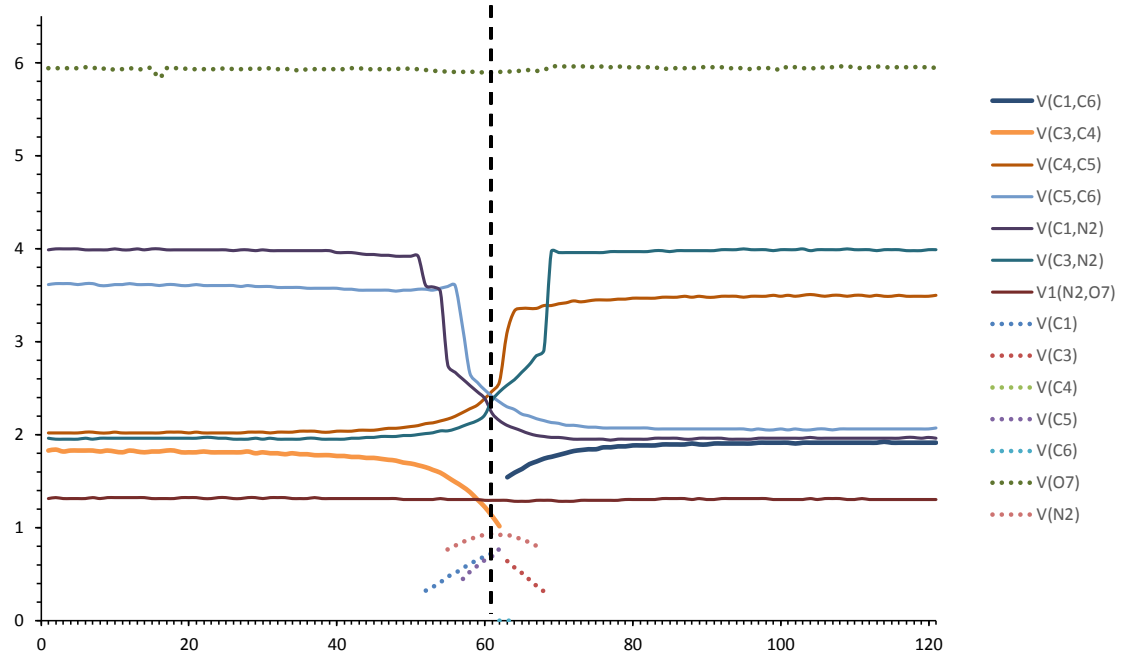

Figura S13. Graphical representation of ELF analysis for the rearrangement of nitrones (*Z*)-**9**.

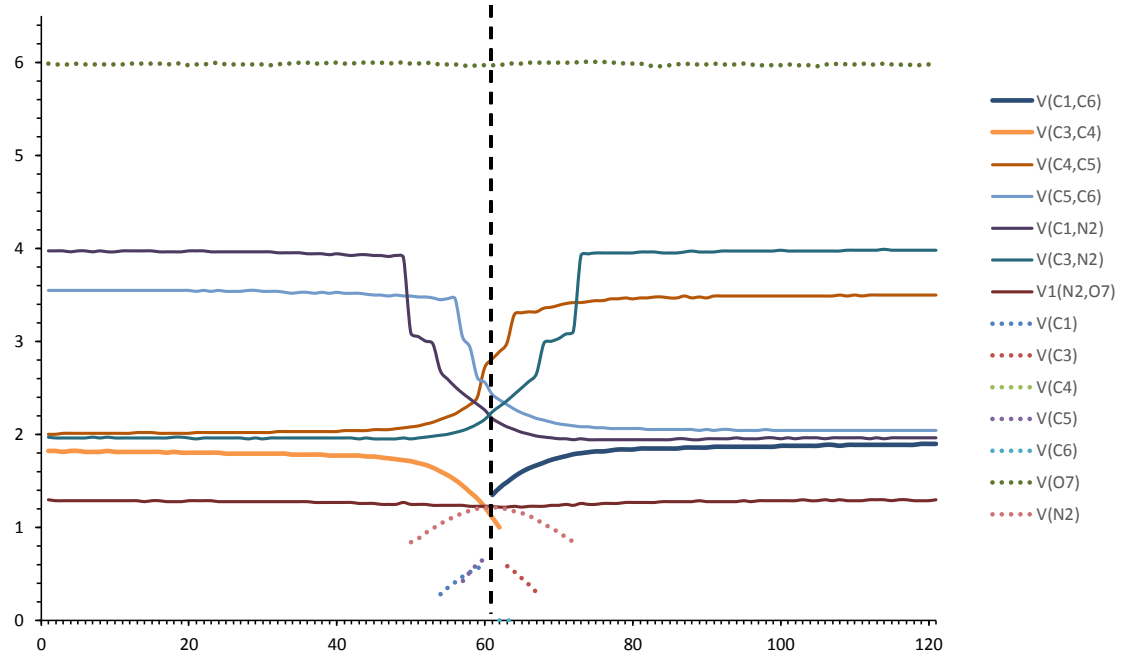

Figura S14. Graphical representation of ELF analysis for the rearrangement of nitrones (*E*)-**9**.

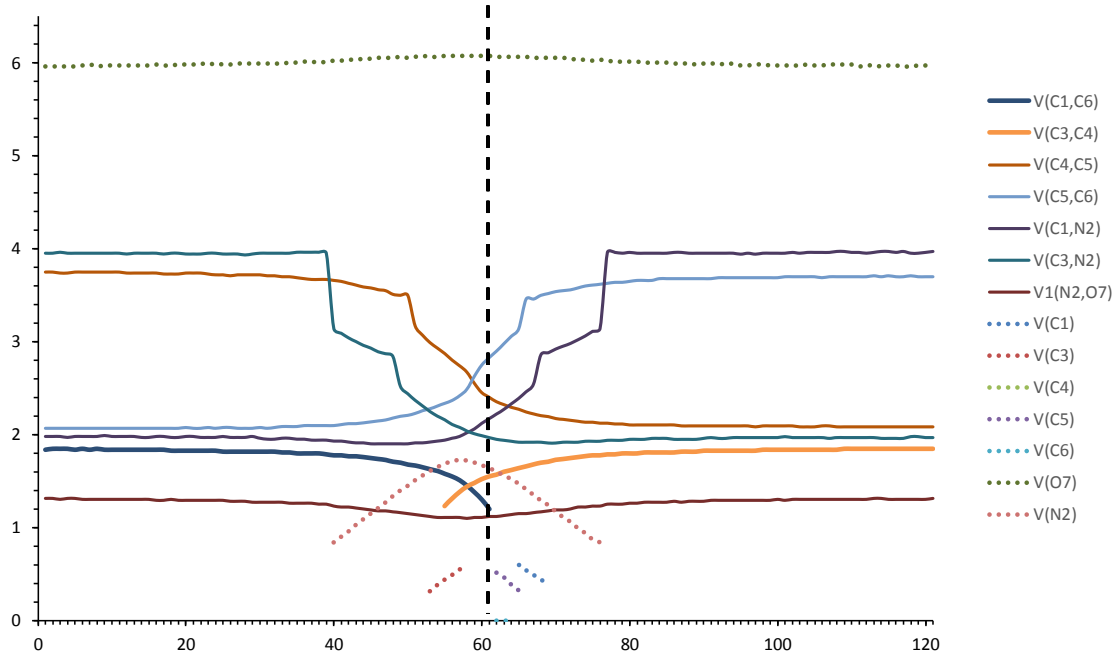

Figura S15. Graphical representation of ELF analysis for the rearrangement of nitrones **10**.

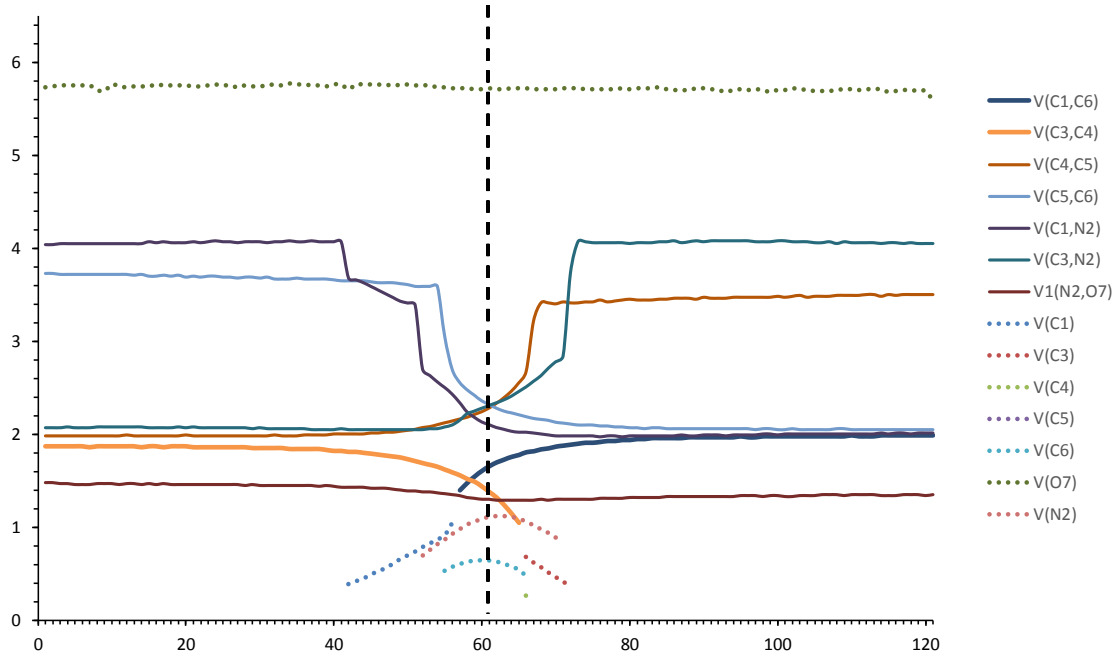

Figura S16. Graphical representation of ELF analysis for the rearrangement of nitrones (*Z*)-**11**.

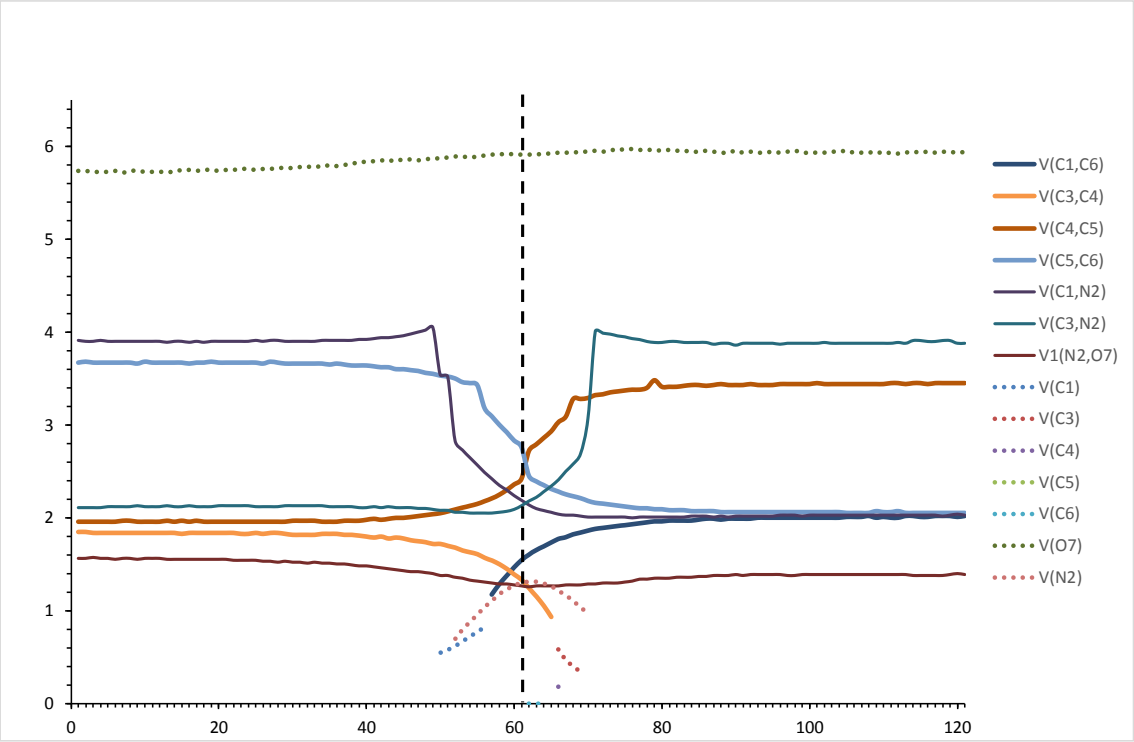

Figura S11. Graphical representation of ELF analysis for the rearrangement of nitrones (*E*)-**11**.

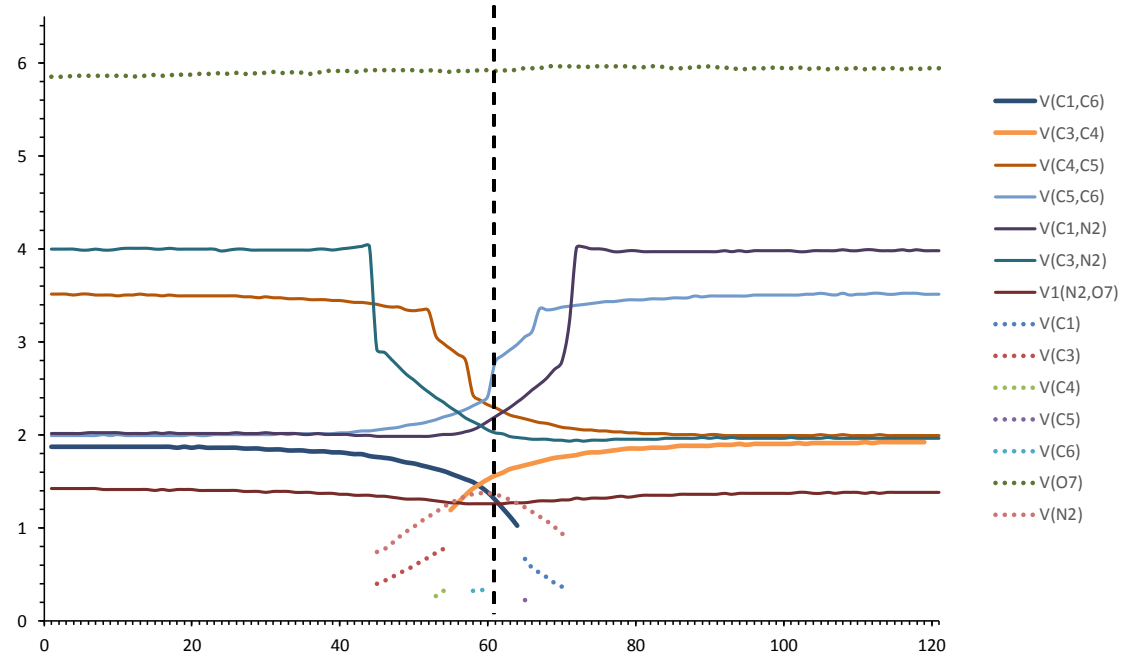

Figura S12. Graphical representation of ELF analysis for the rearrangement of nitrones **12**.

