Deciphering the Molecular Mechanism of Intramolecular Reactions from the Perspective of Bonding Evolution Theory

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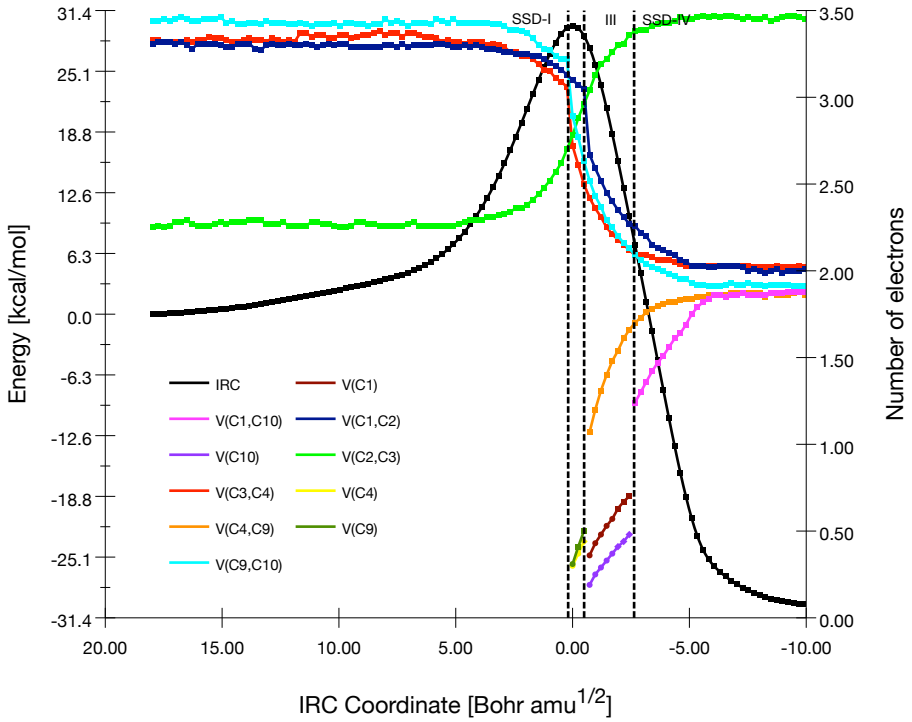

Figure S1. Population evolution (in e) of selected basins along the IRC associated with **TS2-b.**

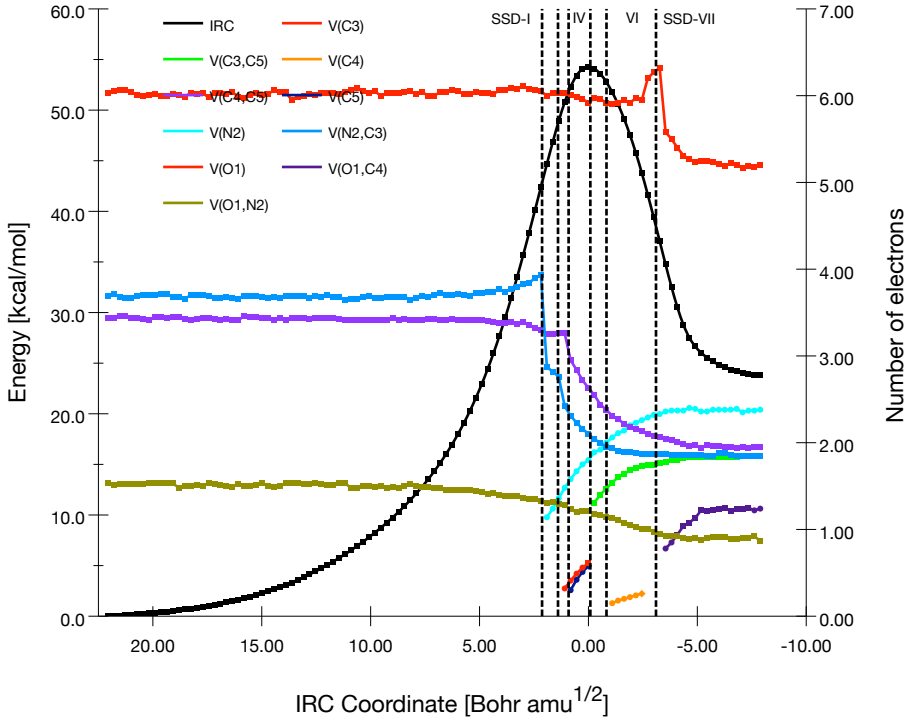

Figure S2. Population evolution (in e) of selected basins along the IRC associated with **TS3-b.**

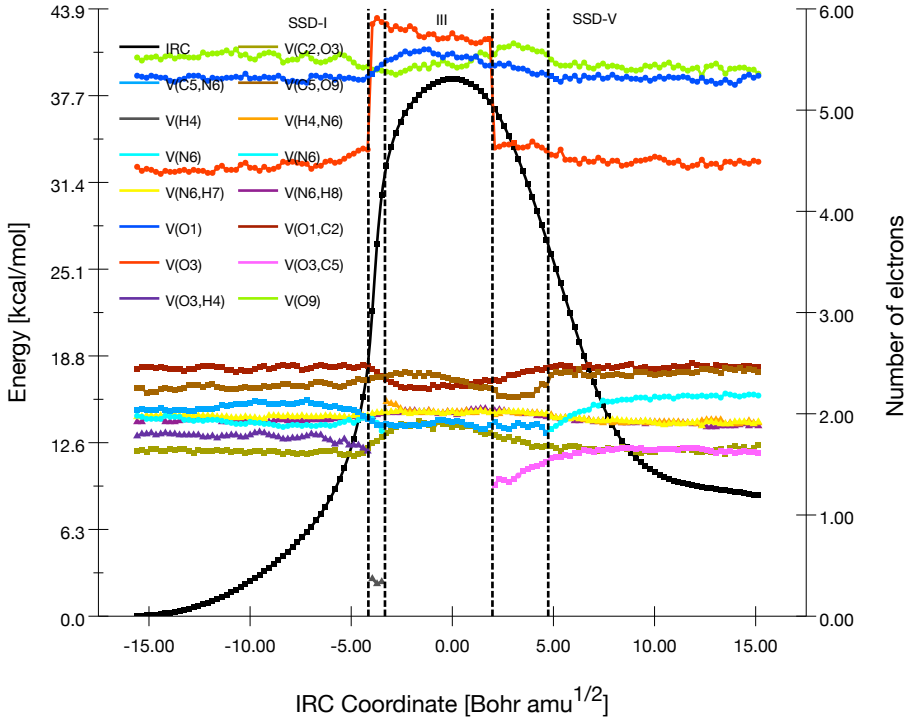

Figure S3. Population evolution (in e) of selected basins along the IRC associated with **TS4-b**.

