Electronic Supplementary Information

Reaction Mechanism of *N*-Cyclopropylglycine Oxidation by Monomeric Sarcosine Oxidase

Mitsuo Shoji,[*ab] Yukihiro Abe,[*c] Mauro Boero,[d] Yasuteru Shigeta[a] and Yoshiaki Nishiya[e]

[a] Center for Computational Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577, Japan.

[b] JST-PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan.

[c] HPC Systems Inc., 646 Nijyohanjikicho, Ayanokojisagaru Karasumadori, Shimogyo-ku, Kyoto 600-8412, Japan.

[d] University of Strasbourg, Institut de Physique et Chimie des Matériaux de Strasbourg, CNRS, UMR 7504, 23 rue du Loess, F-67034 France.

[e] Department of Life Science, Faculty of Science and Engineering, Setsunan University, 17-8 Ikedanaka-machi, Neyagawa, Osaka 572-8508, Japan.

* To whom correspondence should be addressed.
E-mail: mshoji@ccs.tsukuba.ac.jp; yu-abe@hpc.co.jp

Contents

Table S1. Interatomic distances (Å) between CPG and FAD Flavin in states **1**.

States	C1-C4a	C2-C4a	C2-N5	C3-C4a	C3-N5
1a	3.96	4.12	4.03	3.68	3.86
1b	3.27	3.18	3.30	4.46	4.49
1c	4.16	2.98	2.83	2.91	3.35
1d	4.08	3.40	3.23	3.39	3.77

Table S2. Energy contributions for the relative free energies (ΔG/ kcal mol^{-1})

State	ΔE /kcal mol^{-1}	δH/a.u.	S/ cal mol^{-1} K^{-1}	G / kcal mol^{-1}	ΔG /kcal mol^{-1}
1a	0	0.571728	182.460	304.36	0
1b	2.00	0.570737	182.468	305.74	1.37
1c	7.35	0.569605	182.841	310.26	5.90
1d	9.90	0.571007	183.144	313.60	9.24
2a	0.32	0.571755	179.786	305.49	1.13
2b	10.15	0.571080	181.126	314.50	10.14
2c	19.74	0.571834	188.049	322.50	18.14
3a	-12.06	0.573401	179.786	294.15	-10.21
3b	-3.01	0.571863	176.666	303.13	-1.20
4a	-12.75	0.572212	180.099	292.62	-11.74
4b	-9.17	0.572125	178.630	296.59	-7.78
5a	-4.93	0.572119	182.706	299.60	-4.75
5b	-2.94	0.573242	188.998	300.43	-3.94
$\mathbf{1}_{SET}$	17.43	0.570716	186.443	319.97	15.60
$\mathbf{2}_{SET}$	20.52	0.570345	189.331	321.97	17.60
TS(1a,1b)	10.19	0.572089	184.806	314.08	9.71
TS(1a,1c)	15.68	0.570346	187.433	317.69	13.33
TS(1a,1d)	10.73	0.569956	179.692	314.80	10.44
TS(1b,1d)	13.25	0.570004	179.737	317.34	12.98
TS(1d,2c)	46.75	0.568980	182.102	349.49	45.13
TS(1c,2b)	19.55	0.568808	187.122	320.69	16.32
TS(1d,2a)	18.81	0.56962	186.984	322.89	16.14
TS(2a,3a)	10.49	0.567318	176.956	313.72	9.36
TS(2b,3b)	17.31	0.567299	176.739	320.60	16.23
TS(3a,5a)	-3.61	0.571189	178.951	301.46	-2.90
TS(3b,5b)	20.91	0.570608	181.983	324.71	20.34
TS(1_{SET},2_{SET})	21.94	0.570993	188.090	324.16	19.80

Theoretical level for the QM region were UB3LYP-D3//TZVP. $\Delta G(i) = G(i) - G(\mathbf{1a})$, $G(i) = \Delta E(i) + \delta H(i) - T S(i)$, where ΔH is thermal energy correction to enthalpy, S is total entropy and T=298.15 K is temperature.

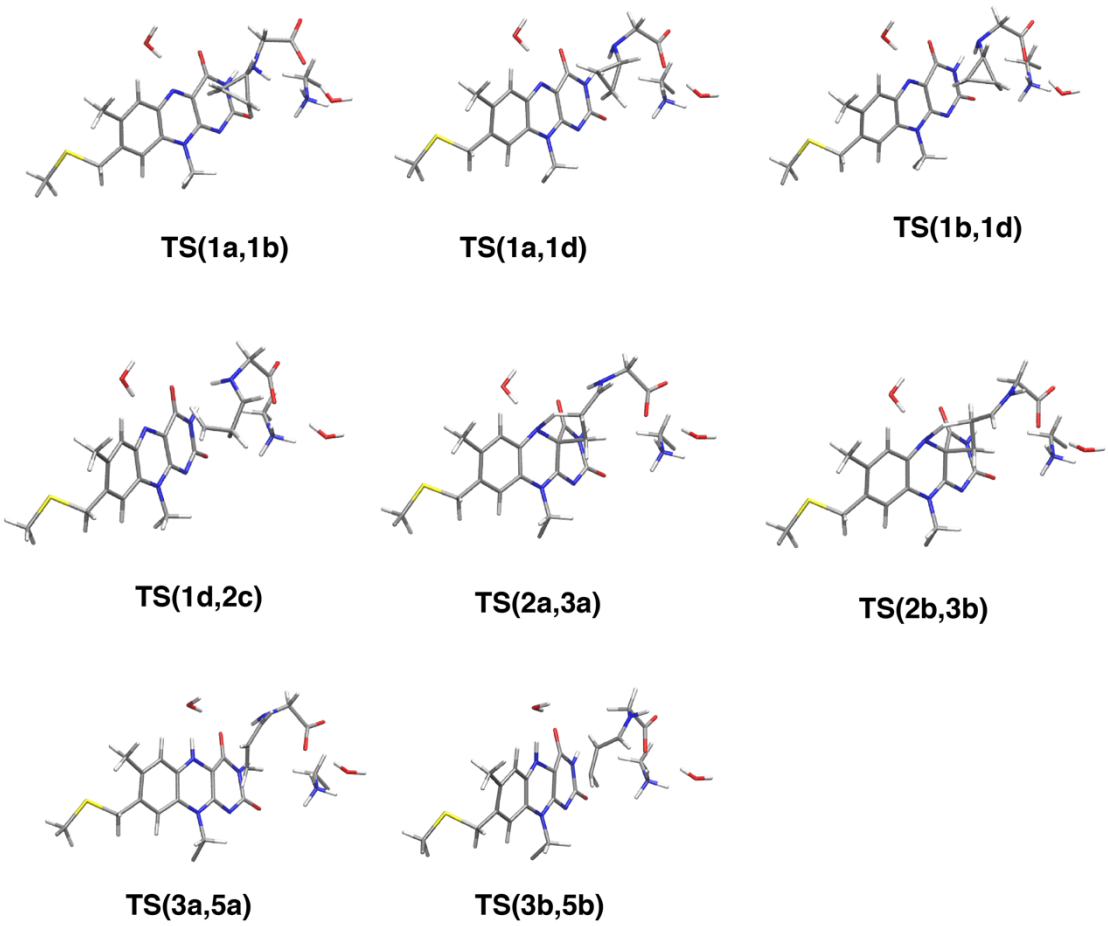
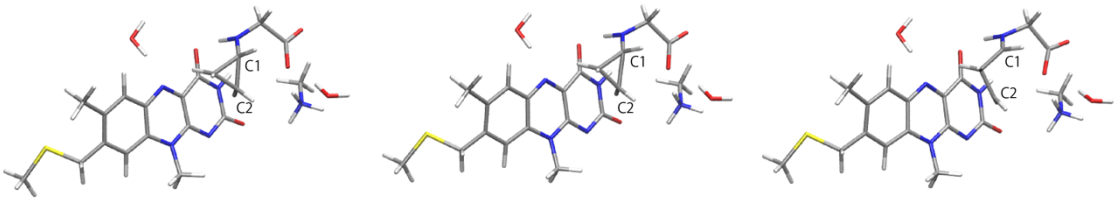


Figure S1. Transition state structures calculated by the QM/MM method. Atoms in the QM regions are only shown for clarity.



1SET **TS(1SET, 2SET)** **2SET**

Figure S2. Intermediate states in the SET mechanism. Structures are calculated by the QM/MM method. Atoms in the QM regions are only shown for clarity.