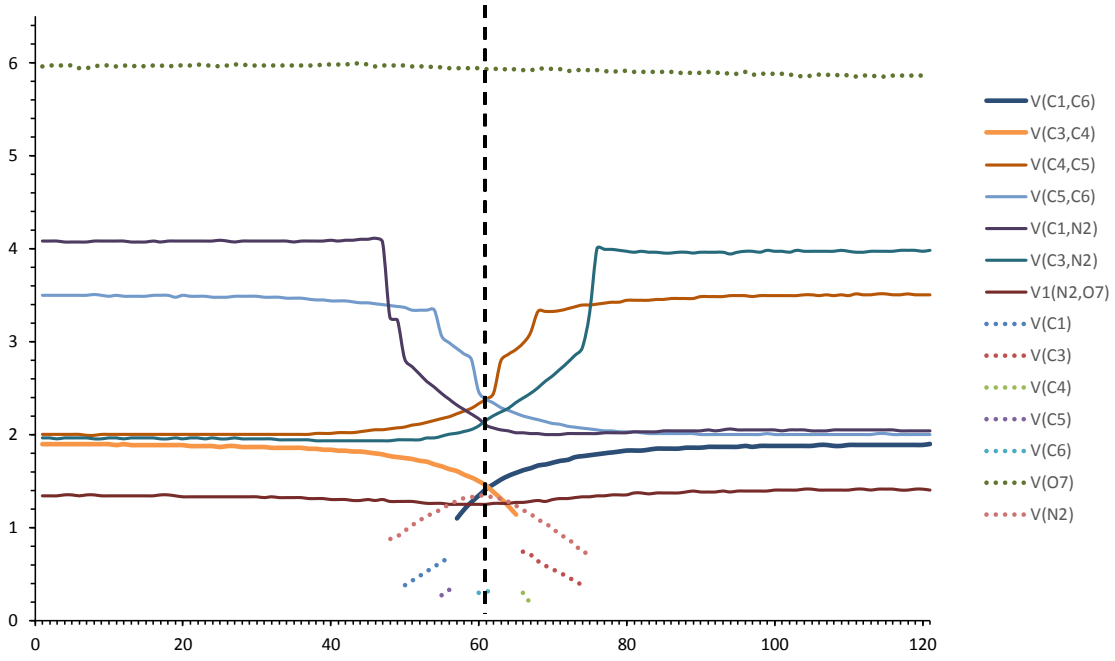

Figura S13. Graphical representation of ELF analysis for the rearrangement of nitrones **13**.

Cartesian coordinates

01a

0 1

C	-1.0571617692	0.2649938284	0.6536293730
C	1.1359111261	1.1268505433	0.0349377037
N	-0.1479378570	0.3994031876	-0.2881431447
C	-0.5850592661	3.3817660465	-2.0299047289
C	1.3989303515	2.1700763630	-1.0730391898
C	2.2806283125	0.1462625679	0.2239718098
O	-0.2429864998	-0.0466568725	-1.4838179974
C	2.6136564132	-0.8020681142	-0.7542140917
C	3.6934865792	-1.6626313680	-0.5578034011
C	4.4606269728	-1.5836130965	0.6066974614
C	4.1366166376	-0.6413127441	1.5828988178
C	3.0503378579	0.2140217963	1.3920315208
H	-0.7973077991	0.7091430314	1.6068810912
H	0.9624987738	1.6478127585	0.9810209455
H	2.0053931006	-0.8755702313	-1.6487870591
H	3.9366457542	-2.3986135474	-1.3196972234
H	5.3034817682	-2.2539263016	0.7527917067
H	4.7235251536	-0.5733634272	2.4950784944
H	2.8006585623	0.9440109584	2.1595431200
C	0.3682988978	3.2680028586	-1.1049956793
H	-1.3128004591	4.1886853148	-2.0042670422
H	-0.6758625493	2.6627784767	-2.8403603776
H	0.4163676785	3.9971973957	-0.2939077482
H	1.4327966656	1.6443747420	-2.0303949070
H	2.3960116795	2.5876212395	-0.8844839596
C	-2.3348515541	-0.4118271262	0.5462503540
C	-2.8103134225	-1.0491975413	-0.6199913430
C	-3.1498350322	-0.4243878673	1.6994900441
C	-4.0565863441	-1.6724696800	-0.6146397487
H	-2.1913120552	-1.0425353642	-1.5062285089
C	-4.3913267882	-1.0488452259	1.6937709194
H	-2.7966384998	0.0632147015	2.6055917276
C	-4.8515744954	-1.6777106778	0.5331795761
H	-4.4095946242	-2.1598791430	-1.5197871029
H	-5.0011607789	-1.0461840395	2.5932877061
H	-5.8219034905	-2.1669914422	0.5255798820

01b

0 1

C	-1.1358577745	1.1268999115	0.0349679422
C	1.0572152755	0.2649652565	0.6535505073
N	0.1479471851	0.3994026065	-0.2881754124
C	-1.3988944538	2.1701305929	-1.0730003204

C	0.5850889009	3.3817509728	-2.0299671656
C	2.3348743739	-0.4119036894	0.5461086986
O	0.2429169269	-0.0466685318	-1.4838523997
C	2.8102516470	-1.0492986447	-0.6201540782
C	4.0565017583	-1.6726169260	-0.6148639967
C	4.8515497173	-1.6778806379	0.5329137920
C	4.3913859951	-1.0489912524	1.6935254698
C	3.1499176860	-0.4244878331	1.6993058475
H	-0.9623772990	1.6478599491	0.9810398943
H	0.7974275969	0.7091299117	1.6068130890
H	2.1912042325	-1.0426187983	-1.5063589422
H	4.4094446335	-2.1600447808	-1.5200269512
H	5.8218601676	-2.1671974336	0.5252662817
H	5.0012671171	-1.0463473885	2.5930103547
H	2.7967866091	0.0631331818	2.6054231139
C	-0.3682267460	3.2680214193	-1.1050102006
H	-2.3959521879	2.5877107582	-0.8843984838
H	-1.4328252102	1.6444265443	-2.0303524627
H	-0.4162297775	3.9972185890	-0.2939207114
H	0.6758268583	2.6627597888	-2.8404269538
H	1.3128589240	4.1886454333	-2.0043668930
C	-2.2806023494	0.1463560937	0.2240654693
C	-2.6137149268	-0.8019688290	-0.7540972319
C	-3.0502512108	0.2141524252	1.3921630522
C	-3.6935677681	-1.6624900108	-0.5576267525
H	-2.0054989054	-0.8755000567	-1.6486999197
C	-4.1365527371	-0.6411398092	1.5830903794
H	-2.8005062317	0.9441374867	2.1596571856
C	-4.4606472065	-1.5834347626	0.6069117312
H	-3.9367926076	-2.3984683015	-1.3195033759
H	-4.7234132360	-0.5731620374	2.4952988292
H	-5.3035199766	-2.2537151975	0.7530526138

02a

0 1

C	0.0591588249	1.4919810128	-0.0662973881
C	2.0660174015	0.3074372094	0.6333279641
N	1.2191685870	0.5691809813	-0.3391646765
C	-0.0020710792	2.5542248177	-1.1878476864
C	2.1925548682	3.4212470956	-2.0506063210
C	3.2281893827	-0.5566433445	0.5732066461
O	1.2822002619	0.1009275494	-1.5306436846
C	3.6404545835	-1.2687176665	-0.5735930882
C	4.7766144495	-2.0735648693	-0.5217532523
C	5.5205639400	-2.1888480129	0.6541863815
C	5.1217293440	-1.4877467203	1.7959677578
C	3.9902259760	-0.6821074334	1.7554857223
H	0.2744601496	1.9880631868	0.8843115713
H	1.8479044779	0.7983948055	1.5741633491

H	3.0612552916	-1.1760740284	-1.4815767442
H	5.0830439211	-2.6167611521	-1.4117843462
H	6.4047704772	-2.8198287172	0.6828811932
H	5.6932478736	-1.5704303909	2.7164023901
H	3.6837264380	-0.1389302533	2.6467835301
C	1.1857502368	3.4805705916	-1.1788589675
H	-0.9304081984	3.1209577991	-1.0429774250
H	-0.0765643177	2.0270236946	-2.1421140914
H	1.2066188592	4.2296554616	-0.3853058253
H	2.2137556401	2.6755992873	-2.8414641450
H	3.0332492505	4.1080567423	-1.9990917282
C	-1.2352684446	0.7094194177	0.0782016476
C	-1.6219159499	-0.2690826749	-0.8514213821
C	-2.0886918170	1.0070852392	1.1505965432
C	-2.8335192128	-0.9387496046	-0.7075280561
H	-0.9538399557	-0.5138390764	-1.6690647946
C	-3.3079674978	0.3530885893	1.3014077059
H	-1.7992164460	1.7612046922	1.8782392909
C	-3.6623518900	-0.6145750620	0.3649878378
H	-3.1444703198	-1.7014456601	-1.4108497071
H	-3.9763572742	0.5736035682	2.1244016916
N	-4.9472469721	-1.3152345525	0.5164242505
O	-5.2384005000	-2.1644864029	-0.3251397316
O	-5.6551953599	-1.0097031195	1.4763515685

02b

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C	0.0247027182	0.6282595516	0.5881206812
C	2.3325102465	1.1481924929	-0.0128401076
N	0.9625720980	0.5919940945	-0.3381967850
C	0.9991437497	3.5556040347	-2.2121279232
C	2.7544395023	2.1014479088	-1.1514506424
C	3.3198526613	0.0221175091	0.2386959511
O	0.8262828654	0.1119032006	-1.5092639547
C	3.5639548251	-0.9761455363	-0.7155567432
C	4.5032912421	-1.9749085839	-0.4604165388
C	5.2166061400	-1.9863408461	0.7403196015
C	4.9806542800	-0.9949960563	1.6928614422
C	4.0341737083	-0.0002519977	1.4430483227
H	0.3242152710	1.0767994467	1.5267959097
H	2.2136663453	1.7231912093	0.9098061539
H	2.9985211803	-0.9786138072	-1.6407449611
H	4.6786917682	-2.7473692979	-1.2043472521
H	5.9502705286	-2.7645251656	0.9324682174
H	5.5275119179	-0.9961749650	2.6318770247
H	3.8530771512	0.7685074821	2.1915711648
C	1.8867731660	3.3290014398	-1.2435970489
H	0.3913914524	4.4563875493	-2.2310053859
H	0.8459408286	2.8434858585	-3.0194465923

H	2.0022016798	4.0608006688	-0.4418093838
H	2.7339003368	1.5422998632	-2.0902263664
H	3.7962094038	2.3838282137	-0.9539393559
C	-1.3280315468	0.1273778903	0.4719169595
C	-1.8577004013	-0.4974778220	-0.6802510594
C	-2.1650088575	0.2818875590	1.6020283569
C	-3.1725378150	-0.9476140405	-0.6921891451
H	-1.2251602043	-0.6193118186	-1.5477029072
C	-3.4764962709	-0.1645169813	1.5946601480
H	-1.7721571517	0.7599856924	2.4955266677
C	-3.9671626005	-0.7777453333	0.4404855910
H	-3.5918365360	-1.4288020295	-1.5672670320
H	-4.1228392991	-0.0498835548	2.4558423897
N	-5.3544113280	-1.2540084228	0.4221401302
O	-5.7637227898	-1.7911484638	-0.6080276261
O	-6.0303482659	-1.0887959431	1.4394500987

03a

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C	-0.3328541066	0.5304410205	0.5675683169
C	1.9866496022	1.1329677301	0.1367078584
N	0.6410138223	0.6213143348	-0.3123791192
C	0.7068831973	3.7676869391	-1.7787837501
C	2.4575957298	2.2132551278	-0.8620722766
C	2.9771553207	-0.0082931048	0.2964204014
O	0.5573270248	0.2953481619	-1.5508819800
C	3.2073654390	-0.9398677125	-0.7264801057
C	4.1509370339	-1.9523792309	-0.5536506677
C	4.8839604969	-2.0442423564	0.6316697617
C	4.6620850087	-1.1195762202	1.6523193838
C	3.7110400011	-0.1118502040	1.4848101318
H	-0.0757912998	0.8532533396	1.5694768669
H	1.8278482101	1.5965874476	1.1149497918
H	2.6234995678	-0.8774028298	-1.6381076260
H	4.3142520691	-2.6730951847	-1.3506963768
H	5.6209766318	-2.8326851049	0.7593993205
H	5.2229354022	-1.1837081104	2.5810970616
H	3.5400070497	0.6033153346	2.2871296404
C	1.5984951716	3.4502550933	-0.8397534850
H	0.1023164705	4.6685806138	-1.7116769995
H	0.5432743993	3.1283710877	-2.6428234699
H	1.7199888666	4.1053236049	0.0252157205
H	2.4645387261	1.7655995449	-1.8588222650
H	3.4928217487	2.4627060213	-0.5976004653
C	-1.6760224924	0.0438965213	0.3360773444
C	-2.1648065578	-0.4241562856	-0.9069152828
C	-2.5600731973	0.0374505980	1.4322672499
C	-3.4708979024	-0.8715256782	-1.0264456800
H	-1.4995163739	-0.4256945202	-1.7591412983

C	-3.8725200085	-0.4102824758	1.3179031346
H	-2.2108670365	0.3916289846	2.3998295056
C	-4.3369189896	-0.8705014125	0.0779696790
H	-3.8504930639	-1.2319058345	-1.9776556076
H	-4.5176754627	-0.3971114099	2.1888374369
O	-5.5981928660	-1.3316317608	-0.1547866205
C	-6.5188346302	-1.3529893885	0.9246753758
H	-7.4487178386	-1.7532803951	0.5167785816
H	-6.1711693131	-2.0022157197	1.7391070509
H	-6.7007638509	-0.3448305660	1.3199854617

03b

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C	-0.3077337245	1.4697874346	-0.0034622509
C	1.6905281984	0.2434080390	0.6663703309
N	0.8812086518	0.5880772337	-0.3121268370
C	-0.3188093597	2.6371929412	-1.0147340870
C	1.8949162438	3.6099446094	-1.7043658357
C	2.8644135247	-0.6027474438	0.5746501226
O	0.9986995681	0.2328304887	-1.5357142935
C	3.3345288697	-1.1969268438	-0.6162139753
C	4.4782063093	-1.9928156927	-0.5937998666
C	5.1743451399	-2.2159775715	0.5957698805
C	4.7179149695	-1.6327368798	1.7813871557
C	3.5786341169	-0.8368543113	1.7701775235
H	-0.1382360481	1.8702859748	1.0004772745
H	1.4273410987	0.6417403114	1.6387713385
H	2.7920806909	-1.0214678972	-1.5346986145
H	4.8283913323	-2.4439421463	-1.5186675976
H	6.0648801007	-2.8388318156	0.6012185944
H	5.2510410156	-1.7992089988	2.7136942846
H	3.2281476590	-0.3853592313	2.6958773767
C	0.8620472116	3.5596415774	-0.8628965346
H	-1.2552991950	3.1859849578	-0.8541050585
H	-0.3486102269	2.2125433918	-2.0211949208
H	0.8560957148	4.2087311700	0.0150338708
H	1.9452360179	2.9644578295	-2.5778209320
H	2.7296460852	4.2877207003	-1.5452288712
C	-1.5895961406	0.6595589098	0.0088374087
C	-1.9960010119	-0.1158854949	-1.0916438703
C	-2.4201514650	0.6996659305	1.1303406872
C	-3.1894049005	-0.8228430414	-1.0585652852
H	-1.3508607646	-0.1816416894	-1.9605731204
C	-3.6299387734	0.0005806087	1.1745202593
H	-2.1280476263	1.2903865911	1.9964044817
C	-4.0186985206	-0.7678420755	0.0726206299
H	-3.5046867301	-1.4301415810	-1.9013990565
H	-4.2464454776	0.0594946194	2.0641344981
O	-5.1713827914	-1.4946561661	-0.0011722191

C	-6.0453806451	-1.4817647294	1.1157835521
H	-6.8880570976	-2.1202256661	0.8443242796
H	-5.5591709613	-1.8857734960	2.0137793292
H	-6.4124750585	-0.4691675471	1.3302253480