Table S1: Basin Populations (in e), IRC coordinates (RX, amu$^{1/2}$. Bohr) and C6-C11/O8-C9 chemical bonds (in Å**)** along the **TS1** reaction pathway.

Basins	SSDI-I		SSD-II		SSD-III		SSD-IV	
	reactant							
V(O8)	4.97	5.36	5.87	5.53	5.53	5.41	5.38	5.22
V(C6,C7)	3.52	3.29	3.29	3.22	2.80	2.66	2.55	2.12
V(C7,O8)	1.42	1.59	1.63	1.77	1.85	1.94	2.01	2.38
V(O8,C9)	1.24	0.54	-	-	-	-	-	-
V(C9,C10)	2.07	2.30	2.39	2.65	2.98	3.08	3.14	3.42
V(C10,C11)	3.44	3.28	3.26	3.14	2.62	2.51	2.41	2.05
V(C6)	-	-	-	-	0.41	0.53	-	-
V(C11)	-	-	-	-	0.28	0.35	-	-
V(C6,C11)	-	-	-	-	-	-	1.05	1.83
d(C6-C11)	3.721	2.210	2.167	2.079	2.035	1.987	1.939	1.546
d(O8-C9)	1.427	1.661	1.711	1.809	1.857	1.904	1.949	3.482
Catastrophes	-	-	*C*	*C*	*FF*	*FF*	*C*	*C*
Ea(kcal/mol)	0.00	22.34	24.14	25.72	25.29	23.99	21.91	-14.87
Rx(amu.bohr)	-13.37	-0.98	-0.65	0.00	0.33	0.65	0.98	14.67

Table S2: Basin Populations (in e), IRC coordinates (RX, amu$^{1/2}$. Bohr) and C1-C9/C4-C10 chemical bonds (in Å**)** along the **TS2-a** reaction pathway.

Basins	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V	
	reactant									
V(C1,C2)	3.30	3.01	2.68	2.68	2.57	2.34	2.29	2.15	2.12	1.99
V(C2,C3)	2.28	2.81	2.90	2.90	2.98	3.19	3.24	3.35	3.37	3.47
V(C3,C4)	3.33	3.06	3.02	3.02	2.69	2.45	2.39	2.24	2.20	2.03
V(C9,C10)	3.42	3.19	2.78	2.78	2.64	2.36	2.29	2.10	2.07	1.92
V(C1)	-	-	0.30	0.30	0.38	0.57	-	-	-	-
V(C4)	-	-	-	-	0.34	0.49	0.54	0.68	-	-
V(C9)	-	-	0.18	0.18	0.27	0.45	-	-	-	-
V(C10)	-	-	0.26	0.26	0.34	0.54	0.51	0.68	-	-
V(C1,C9)	-	-	-	-	-	-	1.20	1.48	1.52	1.84
V(C4,C10)	-	-	-	-	-	-	-	-	1.42	1.87
d(C1-C9)	3.653	2.123	2.085	2.085	2.047	1.935	1.898	1.760	1.728	1.541
d(C4-C10)	3.115	2.358	2.327	2.327	2.296	2.201	2.201	2.168	1.989	1.579
Catastrophes	-	-	*FFF*	*FFF*	*F*	*F*	*C*	*C*	*C*	*C*
Ea(kcal/mol)	0.00	27.56	27.33	27.33	26.57	20.91	18.00	3.60	-0.24	-9.25
Rx(amu.bohr)	10.96	0.00	-0.24	-0.24	-0.48	-1.22	-1.46	-2.44	-2.68	-28.84

Table S3: Basin Populations (in e), IRC coordinates (RX, $amu^{1/2}$. Bohr) and C1-C10/C4-C9 chemical bonds (in Å**)** along the **TS2-b** reaction pathway.

Basins	SSD-I		SSD-II		SSD-III		SSD-IV	
	reactant							
V(C1,C2)	3.31	3.13	3.10	3.05	2.67	2.27	2.26	2.01
V(C2,C3)	2.25	2.70	2.78	2.96	3.04	3.36	3.38	3.45
V(C3,C4)	3.33	3.06	2.72	2.50	2.42	2.12	2.09	2.02
V(C9,C10)	3.44	3.22	2.89	2.63	2.52	2.13	2.09	1.91
V(C1)	-	-	-	-	0.36	0.70	-	-
V(C4)	-	-	0.30	0.44	-	-	-	-
V(C9)	-	-	0.31	0.50	-	-	-	-
V(C10)	-	-	-	-	0.19	0.48	-	-
V(C1,C10)	-	-	-	-	-	-	1.24	1.88
V(C4,C9)	-	-	-	-	1.07	1.66	1.70	1.86
d(C1-C10)	3.741	2.541	2.516	2.465	2.439	2.208	2.166	1.567
d(C4-C9)	3.617	2.052	2.009	1.926	1.885	1.645	1.623	1.538
Catastrophes	-	-	*FF*	*FF*	*FFC*	*FFC*	*C*	*C*
Ea(kcal/mol)	0.00	29.56	29.78	28.78	27.52	10.10	7.18	-29.94
Rx(amu.bohr)	17.97	0.24	0.00	-0.48	-0.73	-2.43	-2.67	-9.95

Table S4: Basin Populations (in e), IRC coordinates (RX, amu$^{1/2}$. Bohr) and C3-C4/O1-C5 chemical bonds (in Å**)** along the **TS3-a** reaction pathway.