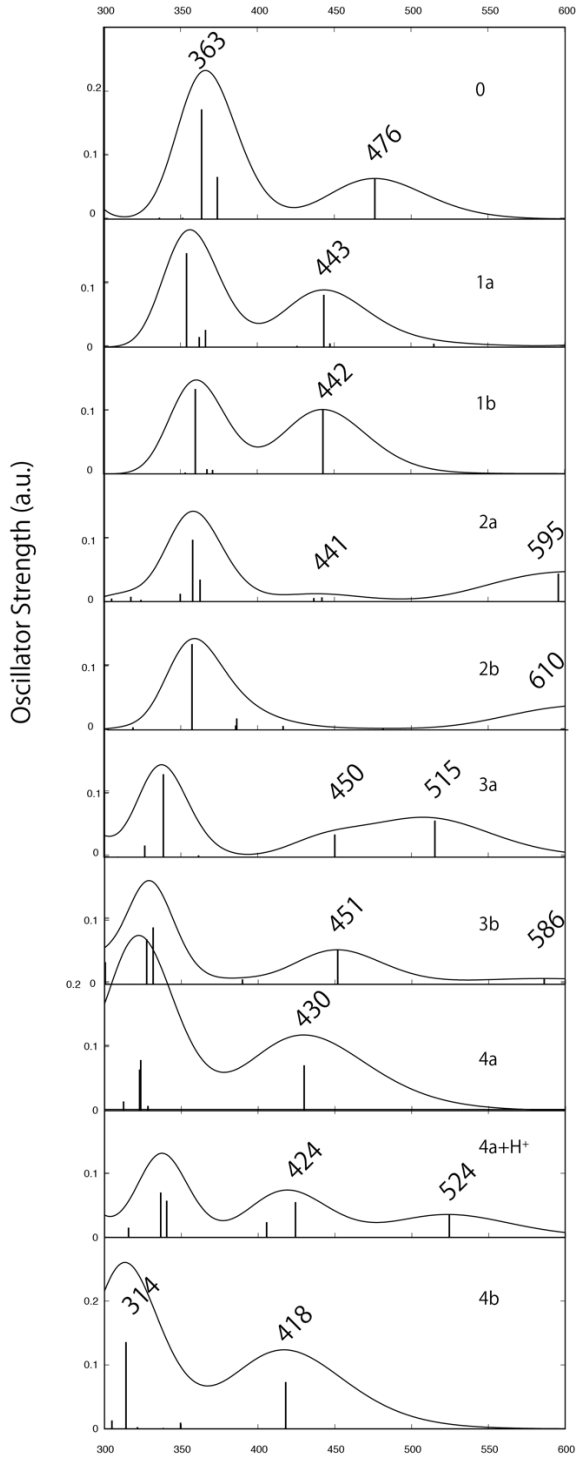


Figure S3. UV/Vis spectra calculated in intermediate states. TDDFT(B3LYP/6-311++G**) method was adapted. Spectra for reduced states (5, no-CPG) are shown in Figure S3.

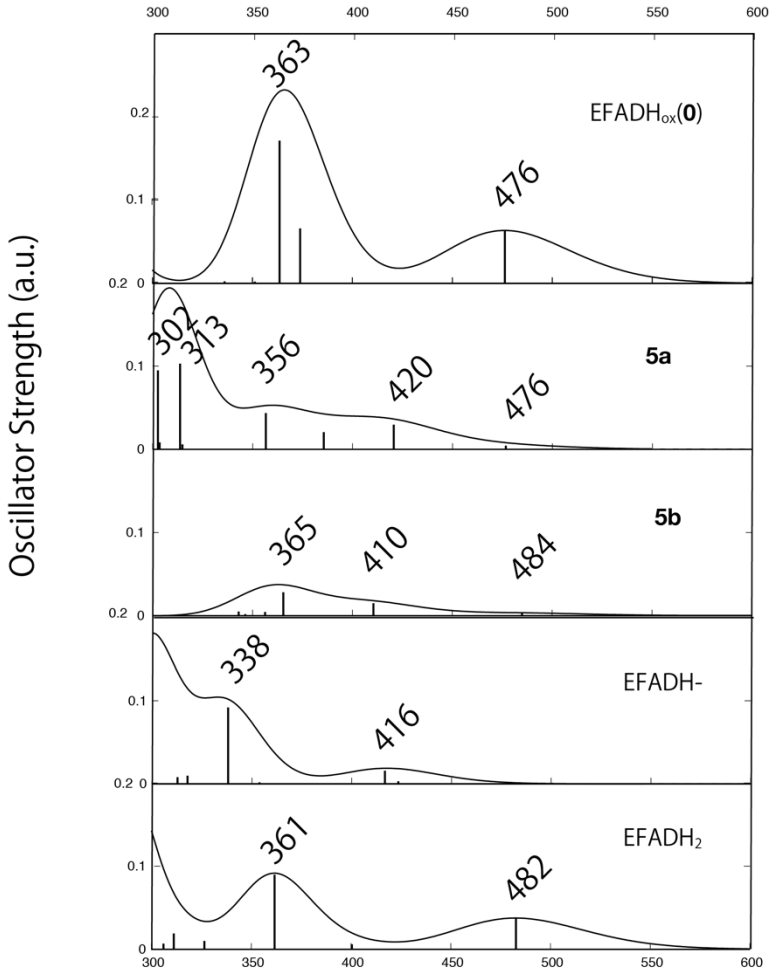


Figure S4. UV/Vis spectra calculated in other states (5, no-CPG). TDDFT(B3LYP/6-311++G**) method was adapted. Spectra for oxidized states are shown in Figure S2.

S1. Validation and benchmark of the QM subsystem

To assess the validity of the size of the QM region better suited to our scopes, five different QM regions, labeled hereafter as QM regions 0-IV, were considered differing in their extension and, hence, in the number of atoms included in the QM subsystem. For these different QM-region sizes we computed the relative energies of the six more relevant states: **1a**, **1b**, **1d**, **2a**, **3a**, and **4a**. All the relative energies and the structures in the QM regions are shown in Figure S5 and Table S3. The minimal size is the QM region 0, containing the FAD flavin ring, the CPG substrate and only one water molecule (W1). The largest QM region, corresponding to the one labeled as IV, contains all the surrounding amino acid residues Lys347, Arg52, Glu57, Ile245 and Met245, plus one water molecule labeled as W2. The relative energies computed by using the QM region IV can be qualitatively reproduced by the minimal QM model 0 within an energy error bar of 5 kcal mol^{-1}. Among the key states considered, the relative energy of state **2a** is the most sensitive and, in this respect, the most stringent test. Indeed, the value ΔE(**2a**)=-3.90 kcal mol^{-1} obtained by using the QM region IV is substantially different from the values obtained using QM region II (ΔE(**2a**, II)=0.41 kcal mol^{-1}) and III (ΔE(**2a**, III)=-1.01 kcal mol^{-1}), in which crucial residues (Ile245 and Met245) and (Lys52 and Glu57) are not included in the QM subsystem.

The relative energies obtained by using the QM regions 0 and III are rather similar especially for states **1**, indicating that the inclusion of the side chains of Ile245 and Met245 does not affect significantly the outcome of the simulations and seems to add just additional computational burden. A comparison of the relative energies obtained by using the QM regions 0, I and IV allows us to conclude that the QM region I, which includes the side chain of Lys347, is particularly well suited to reproduces the relative energy of state **1d,** being the energetics numerically identical to the ones of the more extended QM region IV. Instead, the QM region II does not provide any improvement with respect to QM region I, despite the inclusion of the residues Arg52 and Glu57. Based on this analysis, we selected the QM region I in the present study to cope for both accuracy and the efficiency in terms of computational workload.

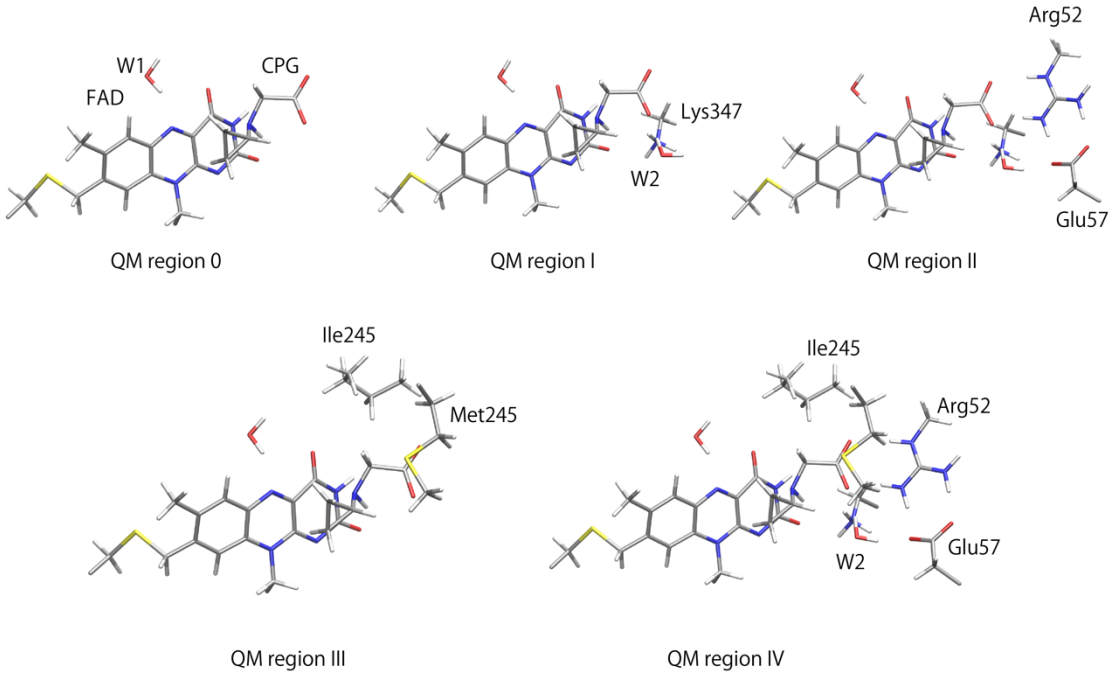


Figure S5. Molecular structures for the different QM regions in state **1a**. Results discussed in the main body are based on the QM region I. Water molecules accessing the CPG and prone to participate to the proton transfer process discussed in the text are labeled as W1 and W2.