04a

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C	-1.8896604017	-0.9160970211	1.3333845845
C	-0.3695405892	0.6408369609	0.2271149404
N	-1.2854873509	-0.5546737644	0.2331210296
C	-3.2240974752	1.7617638171	-1.4508796408
C	-0.7681565792	1.5503135978	-0.9562577932
C	1.0878164940	0.2138741912	0.1903380499
O	-1.4273741159	-1.1739833756	-0.8799515994
C	-2.7846715434	-2.1049987622	1.3190659631
C	1.5711651831	-0.6962983155	-0.7610402900
C	2.9242804160	-1.0343749442	-0.7833497256
C	3.8133675596	-0.4637036497	0.1301769763
C	3.3398937460	0.4448751401	1.0770110918
C	1.9844832747	0.7764217836	1.1074162008
H	-1.7008183745	-0.3256619658	2.2209645318
H	-0.5555777784	1.1706147024	1.1666455232
H	-2.2298352267	-3.0045500074	1.0215949127
H	-3.5795025558	-1.9771564556	0.5729780320
H	-3.2334615846	-2.2679116983	2.3020621880
H	0.8742540872	-1.1511456082	-1.4562942371
H	3.2854249238	-1.7472102748	-1.5201316497
H	4.8674419013	-0.7272826183	0.1053378149
H	4.0214649181	0.8921375465	1.7958066028
H	1.6210537837	1.4823251700	1.8517198239
C	-2.1351502984	2.1618092484	-0.7936368745
H	-4.1919702740	2.2304196840	-1.2917540871
H	-3.1842731727	0.9427704227	-2.1648963313
H	-2.2165376217	2.9735043456	-0.0680323422
H	-0.7195809224	0.9492813255	-1.8676791347
H	-0.0050024227	2.3351255254	-1.0287055602

04b

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C	-2.4245987515	-0.0897237086	0.6050544528
C	0.0024028346	0.0599422254	0.7932213856
N	-1.0336647323	-0.4034053692	0.1256314312
C	-3.1584222540	0.6970119748	-0.4983574616
C	-1.9423028301	2.4199598509	-1.8664076076
C	1.4040607841	-0.1477681728	0.4854013814
O	-0.9837175975	-1.1211709734	-0.9313203075
C	-3.1264108165	-1.4018674938	0.9559456258

C	1.8812950232	-0.8973047574	-0.6113336144
C	3.2526769126	-1.0376270383	-0.8157035579
C	4.1723333402	-0.4450097255	0.0517621505
C	3.7111023339	0.2998949366	1.1410878430
C	2.3455204965	0.4461720374	1.3543463207
H	-2.3190701665	0.5328028136	1.4996363398
H	-0.2439388511	0.6550961700	1.6641682182
H	-2.5943836099	-1.9283078304	1.7553421421
H	-3.1622087991	-2.0503609057	0.0772669507
H	-4.1477600401	-1.2004210155	1.2950748823
H	1.1654459036	-1.3546929783	-1.2800937355
H	3.6054989935	-1.6180686284	-1.6643329155
H	5.2394821314	-0.5612236415	-0.1176494793
H	4.4169672437	0.7661535002	1.8233674847
H	1.9923205518	1.0274204689	2.2035512568
C	-2.5791732949	2.0626001710	-0.7511004753
H	-4.2086703695	0.7864891941	-0.1875998692
H	-3.1313252615	0.0928949039	-1.4102976154
H	-2.6908487728	2.7896752607	0.0558422786
H	-1.8002234730	1.7212251690	-2.6876644892
H	-1.5349899285	3.4189125625	-1.9981580159

05a

0 1

C	-1.2940901898	-0.3548626558	0.8435394325
C	0.6207701792	1.0256620922	0.2387933886
N	-0.5126280271	0.0791718324	-0.1129328534
C	-1.7391763858	3.0751928027	-1.3496389648
C	0.5436096379	2.2364766182	-0.7154892192
C	1.9496707769	0.2942771627	0.2034919058
O	-0.6290144227	-0.2367906670	-1.3299726899
C	-2.4148354680	-1.2986773127	0.5494398777
C	2.3952642435	-0.3766539563	-0.9445347439
C	3.6369056850	-1.0115133664	-0.9466987368
C	4.4518542465	-0.9772327861	0.1870214847
C	4.0158568921	-0.3088825444	1.3312016969
C	2.7693750950	0.3185733182	1.3387184879
H	-1.1214291399	-0.0354596464	1.8597366546
H	0.4253114910	1.3578094516	1.2622817510
H	1.7556188447	-0.4214310097	-1.8188935120
H	3.9682427412	-1.5357238405	-1.8389940776
H	5.4198925556	-1.4707897452	0.1788603502
H	4.6403544962	-0.2791915359	2.2199389927
H	2.4329381484	0.8341924315	2.2358680131
C	-0.6990442449	3.0644345916	-0.5157176628
H	-2.6192451549	3.6827775806	-1.1565108714
H	-1.7499554548	2.4685001332	-2.2518262623
H	-0.7316454547	3.6729235967	0.3898349173
H	0.5999212162	1.8649964144	-1.7418934544

H	1.4412079993	2.8392675397	-0.5295362348
F	-3.3198692824	-0.7859630657	-0.3060905869
F	-3.0574517779	-1.5706652476	1.7107303358
F	-1.9925682458	-2.4698091861	0.0346655813

05b

0 1

C	-1.5327212451	0.5321030703	0.3511263351
C	0.8211003149	0.0826551934	0.7112231755
N	-0.1824164877	0.1247360819	-0.1415453912
C	-2.0920910483	1.6693922746	-0.5190051172
C	-0.5023010955	3.4662057317	-1.2539641910
C	2.1912723835	-0.2854365180	0.4204072539
O	-0.1301452643	-0.1580468179	-1.3872653890
C	-2.4601375825	-0.6883799355	0.3663546073
C	2.6609580771	-0.6865534255	-0.8489153942
C	4.0033069051	-1.0182061717	-1.0205420864
C	4.8988699383	-0.9604171678	0.0490968149
C	4.4441341603	-0.5658423747	1.3108600926
C	3.1075686495	-0.2329302805	1.4938648682
H	-1.4351398556	0.8476644895	1.3928724906
H	0.5714798345	0.3541308934	1.7294498718
H	1.9634772717	-0.7320010754	-1.6736285589
H	4.3520234202	-1.3262646006	-2.0026918687
H	5.9435667494	-1.2214654217	-0.0968624583
H	5.1322947205	-0.5185460780	2.1504615538
H	2.7582274554	0.0732398325	2.4775581369
C	-1.3287069145	2.9549215998	-0.3418043455
H	-3.1439600543	1.8079042005	-0.2404751777
H	-2.0558659238	1.3337012482	-1.5577220939
H	-1.4701961253	3.4744147803	0.6074706783
H	-0.3275604420	2.9672228093	-2.2041316084
H	0.0321625562	4.3965931143	-1.0819963295
F	-2.8220513088	-1.0965457280	-0.8560952753
F	-3.5907952331	-0.3659302952	1.0420046625
F	-1.8875748557	-1.7264124291	1.0066127438

06a

0 1

C	-1.6575418153	-0.2865983087	0.5924843746
C	0.4034235598	0.9537557326	0.1849120685
N	-0.7617241979	0.1129381568	-0.2637806849
C	-1.6437418807	3.2273517710	-1.5397439377
C	0.5004677954	2.1807181994	-0.7481780309
C	1.6812092371	0.1340319736	0.2361079689
O	-0.8201909524	-0.1805308560	-1.5123589250
C	-2.7911532067	-1.1228300982	0.1073796934

C	2.1136135023	-0.6344192892	-0.8545776283
C	3.3117693515	-1.3446139659	-0.7801909648
C	4.0982772155	-1.2897727401	0.3726452208
C	3.6754147869	-0.5249348807	1.4600119266
C	2.4716846620	0.1780544702	1.3913434251
H	-1.5620168840	-0.0131904008	1.6348893311
H	0.1595643353	1.2888453171	1.1978963121
H	-2.4030084748	-2.0426733196	-0.3678224492
H	-3.3392931812	-0.5834758380	-0.6868951017
H	1.4910448318	-0.6895293953	-1.7407262358
H	3.6323815781	-1.9433760787	-1.6287444440
H	5.0331152713	-1.8416641749	0.4237880117
H	4.2766643364	-0.4788790700	2.3641918789
H	2.1449084530	0.7680657947	2.2453461901
C	-0.6800028016	3.1079723147	-0.6261805320
H	-2.4803981840	3.9075347194	-1.4019447015
H	-1.6320710684	2.6408420201	-2.4552253739
H	-0.7351507840	3.6995484608	0.2897151003
H	0.5989675226	1.8144166772	-1.7731807366
H	1.4277148026	2.7067386566	-0.4883847577
C	-4.7310968857	-2.2095721332	0.8560979793
H	-5.3078049405	-2.3843048391	1.7679783488
H	-5.3729612594	-1.7040679256	0.1167623786
H	-4.4190964228	-3.1797410885	0.4371030119
O	-3.6208443019	-1.4146238615	1.2130542833

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C	-1.7499396468	0.3668046746	0.2007240548
C	0.6160112678	0.0187444703	0.6447762888
N	-0.3865154484	-0.0951973085	-0.2016975615
C	-2.1828182811	1.5470655688	-0.6873233546
C	-0.5843406717	3.4028549136	-1.2607361387
C	1.9935738855	-0.3751958670	0.4237781365
O	-0.3191578399	-0.5784988504	-1.3864444882
C	-2.7048783986	-0.8277571270	0.0902923663
C	2.4805261107	-0.9537425025	-0.7682051560
C	3.8263334744	-1.2989156851	-0.8756792821
C	4.7100121092	-1.0812356166	0.1832353519
C	4.2388665666	-0.5082361386	1.3681757847
C	2.8986352492	-0.1600403118	1.4862192419
H	-1.7045841328	0.6755308334	1.2494460118
H	0.3585835838	0.4585210911	1.6005274411
H	-2.2856711689	-1.6911233954	0.6334173688
H	-2.8204052401	-1.1166174732	-0.9633455488
H	1.7919327857	-1.1198609322	-1.5850149705
H	4.1876027102	-1.7435450274	-1.7994179598
H	5.7574437600	-1.3547643186	0.0879796533
H	4.9173043085	-0.3334437293	2.1989692784

H	2.5373685696	0.2860558591	2.4103538600
C	-1.4238012910	2.8149722791	-0.4078506161
H	-3.2542097997	1.6954278381	-0.5046355825
H	-2.0552700279	1.2416872291	-1.7309094806
H	-1.5850192475	3.2630752165	0.5747650103
H	-0.3905674449	2.9861045060	-2.2466950250
H	-0.0601480311	4.3205411034	-1.0073096348
C	-4.9331474313	-1.4257383398	0.5553463489
H	-5.8399054916	-1.0218936916	1.0127732086
H	-5.1430174915	-1.6833708810	-0.4945433932
H	-4.6423149227	-2.3457045491	1.0868300774
O	-3.9370633737	-0.4282058380	0.6576687088

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C	-0.3310450086	-1.1670057776	0.7924803786
C	1.3944600962	0.5245883275	0.4835863544
N	0.3620452330	-0.4370304029	-0.0551001269
C	-1.1933924277	2.5957491595	-0.6282733749
C	1.1779357478	1.9006439288	-0.1844512607
C	2.7987885669	-0.0235881122	0.2954195332
O	0.2462000482	-0.4671705236	-1.3295550114
C	3.2650900418	-0.4618643346	-0.9525741103
C	4.5742486614	-0.9231104399	-1.0896650226
C	5.4377605140	-0.9432357418	0.0078845581
C	4.9817011249	-0.5061571485	1.2516671090
C	3.6688752013	-0.0540436595	1.3925857779
H	-0.0937169017	-1.0037594885	1.8367308470
H	1.1959678240	0.6153154444	1.5554502921
H	2.5879665252	-0.4623208474	-1.7994931414
H	4.9212540562	-1.2676848507	-2.0603309874
H	6.4582085186	-1.2995088749	-0.1055176490
H	5.6430978790	-0.5212888710	2.1139548353
H	3.3182012327	0.2813489333	2.3666879542
C	-0.1366938962	2.5370987333	0.1871049877
H	-0.2007129006	2.9447173180	1.1963017718
H	1.2532371240	1.7637336199	-1.2661491527
H	2.0149869167	2.5374218210	0.1289462320
C	-1.3468619345	-2.1513361072	0.4731183336
C	-1.7516222553	-2.4920709558	-0.8356136572
C	-1.9651211296	-2.8071732975	1.5603662665
C	-2.7390535750	-3.4556923558	-1.0312276110
H	-1.2811232625	-1.9943732756	-1.6720021516
C	-2.9493630821	-3.7663492737	1.3538754918
H	-1.6626539933	-2.5555802462	2.5746324758
C	-3.3418996889	-4.0959397041	0.0532605450
H	-3.0399048363	-3.7085404992	-2.0446652828
H	-3.4109867399	-4.2583363451	2.2058757320
H	-4.1109753977	-4.8458989377	-0.1112945204

H	-1.0913539078	2.1563441749	-1.6227895371
C	-3.6161407427	2.0764113504	-0.5141348709
H	-4.6283125282	2.4771271183	-0.3768292656
H	-3.5642436538	1.6279487531	-1.5132505020
H	-3.4616223166	1.2757233275	0.2176655072
C	-2.5592070717	3.1933154627	-0.3471287568
C	-2.8276240743	4.2996969058	-1.3940510553
H	-2.1048934003	5.1178669522	-1.2962284988
H	-2.7526452045	3.9057623099	-2.4147385036
H	-3.8348654196	4.7160568244	-1.2682095046
C	-2.6688225323	3.7920646252	1.0646612068
H	-3.6679245340	4.2154169081	1.2204732760
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H	-1.9388182941	4.5952926615	1.2187277040

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C	-0.7502819645	0.3288825044	0.3202878959
C	1.6173873679	-0.1264270727	0.7132111397
N	0.6428055603	-0.0269891728	-0.1650830047
C	-1.2156475012	1.5865724159	-0.4853491894
C	0.6981116057	3.0433000901	-1.2653466960
C	3.0034814743	-0.4584972154	0.4464482680
O	0.7545618955	-0.2124519380	-1.4242770349
C	3.5305924631	-0.7350123861	-0.8333901731
C	4.8824626346	-1.0398453068	-0.9797798043
C	5.7337500363	-1.0773192236	0.1262514788
C	5.2227944166	-0.8054732994	1.3987658874
C	3.8760865655	-0.5002497240	1.5560215819
H	-0.6353109783	0.6144842098	1.3690062827
H	1.3297335926	0.0614870188	1.7403838302
H	2.8676325065	-0.7052832781	-1.6867237996
H	5.2740086962	-1.2505817779	-1.9716557445
H	6.7864031402	-1.3161438447	0.0001576853
H	5.8753685542	-0.8317047024	2.2674414797
H	3.4843142360	-0.2893957987	2.5488495430
C	-0.1556316304	2.6582770086	-0.3172258634
H	-0.0944048255	3.1252359449	0.6674875259
H	0.6964691394	2.5881378846	-2.2521854228
H	1.4425271574	3.8141445064	-1.0820752333
C	-1.5975324897	-0.9314580206	0.2604083064
C	-1.8346486731	-1.6105120460	-0.9441890162
C	-2.1266304496	-1.4578338119	1.4460952064
C	-2.5982550404	-2.7768927481	-0.9554771044
H	-1.3990391292	-1.2326374012	-1.8613508832
C	-2.8994921645	-2.6203490714	1.4330176834
H	-1.9364783269	-0.9525872574	2.3908322594
C	-3.1391146127	-3.2827006046	0.2291442480
H	-2.7714099666	-3.2939246406	-1.8956572802