Basins	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V	
	reactant									
V(O1)	5.96	5.94	5.93	5.93	5.95	6.10	5.39	5.39	5.37	5.04
V(O1,N2)	1.52	1.36	1.32	1.32	1.27	1.13	1.10	1.10	1.09	0.98
V(N2,C3)	3.68	3.97	2.94	2.94	2.55	2.15	2.10	2.10	2.06	1.80
V(C4,C5)	3.43	3.32	3.31	3.31	2.94	2.30	2.22	2.22	2.16	1.95
V(N2)			1.12	1.12	1.29	1.88	1.95	1.95	2.02	2.36
V(C3)	-	-	-	-	0.35	0.78	0.81	0.81	-	-
V(C4)	-	-	-	-	0.32	0.61	0.65	0.65	-	-
V(C3,C4)	-	-	-	-	-	-	-	-	1.54	1.92
V(O1,C5)	-	-	-	-	-	-	0.72	0.72	0.81	1.30
d(C3-C4)	2.977	2.308	2.265	2.265	2.220	1.988	1.941	1.941	1.893	1.558
d(O1-C5)	3.057	2.073	2.024	2.024	1.976	1.744	1.698	1.698	1.653	1.420
Catastrophes	-	-	*F*	*F*	*FF*	*FF*	*C*	*C*	*C*	*C*
Ea(kcal/mol)	0.00	13.85	14.48	14.48	14.72	5.96	2.06	2.06	-2.26	-31.20
Rx(amu.bohr)	-8.84	-0.66	-0.33	-0.33	0.00	1.64	1.96	1.96	2.30	13.09

Table S5: Basin Populations (in e), IRC coordinates (RX, amu$^{1/2}$. Bohr) and C3-C5/O1-C4 chemical bonds (in Å**)** along the **TS3-b** reaction pathway.

Basins	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V		SSD-VI		SSD-VII	
	reactant													
V(O1)	6.04	6.05	6.00	6.03	6.03	6.03	6.01	5.92	5.97	5.92	5.90	5.97	5.58	5.20
V(O1,N2)	1.54	1.33	1.31	1.29	1.28	1.28	1.23	1.21	1.18	1.14	1.13	1.01	0.93	0.87
V(N2,C3)	3.69	3.93	2.87	2.76	2.42	2.42	2.31	2.10	2.04	1.95	1.94	1.87	1.87	1.85
V(C4,C5)	3.44	3.30	3.25	3.26	3.26	3.26	2.95	2.63	2.55	2.38	2.31	2.13	2.04	1.95
V(N2)			1.14	1.36	1.48	1.48	1.58	1.80	1.89	2.00	2.06	2.26	2 .36	2.38
V(C3)	-	-	-	-	0.32	0.32	0.41	0.61	-	-	-	-	-	-
V(C4)	-	-	-	-	-	-	-	-	-	-	0.15	0.26	-	-
V(C5)	-	-	-	-	-	-	0.30	0.58	-	-	-	-	-	-
V(C3,C5)	-	-	-	-	-	-	-	-	1.31	1.47	1.54	1.73	1.78	1.85
V(O1,C4)	-	-	-	-	-	-	-	-	-	-	-	-	0.78	1.24
d(C3-C5)	3.810	2.194	2.146	2.049	2.001	2.001	1.953	1.817	1.775	1.705	1.677	1.598	1.570	1.542
d(O1-C4)	3.704	2.502	2.477	2.428	2.404	2.404	2.378	2.294	2.263	2.187	2.144	1.905	1.707	1.465
Catastrophes	-	-	*F*	*F*	*F*	*F*	*F*	*F*	*C*	*C*	*F*	*F*	*C*	*C*
Ea(kcal/mol)	0.00	42.41	44.67	48.93	50.77	50.77	52.30	54.29	54.10	52.79	51.78	43.78	34.75	23.79
Rx(amu.bohr)	22.07	2.18	1.91	1.36	1.09	1.09	0.82	0.00	-0.27	-0.82	-1.90	-2.45	-3.54	-7.89

Table S6: Basin Populations (in e), IRC coordinates (RX, amu$^{1/2}$. Bohr) and C2-N6/O3-H8 chemical bonds (in Å**)** along the **TS4-a** reaction pathway.

Basins	SSDI-I		SSD-II		SSD-III		SSD-IV		SSD-V	
	reactant									
V(O1)	5.38	5.59	5.62	5.68	5.67	5.65	5.66	5.62	5.56	5.47
V(O9)	5.47	5.45	5.43	5.47	5.47	5.49	5.50	5.50	5.51	5.50
V(O1,C2)	2.39	2.19	2.16	2.10	2.12	2.12	2.12	2.19	2.20	2.29
V(C2,O3)	1.58	1.47	1.45	1.07	-	-	-	-	-	-
V(O3)	4.49	4.66	4.70	5.04	6.09	6.00	5.98	5.79	4.30	4.55
V(O3,H4)	1.75	1.72	1.71	1.71	1.72	1.73	1.73	1.78	1.79	1.67
V(C2,N6)	-	-	1.94	1.86	1.84	1.82	1.80	1.78	1.80	1.87
V(C5,N6)	1.98	1.97	1.95	2.01	2.01	2.03	2.02	2.05	2.06	2.02
V(C5,O9)	2.32	2.34	2.36	2.38	2.37	2.37	2.36	2.32	2.32	2.33
V(N6)	2.01	1.88	-	-	-	-	1.85	2.01	2.02	1.99
V(N6,H7)	1.97	2.01	2.00	2.03	2.02	2.04	2.04	2.01	2.00	2.00
V(N6,H8)	1.93	1.98	1.98	2.08	2.11	2.17	-	-	-	-
V(H8)	-	-	-	-			0.36	0.39	-	-
V(O3,H8)	-	-	-	-	-	-			1.86	1.68
d(C2-N6)	2.258	1.902	1.886	1.653	1.647	1.633	1.629	1.611	1.606	1.369
d(O3-H8)	2.311	2.207	2.192	1.588	1.545	1.401	1.163	1.101	1.061	0.963
Catastrophes	-	-	*C*	*C*	*C*	*C*	*FF*	*FF*	*C*	*C*
Ea(kcal/mol)	0.00	11.47	12.00	30.48	31.60	34.51	35.10	31.14	29.33	-16.84
Rx(amu.bohr)	-5.72	-3.30	-3.19	-0.66	-0.55	-0.22	-0.11	0.44	0.55	10.99

Table S7: Basin Populations (in e), IRC coordinates (RX, amu$^{1/2}$. Bohr) and O3-C5/N6-H4 chemical bonds (in Å**)** along the **TS4-b** reaction pathway.