Table S3. Relative QM/MM energies (ΔE/ kcal mol^{-1}) calculated using different QM regions.

	1a	1b	1d	2a	3a	4a
QM region 0	0	1.30	14.42	1.85	-10.34	-11.38
QM region I	0	2.00	9.90	0.32	-12.05	-12.74
QM region II	0	1.85	8.72	0.41	-11.85	-13.10
QM region III	0	1.04	14.91	-1.01	-13.12	-12.97
QM region IV	0	1.24	10.01	-3.90	-15.31	-15.33

Theoretical level applied for the QM regions were UB3LYP-D3//TZVP. Atoms in the QM regions 0-IV are shown in Figure S5. The model used in the main manuscript is QM region I.

38
state 0

C	9.878	-2.658	-1.144
S	8.907	-2.789	-2.679
H	9.273	-2.328	-0.300
H	10.619	-1.889	-1.350
C	2.339	-2.500	-1.212
N	0.694	-0.872	-2.760
C	-0.146	-0.074	-3.504
O	-1.160	0.432	-3.071
N	0.187	0.211	-4.857
C	1.271	-0.275	-5.546
C	2.116	-1.187	-4.724
O	1.540	0.060	-6.684
C	4.073	-2.362	-4.529
N	3.155	-1.722	-5.292
C	5.214	-2.903	-5.151
C	6.258	-3.426	-4.417
C	7.428	-4.044	-5.145
C	6.191	-3.313	-2.997
C	7.371	-3.664	-2.128
C	5.029	-2.861	-2.365
C	3.929	-2.433	-3.115
C	1.789	-1.346	-3.318
N	2.709	-2.037	-2.560
H	-0.401	0.911	-5.312
H	8.084	-3.270	-5.552
H	7.074	-4.645	-5.981
H	8.042	-4.672	-4.504
H	7.173	-3.358	-1.106
H	7.554	-4.740	-2.140
H	5.253	-2.859	-6.230
H	5.009	-2.813	-1.286
H	2.956	-3.349	-0.944
H	1.295	-2.785	-1.228
O	4.577	-0.857	-7.535
H	3.860	-1.079	-6.920
H	4.123	-0.620	-8.350
H_L	10.406	-3.592	-0.909
H_L	2.462	-1.694	-0.417

65
state 1a

C	9.877	-2.659	-1.144
S	8.905	-2.790	-2.677
H	9.271	-2.331	-0.299
H	10.617	-1.889	-1.348
C	2.333	-2.500	-1.215
N	0.704	-0.868	-2.767
C	-0.140	-0.061	-3.517
O	-1.145	0.439	-3.052
N	0.200	0.247	-4.847
C	1.252	-0.288	-5.555
C	2.096	-1.214	-4.743
O	1.555	0.080	-6.676
C	4.062	-2.377	-4.529
N	3.140	-1.732	-5.303
C	5.205	-2.909	-5.147
C	6.255	-3.426	-4.413
C	7.427	-4.043	-5.144
C	6.189	-3.315	-2.999
C	7.369	-3.668	-2.129
C	5.027	-2.863	-2.370
C	3.923	-2.441	-3.121
C	1.776	-1.364	-3.327
N	2.701	-2.047	-2.563
H	-0.429	0.888	-5.331
H	8.085	-3.271	-5.552
H	7.074	-4.644	-5.980
H	8.040	-4.675	-4.505
H	7.174	-3.357	-1.107
H	7.560	-4.741	-2.138
H	5.249	-2.863	-6.226
H	5.006	-2.813	-1.291
H	2.947	-3.352	-0.947
H	1.288	-2.783	-1.228
C	-3.858	0.161	-5.069
H	-4.212	-0.036	-6.079
H	-2.893	0.661	-5.117
N	-3.715	-1.160	-4.393
H	-4.629	-1.607	-4.201
H	-3.285	-1.822	-5.099
H	-3.211	-1.114	-3.496
N	-0.544	-2.370	-6.162
C	-1.064	-1.851	-7.426
C	-2.606	-1.823	-7.526
O	-3.219	-2.443	-6.577
O	-3.135	-1.215	-8.453
C	-0.598	-3.806	-6.092
H	-0.674	-2.454	-8.247
H	-0.676	-0.849	-7.562
H	-1.575	-4.268	-6.175
C	0.562	-4.524	-6.695
C	0.400	-4.459	-5.196
H	-1.120	-2.004	-5.410
H	0.364	-5.464	-7.188
H	1.332	-3.901	-7.131
H	1.068	-3.810	-4.648
H	0.077	-5.336	-4.663
O	-4.034	-5.179	-5.613
H	-3.744	-4.410	-6.125
H	-5.024	-5.059	-5.600
O	4.585	-0.855	-7.534
H	3.875	-1.076	-6.905
H	4.111	-0.619	-8.338
H_L	10.407	-3.593	-0.909
H_L	2.461	-1.695	-0.420
H_L	-4.566	0.779	-4.548

65
state 1b

C	9.875	-2.660	-1.146
S	8.906	-2.792	-2.681
H	9.267	-2.333	-0.302
H	10.614	-1.888	-1.348
C	2.333	-2.496	-1.220
N	0.696	-0.869	-2.775
C	-0.152	-0.065	-3.530
O	-1.158	0.430	-3.063
N	0.190	0.249	-4.856

C	1.253	-0.262	-5.559
C	2.106	-1.181	-4.739
O	1.587	0.120	-6.664
C	4.074	-2.339	-4.529
N	3.157	-1.681	-5.297
C	5.214	-2.874	-5.151
C	6.257	-3.410	-4.421
C	7.426	-4.027	-5.155
C	6.190	-3.309	-3.006
C	7.369	-3.673	-2.139
C	5.027	-2.862	-2.374
C	3.925	-2.426	-3.123
C	1.778	-1.349	-3.329
N	2.703	-2.037	-2.565
H	-0.458	0.864	-5.350
H	8.089	-3.259	-5.561
H	7.069	-4.624	-5.993
H	8.035	-4.667	-4.520
H	7.174	-3.371	-1.114
H	7.559	-4.746	-2.157
H	5.260	-2.813	-6.230
H	5.006	-2.822	-1.295
H	2.946	-3.349	-0.953
H	1.288	-2.778	-1.235
C	-3.857	0.168	-5.080
H	-4.211	-0.027	-6.091
H	-2.895	0.672	-5.130
N	-3.702	-1.155	-4.408
H	-4.611	-1.611	-4.214
H	-3.256	-1.803	-5.108
H	-3.194	-1.105	-3.513
N	-0.418	-2.331	-6.576
C	-1.129	-2.121	-7.845
C	-2.624	-1.891	-7.590
O	-3.098	-2.520	-6.565
O	-3.269	-1.161	-8.342
C	0.562	-3.375	-6.625
H	-1.057	-3.007	-8.490
H	-0.707	-1.282	-8.394
H	1.394	-3.170	-7.290
C	0.866	-4.053	-5.337
C	0.149	-4.819	-6.437
H	-1.147	-2.615	-5.923
H	1.899	-4.231	-5.068
H	0.263	-3.771	-4.488
H	-0.908	-5.013	-6.288
H	0.672	-5.599	-6.967
O	-4.022	-5.217	-5.607
H	-3.673	-4.448	-6.081
H	-5.006	-5.064	-5.613
O	4.588	-0.870	-7.550
H	3.879	-1.043	-6.906
H	4.115	-0.626	-8.352
H_L	10.405	-3.593	-0.909
H_L	2.461	-1.693	-0.422
H_L	-4.565	0.781	-4.553