H	-3.3062399977	-3.0087730419	2.3629468939
H	-3.7378779907	-4.1894852906	0.2137937392
H	-1.2289183231	1.2935831511	-1.5403381237
C	-3.7730067516	1.2100765960	-0.6418332552
H	-4.7443223753	1.7044004863	-0.5161808190
H	-3.6495088102	0.9894587887	-1.7088329073
H	-3.8139590644	0.2610417169	-0.1056322501
C	-2.6521722651	2.1413314022	-0.1312130474
C	-2.8326334941	3.4970333633	-0.8523687476
H	-2.1359952664	4.2577790716	-0.4887420016
H	-2.6732828007	3.3947091371	-1.9325618749
H	-3.8526115504	3.8682742356	-0.6969896153
C	-2.8375167029	2.3599906080	1.3848238939
H	-3.8086856163	2.8306549276	1.5789669968
H	-2.8212422821	1.4152848270	1.9396367747
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C	0.6226821131	-1.2248665729	-0.9655108611
C	-1.3004045315	0.2665594209	-0.8618772089
N	-0.1089545913	-0.4135583934	-0.2329955709
C	1.0349194424	3.0606995063	-0.7859497034
C	-1.2227224910	1.7847189283	-0.5856489595
C	-2.5978197383	-0.3665101829	-0.3883900925
O	0.0938737861	-0.1479398956	1.0050097900
C	-2.9188282921	-0.4751332081	0.9724873843
C	-4.1372021593	-1.0297310855	1.3639493183
C	-5.0545844784	-1.4723259113	0.4082957520
C	-4.7435276509	-1.3649461143	-0.9472212091
C	-3.5204583305	-0.8191768446	-1.3399408786
H	0.3037693628	-1.3235486026	-1.9959601186
H	-1.2078111323	0.1016882554	-1.9393641350
H	-2.1983478375	-0.1496213219	1.7142117941
H	-4.3707772677	-1.1155078410	2.4219435371
H	-6.0043288395	-1.8997821526	0.7187005058
H	-5.4477643249	-1.7091822271	-1.7000255732
H	-3.2827403713	-0.7418683391	-2.3990799589
C	-0.0422152378	2.4261687049	-1.2690038665
H	-0.0789498580	2.3286972330	-2.3573105298
H	-1.2349610289	1.9421359848	0.4899110248
H	-2.1522895708	2.2110702659	-0.9876421102
C	1.7830987414	-1.9834179707	-0.5408615634
C	2.2854468539	-2.0142500565	0.7780623747
C	2.4428686410	-2.7457129719	-1.5298963040
C	3.4087126171	-2.7827139080	1.0782551581
H	1.7806772382	-1.4395949401	1.5418574563
C	3.5632852635	-3.5070121620	-1.2199812335
H	2.0656965356	-2.7333895505	-2.5501980323

C	4.0530262769	-3.5282280647	0.0893238692
H	3.7834749151	-2.7980463317	2.0983824346
H	4.0556057861	-4.0846804415	-1.9977144570
H	4.9291453656	-4.1224970783	0.3346992754
H	1.7425261965	3.3937492236	-1.5496408423
C	1.5282366884	3.4206236679	0.6083533168
C	0.5046742822	3.2499416215	1.7444342331
H	0.9365528223	3.6196561118	2.6827922342
H	-0.4087494643	3.8256448384	1.5538683005
H	0.2430256893	2.1987974940	1.8903761349
C	2.7573576155	2.5275309076	0.9079486541
H	3.5226291651	2.6244210166	0.1280899002
H	3.2143189740	2.8151999694	1.8634760012
H	2.4587638515	1.4762466833	0.9693865242
C	1.9775309392	4.9008354146	0.5665519875
H	2.4151374672	5.1955783586	1.5280332957
H	2.7330571703	5.0692337658	-0.2106941280
H	1.1302143962	5.5659417960	0.3616440800

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C	0.8157552744	0.1613081324	-0.7768570661
C	-1.5160963857	-0.4939261766	-0.6529870379
N	-0.4398463433	-0.0960999188	-0.0039852390
C	1.3210239469	1.6587771820	-0.7781485883
C	-0.8475195310	2.7259067386	-1.6521085967
C	-2.8091387418	-0.8212104708	-0.0854627489
O	-0.3719391209	0.0489129099	1.2710311542
C	-3.1234031186	-0.7767991040	1.2904334268
C	-4.4045533788	-1.1132895119	1.7234203659
C	-5.3920403984	-1.4964510239	0.8140499012
C	-5.0928840622	-1.5441305937	-0.5508913770
C	-3.8188851459	-1.2109037299	-0.9937981627
H	0.5327829472	-0.0036336252	-1.8199102278
H	-1.4058771878	-0.5657584735	-1.7272918354
H	-2.3564620270	-0.4797610795	1.9914122905
H	-4.6323194445	-1.0747459124	2.7854639999
H	-6.3875722770	-1.7562208726	1.1638567968
H	-5.8535783277	-1.8407888003	-1.2679275002
H	-3.5912064237	-1.2493342367	-2.0568077258
C	0.4659317381	2.4952331049	-1.7262040632
H	1.0077589793	2.9421733058	-2.5605533427
H	-1.4718702563	2.3401955431	-0.8523126741
H	-1.3482881486	3.3350974404	-2.4008528142
C	1.8778516209	-0.9008192259	-0.4702613928
C	1.8215895115	-1.7793991607	0.6184256400
C	2.9279003690	-1.0448867134	-1.3903652951
C	2.8013130030	-2.7601472186	0.7875686362
H	1.0169483648	-1.6843821769	1.3377582617

C	3.9105616746	-2.0183572763	-1.2162274163
H	2.9758031155	-0.3954136591	-2.2621561322
C	3.8517839973	-2.8818315609	-0.1212427522
H	2.7393145125	-3.4306019431	1.6408055114
H	4.7142753436	-2.1073775714	-1.9424525180
H	4.6132606628	-3.6447070052	0.0167994189
H	2.2844080864	1.5402105779	-1.2898122692
C	1.7085194415	2.4390652856	0.5449413151
C	0.5069132639	3.0062132415	1.3264999866
H	0.8748675151	3.5201166541	2.2235091158
H	-0.0481940332	3.7393961887	0.7333948347
H	-0.1737600818	2.2142767308	1.6434487902
C	2.5531322891	1.5592024787	1.4855762646
H	3.4126807502	1.1169439225	0.9686857820
H	2.9401860596	2.1736246978	2.3081209083
H	1.9543099658	0.7542996484	1.9151482940
C	2.5826626899	3.6354736862	0.0955738811
H	2.8987877635	4.2174781326	0.9692718729
H	3.4894164251	3.3014076532	-0.4256504350
H	2.0350331227	4.3119367862	-0.5704302380

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C	-0.6901376175	-0.4940900058	0.9113557928
C	1.2802216805	0.8329704561	0.3725356218
N	0.0970358440	-0.0150415764	-0.0270099762
C	-1.0003954696	2.9647363874	-1.0519734845
C	1.2764474567	2.1125695475	-0.4971321219
C	2.5728178103	0.0409815355	0.2804089001
O	-0.0489429287	-0.2049447927	-1.2864082699
C	2.9366516715	-0.6572930566	-0.8802617332
C	4.1505683821	-1.3418803804	-0.9362379532
C	5.0215775011	-1.3311420729	0.1555058807
C	4.6679758465	-0.6360642155	1.3122026569
C	3.4491066968	0.0409967150	1.3731537331
H	-0.4110068937	-0.2251905225	1.9228376044
H	1.1137606967	1.1147231419	1.4160492372
H	2.2509443815	-0.6796787678	-1.7199910246
H	4.4169659788	-1.8861498358	-1.8385593749
H	5.9680075524	-1.8630100808	0.1055244117
H	5.3356729268	-0.6241237272	2.1696847246
H	3.1776400275	0.5775616930	2.2801455900
C	0.0781231057	2.9922927585	-0.2628637334
H	0.0820390697	3.6604447797	0.5967065312
H	1.3353628700	1.7994030640	-1.5427921269
H	2.2025422594	2.6533380537	-0.2678503809
C	-1.8626603842	-1.3280252155	0.7305368057
C	-2.3462209668	-1.7756183709	-0.5178401708
C	-2.5614913629	-1.7079247966	1.8974333070

C	-3.4879769799	-2.5724255132	-0.5782381611
H	-1.8139405446	-1.4906622332	-1.4145950634
C	-3.6993620568	-2.5026591182	1.8258057628
H	-2.2004812475	-1.3705928486	2.8665850515
C	-4.1693962497	-2.9395032447	0.5838527370
H	-3.8477587018	-2.9112486848	-1.5464087250
H	-4.2205671372	-2.7824892838	2.7374273266
H	-5.0585445909	-3.5615152732	0.5246264902
H	-1.0676994392	2.2907975289	-1.9063648858
O	-2.0740681145	3.7767977405	-0.8440845837
C	-3.2241843516	3.4644093503	-1.6185859263
H	-3.9646771737	4.2370122250	-1.4015276361
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H	-3.6352462193	2.4826423515	-1.3484290703

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C	-0.9324720220	0.5792054616	0.3225414352
C	1.3778435946	-0.0420829858	0.7424912579
N	0.4120180394	0.0990152226	-0.1404508438
C	-1.3709718359	1.7503216678	-0.5960271934
C	0.4358909227	3.2100867872	-1.5718312420
C	2.7287810647	-0.5056682788	0.4950362692
O	0.5078555236	-0.1440360309	-1.3957924501
C	3.2280329151	-0.8886222240	-0.7684640051
C	4.5470731869	-1.3198703279	-0.8948147764
C	5.3919216652	-1.3800822678	0.2151814861
C	4.9083420739	-1.0031189868	1.4714818163
C	3.5944035632	-0.5718482642	1.6089815321
H	-0.7994455576	0.9826014679	1.3298985510
H	1.1071317572	0.2129577395	1.7598450135
H	2.5701449879	-0.8408436280	-1.6248644448
H	4.9178685448	-1.6123939729	-1.8737758424
H	6.4188496859	-1.7179320480	0.1045722412
H	5.5563198974	-1.0462942104	2.3428251087
H	3.2229086153	-0.2803618953	2.5890513928
C	-0.3886785970	2.8964555579	-0.5732393865
H	-0.3930588173	3.4808527795	0.3481040337
H	0.4628701594	2.6263408112	-2.4883728043
H	1.1299842538	4.0433475684	-1.4995402062
C	-1.9401644933	-0.5561101503	0.3786000754
C	-2.1207669132	-1.4455079019	-0.6898069844
C	-2.7278936218	-0.7052161690	1.5263956017
C	-3.0681959457	-2.4657503573	-0.6005095407
H	-1.4989767279	-1.3465226717	-1.5725882400
C	-3.6801207406	-1.7209153988	1.6109247733
H	-2.6026408652	-0.0142971314	2.3566074008
C	-3.8519392554	-2.6064467600	0.5462881103
H	-3.1928945431	-3.1540540463	-1.4324660370

H	-4.2842765196	-1.8205983680	2.5088811323
H	-4.5905091450	-3.4012550784	0.6102030528
H	-1.4735919609	1.3587063420	-1.6159469617
O	-2.6330469809	2.1590981626	-0.0808600071
C	-3.3846597312	2.9494148747	-0.9848998474
H	-4.3240394936	3.1926961737	-0.4820457004
H	-2.8643974103	3.8807897799	-1.2498797563
H	-3.6057132733	2.3967027573	-1.9108030144

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C	0.8577931607	-0.6463450740	-0.8930104996
C	-1.2332286327	0.6034716243	-0.8196982584
N	0.0348850902	0.0907020729	-0.1772476569
C	0.7117067886	3.5793885645	-0.5172287016
C	-1.3338219897	2.1264000381	-0.5828290050
C	-2.4434476465	-0.1650249967	-0.3181046605
O	0.2089712418	0.4200630312	1.0467324568
C	-2.7487240568	-0.2559648628	1.0477945678
C	-3.8892122009	-0.9402479001	1.4674644310
C	-4.7446919826	-1.5314563877	0.5349665786
C	-4.4491979183	-1.4423014382	-0.8253602668
C	-3.3026229534	-0.7666146254	-1.2460127256
H	0.5471929986	-0.8185474947	-1.9162027455
H	-1.1236936572	0.4182466673	-1.8923538530
H	-2.0744426143	0.1883718513	1.7711812969
H	-4.1110898146	-1.0103081835	2.5291513510
H	-5.6346095486	-2.0595196429	0.8671605086
H	-5.1057561536	-1.9012119674	-1.5598993155
H	-3.0760777885	-0.7035552180	-2.3085365818
C	-0.1965676122	2.8845618989	-1.2075665406
H	-0.0849980109	2.8508366406	-2.2899804913
H	-1.3611335540	2.3132643616	0.4919118277
H	-2.2977382413	2.4435350752	-1.0024751448
C	2.1090951889	-1.2344520746	-0.4563845085
C	2.6232036839	-1.1489793576	0.8556435101
C	2.8552194298	-1.9416954080	-1.4248915754
C	3.8405700280	-1.7511886917	1.1686044463
H	2.0526092728	-0.6185161719	1.6050557120
C	4.0688931261	-2.5369610168	-1.1024393594
H	2.4705233832	-2.0186097258	-2.4396339181
C	4.5693215027	-2.4432349605	0.1995701336
H	4.2224486521	-1.6789114441	2.1837678568
H	4.6256277085	-3.0749246280	-1.8651354067
H	5.5179848388	-2.9078360392	0.4547630745
H	1.5606793521	4.0689271373	-1.0026072757
O	0.6200030067	3.7811854941	0.8277506521
C	1.8324508713	3.5530300345	1.5399225356
H	2.6665072697	4.1174366031	1.0962971176

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H	2.0732572869	2.4839150217	1.5481412549

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C	0.9278880802	0.4819048886	-0.7529847733
C	-1.3415739497	-0.3793406996	-0.7938581406
N	-0.3615929535	0.1236144142	-0.0678011225
C	1.2599175190	1.9939171512	-0.5698353311
C	-0.6989951684	3.5106700671	-0.1315431918
C	-2.6489461793	-0.7922632742	-0.3236271811
O	-0.4081368129	0.3399190488	1.1883896793
C	-3.0861633536	-0.7053224284	1.0159562910
C	-4.3669448901	-1.1332596640	1.3603491788
C	-5.2348325120	-1.6511082410	0.3971319517
C	-4.8131465754	-1.7414892236	-0.9327433988
C	-3.5381834224	-1.3174125080	-1.2873544490
H	0.7434318454	0.3542397913	-1.8232647998
H	-1.1239089281	-0.4956816135	-1.8481622372
H	-2.4110452159	-0.3042896925	1.7587578624
H	-4.6892164030	-1.0605573244	2.3959567034
H	-6.2312419545	-1.9818285387	0.6779379261
H	-5.4791227837	-2.1431045151	-1.6919128995
H	-3.2156046363	-1.3909037185	-2.3238228977
C	0.0969832483	2.8726500834	-0.9877409966
H	-0.0741502401	2.9480977262	-2.0623398213
H	-0.5457441335	3.4258399980	0.9398474494
H	-1.5280618341	4.1227864931	-0.4752578758
C	2.0534294966	-0.4538351842	-0.3543131001
C	2.4192349588	-0.6608977479	0.9840918138
C	2.7640879167	-1.1158839233	-1.3638630948
C	3.4721918798	-1.5215428708	1.2931159230
H	1.8641743260	-0.1570401948	1.7641445737
C	3.8251312731	-1.9673471016	-1.0521897594
H	2.4864677608	-0.9661566522	-2.4056700953
C	4.1804131276	-2.1733097567	0.2806881578
H	3.7431027214	-1.6812851109	2.3335675329
H	4.3652559259	-2.4721072053	-1.8488389369
H	5.0024597623	-2.8392956560	0.5299469305
H	2.0947962992	2.1631473759	-1.2742591044
O	1.7059226958	2.2469249483	0.7430929741
C	2.5791163877	3.3586187469	0.8409109226
H	2.0939563537	4.2910328625	0.5212789709
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H	3.4888974139	3.2065941116	0.2391396056