Basins	SSD-I		SSD-II		SSD-III		SSD-IV		SSD-V	
	reactant									
V(O1)	5.34	5.33	5.36	5.45	5.49	5.44	5.44	5.35	5.34	5.29
V(O9)	5.52	5.43	5.40	5.39	5.38	5.53	5.55	5.55	5.50	5.42
V(O1,C2)	2.44	2.47	2.44	2.37	2.34	2.32	2.33	2.45	2.46	2.46
V(C2,O3)	1.63	1.66	1.71	1.77	1.81	1.81	1.79	1.68	1.68	1.65
V(O3)	4.44	4.61	5.85	5.87	5.85	5.70	4.63	4.60	4.56	4.50
V(O3,H4)	1.78	1.63	-	-	-	-	-	-	-	-
V(C5,N6)	2.04	1.95	1.93	1.89	1.90	1.89	1.92	1.81	-	-
V(C5,O9)	2.25	2.33	2.35	2.36	2.37	2.25	2.23	2.28	2.38	2.45
V(N6)	1.98	1.97	1.95	1.83	-	-	-	-	1.85	2.17
V(N6,H7)	1.92	1.96	1.97	2.00	2.01	2.02	2.03	1.97	1.97	1.89
V(N6,H8)	1.97	1.98	2 .00	2.01	2.01	2.01	2.00	2.00	1.97	1.92
V(H4)	-	-	0.37	0.34	-	-	-	-	-	-
V(O3,C5)	-	-	-	-	-	-	1.30	1.52	1.56	1.62
V(H4,N6)	-	-	-	-	2.12	2.01	1.99	1.99	1.99	1.90
d(O3-C5)	3.158	2.452	2.442	2.431	2.422	1.799	1.766	1.475	1.462	1.384
d(H4,N6)	1.938	1.482	1.388	1.202	1.135	1.017	1.017	1.013	1.013	1.012
Catastrophes			*CF*	*CF*	*CFF*	*FFC*	*C*	*C*	*CF*	*CF*
Ea(kcal/mol)	0.00	18.07	22.05	30.45	32.56	37.18	36.68	27.25	26.19	8.95
Rx(amu.bohr)	-15.58	-4.18	-3.96	-3.49	-3.26	1.86	2.09	4.66	4.90	12.20

Table S8: Relative electronic energies (ΔE, kcal/mol), enthalpies (ΔH, kcal/mol), entropies (ΔS, cal/mol.K) and Gibbs free energies (ΔG, kcal/mol) of activation and reaction for the thermal sigmatropic rearrangement of allyloxycycloheptatriene

Species	ΔE	ΔH	ΔS	ΔG
TS1	27.0	25.4	30.0	-9.6
2	-16.7	-16.3	-14.8	-3.2
TS2-a	12.5	11.4	18.1	-14.1
TS2-b	14.6	13.5	19.8	-13.3
3	-43.9	-42.5	-33.7	-18.4
4	-45.1	-43.8	-35.0	-18.7

Table S9. Electronic energies, enthalpies, entropies and Gibbs free energies (in a.u) of all species involved in the thermal sigmatropic rearrangement of allyloxycycloheptatriene

Species	E	H	S	G
1	-463.38583	-463.164531	125.870	-463.25944
TS1	-463.34283	-463.124011	116.249	-463.21167
2	-463.41242	-463.190459	122.705	-463.28298
TS2-a	-463.36592	-463.146305	111.785	-463.23059
TS2-b	-463.36257	-463.143001	112.565	-463.22788
3	-463.45582	-463.232205	107.443	-463.31322
4	-463.45775	-463.234391	107.186	-463.31521

Table S10. Relative electronic energies (ΔE, kcal/mol), enthalpies (ΔH°, kcal/mol), entropies (ΔS°, cal/mol.K) and Gibbs free energies (ΔG°, kcal/mol) of activation and reaction for the IM32CA of nitrone-alkene 5

Species	ΔE°(gas)	ΔE°(Toluene)	ΔH°(Toluene)	ΔS°(Toluene)	ΔG°(Toluene)
TS3-a	15.9	17.8	17.3	-13.8	21.4
TS3-b	53.4	54.3	53.6	-15.4	58.2
6	-28.5	-26.9	-25.3	-13.9	-21.1
7	-26.8	-25.4	-23.9	-16.8	-18.9

Table S11 Electronic energies, enthalpies, entropies and Gibbs free energies (in a.u) of all species involved in the IM32CA of nitrone-alkene 5

Species	E(gas)	E(Toluene)	H(Toluene)	S(Toluene)	G(Toluene)
5	-955.02011	-955.02662	-954.79235	121.165	-954.84992
TS3-a	-954.99479	-954.99827	-954.76484	107.382	-954.81586
TS3-b	-954.93503	-954.94004	-954.70686	105.801	-954.75713
6	-955.06554	-955.06945	-954.83260	107.222	-954.88354
7	-955.06284	-955.06716	-954.83040	104.389	-954.88000

Table S12 Relative electronic energies (ΔE, kcal/mol), enthalpies (ΔH, kcal/mol), entropies (ΔS, cal/mol.K) and Gibbs free energies (ΔG, kcal/mol) of activation and reaction for the Thermal decomposition of N-carbamoyl-L-proline

Species	ΔE	ΔH	ΔS	ΔG
TS4-a	54.1	49.9	-6.0	52.7
TS4-b	40.3	38.9	-6.0	41.8
9(H_2O)	16.0	13.3	34.4	-3.1
10(NH_3)	8.0	5.3	32.4	-10.1

Table S13. Electronic energies, enthalpies, entropies and Gibbs free energies (in a.u) of all species involved in the Thermal decomposition of N-carbamoyl-L-proline