65

state 1c

C	9.888	-2.657	-1.133
S	8.923	-2.779	-2.669
H	9.280	-2.332	-0.289
H	10.633	-1.890	-1.331
C	2.362	-2.507	-1.202
N	0.721	-0.878	-2.719
C	-0.124	-0.072	-3.449
O	-1.130	0.436	-2.992
N	0.180	0.206	-4.804
C	1.279	-0.241	-5.487
C	2.163	-1.112	-4.674
O	1.530	0.083	-6.638
C	4.145	-2.250	-4.491
N	3.243	-1.560	-5.237
C	5.278	-2.788	-5.125
C	6.297	-3.377	-4.405
C	7.447	-4.020	-5.147
C	6.221	-3.311	-2.987
C	7.400	-3.683	-2.130
C	5.059	-2.874	-2.349
C	3.968	-2.408	-3.093
C	1.814	-1.341	-3.288
N	2.737	-2.037	-2.538
H	-0.471	0.825	-5.289
H	8.112	-3.265	-5.575
H	7.067	-4.623	-5.970
H	8.061	-4.656	-4.513
H	7.208	-3.400	-1.101
H	7.595	-4.756	-2.171
H	5.324	-2.705	-6.203
H	5.033	-2.863	-1.268
H	2.988	-3.346	-0.925
H	1.321	-2.803	-1.225
C	-3.850	0.169	-5.067
H	-4.194	-0.029	-6.081
H	-2.890	0.675	-5.110
N	-3.695	-1.148	-4.391
H	-4.603	-1.603	-4.202
H	-3.203	-1.825	-5.062
H	-3.201	-1.087	-3.490
N	-0.662	-3.853	-7.850
C	-1.203	-2.528	-8.102
C	-2.507	-2.200	-7.340
O	-2.630	-2.743	-6.187
O	-3.337	-1.433	-7.864
C	0.203	-4.134	-6.764
H	-1.398	-2.426	-9.171
H	-0.459	-1.763	-7.857
H	0.279	-5.202	-6.592
C	1.434	-3.320	-6.548
C	0.339	-3.256	-5.510
H	-1.389	-4.551	-7.942
H	2.364	-3.814	-6.294
H	1.584	-2.463	-7.193
H	-0.331	-2.409	-5.492
H	0.490	-3.755	-4.562
O	-4.048	-5.319	-5.629
H	-3.560	-4.501	-5.812
H	-5.008	-5.075	-5.649
O	4.583	-0.878	-7.555
H	3.919	-1.005	-6.853

H	4.062	-0.762	-8.356
C_MM	10.626	-3.978	-0.808
C_MM	2.515	-1.362	-0.091
C_MM	-4.856	1.031	-4.333

65

state 1d

C	9.889	-2.646	-1.132
S	8.906	-2.761	-2.660
H	9.293	-2.313	-0.282
H	10.635	-1.882	-1.340
C	2.318	-2.463	-1.213
N	0.677	-0.857	-2.754
C	-0.170	-0.065	-3.491
O	-1.163	0.471	-3.038
N	0.125	0.173	-4.857
C	1.223	-0.287	-5.532
C	2.091	-1.162	-4.718
O	1.474	0.031	-6.690
C	4.075	-2.306	-4.518
N	3.158	-1.659	-5.283
C	5.219	-2.842	-5.135
C	6.258	-3.380	-4.400
C	7.423	-4.007	-5.131
C	6.190	-3.271	-2.984
C	7.366	-3.638	-2.115
C	5.023	-2.822	-2.356
C	3.922	-2.393	-3.108
C	1.763	-1.337	-3.321
N	2.691	-2.014	-2.558
H	-0.511	0.803	-5.346
H	8.089	-3.245	-5.544
H	7.058	-4.606	-5.964
H	8.032	-4.644	-4.493
H	7.172	-3.343	-1.089
H	7.551	-4.713	-2.140
H	5.269	-2.791	-6.214
H	4.998	-2.776	-1.276
H	2.963	-3.281	-0.917
H	1.286	-2.786	-1.237
C	-3.854	0.193	-5.071
H	-4.194	-0.006	-6.086
H	-2.892	0.696	-5.108
N	-3.698	-1.128	-4.397
H	-4.602	-1.596	-4.217
H	-3.205	-1.775	-5.075
H	-3.203	-1.071	-3.495
N	-0.193	-2.376	-7.883
C	-1.470	-2.014	-8.442
C	-2.678	-1.883	-7.493
O	-2.685	-2.568	-6.421
O	-3.586	-1.118	-7.878
C	-0.109	-3.585	-7.158
H	-1.736	-2.753	-9.195
H	-1.383	-1.085	-8.995
H	-0.663	-4.387	-7.635
C	1.161	-3.935	-6.449
C	-0.061	-3.630	-5.632
H	0.362	-1.610	-7.533
H	1.434	-4.973	-6.522
H	1.983	-3.232	-6.514
H	-0.154	-2.669	-5.144
H	-0.555	-4.450	-5.131
O	-4.108	-5.359	-5.617
H	-3.647	-4.593	-5.987
H	-5.063	-5.097	-5.599
O	4.556	-0.791	-7.509
H	3.886	-1.027	-6.843
H	4.041	-0.611	-8.302
C_MM	10.629	-3.968	-0.805
C_MM	2.435	-1.295	-0.119
C_MM	-4.862	1.061	-4.349

65

state 2a

C	9.896	-2.637	-1.116
S	8.903	-2.733	-2.637
H	9.306	-2.307	-0.261
H	10.645	-1.876	-1.320
C	2.309	-2.421	-1.234
N	0.680	-0.797	-2.750
C	-0.173	-0.034	-3.484
O	-1.195	0.481	-3.061
N	0.160	0.267	-4.841
C	1.118	-0.356	-5.567
C	1.852	-1.488	-4.848
O	1.323	-0.056	-6.746
C	4.073	-2.205	-4.562
N	3.178	-1.550	-5.340
C	5.253	-2.728	-5.143
C	6.275	-3.288	-4.401
C	7.429	-3.939	-5.137
C	6.189	-3.249	-2.989
C	7.356	-3.629	-2.117
C	4.999	-2.818	-2.394
C	3.910	-2.390	-3.164
C	1.726	-1.354	-3.335
N	2.664	-1.971	-2.586
H	-0.455	0.934	-5.309
H	8.115	-3.194	-5.549
H	7.051	-4.527	-5.973
H	8.022	-4.596	-4.502
H	7.157	-3.341	-1.088
H	7.571	-4.698	-2.148
H	5.334	-2.674	-6.220
H	4.947	-2.797	-1.314
H	2.979	-3.220	-0.943
H	1.287	-2.780	-1.248
C	-3.843	0.212	-5.078
H	-4.181	0.002	-6.089
H	-2.886	0.724	-5.112
N	-3.665	-1.104	-4.393
H	-4.557	-1.606	-4.240
H	-3.087	-1.722	-5.007
H	-3.203	-1.017	-3.472
N	-0.115	-2.137	-8.038
C	-1.457	-1.939	-8.558
C	-2.515	-1.932	-7.420
O	-2.205	-2.489	-6.332
O	-3.582	-1.375	-7.724

C	0.213	-3.238	-7.454
H	-1.698	-2.747	-9.239
H	-1.530	-1.020	-9.123
H	-0.469	-4.072	-7.593
C	1.379	-3.366	-6.569
C	1.026	-2.832	-5.155
H	0.476	-1.315	-7.867
H	1.647	-4.417	-6.512
H	2.253	-2.801	-6.923
H	-0.048	-2.674	-5.035
H	1.345	-3.565	-4.418
O	-4.172	-5.425	-5.620
H	-3.666	-4.650	-5.887
H	-5.120	-5.127	-5.599
O	4.527	-0.724	-7.497
H	3.929	-0.935	-6.728
H	3.933	-0.391	-8.176
C_MM	10.632	-3.964	-0.795
C_MM	2.394	-1.259	-0.132
C_MM	-4.862	1.075	-4.362

65

state 2b

C	9.894	-2.651	-1.119
S	8.909	-2.749	-2.643
H	9.299	-2.327	-0.265
H	10.643	-1.889	-1.318
C	2.347	-2.488	-1.212
N	0.707	-0.834	-2.708
C	-0.136	-0.049	-3.435
O	-1.172	0.442	-3.011
N	0.220	0.311	-4.766
C	1.228	-0.255	-5.492
C	1.886	-1.463	-4.812
O	1.510	0.122	-6.620
C	4.075	-2.293	-4.548
N	3.178	-1.651	-5.330
C	5.245	-2.828	-5.136
C	6.277	-3.371	-4.396
C	7.439	-4.005	-5.130
C	6.205	-3.298	-2.983
C	7.378	-3.657	-2.112
C	5.023	-2.861	-2.381
C	3.929	-2.445	-3.147
C	1.759	-1.383	-3.296
N	2.690	-2.024	-2.564
H	-0.373	1.010	-5.214
H	8.112	-3.249	-5.543
H	7.071	-4.602	-5.964
H	8.044	-4.648	-4.494
H	7.177	-3.360	-1.087
H	7.597	-4.725	-2.134
H	5.310	-2.794	-6.215
H	4.983	-2.821	-1.300
H	2.988	-3.321	-0.955
H	1.309	-2.793	-1.210
C	-3.844	0.169	-5.069
H	-4.193	-0.032	-6.080
H	-2.883	0.675	-5.109
N	-3.678	-1.147	-4.385
H	-4.581	-1.615	-4.192
H	-3.194	-1.793	-5.043
H	-3.175	-1.075	-3.485
N	-0.824	-3.612	-7.841
C	-1.239	-2.265	-8.228
C	-2.623	-1.959	-7.587
O	-2.896	-2.629	-6.538
O	-3.317	-1.104	-8.143
C	0.196	-3.985	-7.136
H	-1.309	-2.209	-9.314
H	-0.505	-1.533	-7.892
H	0.205	-5.040	-6.878
C	1.253	-3.094	-6.654
C	0.900	-2.687	-5.212
H	-1.507	-4.323	-8.081
H	2.220	-3.596	-6.658
H	1.371	-2.213	-7.284
H	-0.149	-2.387	-5.126
H	1.078	-3.510	-4.519
O	-4.054	-5.265	-5.638
H	-3.656	-4.441	-5.954
H	-5.031	-5.073	-5.630
O	4.546	-0.806	-7.495
H	3.954	-1.033	-6.731
H	3.941	-0.468	-8.162
C_MM	10.628	-3.978	-0.807
C_MM	2.512	-1.356	-0.093
C_MM	-4.852	1.029	-4.334