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C	-0.5643909830	-0.5857266428	0.8315752185
C	1.3776584272	0.7735557541	0.2787598019
N	0.2135818664	-0.1037366728	-0.1125113376
C	-0.8720463280	2.7595826364	-1.2978249880
C	1.4223870555	1.9779666326	-0.6916985140
C	2.6776439631	-0.0123573434	0.2939336992
O	0.0871290800	-0.3246864344	-1.3716444025
C	3.0607110140	-0.8297268640	-0.7789883762
C	4.2771132842	-1.5109722461	-0.7392649647
C	5.1283506303	-1.3777255621	0.3599650026
C	4.7533811424	-0.5639571849	1.4292839111
C	3.5322505371	0.1108024583	1.3964316010
H	-0.2980775656	-0.2862124021	1.8384803133
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H	2.3903192589	-0.9444741836	-1.6241342043
H	4.5605300172	-2.1486687829	-1.5722707027
H	6.0765870242	-1.9078141157	0.3839982749
H	5.4055922022	-0.4576638484	2.2918827346
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C	0.2273052966	2.8784681168	-0.5542983637
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H	1.4999070499	1.5811886797	-1.7057927792
H	2.3366911808	2.5382210059	-0.4701360422
C	-1.7053045203	-1.4639172837	0.6648002330
C	-2.1617142698	-1.9606077717	-0.5750333957
C	-2.3984950383	-1.8353076394	1.8377708956
C	-3.2742747269	-2.7978446071	-0.6216073049
H	-1.6349134813	-1.6810554101	-1.4765886132
C	-3.5072268321	-2.6707761975	1.7795104650
H	-2.0574374751	-1.4591065733	2.7997482904
C	-3.9509346171	-3.1562433437	0.5459720001
H	-3.6163289164	-3.1727456715	-1.5825338495
H	-4.0268659787	-2.9432176664	2.6939922321
H	-4.8186023674	-3.8085205841	0.4970410054
H	-1.0472666293	2.0213943628	-2.0685816965
N	-2.0055003923	3.6584545320	-1.1040188098
O	-2.9639892612	3.4835923811	-1.8581893678
O	-1.9459229718	4.5206606308	-0.2251481364

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C	-0.7802878032	0.5524762798	0.2195390831
C	1.5206712896	-0.0435375072	0.7081380575
N	0.5735577121	0.0548250879	-0.1996131957
C	-1.1835810516	1.6443017960	-0.8097057938
C	0.6087235513	3.0895551403	-1.7693509459
C	2.8724864875	-0.5273671484	0.5115195762
O	0.6873697374	-0.2480804400	-1.4414653354

C	3.3899241915	-0.9859550105	-0.7190198482
C	4.7072263183	-1.4331630563	-0.7961781799
C	5.5311354896	-1.4341931619	0.3311653150
C	5.0292092221	-0.9814884228	1.5548655195
C	3.7166139396	-0.5341084013	1.6436535684
H	-0.6650757548	1.0345311464	1.1916358462
H	1.2307643707	0.2649316928	1.7053920580
H	2.7479396767	-0.9839576303	-1.5887527621
H	5.0931825296	-1.7848757698	-1.7492880861
H	6.5570102463	-1.7851046948	0.2589712623
H	5.6616031355	-0.9787011640	2.4384352864
H	3.3300468399	-0.1842926825	2.5983397109
C	-0.2676195621	2.8378648610	-0.7984285087
H	-0.3448092121	3.4811160220	0.0759725701
H	0.7063665806	2.4389235612	-2.6337454667
H	1.2752291832	3.9458067804	-1.7166323362
C	-1.7783275624	-0.5866572769	0.3404646530
C	-1.9588239860	-1.5273968047	-0.6839878522
C	-2.5551918389	-0.6821397190	1.5021352451
C	-2.8967001621	-2.5485287366	-0.5366404755
H	-1.3450967455	-1.4676383922	-1.5759382156
C	-3.4985434865	-1.7004495399	1.6420130894
H	-2.4314888681	0.0507126917	2.2953339278
C	-3.6700889137	-2.6371779971	0.6227587555
H	-3.0245047152	-3.2763834744	-1.3332487865
H	-4.0966149973	-1.7598140176	2.5471223320
H	-4.4035048907	-3.4317829216	0.7300847421
H	-1.2694226526	1.2030997299	-1.7994462095
N	-2.5838288373	2.1133215642	-0.4421813963
O	-3.4591240367	2.0058925535	-1.2887167703
O	-2.7303784246	2.5828930627	0.6865315661

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C	-0.8389330965	-0.6969107488	0.7216228486
C	1.0611815213	0.7075724563	0.1585985731
N	-0.1651387961	-0.0811662487	-0.2251761440
C	-0.4830236776	3.7447549004	0.2465429484
C	1.1301787248	1.9843262468	-0.7101735121
C	2.3161657310	-0.1376886880	0.0331759504
O	-0.4410580428	-0.1045822992	-1.4796479646
C	2.5349507899	-0.9720596807	-1.0716240710
C	3.7124454821	-1.7136345639	-1.1652243122
C	4.6862754136	-1.6225821836	-0.1680228032
C	4.4752839750	-0.7886982726	0.9306378870
C	3.2936371668	-0.0531722975	1.0322027418
H	-0.4488153140	-0.5534889449	1.7225791102
H	0.9295168336	1.0133482724	1.1977231489
H	1.7721543841	-1.0461748046	-1.8405462798

H	3.8695356582	-2.3642613151	-2.0214153691
H	5.6037182707	-2.1996616235	-0.2466241012
H	5.2260844887	-0.7130622197	1.7125720671
H	3.1321456872	0.5966985914	1.8893592992
C	-0.1261557554	2.8047011240	-0.6361984066
H	-1.4054763589	4.3071967902	0.1918256715
H	-0.8670617602	2.5908613183	-1.4031376457
H	1.2924969484	1.6844288082	-1.7471061418
H	1.9918723879	2.5528347088	-0.3567792446
C	-2.0080475731	-1.5382116231	0.5603241840
C	-2.6122967285	-1.8430998276	-0.6784599517
C	-2.5689546607	-2.0823805254	1.7366154329
C	-3.7367499762	-2.6647588394	-0.7206387077
H	-2.1858654227	-1.4313028289	-1.5825480817
C	-3.6910273813	-2.9004163829	1.6827955484
H	-2.1125233930	-1.8561618304	2.6977115004
C	-4.2814310485	-3.1954535578	0.4504608938
H	-4.1916610897	-2.8928745063	-1.6809874485
H	-4.1059424148	-3.3088221546	2.6002441444
H	-5.1589496124	-3.8347832281	0.4052600538
N	0.3305553103	4.1883465785	1.3666203054
O	-0.0300608190	5.2296374586	1.9161209788
O	1.3102421480	3.5173829416	1.7139468978

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C	-0.8935735415	0.4497986516	0.8484143109
C	1.3596563811	-0.4466013085	0.7794845721
N	0.3940868150	0.1798705676	0.1426677530
C	-1.2839154410	1.9554332164	0.7012026452
C	0.9349747980	3.1716094196	0.8042968865
C	2.6493184795	-0.8324881276	0.2438492738
O	0.4340098276	0.5863146362	-1.0745876325
C	3.0697072063	-0.5969781921	-1.0832347815
C	4.3334885777	-1.0140590259	-1.4960198449
C	5.1981798584	-1.6634099346	-0.6128283001
C	4.7924649875	-1.9008863870	0.7039018239
C	3.5339689577	-1.4908058157	1.1263360982
H	-0.6900365515	0.3452920233	1.9181996744
H	1.1396844560	-0.6999533464	1.8096450858
H	2.3970743190	-0.0943485527	-1.7641511277
H	4.6448117514	-0.8280924069	-2.5204404523
H	6.1817174523	-1.9832606910	-0.9461863119
H	5.4575165930	-2.4062177344	1.3988408530
H	3.2216354738	-1.6794725348	2.1510713524
C	-0.2701523246	2.8942009860	1.3036280307
H	-2.2337470102	2.0460100795	1.2325990987
H	-0.5850226579	3.3557288548	2.2383269865
H	1.2801715025	2.7502760442	-0.1336180479

H	1.6017868803	3.8556310684	1.3225552160
C	-1.9547084655	-0.5788774469	0.4832407462
C	-2.0640515161	-1.1371871635	-0.7965183830
C	-2.8372680577	-0.9950613334	1.4876135705
C	-3.0427618085	-2.0948695640	-1.0577922030
H	-1.3817729839	-0.8190424441	-1.5764725035
C	-3.8257561997	-1.9422443214	1.2195392243
H	-2.7528870477	-0.5781412742	2.4898567047
C	-3.9287527956	-2.4968389334	-0.0562473407
H	-3.1168332085	-2.5231877937	-2.0535878539
H	-4.5043674974	-2.2526661524	2.0094203129
H	-4.6926634839	-3.2400444152	-0.2681227578
N	-1.7039323258	2.3287280301	-0.7388991431
O	-2.7374155914	1.7881909818	-1.1238829272
O	-1.0590788088	3.1509713403	-1.3658326087

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C	-1.0676455131	0.7011509132	-0.0143115455
C	1.0527255297	-0.2890593616	0.6534387398
N	0.1565432754	-0.1350715452	-0.2982611052
C	-1.2545520299	1.7034358374	-1.1714392948
C	0.7399694193	2.8056604648	-2.2378325508
C	2.2765851568	-1.0633188048	0.5860549389
O	0.2183601274	-0.6472278721	-1.4697428667
C	2.7092071287	-1.7835068838	-0.5481832135
C	3.9063288830	-2.4954994108	-0.5068128540
C	4.6930924716	-2.5103068150	0.6466185738
C	4.2746523469	-1.8005395141	1.7759715259
C	3.0826987137	-1.0865780152	1.7453936213
H	-0.8558436823	1.2628521532	0.8977812763
H	0.8249990831	0.2215439895	1.5812380424
H	2.0963889940	-1.7687481770	-1.4386482389
H	4.2269169564	-3.0455537462	-1.3878020266
H	5.6246354054	-3.0696003183	0.6676317422
H	4.8783262308	-1.8049603422	2.6796740944
H	2.7615909812	-0.5364523850	2.6273271165
C	-0.1543679936	2.7296460490	-1.2448194841
H	0.7018238122	2.0790320953	-3.0398046962
H	1.5265476484	3.5495300791	-2.2787766676
C	-2.2853247837	-0.1763574375	0.2190596088
C	-2.6660933208	-1.1783550764	-0.6851898173
C	-3.0755259127	0.0494984121	1.3531899170
C	-3.8128519865	-1.9367132114	-0.4498821778
H	-2.0438346630	-1.3720901959	-1.5518700624
C	-4.2281854609	-0.7034326308	1.5819121872
H	-2.7899043694	0.8239905385	2.0620444993
C	-4.5995263597	-1.7005587552	0.6796925420
H	-4.0929177388	-2.7158312210	-1.1540632564

H	-4.8303103941	-0.5133565840	2.4665192815
H	-5.4943659367	-2.2914781073	0.8563300251
H	-1.3154246289	1.1490138345	-2.1088505829
H	-2.2115926757	2.2119197205	-1.0061197658
O	-0.2077367686	3.5502784859	-0.1477244731
C	0.7816428722	4.5617122258	-0.0405757348
H	0.5784560097	5.0912082207	0.8923738448
H	1.7900949716	4.1288272418	-0.0086937506
H	0.7220762009	5.2645581497	-0.8817804119

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C	-1.1940532354	-0.1191762627	0.6025490042
C	1.0240206118	0.6279695872	-0.0700550657
N	-0.2792670851	-0.0860626459	-0.3425215702
C	-0.5753225366	2.9258526985	-2.2190562930
C	1.3130319632	1.5742271488	-1.2550762750
C	2.1410294776	-0.3649147603	0.1974100011
O	-0.3815012838	-0.6275073149	-1.4985743938
C	2.4505240555	-1.3968928495	-0.7005203664
C	3.5086780600	-2.2652023831	-0.4329034714
C	4.2776471902	-2.1113422479	0.7229627773
C	3.9768624681	-1.0860471505	1.6196317968
C	2.9118699968	-0.2225386210	1.3582500286
H	-0.9284916473	0.4022967957	1.5140136714
H	0.8629783203	1.2306688216	0.8268622122
H	1.8407762052	-1.5274256251	-1.5875475958
H	3.7337618766	-3.0660293854	-1.1323911349
H	5.1036550229	-2.7882592270	0.9243701887
H	4.5646121087	-0.9600412250	2.5250969945
H	2.6776514698	0.5710360126	2.0652030865
C	0.3685182172	2.7506760823	-1.2924786381
H	1.2275851895	1.0011338413	-2.1798678375
H	2.3544102910	1.9040683135	-1.1669359952
C	-2.4873163258	-0.7718965820	0.5446972996
C	-2.9731135480	-1.4934865148	-0.5668291139
C	-3.3067326754	-0.6680434847	1.6900657586
C	-4.2344579271	-2.0836229898	-0.5171909550
H	-2.3505086875	-1.5756920430	-1.4466976583
C	-4.5632361934	-1.2606203859	1.7288758262
H	-2.9455321325	-0.1138396706	2.5536415736
C	-5.0339903119	-1.9731456886	0.6221179403
H	-4.5957585093	-2.6363614248	-1.3805663117
H	-5.1766989928	-1.1675212033	2.6210678527
H	-6.0161420112	-2.4375336183	0.6494173234
H	-0.7203543084	2.1926591250	-3.0040590725
H	-1.2414233234	3.7813282788	-2.1786705731
O	0.4228080796	3.6290747232	-0.2220981774
C	1.6843120781	4.2298985044	0.0510966157

H	1.5025507161	4.9765353092	0.8276231526
H	2.4240904707	3.5083267504	0.4241723264
H	2.0900848658	4.7280783113	-0.8395909319

11Ea

0 1

C	-0.4384398760	-1.5768435075	-0.7679471622
C	-2.0907011137	0.1637144973	-0.4383055102
N	-1.0992286892	-0.8469017748	0.1115501799
C	0.8144820760	2.0012184615	0.2365522304
C	-1.6281711153	1.5654391083	0.0113981188
O	-0.9922153691	-0.8786020719	1.3571137781
H	-0.6180784020	-1.4577611286	-1.8221594858
H	-2.0438799411	0.0843709757	-1.5282785432
C	-0.2842847562	1.9683635121	-0.5261783339
H	-0.2000799022	2.2294329298	-1.5796043923
H	-1.6290234100	1.5763119968	1.1062900966
H	-2.4048079443	2.2691828633	-0.3173574586
H	0.7870563862	1.7361051482	1.2948956051
O	2.0233127336	2.3812298008	-0.2494647545
C	3.1266621425	2.1729559424	0.6267581889
H	4.0023592935	2.5865253127	0.1234947448
H	2.9798555313	2.6936049097	1.5825646523
H	3.2883625053	1.1044457359	0.8175350854
C	-3.4827044425	-0.2055484518	0.0698971048
H	-3.4988705183	-0.2024581319	1.1626611018
H	-4.2085620635	0.5269268278	-0.2968221483
H	-3.7861535337	-1.1964898806	-0.2830893698
N	0.5493685003	-2.5541851521	-0.4319248558
O	1.0173621418	-3.1521642195	-1.4135412476
O	0.8734217665	-2.7407467036	0.7388403756