Species	E	H	S	G
8	-569.87326	-569.67368	123.392	-569.76731
TS4-a	-569.78699	-569.59417	117.423	-569.68327
TS4-b	-569.80910	-569.61167	117.420	-569.70077
9(H_2O)	-569.84777	-569.65254	157.834	-569.77230
10(NH_3)	-569.86051	-569.66527	155.755	-569.78346

Cartesian coordinates

1

C	-2.5952950000	1.1101830000	-0.6294860000
C	-2.9634680000	-0.1695560000	-0.7510130000
C	-1.6539420000	1.6028480000	0.3570950000
C	-1.0356400000	-1.3933760000	0.1144870000
C	-0.5845580000	0.9310830000	0.8295770000
C	-0.1878130000	-0.4132780000	0.4465200000
H	-3.0086480000	1.8440850000	-1.3115450000
H	-3.6077510000	-0.4663620000	-1.5698070000
H	-1.7655030000	2.6373270000	0.6612900000
H	-0.6246470000	-2.3377740000	-0.2184550000
H	0.1091420000	1.4516660000	1.4808410000
O	1.1628510000	-0.6790070000	0.4813140000
C	1.9382090000	0.0991890000	-0.4242820000
C	3.3572900000	-0.3544860000	-0.3337340000
H	1.5506290000	-0.0550680000	-1.4385170000
H	3.5114010000	-1.4242680000	-0.4224790000
C	4.3833500000	0.4641020000	-0.1743750000
H	5.4005560000	0.0988670000	-0.1443120000
H	4.2391060000	1.5330130000	-0.0716280000
H	1.8595040000	1.1649070000	-0.1908230000
C	-2.5193210000	-1.2099760000	0.2401890000
H	-2.7617160000	-0.8639970000	1.2501380000
H	-3.0377580000	-2.1507440000	0.0749130000

TS1

C	0.6496530000	-1.3903110000	0.4438390000
C	1.9887270000	-1.2827080000	0.5586270000

C	2.8190270000	-0.2866780000	-0.0933110000
C	-0.2036910000	-0.5668610000	-0.4088650000
C	2.4351560000	0.9675600000	-0.3514160000
C	-0.0402070000	0.8199820000	-0.5166610000
C	1.1285380000	1.5052020000	0.1494310000
H	0.1614120000	-2.2657680000	0.8592400000
H	2.5086500000	-2.0722910000	1.0890930000
H	3.8103940000	-0.6059920000	-0.3926850000
H	3.0921590000	1.6240620000	-0.9084590000
H	-0.4828450000	1.2916370000	-1.3830610000
H	1.0728670000	1.3193990000	1.2277730000
H	1.0645250000	2.5808450000	-0.0026880000
O	-1.2492670000	-1.1298300000	-0.9148460000
C	-2.6859790000	-0.7680150000	0.1238720000
H	-3.4337610000	-1.3107070000	-0.4361230000
H	-2.3274740000	-1.2862370000	1.0053060000
C	-2.6998470000	0.6286410000	0.1292590000
H	-3.2641130000	1.1433400000	-0.6379370000
C	-1.6380360000	1.2771270000	0.7338320000
H	-1.1828360000	0.8421670000	1.6162490000
H	-1.5448890000	2.3545510000	0.6704150000

2

C	2.4259930000	-0.3674800000	-0.6685810000
C	2.0722760000	-1.1637030000	0.3421610000
C	1.8612090000	0.9298410000	-1.0235790000
C	-0.3450060000	-0.3829140000	0.7591000000
C	0.7655880000	1.5565140000	-0.5746810000
C	-0.2271510000	1.0934220000	0.4233460000
H	3.2622340000	-0.6812000000	-1.2811460000
H	2.6499340000	-2.0700800000	0.4820790000
H	2.4491450000	1.4783530000	-1.7516260000
H	-1.0918950000	-0.4335740000	1.5518600000
H	0.5560050000	2.5565960000	-0.9328770000
O	-0.9423800000	1.9115340000	0.9579610000
C	-3.1216290000	-0.1529360000	-0.3272490000
C	-2.2395090000	-0.9746830000	-0.8760960000
H	-4.1200470000	-0.0715300000	-0.7351500000
H	-2.5418320000	-1.5583530000	-1.7403150000
C	-0.8255330000	-1.2138770000	-0.4327240000
H	-0.7192090000	-2.2732540000	-0.1746560000
H	-0.1587550000	-1.0585870000	-1.2845030000
H	-2.8875570000	0.4723360000	0.5239040000
C	0.9743340000	-0.9192530000	1.3328130000
H	0.7568260000	-1.8542600000	1.8503730000
H	1.3407690000	-0.2283050000	2.1013060000

TS2-a

C	-2.0638610000	-0.4991160000	0.4025220000
C	-1.5916630000	0.7955950000	0.4843550000

C	-1.2225110000	-1.5934900000	0.2878300000
C	0.9330590000	0.9117150000	0.6538450000
C	0.1377020000	-1.5146190000	-0.0206330000
C	1.1993420000	-0.5750480000	0.4740860000
H	-3.1230560000	-0.6593420000	0.2385310000
H	-2.3225110000	1.5839650000	0.3423540000
H	-1.6775330000	-2.5676070000	0.1571020000
H	1.7686920000	1.3036450000	1.2314810000
H	0.6153150000	-2.4568210000	-0.2686210000
O	2.3150180000	-1.0123010000	0.6409960000
C	0.0071020000	-0.4361410000	-1.8440580000
C	-0.2589570000	0.8650610000	-1.4602440000
H	-0.7336260000	-1.0083470000	-2.3861060000
H	-1.1055980000	1.4000370000	-1.8610500000
C	0.8435930000	1.5788450000	-0.7340720000
H	1.7935940000	1.4803700000	-1.2625290000
H	0.6362750000	2.6406980000	-0.6021590000
H	1.0342650000	-0.7303740000	-2.0270050000
C	-0.3991860000	1.1755820000	1.3331560000
H	-0.4549440000	2.2373370000	1.5742950000
H	-0.4587410000	0.6245410000	2.2750120000