65

state 2c

C	9.913	-2.637	-1.102
S	8.923	-2.720	-2.619
H	9.326	-2.310	-0.243
H	10.667	-1.882	-1.302
C	2.345	-2.466	-1.215
N	0.690	-0.922	-2.775
C	-0.137	-0.138	-3.493
O	-1.137	0.432	-3.074
N	0.185	0.112	-4.870
C	1.108	-0.545	-5.606
C	1.963	-1.584	-4.872
O	1.225	-0.330	-6.816
C	4.214	-2.005	-4.471
N	3.323	-1.277	-5.197
C	5.403	-2.478	-5.075
C	6.365	-3.175	-4.373
C	7.471	-3.868	-5.142
C	6.240	-3.256	-2.963
C	7.409	-3.662	-2.109
C	5.042	-2.886	-2.360
C	3.978	-2.374	-3.122
C	1.748	-1.486	-3.360
N	2.700	-2.045	-2.578
H	-0.421	0.782	-5.343
H	8.164	-3.156	-5.595
H	7.034	-4.456	-5.950
H	8.062	-4.542	-4.523
H	7.212	-3.404	-1.073

H	7.632	-4.727	-2.178
H	5.498	-2.343	-6.145
H	4.964	-2.970	-1.284
H	3.011	-3.266	-0.914
H	1.323	-2.818	-1.222
C	-3.848	0.198	-5.067
H	-4.190	-0.022	-6.077
H	-2.891	0.710	-5.108
N	-3.671	-1.105	-4.362
H	-4.565	-1.596	-4.184
H	-3.141	-1.737	-4.996
H	-3.181	-1.010	-3.456
N	-0.234	-2.591	-7.608
C	-1.343	-2.142	-8.436
C	-2.608	-1.954	-7.545
O	-2.610	-2.553	-6.424
O	-3.495	-1.243	-8.018
C	-0.424	-3.552	-6.768
H	-1.564	-2.840	-9.233
H	-1.087	-1.198	-8.894
H	-1.190	-4.277	-7.007
C	1.699	-3.048	-5.413
C	0.292	-3.658	-5.478
H	0.490	-1.884	-7.426
H	2.304	-3.680	-4.764
H	2.182	-3.056	-6.394
H	-0.391	-3.128	-4.799
H	0.274	-4.695	-5.139
O	-4.129	-5.329	-5.638
H	-3.698	-4.517	-5.920
H	-5.098	-5.097	-5.606
O	4.522	-0.714	-7.500
H	3.956	-0.854	-6.688
H	3.897	-0.644	-8.226
C_MM	10.638	-3.969	-0.796
C_MM	2.440	-1.297	-0.121
C_MM	-4.864	1.063	-4.354

65

state 3a

C	9.899	-2.650	-1.122
S	8.923	-2.753	-2.650
H	9.298	-2.326	-0.272
H	10.649	-1.888	-1.317
C	2.369	-2.495	-1.205
N	0.747	-0.822	-2.674
C	-0.124	-0.042	-3.397
O	-1.145	0.435	-2.952
N	0.210	0.312	-4.735
C	1.260	-0.207	-5.415
C	1.864	-1.442	-4.775
O	1.629	0.241	-6.497
C	4.123	-2.304	-4.518
N	3.202	-1.600	-5.248
C	5.249	-2.858	-5.127
C	6.299	-3.394	-4.390
C	7.454	-4.030	-5.133
C	6.234	-3.310	-2.988
C	7.406	-3.676	-2.121
C	5.059	-2.857	-2.374
C	3.970	-2.420	-3.126
C	1.791	-1.350	-3.268
N	2.722	-2.016	-2.545
H	-0.379	1.019	-5.177
H	8.115	-3.273	-5.567
H	7.081	-4.645	-5.952
H	8.075	-4.655	-4.494
H	7.206	-3.387	-1.093
H	7.624	-4.744	-2.152
H	5.306	-2.837	-6.208
H	5.023	-2.827	-1.293
H	3.014	-3.324	-0.940
H	1.335	-2.812	-1.211
C	-3.841	0.178	-5.067
H	-4.181	-0.005	-6.083
H	-2.881	0.686	-5.098
N	-3.678	-1.156	-4.418
H	-4.577	-1.644	-4.268
H	-3.122	-1.768	-5.088
H	-3.213	-1.109	-3.499
N	-0.116	-1.900	-7.896
C	-1.432	-1.914	-8.508
C	-2.554	-1.883	-7.465
O	-2.334	-2.443	-6.344
O	-3.584	-1.263	-7.789
C	0.455	-3.093	-7.545
H	-1.523	-2.815	-9.109
H	-1.577	-1.071	-9.180
H	0.338	-3.845	-8.314
C	0.884	-2.680	-5.113
C	1.090	-3.401	-6.398
H	-0.024	-1.165	-7.213
H	-0.152	-2.330	-5.059
H	1.037	-3.391	-4.303
H	1.613	-4.346	-6.369
H	3.334	-1.576	-6.257
O	-4.052	-5.273	-5.593
H	-3.581	-4.506	-5.941
H	-5.021	-5.048	-5.629
O	3.668	-1.020	-7.963
H	2.901	-0.455	-7.787
H	3.291	-1.803	-8.389
C_MM	10.630	-3.978	-0.808
C_MM	2.517	-1.358	-0.088
C_MM	-4.855	1.028	-4.331

65

state 3b

C	9.907	-2.649	-1.118
S	8.935	-2.748	-2.647
H	9.306	-2.323	-0.269
H	10.659	-1.890	-1.312
C	2.398	-2.499	-1.193
N	0.785	-0.809	-2.651
C	-0.112	-0.070	-3.384
O	-1.120	0.427	-2.927
N	0.172	0.229	-4.746
C	1.257	-0.226	-5.411
C	1.943	-1.417	-4.745
O	1.640	0.264	-6.468

C	4.193	-2.230	-4.487
N	3.304	-1.446	-5.189
C	5.305	-2.792	-5.111
C	6.333	-3.383	-4.386
C	7.476	-4.028	-5.138
C	6.260	-3.329	-2.982
C	7.435	-3.696	-2.122
C	5.088	-2.884	-2.359
C	4.011	-2.410	-3.106
C	1.835	-1.337	-3.237
N	2.763	-2.006	-2.523
H	-0.429	0.923	-5.192
H	8.135	-3.276	-5.581
H	7.088	-4.642	-5.950
H	8.100	-4.654	-4.505
H	7.233	-3.420	-1.091
H	7.662	-4.761	-2.167
H	5.360	-2.750	-6.192
H	5.049	-2.886	-1.279
H	3.051	-3.318	-0.920
H	1.367	-2.828	-1.214
C	-3.840	0.174	-5.077
H	-4.181	-0.007	-6.095
H	-2.881	0.682	-5.112
N	-3.669	-1.162	-4.435
H	-4.569	-1.645	-4.278
H	-3.122	-1.795	-5.104
H	-3.204	-1.114	-3.516
N	-0.580	-3.537	-8.255
C	-1.319	-2.291	-8.415
C	-2.481	-2.083	-7.414
O	-2.395	-2.642	-6.273
O	-3.419	-1.355	-7.801
C	0.107	-3.746	-7.086
H	-1.724	-2.245	-9.419
H	-0.644	-1.438	-8.328
H	-0.077	-4.689	-6.572
C	0.903	-2.809	-6.562
C	1.131	-2.706	-5.094
H	-1.122	-4.329	-8.566
H	3.445	-1.414	-6.196
H	1.045	-1.912	-7.148
H	0.159	-2.634	-4.596
H	1.659	-3.553	-4.643
O	-4.045	-5.303	-5.610
H	-3.559	-4.522	-5.908
H	-5.006	-5.056	-5.630
O	3.713	-1.004	-7.947
H	2.944	-0.435	-7.800
H	3.350	-1.821	-8.319
C_MM	10.632	-3.978	-0.804
C_MM	2.519	-1.357	-0.082
C_MM	-4.851	1.024	-4.330