11Eb

0 1

C	0.0635893102	-0.2709496097	-0.5007277157
C	-2.2663822087	-0.7864179687	-0.8615249813
N	-1.2990946374	-0.5619150484	-0.0078380098
C	0.6465792896	0.9889780521	0.1403310785
C	-1.0105776574	2.7621250372	0.7942968474
O	-1.4346784426	-0.5703538140	1.2634830532
H	0.0709979430	-0.2180478210	-1.5877374212
H	-2.0143145886	-0.7746836882	-1.9137116170
C	-0.2157299008	2.2021414222	-0.1170664644
H	-0.1404503253	2.6122273753	-1.1241885486
H	-1.1004890095	2.3533877941	1.7973617585
H	-1.6126939195	3.6368573917	0.5632485661
H	0.7352959499	0.7945243775	1.2139599409

O	1.9212585408	1.1267035860	-0.4739204627
C	2.8620417013	1.8289140627	0.3257033235
H	3.7816374015	1.8927255209	-0.2605462942
H	2.5146434495	2.8437987941	0.5640717019
H	3.0648368348	1.2883193591	1.2605488170
C	-3.6307747465	-1.0652789764	-0.3437576216
H	-3.9677675423	-0.2462575549	0.3046222598
H	-4.3399299524	-1.1979424695	-1.1636375381
H	-3.6270809352	-1.9673012032	0.2823724757
N	0.9110431375	-1.5053159648	-0.1636416121
O	0.8067391139	-2.4352083081	-0.9570969065
O	1.5880231942	-1.4907503461	0.8513443706

11Za

0 1

C	0.2798095237	-1.2130870612	-0.8511528111
C	-1.9148802800	-0.2247882395	-0.5736301023
N	-0.6081528073	-0.7398499027	0.0061281657
C	0.2324648681	2.5319663482	-0.4311145259
C	-1.9538953489	1.3037713369	-0.3542968759
O	-0.4827936659	-0.6422133442	1.2446873509
H	0.0481530582	-1.2762368878	-1.8998251883
H	-1.8867745833	-0.4499915514	-1.6438328785
C	-0.8414837954	2.0343493320	-1.0559621403
H	-0.8925433151	2.1466415218	-2.1365346596
H	-1.9110412906	1.4914193202	0.7216090458
H	-2.9335769089	1.6454328003	-0.7130978642
H	1.0505589781	3.0083882828	-0.9774545643
O	0.3558272361	2.5331914066	0.9209550841
C	1.6671273349	2.2570073330	1.4151270325
H	2.4190670271	2.8745460161	0.9033810063
H	1.6566614254	2.5057371886	2.4777619245
H	1.9090119222	1.1955156299	1.2897402831
N	1.5891436385	-1.6556478542	-0.4961577276
O	2.0184774144	-1.4958872468	0.6471692453
O	2.2184819945	-2.1740544803	-1.4311356815
C	-3.0678102378	-0.9631609115	0.1006352424
H	-3.0460932287	-0.7935874436	1.1796913140
H	-4.0172104203	-0.5916945813	-0.2974100544
H	-3.0145765391	-2.0405730118	-0.0869346206

11Zb

0 1

C	0.1160498983	-0.2992642350	-0.6677534521
C	-2.0123653715	-1.4062937785	-0.6058831749
N	-1.1097647669	-0.7048612735	0.0407273601
C	0.4739471356	1.1970601475	-0.5305510416

C	-1.4957952799	2.6859225851	-0.0816492352
O	-1.2245592587	-0.3392907951	1.2542008833
H	0.0156932772	-0.5506830339	-1.7253192897
H	-1.8024752527	-1.6744852515	-1.6333884244
C	-0.6971018725	2.0660867353	-0.9483624093
H	-0.8562473164	2.1625578034	-2.0226285351
H	-1.3459428577	2.5770083318	0.9876878439
H	-2.3194944580	3.3096021187	-0.4174476565
H	1.2984421519	1.3449019452	-1.2449981828
O	0.9334541111	1.4336591023	0.7777233724
C	1.8689993125	2.4987920605	0.8606788605
H	1.4318789981	3.4512928685	0.5313528427
H	2.1511555047	2.5783993329	1.9126671775
H	2.7662020222	2.2851244556	0.2612737026
N	1.2955688479	-1.1582871128	-0.1884306225
O	1.0673233410	-2.1144208685	0.5296976750
O	2.3877195756	-0.8264007486	-0.6380477107
C	-3.2474762668	-1.8117226573	0.1115786270
H	-3.7599066886	-0.9298695009	0.5177776331
H	-3.9249868682	-2.3559863820	-0.5502689137
H	-2.9982729181	-2.4419928493	0.9758096706

12a

0 1

C	-1.8934385019	0.0018789734	-0.7336289305
C	0.2991917465	0.6604612000	-0.1907233033
N	-0.4106225871	-0.3000281234	-0.7658590602
C	-2.5936507676	-1.0528728367	0.1465788597
C	-1.4454412551	-1.8714064539	2.2241140926
C	-2.2368830816	-0.9914163567	1.6089150673
O	-0.0448524631	-1.3871945533	-1.2737224034
H	-3.6752783362	-0.9142081088	0.0129308678
H	-2.3350345913	-2.0340767922	-0.2646342792
H	-1.0046384659	-2.7101458246	1.6899246283
H	-1.2082313091	-1.7857821295	3.2812023927
H	-2.6558252471	-0.1634584424	2.1821727967
C	-1.9579392305	1.4683190506	-0.2779975418
C	-0.5670042714	1.7676513663	0.3348737744
H	-2.1365549562	2.1168916524	-1.1408943751
H	-0.5866942870	1.7499212641	1.4321899760
H	-0.1797395355	2.7503037972	0.0484167067
H	-2.7702789756	1.6425369934	0.4328662425
C	1.7541153746	0.6782160942	-0.0028428763
O	2.3035497772	1.5943659304	0.5891703153
O	2.4039800282	-0.3736240764	-0.5319933478
C	3.8278420157	-0.3581214735	-0.3495596988
H	4.0806171890	-0.3524029775	0.7143121936
H	4.1884100884	-1.2698924111	-0.8261429779
H	4.2684600139	0.5244249254	-0.8217475183

H	-2.2275353713	-0.1386566873	-1.7652806010

12b

0 1

C	-1.5957451755	0.8310216008	-1.4045616403
C	-0.0601179298	0.2675664644	0.2802352314
N	-0.6390146461	-0.0043586207	-1.1028154526
C	-2.6686568312	-1.9851948440	0.8384201261
C	-0.4118005025	-0.9419939849	1.1768592080
C	-1.8855550211	-1.0963630550	1.4520051598
O	-0.1876829499	-0.9851416037	-1.7652601190
H	-3.7285998717	-2.0666874673	1.0649858932
H	-2.2740446393	-2.6617961468	0.0837202983
H	-0.0261119956	-1.8330502898	0.6761074968
H	0.1400767713	-0.8306899009	2.1181825531
H	-2.3205785013	-0.4328044233	2.2004617324
C	-1.8838886046	1.8192705172	-0.3261722599
C	-0.7052575257	1.6160467350	0.6645291252
H	-1.9261948443	2.8484281069	-0.7033970834
H	-1.0332409809	1.6228569930	1.7070879615
H	0.0306615085	2.4104507732	0.5300474138
H	-2.8552669031	1.6149365330	0.1458880882
C	1.4579903469	0.4234074403	0.0445240269
O	1.9515887841	1.4143710019	-0.4477205667
O	2.1596146607	-0.6490047966	0.4344853899
C	3.5719048316	-0.5931977300	0.1631341881
H	4.0242753232	0.2644307704	0.6674562540
H	3.9781524482	-1.5284550734	0.5480987802
H	3.7432608346	-0.5106229255	-0.9127055143
H	-2.1063605867	0.7123259259	-2.3514222909

13a

0 1

C	1.3200990867	-0.2186086454	0.4309943325
C	-0.8753630130	0.5536850071	0.0935108456
N	0.2221829112	-0.4320047504	-0.2400578804
C	0.8440101266	2.0009812533	-2.5874946967
C	-1.1384716867	1.4076447768	-1.1680041837
C	0.0245853199	2.2767337100	-1.5713928795
O	0.0237063339	-1.3169090537	-1.1389287342
H	1.6718978997	2.6551906330	-2.8484272414
H	0.7144679670	1.1062809969	-3.1923126813
H	-1.3887876616	0.7167958289	-1.9765671642
H	-2.0255025041	2.0241646327	-0.9774600629
H	0.1909139816	3.1822153177	-0.9866188433
C	2.5029797061	-1.0843494619	0.1530444019
C	1.2195496693	0.9533629979	1.3499981228

C	-0.2941053153	1.2993402537	1.3172302314
C	4.7087180377	-1.5023699485	0.8357812564
O	3.5448001594	-0.7283714722	1.0373181617
H	2.2152893393	-2.1452490561	0.2625733785
H	2.8091716264	-0.9633690937	-0.9030700751
H	1.5718288627	0.7135632095	2.3588080205
H	-0.4722629415	2.3758758636	1.2532371980
H	4.5174903787	-2.5743524754	1.0021846633
H	5.4529767823	-1.1562988374	1.5573622885
H	5.1091191794	-1.3760145721	-0.1828514408
H	-0.7775167813	0.9257444257	2.2214995502
H	1.8433017861	1.7823884771	0.9894914304
C	-2.0841937434	-0.3187285111	0.4968372068
O	-2.1389512645	-0.9269200889	1.5430639793
O	-3.0532062655	-0.3324372339	-0.4292343725
C	-4.1720818637	-1.1886391910	-0.1357199431
H	-4.6514143398	-0.8839819037	0.7981061835
H	-4.8545436452	-1.0731183260	-0.9776909833
H	-3.8379601286	-2.2250567624	-0.0473580690

13b

0 1

C	1.2314398679	0.2403429041	-0.0538934485
C	-1.0126057138	0.0098818771	0.6464520958
N	-0.1318728193	-0.4067211156	-0.2507143541
C	1.4744946082	1.1973594901	-1.2468848488
C	-0.4200176014	2.5680533191	-2.1637088465
C	0.5798585762	2.4069354489	-1.2952567344
O	-0.2759644932	-1.1989046195	-1.2166971941
H	2.5265161368	1.5006479517	-1.1851581155
H	1.3511618079	0.6063676690	-2.1609887381
H	-0.6538348204	1.8111348770	-2.9093352455
H	-1.0395892644	3.4608963727	-2.1634140830
H	0.7795743150	3.1938193961	-0.5670127929
C	2.2666298892	-0.8930303853	-0.0706067943
C	1.0984072247	0.9139229241	1.3253983533
C	-0.4207505421	1.0063706458	1.5984112168
C	4.5710491612	-1.2691532722	0.2273454839
O	3.5222467270	-0.3207510121	0.2361251130
H	1.9910528772	-1.6544092070	0.6788393317
H	2.2761834624	-1.3796264248	-1.0555952224
H	1.5847242499	0.2922642195	2.0830270690
H	-0.8188757399	2.0085411025	1.3954024941
H	4.4109782889	-2.0570063419	0.9801182728
H	5.4919059990	-0.7307106325	0.4648174905
H	4.6766897654	-1.7471190495	-0.7588864619
H	-0.6811096778	0.7729010810	2.6354063267
H	1.5910613419	1.8884293483	1.3500142943
C	-2.4294276123	-0.3682458116	0.7203974251

O	-3.1692631300	0.1181594003	1.5612304117
O	-2.8202789828	-1.2759284941	-0.1917662337
C	-4.2056725226	-1.6457267135	-0.1204417177
H	-4.8465134214	-0.7744176284	-0.2817178994
H	-4.3481327850	-2.3799835644	-0.9135737067
H	-4.4398961723	-2.0804887550	0.8552650588

TS01

0 1

C	-1.1852290000	0.6631950000	0.33108800
C	1.1851910000	0.6629340000	0.33116100
N	-0.0000320000	-0.0156360000	-0.02631300
C	-1.2136280000	1.9940930000	-0.85311500
C	1.2136990000	1.9940060000	-0.85330500
C	2.5003800000	-0.0557050000	0.27231500
O	-0.0000980000	-0.7012110000	-1.12943500
C	2.8604440000	-0.9494880000	-0.74930300
C	4.1202570000	-1.5495560000	-0.74023200
C	5.0416460000	-1.2614460000	0.26764100
C	4.6944980000	-0.3672770000	1.28176600
C	3.4341600000	0.2273770000	1.28221200
H	-1.0568220000	1.1389340000	1.30206500
H	1.0568450000	1.1388240000	1.30206300
H	2.1399080000	-1.1823940000	-1.52159600
H	4.3820210000	-2.2475180000	-1.53126000
H	6.0221110000	-1.7303320000	0.26430500
H	5.4004580000	-0.1365620000	2.07515100
H	3.1683970000	0.9185620000	2.07948400

C	0.0001250000	2.7238300000	-0.70235900
H	-2.1429890000	2.5391270000	-0.68572000
H	-1.2602660000	1.3443780000	-1.73711000
H	0.0002100000	3.6707860000	-0.16600400
H	1.2600750000	1.3440210000	-1.73711500
H	2.1432000000	2.5388290000	-0.68604000
C	-2.5004130000	-0.0555090000	0.27232800
C	-2.8608940000	-0.9484010000	-0.74992200
C	-3.4337520000	0.2266340000	1.28288400
C	-4.1206760000	-1.5485280000	-0.74083600
H	-2.1406960000	-1.1806320000	-1.52273200
C	-4.6940610000	-0.3680930000	1.28248000
H	-3.1676710000	0.9171250000	2.08065100
C	-5.0416240000	-1.2613690000	0.26771400
H	-4.3827650000	-2.2457910000	-1.53237500
H	-5.3996750000	-0.1381170000	2.07638800
H	-6.0220660000	-1.7303010000	0.26440000

TS02

0 1

C	-0.1116700000	0.9855540000	0.27136100
C	2.2357910000	0.6702630000	0.32093000
N	0.9761980000	0.1445570000	-0.04150200
C	0.0511790000	2.2773580000	-0.95718800
C	2.4561820000	1.9537410000	-0.89930700
C	3.4446830000	-0.2163160000	0.30235700

O	0.9011490000	-0.5700500000	-1.12299500
C	3.7111480000	-1.1570830000	-0.70569500
C	4.8788940000	-1.9191810000	-0.65798400
C	5.8008800000	-1.7491200000	0.37591400
C	5.5475660000	-0.8094490000	1.37648700
C	4.3784800000	-0.0520530000	1.33822000
H	0.0596340000	1.4730750000	1.22926300
H	2.1569590000	1.1860240000	1.27662300
H	2.9908290000	-1.2994130000	-1.49987900
H	5.0679540000	-2.6510560000	-1.43883200
H	6.7096020000	-2.3444460000	0.40287100
H	6.2549640000	-0.6691090000	2.18930800
H	4.1848940000	0.6738310000	2.12534500
C	1.3474110000	2.8404770000	-0.79172400
H	-0.8004050000	2.9452010000	-0.82501400
H	-0.0634600000	1.6114360000	-1.82235400
H	1.4621010000	3.7930850000	-0.27859900
H	2.4317910000	1.2789560000	-1.76476000
H	3.4459950000	2.3757300000	-0.72502400
C	-1.5069910000	0.4445860000	0.20156800
C	-1.9461920000	-0.4684290000	-0.77319100
C	-2.4297800000	0.9234360000	1.14894100
C	-3.2700800000	-0.8995150000	-0.78620300
H	-1.2356430000	-0.8482580000	-1.49410000
C	-3.7555910000	0.5077980000	1.13923800