TS2-b

C	1.5640860000	1.3711290000	0.4193420000
C	1.5708510000	0.0497000000	0.8676960000
C	0.5528470000	1.8949620000	-0.3723820000
C	-0.8892500000	-0.8642440000	0.7122710000
C	-0.6230730000	1.2627300000	-0.7231420000
C	-1.4776330000	0.4039610000	0.1371800000
H	2.4966750000	1.9185150000	0.4683390000
H	2.5077550000	-0.2505200000	1.3271590000
H	0.7726120000	2.8189630000	-0.8952180000
H	-1.6417300000	-1.3228680000	1.3515960000
H	-1.2235420000	1.7464260000	-1.4861750000
O	-2.6584240000	0.6436800000	0.2373770000
C	1.6553420000	-0.9376350000	-0.8806110000
C	0.3633220000	-0.9596450000	-1.3702520000
H	1.9910920000	-1.8024690000	-0.3177420000
H	0.1221760000	-0.5831320000	-2.3512380000
C	-0.6470000000	-1.7120510000	-0.5528830000
H	-1.5866920000	-1.8538570000	-1.0845960000
H	-0.2650910000	-2.6958040000	-0.2661910000
H	2.4350290000	-0.4377770000	-1.4383350000
C	0.3929810000	-0.6638230000	1.5170120000
H	0.7301270000	-1.6516610000	1.8421040000
H	0.1541490000	-0.1057650000	2.4258980000

3

C	-1.3685030000	1.2317110000	-0.8197440000
C	-1.5245760000	-0.2285780000	-0.4850900000

C	-0.2901520000	1.8771650000	-0.3970610000
C	0.6785970000	-1.2360860000	-0.4637800000
C	0.6196740000	1.1664180000	0.5822730000
C	1.4095440000	0.0668620000	-0.1430160000
H	-2.0838840000	1.6975270000	-1.4858470000
H	-2.5470030000	-0.5535160000	-0.6635100000
H	-0.0711650000	2.8964060000	-0.6842530000
H	1.4102980000	-1.9324650000	-0.8676650000
H	1.3506350000	1.8503160000	1.0060300000
O	2.5671780000	0.2247800000	-0.4364330000
C	-0.3185710000	0.5607380000	1.6439660000
C	-1.0750370000	-0.5933760000	0.9842230000
H	-0.9917820000	1.3415620000	1.9953090000
H	-1.9276220000	-0.8919380000	1.5902640000
C	-0.0581940000	-1.7268600000	0.7898540000
H	0.5843300000	-1.8637270000	1.6589240000
H	-0.5408830000	-2.6800840000	0.5700370000
H	0.2396980000	0.1864350000	2.5029820000
C	-0.5290900000	-1.0142970000	-1.3867860000
H	-0.9295400000	-1.9928020000	-1.6567570000
H	-0.2926480000	-0.4781440000	-2.3030910000

4

C	1.1222850000	1.5763160000	0.4618510000
C	1.5366560000	0.1475080000	0.7267300000
C	0.1891010000	1.8048890000	-0.4529020000
C	-0.7848270000	-1.0261380000	0.7380140000
C	-0.5339600000	0.6229230000	-1.0507640000
C	-1.4526490000	0.1774300000	0.0973300000
H	1.6204680000	2.3865970000	0.9783770000
H	2.4703720000	0.1388580000	1.2881170000
H	-0.1458110000	2.8020000000	-0.7033670000
H	-1.4899320000	-1.5597220000	1.3711180000
H	-1.1288940000	0.9042200000	-1.9162020000
O	-2.5122180000	0.6607690000	0.3808820000
C	1.7364860000	-0.4958700000	-0.6565640000
C	0.3591140000	-0.6388250000	-1.3051040000
H	2.1980660000	-1.4814340000	-0.5696000000
H	0.4473190000	-0.8447950000	-2.3692980000
C	-0.3866160000	-1.7572390000	-0.5489600000
H	-1.2752750000	-2.0846820000	-1.0915160000
H	0.2455250000	-2.6266470000	-0.3683600000
H	2.3985330000	0.1317510000	-1.2518440000
C	0.4840040000	-0.6441920000	1.5371830000
H	0.9380560000	-1.5778710000	1.8808980000
H	0.2017480000	-0.0752410000	2.4237340000

5

C	1.7106260000	-2.7521070000	-0.1273850000
C	0.3774760000	-3.0531180000	0.1034790000

C	-0.5716510000	-2.0428790000	0.1403710000
C	-0.2009750000	-0.7147170000	-0.0502860000
C	1.1522770000	-0.3969190000	-0.2752700000
C	2.0846730000	-1.4332080000	-0.3220900000
C	1.5315340000	0.9911570000	-0.5436820000
C	-2.9571730000	-0.2076500000	-0.0864590000
C	-3.9950140000	0.8311080000	-0.3662660000
C	-4.9463110000	1.1671950000	0.4897420000
O	2.8935270000	2.7860220000	-0.3830300000
N	2.5495880000	1.6219100000	-0.0346940000
C	3.3858440000	1.0533270000	1.0374960000
S	-1.3437920000	0.6311360000	0.0314100000
H	2.4512760000	-3.5378300000	-0.1722440000
H	0.0681890000	-4.0781910000	0.2551590000
H	-1.6020050000	-2.2988970000	0.3364020000
H	3.1161110000	-1.1942020000	-0.5455260000
H	0.9587020000	1.5850610000	-1.2431240000
H	-2.8987190000	-0.9276910000	-0.9030680000
H	-3.1758850000	-0.7291950000	0.8439590000
H	-3.9254040000	1.3272200000	-1.3279450000
H	-5.0231210000	0.6926810000	1.4605280000
H	-5.6786230000	1.9251880000	0.2495570000
H	2.9179180000	0.1876490000	1.4918560000
H	3.5177760000	1.8585240000	1.7528780000
H	4.3512830000	0.7968240000	0.6081980000