65
state 4a

C	9.895	-2.653	-1.122
S	8.912	-2.762	-2.645
H	9.299	-2.327	-0.270
H	10.643	-1.891	-1.324
C	2.355	-2.475	-1.231
N	0.725	-0.830	-2.750
C	-0.183	-0.110	-3.503
O	-1.160	0.432	-3.030
N	0.072	0.112	-4.879
C	1.187	-0.324	-5.525
C	1.881	-1.503	-4.843
O	1.607	0.212	-6.537
C	4.163	-2.225	-4.522
N	3.259	-1.478	-5.242
C	5.297	-2.761	-5.129
C	6.318	-3.351	-4.394
C	7.464	-4.003	-5.137
C	6.227	-3.304	-2.991
C	7.391	-3.679	-2.115
C	5.044	-2.863	-2.383
C	3.970	-2.393	-3.140
C	1.769	-1.368	-3.323
N	2.717	-1.989	-2.571
H	-0.512	0.812	-5.338
H	8.136	-3.259	-5.574
H	7.077	-4.614	-5.953
H	8.075	-4.638	-4.499
H	7.186	-3.385	-1.091
H	7.603	-4.748	-2.139
H	5.369	-2.713	-6.209
H	4.993	-2.863	-1.303
H	2.987	-3.317	-0.974
H	1.318	-2.782	-1.243
C	-3.846	0.178	-5.074
H	-4.190	-0.011	-6.088
H	-2.890	0.691	-5.112
N	-3.671	-1.152	-4.420
H	-4.567	-1.647	-4.277
H	-3.094	-1.766	-5.071
H	-3.219	-1.090	-3.495
N	-0.029	-2.095	-7.787
C	-1.318	-1.982	-8.437
C	-2.458	-1.935	-7.399
O	-2.267	-2.499	-6.275
O	-3.502	-1.357	-7.760
C	0.294	-3.270	-7.456
H	-1.528	-2.833	-9.089
H	-1.399	-1.093	-9.051
H	-0.294	-4.143	-7.774
C	1.136	-2.868	-5.124
C	1.416	-3.526	-6.487
H	2.376	-3.210	-6.900
H	0.059	-2.726	-5.008
H	1.471	-3.542	-4.338
H	1.482	-4.605	-6.340
H	3.443	-1.384	-6.240
O	-4.046	-5.284	-5.606
H	-3.574	-4.508	-5.932
H	-5.011	-5.055	-5.632
O	3.621	-0.979	-7.989
H	2.804	-0.481	-7.819
H	3.333	-1.755	-8.487
C_MM	10.629	-3.978	-0.807
C_MM	2.513	-1.358	-0.093

C_MM	-4.857	1.027	-4.333

65
state 4b

C	9.902	-2.651	-1.118
S	8.924	-2.754	-2.642
H	9.305	-2.325	-0.266
H	10.653	-1.891	-1.316
C	2.372	-2.481	-1.215
N	0.753	-0.812	-2.707
C	-0.128	-0.057	-3.451
O	-1.131	0.448	-2.996
N	0.180	0.241	-4.802
C	1.192	-0.310	-5.506
C	1.928	-1.444	-4.795
O	1.491	0.067	-6.636
C	4.199	-2.172	-4.492
N	3.309	-1.379	-5.189
C	5.320	-2.719	-5.112
C	6.332	-3.338	-4.385
C	7.469	-3.994	-5.136
C	6.243	-3.305	-2.982
C	7.410	-3.682	-2.114
C	5.063	-2.867	-2.367
C	3.994	-2.381	-3.118
C	1.801	-1.343	-3.283
N	2.739	-1.988	-2.547
H	-0.472	0.857	-5.285
H	8.142	-3.255	-5.579
H	7.072	-4.603	-5.949
H	8.081	-4.634	-4.503
H	7.208	-3.396	-1.086
H	7.626	-4.750	-2.149
H	5.400	-2.644	-6.190
H	5.011	-2.881	-1.287
H	3.011	-3.315	-0.952
H	1.337	-2.795	-1.234
C	-3.842	0.182	-5.057
H	-4.176	-0.031	-6.069
H	-2.889	0.702	-5.101
N	-3.647	-1.124	-4.376
H	-4.498	-1.707	-4.349
H	-2.872	-1.616	-4.929
H	-3.315	-1.031	-3.405
N	-0.715	-3.986	-7.548
C	-1.042	-2.647	-8.020
C	-2.079	-2.055	-7.044
O	-1.651	-1.896	-5.859
O	-3.223	-1.780	-7.456
C	0.367	-4.226	-6.941
H	-1.489	-2.723	-9.008
H	-0.195	-1.951	-8.071
H	0.503	-5.255	-6.591
C	1.466	-3.260	-6.575
C	1.216	-2.794	-5.135
H	2.446	-3.737	-6.671
H	3.481	-1.308	-6.188
H	1.455	-2.409	-7.254
H	0.143	-2.666	-4.992
H	1.575	-3.543	-4.428
O	-4.070	-5.334	-5.580
H	-3.674	-4.942	-6.365
H	-5.034	-5.090	-5.617
O	3.804	-0.989	-7.949
H	2.963	-0.510	-7.881
H	3.574	-1.837	-8.352
C_MM	10.631	-3.979	-0.805
C_MM	2.516	-1.356	-0.089
C_MM	-4.863	1.032	-4.332

65
state 5a

C	9.910	-2.643	-1.111
S	8.930	-2.726	-2.634
H	9.315	-2.319	-0.257
H	10.666	-1.887	-1.303
C	2.351	-2.483	-1.242
N	0.727	-0.798	-2.732
C	-0.156	-0.047	-3.453
O	-1.182	0.457	-2.999
N	0.125	0.175	-4.809
C	1.178	-0.390	-5.496
C	2.037	-1.193	-4.737
O	1.236	-0.198	-6.768
C	4.107	-2.393	-4.549
N	3.083	-1.902	-5.338
C	5.246	-2.932	-5.135
C	6.313	-3.420	-4.381
C	7.476	-4.058	-5.110
C	6.247	-3.277	-2.989
C	7.407	-3.636	-2.105
C	5.076	-2.776	-2.390
C	3.976	-2.388	-3.146
C	1.803	-1.303	-3.336
N	2.717	-2.005	-2.573
H	-0.504	0.790	-5.319
H	8.128	-3.302	-5.557
H	7.114	-4.695	-5.917
H	8.105	-4.660	-4.458
H	7.199	-3.340	-1.081
H	7.619	-4.705	-2.127
H	5.291	-2.983	-6.215
H	5.043	-2.701	-1.312
H	2.981	-3.328	-0.983
H	1.311	-2.783	-1.247
C	-3.835	0.180	-5.063
H	-4.178	-0.016	-6.075
H	-2.879	0.693	-5.088
N	-3.654	-1.145	-4.393
H	-4.551	-1.629	-4.206
H	-3.140	-1.772	-5.047
H	-3.154	-1.068	-3.490
N	-0.276	-2.307	-7.921
C	-1.491	-1.945	-8.616
C	-2.656	-1.844	-7.594
O	-2.571	-2.561	-6.557
O	-3.561	-1.065	-7.919
C	-0.074	-3.538	-7.567
H	-1.730	-2.713	-9.340
H	-1.400	-1.013	-9.152

H	-0.569	-4.305	-8.157
C	0.362	-3.276	-5.236
C	0.662	-3.893	-6.394
H	0.250	-1.545	-7.447
H	-0.441	-2.554	-5.192
H	0.836	-3.584	-4.321
H	1.307	-4.757	-6.443
H	3.340	-1.631	-6.283
O	-4.063	-5.286	-5.604
H	-3.620	-4.546	-6.035
H	-5.031	-5.058	-5.612
O	3.604	-0.870	-7.931
H	2.742	-0.483	-7.659
H	3.359	-1.642	-8.456
C_MM	10.632	-3.978	-0.805
C_MM	2.515	-1.364	-0.099
C_MM	-4.855	1.026	-4.330