H	-2.1037750000	1.6291560000	1.90885600
C	-4.1580930000	-0.4043710000	0.16565800
H	-3.6219490000	-1.6093470000	-1.52476400
H	-4.4721750000	0.8682080000	1.86663800
N	-5.5578500000	-0.8540430000	0.14571900
O	-5.8889970000	-1.6580840000	-0.72526000
O	-6.3169820000	-0.3984730000	1.00183200

TS03

0 1

C	-0.3785380000	0.8752140000	0.31911300
C	1.9790940000	0.6255090000	0.39452800
N	0.7481580000	0.1118060000	-0.06176800
C	-0.2192490000	2.3037810000	-0.73061700
C	2.1936700000	2.0522470000	-0.66122900
C	3.2168380000	-0.2164530000	0.30848400
O	0.7216400000	-0.4705140000	-1.22272400
C	3.5216610000	-1.0557770000	-0.77537800
C	4.7144770000	-1.7799690000	-0.78423200
C	5.6250540000	-1.6703490000	0.26775400
C	5.3336590000	-0.8309870000	1.34434800
C	4.1392460000	-0.1134530000	1.36252800
H	-0.2458870000	1.2430270000	1.33557500
H	1.8604800000	1.0254780000	1.40020600
H	2.8088310000	-1.1495670000	-1.58348000
H	4.9324780000	-2.4339850000	-1.62459300

H	6.5537250000	-2.2346800000	0.25014900
H	6.0314110000	-0.7385420000	2.17245500
H	3.9162880000	0.5336640000	2.20847400
C	1.0559250000	2.8873550000	-0.47703200
H	-1.0942060000	2.9255540000	-0.53911200
H	-0.2972920000	1.7496970000	-1.67534800
H	1.1310680000	3.7740010000	0.14968200
H	2.2081480000	1.4810670000	-1.59880600
H	3.1669700000	2.4769510000	-0.41432500
C	-1.7511240000	0.3017480000	0.14650000
C	-2.1679060000	-0.4240890000	-0.98598300
C	-2.6919660000	0.5454270000	1.15390400
C	-3.4705320000	-0.8930310000	-1.08362300
H	-1.4512180000	-0.6362490000	-1.76788600
C	-4.0069520000	0.0861950000	1.06272600
H	-2.3975040000	1.1053070000	2.03927800
C	-4.4019270000	-0.6414680000	-0.06545700
H	-3.7940300000	-1.4624810000	-1.94952300
H	-4.7004630000	0.2940390000	1.86953500
O	-5.6545310000	-1.1436350000	-0.26793900
C	-6.6376640000	-0.9195780000	0.72932900
H	-7.5478830000	-1.4002840000	0.36615100
H	-6.3495440000	-1.3684440000	1.68924900
H	-6.8279270000	0.1520610000	0.87602400

TS04

0 1

C	-2.4133940000	-0.3337860000	0.77296300
C	-0.2061620000	0.4523840000	0.35897900
N	-1.1388650000	-0.6278130000	0.29241800
C	-3.0181520000	0.8310310000	-0.51005300
C	-0.7178310000	1.5014330000	-0.88449800
C	1.2559980000	0.1323230000	0.19730100
O	-1.0484760000	-1.4581940000	-0.69925000
C	-3.3876040000	-1.4906970000	0.80391100
C	1.7563890000	-0.6989590000	-0.81710600
C	3.1300500000	-0.9189760000	-0.92641700
C	4.0227810000	-0.3090280000	-0.04354800
C	3.5333430000	0.5251430000	0.96253800
C	2.1609020000	0.7409610000	1.07990100
H	-2.3731700000	0.2413880000	1.69697100
H	-0.3632660000	0.9873960000	1.29613900
H	-3.0610140000	-2.2392860000	1.53471800
H	-3.4387300000	-1.9731350000	-0.17334900
H	-4.3819010000	-1.1376750000	1.09355100
H	1.0621470000	-1.1850560000	-1.48974300
H	3.5035010000	-1.5725390000	-1.71055000
H	5.0915010000	-0.4827520000	-0.13798800
H	4.2166220000	1.0040560000	1.65893100
H	1.7863570000	1.3886200000	1.87008600
C	-2.0811020000	1.8811650000	-0.61367300
H	-4.0416430000	1.0913560000	-0.23664600

H	-2.9614150000	0.0694700000	-1.29999400
H	-2.2928330000	2.8511940000	-0.16868100
H	-0.6005760000	0.8195160000	-1.73806200
H	0.0029800000	2.3197340000	-0.93009700

TS05

0 1

C	-1.6954810000	0.1562530000	0.50713000
C	0.6184530000	0.6221230000	0.41150200
N	-0.4689730000	-0.2249990000	0.00572400
C	-2.0287880000	1.7378240000	-0.45991100
C	0.3843240000	2.0245310000	-0.50656100
C	2.0163230000	0.0958690000	0.22143100
O	-0.4255550000	-0.7692960000	-1.16351100
C	-2.8772600000	-0.7615860000	0.24739900
C	2.4685320000	-0.4728320000	-0.97945500
C	3.7907530000	-0.9034770000	-1.09307500
C	4.6799320000	-0.7637410000	-0.02618000
C	4.2390310000	-0.1923770000	1.16818300
C	2.9165750000	0.2323850000	1.28837700
H	-1.6698020000	0.4413650000	1.55481100
H	0.4693720000	0.8996920000	1.45562300
H	1.7762390000	-0.5983940000	-1.80130100
H	4.1264270000	-1.3510040000	-2.02478200
H	5.7091020000	-1.0986840000	-0.12426400
H	4.9201620000	-0.0810110000	2.00750100

H	2.5782390000	0.6726440000	2.22410300
C	-0.9228260000	2.5654560000	-0.20560000
H	-3.0177520000	2.0815530000	-0.15926100
H	-2.0192810000	1.1914110000	-1.41003300
H	-1.0130740000	3.4024660000	0.48334900
H	0.4677550000	1.5969740000	-1.51485100
H	1.2254140000	2.6851710000	-0.28939900
F	-3.2361390000	-0.8611450000	-1.03816700
F	-3.9431670000	-0.2649750000	0.92697700
F	-2.6432460000	-2.0022560000	0.71420000

TS06

0 1

C	-1.7543430000	0.0363620000	0.40928200
C	0.5689950000	0.5273300000	0.37648400
N	-0.4955940000	-0.3381270000	-0.02684600
C	-2.0526830000	1.5752270000	-0.56387700
C	0.3489730000	1.9165610000	-0.58114600
C	1.9786030000	0.0168710000	0.23825000
O	-0.4180970000	-0.9336040000	-1.17916000
C	-2.8708900000	-0.9218470000	0.04570000
C	2.4616830000	-0.6061370000	-0.92315800
C	3.7931010000	-1.0178930000	-0.99302400
C	4.6622040000	-0.8058970000	0.07853900
C	4.1909950000	-0.1802590000	1.23359500
C	2.8593370000	0.2257380000	1.30996500

H	-1.7801140000	0.3384890000	1.45430100
H	0.3893300000	0.8350760000	1.40717600
H	-2.6253730000	-1.9277840000	0.42650700
H	-2.9675370000	-1.0024670000	-1.04512600
H	1.7821590000	-0.7860420000	-1.74560500
H	4.1523600000	-1.5074370000	-1.89453300
H	5.6987500000	-1.1264710000	0.01467500
H	4.8559780000	-0.0119750000	2.07657400
H	2.4974800000	0.7089260000	2.21528600
C	-0.9693440000	2.4392830000	-0.31285800
H	-3.0555730000	1.9019930000	-0.29308600
H	-2.0101370000	1.0321480000	-1.51749300
H	-1.0854040000	3.2814720000	0.36641000
H	0.4606730000	1.4652100000	-1.57619300
H	1.1796160000	2.5890280000	-0.35921100
C	-5.1786690000	-1.2378330000	0.36168200
H	-6.0376720000	-0.7778830000	0.85677200
H	-5.3769500000	-1.2987700000	-0.72002800
H	-5.0476430000	-2.2612210000	0.74779700
O	-4.0554750000	-0.4277000000	0.64129700

TS07E

0 1

C	-0.6551880000	-0.1503430000	0.47442300
C	1.6793520000	0.2791060000	0.50212600
N	0.6259240000	-0.4492870000	-0.03803400

C	-1.0403500000	1.4662650000	-0.39394600
C	1.3780220000	1.9155240000	-0.37658800
C	3.1005980000	-0.0976890000	0.25617600
O	0.7137580000	-0.8679420000	-1.26331300
C	3.5723860000	-0.6855830000	-0.92981900
C	4.9292140000	-0.9787930000	-1.07188700
C	5.8362370000	-0.6812640000	-0.05392300
C	5.3770560000	-0.0891360000	1.12432000
C	4.0224860000	0.1970360000	1.27589500
H	-0.5773290000	0.1276090000	1.52328000
H	1.4993560000	0.5071120000	1.54954500
H	2.8649630000	-0.9252590000	-1.71174700
H	5.2782510000	-1.4430260000	-1.99065000
H	6.8918210000	-0.9093230000	-0.17586600
H	6.0710120000	0.1442990000	1.92746000
H	3.6715260000	0.6522410000	2.19985300
C	0.0684140000	2.2998070000	-0.04048500
H	-0.0683080000	3.0664320000	0.72039800
H	1.5254250000	1.4665960000	-1.36428200
H	2.1948000000	2.5637750000	-0.06191700
C	-1.7045770000	-1.2033670000	0.28641100
C	-1.9512500000	-1.8518380000	-0.93516200
C	-2.4654640000	-1.5722550000	1.40823000
C	-2.9393190000	-2.8328890000	-1.02071000
H	-1.3556860000	-1.5934130000	-1.79952200

C	-3.4571460000	-2.5476730000	1.31686400
H	-2.2735480000	-1.0945670000	2.36649500
C	-3.6992780000	-3.1816790000	0.09713800
H	-3.1163310000	-3.3272700000	-1.97236900
H	-4.0324530000	-2.8163100000	2.19888800
H	-4.4699910000	-3.9440440000	0.02029200
H	-0.9419500000	1.0265820000	-1.39554800
C	-3.5740440000	1.2040580000	-0.79010800
H	-4.5239210000	1.7510930000	-0.74821100
H	-3.3555840000	1.0015030000	-1.84534600
H	-3.7205170000	0.2474690000	-0.28803200
C	-2.4608010000	2.0563950000	-0.14593400
C	-2.5097240000	3.4451590000	-0.83379800
H	-1.7959970000	4.1481130000	-0.39325100
H	-2.2791140000	3.3624800000	-1.90244300
H	-3.5136780000	3.8776800000	-0.73950200
C	-2.7601220000	2.2338830000	1.35619000
H	-3.7286190000	2.7294850000	1.49261800
H	-2.8101010000	1.2700800000	1.87356200
H	-2.0045620000	2.8508500000	1.85656100

TS07Z

0 1

C	0.7906810000	-0.4822530000	-0.78186800
C	-1.5556040000	-0.3035250000	-0.79122100
N	-0.4074940000	-0.6028030000	-0.09315800

C	1.1117700000	1.6586400000	-0.86097600
C	-1.3770930000	1.8111690000	-0.91452500
C	-2.9141200000	-0.5284610000	-0.26776300
O	-0.4237210000	-0.7201910000	1.19772400
C	-3.2659260000	-0.5278580000	1.09579200
C	-4.5957490000	-0.7109180000	1.47476200
C	-5.5967780000	-0.8894970000	0.51899000
C	-5.2598980000	-0.8860200000	-0.83668300
C	-3.9352120000	-0.7065910000	-1.22269400
H	0.6307090000	-0.5295160000	-1.85269200
H	-1.4555270000	-0.4837650000	-1.85454900
H	-2.4887480000	-0.4038090000	1.83608000
H	-4.8490860000	-0.7143450000	2.53179600
H	-6.6296100000	-1.0315130000	0.82574900
H	-6.0275810000	-1.0275050000	-1.59281600
H	-3.6816040000	-0.7075720000	-2.28092300
C	-0.1221170000	1.9379500000	-1.49945100
H	-0.1059000000	1.9025190000	-2.59099100
H	-1.5203970000	1.9355590000	0.15251600
H	-2.2613270000	2.0070730000	-1.51576700
C	2.0149310000	-1.2053070000	-0.37223000
C	2.2064820000	-1.8261810000	0.87577500
C	3.0372060000	-1.3106160000	-1.33523100
C	3.3838760000	-2.5275660000	1.13592000
H	1.4216240000	-1.7571360000	1.61691600

C	4.2166060000	-1.9974570000	-1.06271600
H	2.9004140000	-0.8505890000	-2.31200400
C	4.3964250000	-2.6112750000	0.17898900
H	3.5102220000	-3.0092890000	2.10219100
H	4.9907600000	-2.0614100000	-1.82292000
H	5.3140760000	-3.1517030000	0.39522900
H	1.9460850000	1.5903160000	-1.56319200
C	1.6084570000	2.3194010000	0.44514300
C	0.6123410000	2.3439170000	1.62068500
H	1.1150630000	2.7519020000	2.50628500
H	-0.2442930000	2.9943730000	1.41502600
H	0.2483030000	1.3411930000	1.85861700
C	2.9255600000	1.6780190000	0.92571300
H	3.6460220000	1.5656170000	0.10666400
H	3.3857180000	2.3162780000	1.68940900
H	2.7629240000	0.6934780000	1.36670400
C	1.9218370000	3.7876460000	0.04182800
H	2.3235140000	4.3311390000	0.90611200
H	2.6691000000	3.8367280000	-0.75978400
H	1.0197230000	4.3038330000	-0.30278800

TS08E

0 1

C	-0.8692920000	0.1521500000	0.54239100
C	1.4826840000	0.3523220000	0.53488900
N	0.3600770000	-0.2904400000	0.03526300

C	-1.1265890000	1.7562200000	-0.40335000
C	1.2957600000	2.0203440000	-0.44566900
C	2.8607170000	-0.1404670000	0.27824200
O	0.3919600000	-0.7803100000	-1.16787000
C	3.2594760000	-0.8317480000	-0.87928100
C	4.5868360000	-1.2348220000	-1.02964600
C	5.5382480000	-0.9476420000	-0.05007300
C	5.1531130000	-0.2530900000	1.09862100
C	3.8281740000	0.1433950000	1.25941600
H	-0.7617130000	0.5007200000	1.56673500
H	1.3375180000	0.6590520000	1.56655700
H	2.5187940000	-1.0622410000	-1.63254500
H	4.8776940000	-1.7777380000	-1.92528200
H	6.5704720000	-1.2623810000	-0.17864200
H	5.8817760000	-0.0256850000	1.87221100
H	3.5348420000	0.6775960000	2.16086900
C	0.0327120000	2.5328570000	-0.12026600
H	-0.0733370000	3.3363780000	0.60580500
H	1.3955700000	1.4902030000	-1.39679200
H	2.1718400000	2.6026100000	-0.16714100
C	-2.1039230000	-0.6690100000	0.37664500
C	-2.3456780000	-1.5368290000	-0.70260100
C	-3.0983260000	-0.5243550000	1.36004200
C	-3.5446840000	-2.2479030000	-0.77343000
H	-1.5813900000	-1.6573140000	-1.45845900

C	-4.2981320000	-1.2272980000	1.27686800
H	-2.9283210000	0.1503290000	2.19501300
C	-4.5258270000	-2.0957860000	0.20765800
H	-3.7115930000	-2.9245630000	-1.60765200
H	-5.0514900000	-1.1004330000	2.04992200
H	-5.4587690000	-2.6493790000	0.14113900
H	-1.1677880000	1.2667310000	-1.38468300
O	-2.3267690000	2.2843490000	0.04362800
C	-3.3874820000	2.2534690000	-0.90493500
H	-4.2724320000	2.6366770000	-0.39187200
H	-3.1635080000	2.8961920000	-1.76786300
H	-3.5869520000	1.2331710000	-1.25335000