TS3-a

C	-3.187404000	-1.184611000	-0.555652000
C	-3.526079000	0.042049000	0.000713000
C	-2.532897000	0.935187000	0.365010000
C	-1.186405000	0.604974000	0.215580000
C	-0.839504000	-0.652387000	-0.300201000
C	-1.853753000	-1.516917000	-0.714092000
C	0.561745000	-1.070565000	-0.475215000
C	1.082396000	1.859147000	-0.830800000
C	1.763662000	0.604020000	-1.299725000
C	2.988579000	0.197503000	-0.800674000
O	2.628441000	-1.466863000	0.202285000
N	1.390111000	-1.316825000	0.535785000
C	1.162475000	-0.977444000	1.930937000
S	0.030526000	1.797955000	0.685694000
H	-3.958364000	-1.877396000	-0.862747000
H	-4.564969000	0.313853000	0.128564000
H	-2.790118000	1.910239000	0.755505000
H	-1.579393000	-2.473159000	-1.141294000
H	0.803614000	-1.637163000	-1.362174000
H	0.452612000	2.265908000	-1.618506000
H	1.804718000	2.628345000	-0.556730000
H	1.516960000	0.319894000	-2.314294000

H	3.434363000	0.739476000	0.024813000
H	3.681375000	-0.346438000	-1.423387000
H	0.099234000	-0.874151000	2.125956000
H	1.675389000	-0.045018000	2.162239000
H	1.580964000	-1.784745000	2.526890000

TS3-b

C	-2.903604000	-1.710522000	0.029326000
C	-3.499645000	-0.459337000	0.051119000
C	-2.727767000	0.693509000	-0.011932000
C	-1.344737000	0.602544000	-0.096334000
C	-0.741450000	-0.671663000	-0.120819000
C	-1.521454000	-1.813493000	-0.057288000
C	1.358841000	2.184499000	-0.246845000
C	2.120881000	1.193110000	0.587584000
C	1.322956000	0.269486000	1.254904000
O	2.801063000	-0.510246000	-0.790346000
N	1.798648000	-1.330145000	-0.530914000
C	2.120417000	-2.506058000	0.253696000
S	-0.508823000	2.211507000	-0.105603000
H	-3.510570000	-2.603803000	0.070590000
H	-4.575508000	-0.372090000	0.113979000
H	-3.202809000	1.665896000	0.004421000
H	-1.048306000	-2.785220000	-0.099819000
H	1.623641000	2.060328000	-1.299265000
H	1.596644000	3.213938000	0.026539000
H	3.180874000	1.328056000	0.726719000
H	0.389006000	0.631313000	1.663331000
H	1.808592000	-0.469959000	1.878865000
H	1.201574000	-2.979520000	0.596367000
H	2.740919000	-2.230730000	1.109196000
H	2.679817000	-3.200705000	-0.368436000
C	0.720554000	-0.532008000	-0.260658000
H	0.828299000	0.250973000	-0.990188000

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C	-2.4236230000	2.0985790000	-0.3436070000
C	-3.3348900000	1.0536440000	-0.2923780000
C	-2.8967970000	-0.2433700000	-0.0768860000
C	-1.5432340000	-0.4987880000	0.1223470000
C	-0.6244760000	0.5546860000	0.0907080000
C	-1.0721140000	1.8429700000	-0.1628990000
C	0.8189450000	0.2116520000	0.2971140000
C	0.6994620000	-2.2669450000	-0.0253410000
C	1.2169020000	-0.9666080000	-0.5905010000
C	2.7202490000	-0.7615580000	-0.6076040000

O	2.8507510000	0.6402770000	-0.7607370000
N	1.7707300000	1.2719680000	-0.0412750000
C	2.3458440000	1.8960640000	1.1369020000
S	-1.0752440000	-2.1762910000	0.4551030000
H	-2.7622840000	3.1078300000	-0.5317670000
H	-4.3896500000	1.2425610000	-0.4381190000
H	-3.6012210000	-1.0646640000	-0.0688860000
H	-0.3428530000	2.6388590000	-0.2290410000
H	0.9568360000	-0.1080620000	1.3435450000
H	1.2539460000	-2.5348940000	0.8738410000
H	0.7883010000	-3.0775830000	-0.7448630000
H	0.8194500000	-0.7961810000	-1.5923370000
H	3.1693220000	-1.1093400000	0.3319270000
H	3.2336000000	-1.2257800000	-1.4470160000
H	1.5335360000	2.3603460000	1.6973080000
H	3.0476720000	2.6658330000	0.8267820000
H	2.8585180000	1.1738030000	1.7846860000

7

C	3.1772140000	-1.2420350000	0.2723930000
C	3.5060560000	0.0388530000	-0.1388860000
C	2.5001210000	0.9633660000	-0.3700850000
C	1.1570340000	0.6247700000	-0.2133560000
C	0.8162680000	-0.6764370000	0.1815060000
C	1.8424650000	-1.5828190000	0.4295840000
C	-0.6058130000	-1.1465760000	0.3822800000
C	-1.2327870000	1.9127450000	0.6600590000
C	-2.0604970000	0.6454370000	0.8771520000
C	-1.3118530000	-0.4807590000	1.5695100000
O	-2.4953460000	0.0669210000	-0.3313330000
N	-1.4706420000	-0.8536650000	-0.7814320000
C	-2.2008000000	-2.0224520000	-1.2379380000
S	-0.0070630000	1.8835810000	-0.6718660000
H	3.9498820000	-1.9732750000	0.4653420000
H	4.5404150000	0.3257150000	-0.2696880000
H	2.7484360000	1.9721030000	-0.6716560000
H	1.5828510000	-2.5878820000	0.7400790000
H	-0.5733040000	-2.2270410000	0.5287600000
H	-0.7610110000	2.2126550000	1.5963140000
H	-1.8964340000	2.7179830000	0.3453820000
H	-2.9625820000	0.9223310000	1.4254120000
H	-2.0278030000	-1.1708460000	2.0135130000
H	-0.6169650000	-0.1446870000	2.3351720000
H	-1.4820310000	-2.7256980000	-1.6554360000
H	-2.8871020000	-1.7170570000	-2.0237390000
H	-2.7685260000	-2.5058680000	-0.4322180000