65

State 5b

C	9.906	-2.645	-1.114
S	8.918	-2.734	-2.633
H	9.315	-2.316	-0.259
H	10.661	-1.889	-1.314
C	2.329	-2.479	-1.240
N	0.703	-0.763	-2.722
C	-0.164	-0.003	-3.449
O	-1.225	0.457	-3.018
N	0.169	0.292	-4.778
C	1.233	-0.256	-5.465
C	2.061	-1.090	-4.700
O	1.353	-0.012	-6.713
C	4.097	-2.353	-4.533
N	3.068	-1.857	-5.320
C	5.232	-2.895	-5.124
C	6.295	-3.397	-4.373
C	7.452	-4.041	-5.105
C	6.227	-3.262	-2.980
C	7.388	-3.629	-2.097
C	5.057	-2.763	-2.378
C	3.957	-2.363	-3.132
C	1.785	-1.262	-3.325
N	2.690	-2.001	-2.568
H	-0.468	0.899	-5.289
H	8.108	-3.291	-5.555
H	7.082	-4.675	-5.912
H	8.078	-4.650	-4.457
H	7.184	-3.327	-1.074
H	7.592	-4.700	-2.115
H	5.276	-2.938	-6.205
H	5.022	-2.702	-1.299
H	2.950	-3.331	-0.985
H	1.285	-2.764	-1.239
C	-3.839	0.182	-5.060
H	-4.195	-0.043	-6.062
H	-2.889	0.706	-5.112
N	-3.632	-1.115	-4.355
H	-4.515	-1.624	-4.179
H	-3.062	-1.736	-4.967
H	-3.151	-0.994	-3.446
N	-0.713	-3.276	-8.360
C	-1.165	-1.896	-8.271
C	-2.470	-1.908	-7.399
O	-2.385	-2.567	-6.327
O	-3.439	-1.287	-7.858
C	-0.178	-3.964	-7.391
H	-1.390	-1.538	-9.270
H	-0.409	-1.262	-7.804
H	-0.290	-5.042	-7.451
C	0.574	-3.379	-6.342
C	0.861	-4.054	-5.224
H	-1.189	-3.814	-9.073
H	3.358	-1.543	-6.245
H	0.919	-2.367	-6.480
H	1.452	-3.614	-4.438
H	0.459	-5.045	-5.048
O	-4.055	-5.284	-5.657
H	-3.594	-4.451	-5.809
H	-5.024	-5.061	-5.650
O	3.615	-0.882	-7.932
H	2.769	-0.460	-7.656
H	3.344	-1.671	-8.415
C_MM	10.630	-3.978	-0.804
C_MM	2.513	-1.364	-0.097
C_MM	-4.857	1.032	-4.330

65

state TS(1a, 1b)

C	9.887	-2.655	-1.134
S	8.909	-2.774	-2.663
H	9.290	-2.324	-0.285
H	10.633	-1.893	-1.342
C	2.342	-2.489	-1.217
N	0.685	-0.878	-2.766
C	-0.158	-0.073	-3.513
O	-1.172	0.419	-3.058
N	0.176	0.241	-4.846
C	1.278	-0.208	-5.528
C	2.165	-1.068	-4.692
O	1.579	0.149	-6.650
C	4.156	-2.185	-4.488
N	3.265	-1.484	-5.232
C	5.292	-2.721	-5.121
C	6.293	-3.335	-4.400
C	7.435	-3.993	-5.140
C	6.206	-3.281	-2.980
C	7.380	-3.665	-2.119
C	5.039	-2.850	-2.345
C	3.958	-2.366	-3.094
C	1.797	-1.315	-3.311
N	2.719	-2.012	-2.554
H	-0.482	0.843	-5.342
H	8.116	-3.250	-5.563
H	7.044	-4.584	-5.967
H	8.032	-4.646	-4.508
H	7.188	-3.377	-1.090
H	7.566	-4.739	-2.158
H	5.352	-2.612	-6.196
H	5.003	-2.857	-1.265
H	2.958	-3.339	-0.952

H	1.298	-2.774	-1.241
C	-3.859	0.176	-5.083
H	-4.221	-0.022	-6.091
H	-2.901	0.684	-5.138
N	-3.691	-1.147	-4.416
H	-4.594	-1.605	-4.203
H	-3.260	-1.776	-5.137
H	-3.159	-1.100	-3.533
N	-0.564	-2.423	-6.626
C	-1.152	-1.986	-7.893
C	-2.655	-1.717	-7.721
O	-3.196	-2.322	-6.712
O	-3.245	-0.996	-8.524
C	0.040	-3.727	-6.687
H	-1.078	-2.764	-8.662
H	-0.632	-1.124	-8.291
H	-0.163	-4.309	-7.582
C	1.364	-3.967	-6.025
C	0.091	-4.480	-5.410
H	-1.375	-2.534	-6.024
H	2.071	-4.607	-6.507
H	1.801	-3.122	-5.541
H	-0.224	-3.943	-4.533
H	-0.201	-5.508	-5.431
O	-4.029	-5.220	-5.610
H	-3.645	-4.499	-6.126
H	-5.005	-5.033	-5.624
O	4.604	-0.860	-7.565
H	3.902	-0.944	-6.896
H	4.138	-0.911	-8.404
C_MM	10.626	-3.976	-0.810
C_MM	2.513	-1.360	-0.093
C_MM	-4.858	1.033	-4.335

65

TS(1a,1d)

C	9.897	-2.645	-1.129
S	8.912	-2.756	-2.656
H	9.304	-2.309	-0.279
H	10.647	-1.887	-1.340
C	2.345	-2.486	-1.194
N	0.717	-0.880	-2.744
C	-0.126	-0.083	-3.489
O	-1.121	0.446	-3.038
N	0.190	0.182	-4.848
C	1.333	-0.217	-5.496
C	2.163	-1.153	-4.690
O	1.669	0.189	-6.591
C	4.112	-2.337	-4.495
N	3.210	-1.663	-5.254
C	5.251	-2.873	-5.120
C	6.286	-3.417	-4.388
C	7.452	-4.042	-5.121
C	6.213	-3.313	-2.970
C	7.396	-3.665	-2.109
C	5.050	-2.870	-2.336
C	3.952	-2.433	-3.087
C	1.814	-1.346	-3.296
N	2.728	-2.043	-2.539
H	-0.433	0.836	-5.324
H	8.099	-3.276	-5.555
H	7.088	-4.662	-5.939
H	8.079	-4.656	-4.479
H	7.200	-3.376	-1.081
H	7.598	-4.736	-2.144
H	5.301	-2.800	-6.198
H	5.028	-2.832	-1.256
H	2.988	-3.302	-0.889
H	1.314	-2.809	-1.223
C	-3.856	0.186	-5.085
H	-4.203	-0.003	-6.100
H	-2.894	0.689	-5.128
N	-3.697	-1.144	-4.427
H	-4.604	-1.599	-4.225
H	-3.251	-1.801	-5.135
H	-3.180	-1.105	-3.537
N	-0.284	-2.257	-7.429
C	-1.429	-2.049	-8.304
C	-2.759	-1.894	-7.562
O	-2.940	-2.611	-6.513
O	-3.558	-1.042	-7.988
C	-0.229	-3.578	-6.843
H	-1.483	-2.877	-9.008
H	-1.288	-1.159	-8.909
H	-0.949	-4.275	-7.252
C	1.116	-4.121	-6.452
C	0.110	-3.742	-5.392
H	-0.346	-1.573	-6.687
H	1.247	-5.178	-6.616
H	1.969	-3.486	-6.657
H	0.263	-2.838	-4.817
H	-0.338	-4.550	-4.838
O	-4.083	-5.339	-5.617
H	-3.630	-4.571	-5.993
H	-5.042	-5.087	-5.618
O	4.601	-0.869	-7.530
H	3.904	-1.025	-6.870
H	4.130	-0.882	-8.368
C_MM	10.629	-3.969	-0.804
C_MM	2.458	-1.313	-0.108
C_MM	-4.858	1.051	-4.348

65

TS(1a, 1c)

C	9.886	-2.657	-1.138
S	8.915	-2.779	-2.671
H	9.283	-2.327	-0.292
H	10.631	-1.892	-1.342
C	2.358	-2.508	-1.196
N	0.708	-0.895	-2.726
C	-0.144	-0.102	-3.466
O	-1.138	0.422	-3.007
N	0.151	0.157	-4.828
C	1.288	-0.228	-5.483
C	2.168	-1.108	-4.668
O	1.580	0.143	-6.607
C	4.141	-2.250	-4.486
N	3.248	-1.549	-5.226
C	5.276	-2.784	-5.124
C	6.291	-3.377	-4.405

C	7.441	-4.015	-5.149
C	6.214	-3.311	-2.984
C	7.394	-3.683	-2.129
C	5.051	-2.879	-2.343
C	3.962	-2.410	-3.087
C	1.811	-1.343	-3.284
N	2.732	-2.043	-2.537
H	-0.494	0.782	-5.313
H	8.105	-3.258	-5.572
H	7.060	-4.613	-5.975
H	8.053	-4.657	-4.519
H	7.202	-3.398	-1.099
H	7.589	-4.755	-2.169
H	5.329	-2.684	-6.200
H	5.026	-2.873	-1.262
H	2.984	-3.346	-0.918
H	1.318	-2.803	-1.217
C	-3.850	0.181	-5.077
H	-4.201	-0.021	-6.089
H	-2.895	0.695	-5.127
N	-3.678	-1.141	-4.411
H	-4.580	-1.613	-4.224
H	-3.225	-1.762	-5.132
H	-3.170	-1.093	-3.516
N	-1.131	-3.694	-7.213
C	-1.294	-2.489	-8.010
C	-2.688	-1.910	-7.739
O	-3.237	-2.333	-6.648
O	-3.187	-1.095	-8.514
C	0.143	-4.181	-6.800
H	-1.185	-2.670	-9.082
H	-0.589	-1.678	-7.760
H	0.352	-5.218	-7.063
C	1.319	-3.262	-6.718
C	0.658	-3.721	-5.444
H	-1.790	-3.658	-6.457
H	2.305	-3.643	-6.935
H	1.182	-2.245	-7.052
H	0.007	-3.029	-4.919
H	1.176	-4.415	-4.798
O	-4.055	-5.313	-5.620
H	-3.696	-4.693	-6.250
H	-5.025	-5.088	-5.607
O	4.585	-0.862	-7.550
H	3.898	-0.976	-6.870
H	4.095	-0.761	-8.372
C	10.625	-3.976	-0.811
C	2.516	-1.361	-0.089
C	-4.857	1.033	-4.335