TS08Z

0 1

C	1.0007800000	-0.0457650000	-0.78479800
C	-1.3693110000	0.1035360000	-0.74009900
N	-0.1976420000	-0.3394040000	-0.09734100
C	1.1558580000	1.7861840000	-0.63283900
C	-1.2647270000	1.9279560000	-0.56354700
C	-2.7042850000	-0.3432450000	-0.24319900
O	-0.2031660000	-0.5825880000	1.15884600
C	-3.0581840000	-0.4030130000	1.11553300
C	-4.3483070000	-0.7838340000	1.48599300
C	-5.3048810000	-1.1008640000	0.52044800
C	-4.9648610000	-1.0351680000	-0.83192400

C	-3.6771850000	-0.6579010000	-1.20685900
H	0.8497090000	-0.1668280000	-1.85498600
H	-1.2818790000	-0.0290120000	-1.81566700
H	-2.3150140000	-0.1738530000	1.86642600
H	-4.6051450000	-0.8332250000	2.54094700
H	-6.3071450000	-1.3971970000	0.81845100
H	-5.6988370000	-1.2811010000	-1.59473400
H	-3.4191890000	-0.6112260000	-2.26290900
C	-0.0495510000	2.3127010000	-1.18730400
H	-0.0524950000	2.5280280000	-2.25500800
H	-1.2841960000	1.9663880000	0.52807600
H	-2.1925460000	2.2808140000	-1.01292900
C	2.2803890000	-0.6795320000	-0.34780700
C	2.6623230000	-0.8395320000	0.99484400
C	3.1662210000	-1.0940460000	-1.35629500
C	3.8938980000	-1.4167900000	1.30426900
H	1.9862680000	-0.5220430000	1.77447700
C	4.3984840000	-1.6637700000	-1.04141800
H	2.8838190000	-0.9738900000	-2.40043600
C	4.7656580000	-1.8293000000	0.29486500
H	4.1742450000	-1.5424750000	2.34694400
H	5.0656500000	-1.9824710000	-1.83796100
H	5.7235080000	-2.2768720000	0.54710900
H	2.0794520000	1.9910510000	-1.18910600
O	1.3377990000	1.9007840000	0.75183800

C	1.8651180000	3.1615960000	1.13090400
H	1.1931900000	3.9799420000	0.83696400
H	1.9692540000	3.1426500000	2.21840600
H	2.8531740000	3.3363130000	0.67725200

TS09E

0 1

C	-0.8155860000	0.0725610000	0.43980200
C	1.5342670000	0.3770460000	0.42853000
N	0.4397060000	-0.3731270000	-0.00982000
C	-1.0279510000	1.5354140000	-0.65076500
C	1.3584790000	1.8712390000	-0.69427800
C	2.9307350000	-0.1220290000	0.27147200
O	0.5086730000	-0.9691340000	-1.15744300
C	3.3780130000	-0.8999160000	-0.80988400
C	4.7131350000	-1.2995630000	-0.87476900
C	5.6212130000	-0.9223690000	0.11555400
C	5.1864470000	-0.1411520000	1.18802900
C	3.8529860000	0.2532470000	1.26390500
H	-0.7350080000	0.5191160000	1.42798600
H	1.3573240000	0.7714580000	1.42561500
H	2.6712520000	-1.2004650000	-1.57109800
H	5.0443180000	-1.9100030000	-1.71060700
H	6.6601070000	-1.2348550000	0.05349500
H	5.8821680000	0.1559690000	1.96792900
H	3.5195660000	0.8560940000	2.10599800

C	0.0796370000	2.3986970000	-0.43278600
H	-0.0583060000	3.2632980000	0.20913400
H	1.4704290000	1.2674190000	-1.60099100
H	2.2181570000	2.5032030000	-0.47949100
C	-2.0170200000	-0.8092690000	0.33344000
C	-2.2562170000	-1.6948270000	-0.73069200
C	-2.9696650000	-0.7065550000	1.36159600
C	-3.4149090000	-2.4707690000	-0.74168000
H	-1.5254090000	-1.7810950000	-1.52289700
C	-4.1293810000	-1.4774420000	1.33805300
H	-2.8023940000	-0.0136390000	2.18239300
C	-4.3539530000	-2.3658690000	0.28549000
H	-3.5852410000	-3.1589090000	-1.56524000
H	-4.8539860000	-1.3844440000	2.14210200
H	-5.2569970000	-2.9699620000	0.26449000
H	-1.0930740000	0.9974330000	-1.59837900
N	-2.3489500000	2.1195710000	-0.31172400
O	-3.2615530000	1.9447750000	-1.11123000
O	-2.4433180000	2.7123090000	0.76545500

TS09Z

0 1

C	-0.9292360000	-0.0817630000	0.81705500
C	1.4462910000	0.0706410000	0.76810900
N	0.2737280000	-0.3486780000	0.12383500
C	-1.0920400000	1.7803900000	0.82061400

C	1.3532860000	1.9382000000	0.58302300
C	2.7791740000	-0.3610100000	0.26339500
O	0.2708380000	-0.6059510000	-1.12746200
C	3.1263110000	-0.4127250000	-1.09774500
C	4.4167840000	-0.7853630000	-1.47406400
C	5.3779360000	-1.1019080000	-0.51278800
C	5.0440560000	-1.0433570000	0.84159700
C	3.7568390000	-0.6732230000	1.22366100
H	-0.7725210000	-0.2066050000	1.88550000
H	1.3584390000	-0.0495500000	1.84400300
H	2.3810840000	-0.1811420000	-1.84591300
H	4.6702180000	-0.8281210000	-2.52987500
H	6.3804170000	-1.3917220000	-0.81594000
H	5.7827200000	-1.2883470000	1.59990700
H	3.5030750000	-0.6307370000	2.28085100
C	0.1603400000	2.3082730000	1.24199600
H	-1.9488500000	1.9572420000	1.46409100
H	0.2128110000	2.5971570000	2.28980600
H	1.3564730000	1.9457710000	-0.50575100
H	2.2868730000	2.2878640000	1.02153700
C	-2.1962750000	-0.7383330000	0.38018400
C	-2.5744370000	-0.9172770000	-0.96129000
C	-3.0681550000	-1.1704470000	1.39443600
C	-3.7892230000	-1.5317660000	-1.26475000
H	-1.9147360000	-0.5886910000	-1.75178500

C	-4.2814300000	-1.7789610000	1.08455800
H	-2.7884150000	-1.0344470000	2.43727700
C	-4.6443950000	-1.9640220000	-0.25087300
H	-4.0682120000	-1.6678390000	-2.30589400
H	-4.9383460000	-2.1117680000	1.88346700
H	-5.5892460000	-2.4403260000	-0.49839200
N	-1.5705870000	2.0811550000	-0.57238800
O	-2.7818460000	2.2498590000	-0.68934200
O	-0.7575830000	2.1410690000	-1.49016000

TS10

0 1

C	-1.2273080000	0.2125620000	0.35717400
C	1.1323340000	0.1835310000	0.27878900
N	-0.0908470000	-0.5070820000	-0.01260200
C	-1.2149990000	1.5839100000	-0.89203100
C	1.2129100000	1.3974950000	-0.87577500
C	2.4126790000	-0.6166110000	0.26316900
O	-0.1246310000	-1.1339940000	-1.17748200
C	2.7051920000	-1.5878210000	-0.70652200
C	3.9269130000	-2.2615720000	-0.67354300
C	4.8771100000	-1.9702640000	0.30672900
C	4.5957110000	-1.0008800000	1.27045100
C	3.3712780000	-0.3338750000	1.24770200
H	-1.0734320000	0.7155180000	1.31157400
H	1.0338090000	0.6678860000	1.25335100

H	1.9546760000	-1.8193970000	-1.45145500
H	4.1364430000	-3.0203270000	-1.42324500
H	5.8281150000	-2.4963320000	0.32210100
H	5.3231380000	-0.7688280000	2.04399800
H	3.1545900000	0.4128980000	2.00949600
C	0.0300720000	2.2321250000	-0.75145000
H	1.1759090000	0.7837840000	-1.78498800
H	2.1739010000	1.9015850000	-0.77899900
C	-2.5854050000	-0.4110340000	0.29500600
C	-2.9426520000	-1.4234730000	-0.61015700
C	-3.5563880000	0.0710350000	1.18895400
C	-4.2378630000	-1.9428970000	-0.59960000
H	-2.1876330000	-1.7993660000	-1.28845300
C	-4.8516390000	-0.4418290000	1.18590100
H	-3.2915260000	0.8536860000	1.89731800
C	-5.1970180000	-1.4550220000	0.28929300
H	-4.4980780000	-2.7352860000	-1.29680700
H	-5.5867970000	-0.0563730000	1.88752300
H	-6.2051210000	-1.8613530000	0.28582500
H	-1.2710290000	0.8872720000	-1.73501200
H	-2.1035580000	2.1918370000	-0.73316800
O	0.0189180000	3.4613350000	-0.17185500
C	1.2544070000	4.1214760000	0.07839100
H	0.9901750000	5.1105670000	0.45612300
H	1.8517060000	3.5945480000	0.83312300

H	1.8443480000	4.2273980000	-0.84027300

TS11E

0 1

C	0.1527310000	-0.4633750000	-0.53340200
C	-2.1238230000	0.1367940000	-0.51768200
N	-1.1340610000	-0.7006990000	0.01536300
C	0.7065190000	0.9835420000	0.05635200
C	-1.6228410000	1.7137030000	0.16779200
O	-1.1940910000	-1.0087940000	1.27072600
H	0.1495200000	-0.4458300000	-1.61970000
H	-2.0327820000	0.2172680000	-1.60075900
C	-0.2950500000	1.9909770000	-0.23492100
H	-0.0633640000	2.7363260000	-0.99052400
H	-1.7295740000	1.3611570000	1.20652200
H	-2.3779060000	2.4491980000	-0.11179600
H	0.7777250000	0.7124700000	1.12407200
O	1.9534180000	1.1840470000	-0.55325500
C	2.9897850000	1.5647920000	0.34658800
H	3.9000020000	1.6519090000	-0.25088400
H	2.7721510000	2.5335730000	0.81738400
H	3.1354980000	0.8053270000	1.12494300
C	-3.5321620000	-0.1461840000	-0.03864700
H	-4.2154470000	0.6253320000	-0.40505800
H	-3.8693040000	-1.1159970000	-0.42040900
H	-3.5638330000	-0.1785050000	1.05152900

N	1.1213260000	-1.5617120000	-0.14170000
O	1.7139660000	-1.4761770000	0.92286700
O	1.2211470000	-2.4736830000	-0.95501800

TS11Z

0 1

C	0.3617930000	-0.6166620000	-0.68259900
C	-1.9826890000	-0.3994440000	-0.47206100
N	-0.7894590000	-0.9148840000	0.09529400
C	0.6225380000	1.0945520000	-0.60711900
C	-1.7863630000	1.3331900000	-0.35696700
O	-0.7401700000	-1.1240300000	1.34688500
H	0.2143490000	-0.8568860000	-1.73164100
H	-2.0263560000	-0.6183920000	-1.53956700
C	-0.5992840000	1.7035990000	-1.06488000
H	-0.6669120000	1.9617340000	-2.11963200
H	-1.7215640000	1.4144620000	0.73429600
H	-2.7203090000	1.7515350000	-0.73754900
H	1.5004940000	1.2594120000	-1.24277600
O	0.9412320000	1.2154900000	0.76077600
C	1.5091330000	2.4767540000	1.08167000
H	0.8158190000	3.2964770000	0.84934600
H	1.7153880000	2.4584390000	2.15391800
H	2.4496150000	2.6417460000	0.53444200
N	1.6452650000	-1.2927140000	-0.28243600
O	1.6698790000	-2.0884340000	0.63633700

O	2.5975650000	-0.9824040000	-1.00063800
C	-3.2347830000	-0.8057950000	0.27978200
H	-3.2065910000	-0.4389360000	1.30727000
H	-4.1153340000	-0.4017090000	-0.22805000
H	-3.3193610000	-1.8968270000	0.31610300

TS12

0 1

C	-1.9366760000	0.1692960000	-0.93006900
C	0.0340390000	0.3313620000	0.20718500
N	-0.5719850000	-0.1273290000	-1.01550900
C	-2.4911860000	-1.1457570000	0.15066100
C	-0.3636960000	-0.9057540000	1.29965900
C	-1.8053940000	-0.9699590000	1.38078600
O	-0.1486980000	-1.1689210000	-1.62771600
H	-3.5819770000	-1.1156130000	0.18197900
H	-2.1014620000	-1.9487150000	-0.49442500
H	0.0907380000	-1.7541410000	0.77078800
H	0.1488400000	-0.7083440000	2.24433600
H	-2.3237570000	-0.5812620000	2.25347300
C	-2.0463230000	1.5238760000	-0.25083900
C	-0.7026130000	1.6382870000	0.52828400
H	-2.1481790000	2.3267640000	-0.98835200
H	-0.8576750000	1.7410510000	1.60561900
H	-0.1079630000	2.4885270000	0.18915500
H	-2.9140360000	1.5675020000	0.41322800

C	1.5512730000	0.4859600000	0.10251500
O	2.1033820000	1.5602160000	-0.00991500
O	2.1947760000	-0.6859340000	0.15121600
C	3.6221600000	-0.6146400000	-0.01396300
H	4.0687920000	-0.0057590000	0.77644000
H	3.9714960000	-1.6451710000	0.04560500
H	3.8682990000	-0.1792720000	-0.98543100
H	-2.4743920000	-0.0131680000	-1.85783400

TS13

0 1

C	1.2460120000	0.0353570000	0.12040100
C	-1.0086200000	0.4069260000	0.29285300
N	-0.0265090000	-0.5553600000	-0.07457100
C	1.3526650000	1.0776240000	-1.28452600
C	-1.0398830000	1.4463070000	-1.11801700
C	0.2710160000	2.0098140000	-1.22402700
O	-0.2135210000	-1.4185600000	-1.00498700
H	2.3608500000	1.4919810000	-1.29128300
H	1.2193620000	0.2811610000	-2.03292800
H	-1.2728000000	0.6661290000	-1.85425700
H	-1.8626570000	2.1544480000	-0.99798900
H	0.4497490000	3.0429950000	-0.93718400
C	2.3953710000	-0.9539100000	0.03572000
C	1.1137120000	0.8672710000	1.39292700
C	-0.4136020000	1.1371490000	1.49964200

C	4.7411430000	-1.0712250000	0.14193200
O	3.6027550000	-0.2353970000	0.19722500
H	2.2802790000	-1.7056090000	0.83571600
H	2.3626810000	-1.4841200000	-0.92599900
H	1.4804420000	0.3040200000	2.25794100
H	-0.6496810000	2.2038330000	1.46105900
H	4.7278410000	-1.8277270000	0.94251400
H	5.6164870000	-0.4299560000	0.27205600
H	4.8160800000	-1.5915440000	-0.82573200
H	-0.8380280000	0.7354410000	2.42199700
H	1.7002950000	1.7860970000	1.32689800
C	-2.4081840000	-0.1493700000	0.51840800
O	-2.9558270000	-0.1442360000	1.60168600
O	-2.9682460000	-0.6194250000	-0.60245500
C	-4.2745340000	-1.1999160000	-0.44370500
H	-4.9812630000	-0.4554920000	-0.06736900
H	-4.5619810000	-1.5392580000	-1.43862700
H	-4.2339780000	-2.0400890000	0.25379200