8

C	-0.9216060000	1.6637580000	0.7826390000
C	0.3516630000	2.3871420000	0.3386580000

C	0.8683320000	1.4859870000	-0.7762390000
C	-0.6010640000	0.1713420000	0.5876200000
C	1.6468220000	-0.7300730000	-0.0644200000
C	-1.7259260000	-0.5647640000	-0.1279340000
N	0.5935650000	0.1426280000	-0.2638480000
N	1.3358430000	-1.8655980000	0.6536710000
O	2.7688750000	-0.5050310000	-0.4695490000
O	-2.5909390000	-0.0711020000	-0.7895330000
O	-1.6175110000	-1.9029310000	0.0309390000
H	-1.7549340000	1.9311390000	0.1350750000
H	-1.2051710000	1.8772310000	1.8103070000
H	0.1584500000	3.4056120000	0.0094460000
H	1.0826390000	2.4166290000	1.1473810000
H	1.9303980000	1.5740450000	-0.9787280000
H	0.3100100000	1.6512280000	-1.7003150000
H	-0.3944040000	-0.3409000000	1.5273990000
H	2.0826900000	-2.5402350000	0.6337370000
H	0.4065970000	-2.2461890000	0.5676560000
H	-2.3148580000	-2.3156240000	-0.4975060000

TS4-a

C	-2.1963830000	-1.0064260000	-0.4625790000
C	-2.1687800000	0.1595650000	0.5313800000
C	0.0106280000	-0.8229210000	0.5682630000
C	-0.9449280000	-1.8278640000	-0.1056720000
H	-3.1124840000	-1.5894900000	-0.4049320000
H	-2.1115260000	-0.6060060000	-1.4733530000
H	-2.5572580000	-0.1334250000	1.5071230000
H	-2.6820380000	1.0555050000	0.1944430000
H	0.3095940000	-1.1515300000	1.5602540000
H	-0.4692720000	-2.2769710000	-0.9746330000
H	-1.1910820000	-2.6242370000	0.5939310000
N	-0.7386370000	0.4334010000	0.6403960000
C	-0.1970470000	1.4613460000	-0.0706450000
O	-0.7341890000	2.4722630000	-0.4374590000
N	1.1611640000	1.1177440000	-0.3667920000
H	1.4809040000	1.5047240000	-1.2484780000
H	1.9847850000	0.9740520000	0.5009070000
C	1.2904270000	-0.4963600000	-0.2254250000
O	1.7590900000	-1.1337500000	-1.1342050000
O	2.3975990000	-0.1343610000	1.0357430000
H	3.2471830000	-0.4478810000	0.7049560000

TS4-b

C	1.901510000	-1.260270000	-0.516280000
C	2.114820000	-0.218390000	0.580820000
C	0.583090000	-1.908850000	-0.106720000
H	2.711440000	-1.981830000	-0.591870000
H	1.787450000	-0.762120000	-1.479870000
H	2.466860000	-0.694590000	1.497140000
H	2.795610000	0.583510000	0.309270000

H	0.013340000	-2.322630000	-0.933340000
H	0.742140000	-2.688680000	0.638910000
C	0.380410000	1.457140000	-0.276360000
O	1.146870000	2.399550000	-0.354420000
H	-2.529920000	1.191660000	0.173080000
C	-1.383190000	-0.517320000	-0.045500000
O	-2.076320000	-1.162430000	-0.770390000
C	0.709420000	0.341710000	0.767510000
H	0.576530000	0.757430000	1.770020000
N	-0.181400000	-0.806140000	0.525730000
N	-2.206930000	0.496760000	0.847820000
H	-2.980980000	-0.007840000	1.275770000
H	-1.640630000	0.967300000	1.550500000
O	-0.703040000	1.232790000	-0.905840000

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C	-0.9528880000	-1.5093980000	-0.5073610000
C	-2.2803030000	-0.8155170000	-0.1785950000
C	-1.8831810000	0.6362210000	0.1477730000
C	-0.0104430000	-0.8570030000	0.5059070000
C	0.4619360000	1.3717910000	0.0271430000
C	1.4437620000	-0.7259160000	0.0881940000
N	-0.4796060000	0.5248710000	0.5658330000
N	1.6363220000	0.6199660000	-0.1252740000
O	0.3202960000	2.5227060000	-0.2865920000
O	2.2532820000	-1.6031120000	-0.0345050000
H	-0.6282440000	-1.2557220000	-1.5185970000
H	-0.9879720000	-2.5914320000	-0.4170310000
H	-2.9998610000	-0.8694280000	-0.9918340000
H	-2.7299040000	-1.2834830000	0.6976530000
H	-2.4956180000	1.0644970000	0.9379100000
H	-1.9417240000	1.2931770000	-0.7204580000
H	-0.0652830000	-1.3522470000	1.4767920000
H	2.4896810000	1.0229570000	-0.4779400000

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C	-0.9761990000	-1.4890580000	-0.5190530000
C	-2.2890330000	-0.7719880000	-0.1777160000
C	-1.8666680000	0.6666030000	0.1796030000
C	-0.0201250000	-0.8617960000	0.5001530000
C	0.4922200000	1.3382740000	0.0140150000
C	1.4255350000	-0.7214450000	0.0850400000
N	-0.4563000000	0.5226060000	0.5697420000
O	0.3981360000	2.4770590000	-0.3126930000
O	2.2524630000	-1.5614050000	-0.0329060000
O	1.6616880000	0.6048740000	-0.1542090000
H	-0.6498530000	-1.2339270000	-1.5289280000
H	-1.0332960000	-2.5705610000	-0.4362290000
H	-3.0057320000	-0.7950490000	-0.9946350000

H	-2.7515570000	-1.2481510000	0.6870150000
H	-2.4563910000	1.0805360000	0.9936780000
H	-1.9271740000	1.3487030000	-0.6680500000
H	-0.0745740000	-1.3675550000	1.4651680000

H_2O

H	0.0000000000	-0.7599420000	-0.4678220000
H	0.0000000000	0.7599420000	-0.4678220000
O	0.0000000000	0.0000000000	0.1169560000

NH_3

N	0.0000000000	0.1150260000	0.0000000000
H	-0.4685760000	-0.2683680000	0.8116150000
H	-0.4685760000	-0.2683680000	-0.8116150000
H	0.9371510000	-0.2684470000	0.0000000000