65
TS(1b,1d)

C	9.895	-2.646	-1.129
S	8.911	-2.757	-2.655
H	9.303	-2.310	-0.278
H	10.645	-1.887	-1.340
C	2.342	-2.488	-1.195
N	0.705	-0.887	-2.747
C	-0.144	-0.096	-3.496
O	-1.130	0.441	-3.038
N	0.158	0.149	-4.860
C	1.306	-0.236	-5.506
C	2.153	-1.150	-4.691
O	1.636	0.168	-6.604
C	4.116	-2.312	-4.493
N	3.214	-1.639	-5.251
C	5.257	-2.845	-5.120
C	6.287	-3.400	-4.389
C	7.449	-4.031	-5.122
C	6.210	-3.304	-2.970
C	7.392	-3.661	-2.108
C	5.046	-2.865	-2.336
C	3.950	-2.422	-3.086
C	1.801	-1.352	-3.300
N	2.720	-2.045	-2.541
H	-0.471	0.794	-5.340
H	8.101	-3.269	-5.556
H	7.080	-4.648	-5.940
H	8.072	-4.650	-4.480
H	7.197	-3.372	-1.080
H	7.590	-4.733	-2.144
H	5.308	-2.764	-6.197
H	5.021	-2.835	-1.255
H	2.981	-3.309	-0.894
H	1.309	-2.807	-1.220
C	-3.857	0.192	-5.072
H	-4.197	-0.001	-6.088
H	-2.896	0.697	-5.110
N	-3.706	-1.131	-4.405
H	-4.613	-1.584	-4.206
H	-3.255	-1.784	-5.119
H	-3.192	-1.089	-3.513
N	-0.253	-2.331	-7.592
C	-1.461	-2.016	-8.341
C	-2.742	-1.856	-7.523
O	-2.856	-2.533	-6.442
O	-3.584	-1.045	-7.945
C	-0.085	-3.729	-7.307
H	-1.616	-2.794	-9.085
H	-1.337	-1.103	-8.915
H	-0.072	-4.316	-8.217
C	0.857	-4.151	-6.230
C	-0.623	-4.425	-6.080
H	-0.265	-1.811	-6.722
H	1.517	-4.956	-6.487
H	1.301	-3.386	-5.609
H	-1.168	-3.786	-5.406
H	-1.010	-5.433	-6.163
O	-4.074	-5.329	-5.619
H	-3.624	-4.575	-6.023
H	-5.034	-5.080	-5.615
O	4.603	-0.855	-7.530
H	3.899	-1.008	-6.877
H	4.151	-0.934	-8.376
C_MM	10.629	-3.970	-0.805
C_MM	2.464	-1.318	-0.107
C_MM	-4.864	1.055	-4.345

65
TS(1c,2b)

C	9.895	-2.652	-1.127
S	8.917	-2.758	-2.654
H	9.298	-2.323	-0.276
H	10.644	-1.891	-1.328
C	2.362	-2.498	-1.208
N	0.718	-0.870	-2.720
C	-0.131	-0.073	-3.447
O	-1.150	0.422	-2.995
N	0.187	0.235	-4.787
C	1.255	-0.262	-5.492
C	2.122	-1.172	-4.706
O	1.483	0.060	-6.652
C	4.144	-2.249	-4.502
N	3.246	-1.552	-5.261
C	5.282	-2.788	-5.122
C	6.302	-3.375	-4.395
C	7.454	-4.017	-5.136
C	6.224	-3.307	-2.982
C	7.401	-3.676	-2.120
C	5.056	-2.863	-2.355
C	3.970	-2.404	-3.107
C	1.806	-1.348	-3.296
N	2.730	-2.025	-2.544
H	-0.452	0.867	-5.268
H	8.112	-3.263	-5.575
H	7.074	-4.631	-5.952
H	8.074	-4.644	-4.499
H	7.204	-3.392	-1.091
H	7.611	-4.745	-2.160
H	5.344	-2.706	-6.199
H	5.024	-2.849	-1.275
H	2.995	-3.334	-0.936
H	1.324	-2.800	-1.223
C	-3.846	0.171	-5.071
H	-4.196	-0.037	-6.082
H	-2.889	0.684	-5.123
N	-3.673	-1.141	-4.384
H	-4.576	-1.600	-4.173
H	-3.210	-1.805	-5.055
H	-3.156	-1.068	-3.494
N	-0.804	-3.801	-7.738
C	-1.247	-2.475	-8.143
C	-2.605	-2.111	-7.496
O	-2.881	-2.720	-6.405
O	-3.305	-1.260	-8.059
C	0.233	-4.090	-6.939
H	-1.342	-2.421	-9.227
H	-0.517	-1.720	-7.848
H	0.310	-5.131	-6.651
C	1.307	-3.172	-6.606
C	0.501	-2.996	-5.354
H	-1.543	-4.490	-7.768
H	2.276	-3.631	-6.437
H	1.428	-2.293	-7.235
H	-0.428	-2.447	-5.379
H	0.683	-3.645	-4.514
O	-4.042	-5.315	-5.655
H	-3.582	-4.486	-5.857
H	-5.008	-5.084	-5.665
O	4.577	-0.838	-7.537
H	3.946	-0.985	-6.801
H	4.023	-0.666	-8.300
C_MM	10.628	-3.977	-0.808
C_MM	2.516	-1.360	-0.091
C_MM	-4.854	1.030	-4.335

65

TS(1d, 2a)

C	9.900	-2.641	-1.122
S	8.909	-2.744	-2.643
H	9.312	-2.305	-0.268
H	10.651	-1.884	-1.333
C	2.329	-2.456	-1.212
N	0.688	-0.864	-2.751
C	-0.152	-0.065	-3.480
O	-1.157	0.460	-3.035
N	0.163	0.211	-4.836
C	1.250	-0.263	-5.514
C	2.124	-1.138	-4.708
O	1.494	0.047	-6.681
C	4.135	-2.228	-4.499
N	3.244	-1.533	-5.263
C	5.280	-2.760	-5.114
C	6.295	-3.347	-4.383
C	7.447	-3.995	-5.121
C	6.209	-3.277	-2.969
C	7.384	-3.649	-2.103
C	5.037	-2.835	-2.347
C	3.949	-2.381	-3.102
C	1.780	-1.342	-3.320
N	2.709	-2.004	-2.551
H	-0.480	0.832	-5.325
H	8.109	-3.245	-5.560
H	7.065	-4.607	-5.937
H	8.062	-4.624	-4.482
H	7.189	-3.363	-1.075
H	7.585	-4.720	-2.142
H	5.349	-2.673	-6.190
H	4.999	-2.821	-1.266
H	2.981	-3.266	-0.907
H	1.302	-2.794	-1.240
C	-3.848	0.203	-5.072
H	-4.185	-0.001	-6.085
H	-2.890	0.714	-5.107
N	-3.679	-1.113	-4.393
H	-4.576	-1.597	-4.220
H	-3.143	-1.748	-5.053
H	-3.193	-1.042	-3.485
N	-0.129	-2.271	-7.955
C	-1.459	-2.015	-8.466
C	-2.588	-1.920	-7.426
O	-2.425	-2.500	-6.312
O	-3.593	-1.281	-7.792
C	0.213	-3.416	-7.330
H	-1.725	-2.795	-9.171
H	-1.461	-1.097	-9.043
H	-0.343	-4.307	-7.586
C	1.417	-3.463	-6.510
C	0.407	-3.255	-5.439
H	0.450	-1.461	-7.770

H	1.861	-4.447	-6.459
H	2.181	-2.703	-6.700
H	-0.207	-2.380	-5.377
H	0.153	-4.079	-4.786
O	-4.128	-5.394	-5.624
H	-3.617	-4.613	-5.860
H	-5.076	-5.104	-5.617
O	4.567	-0.795	-7.529
H	3.938	-0.948	-6.793
H	4.005	-0.666	-8.300
C_MM	10.632	-3.967	-0.800
C_MM	2.426	-1.287	-0.120
C_MM	-4.864	1.067	-4.354

65

TS(1d,2c)

C	9.900	-2.645	-1.121
S	8.921	-2.760	-2.646
H	9.303	-2.316	-0.270
H	10.647	-1.883	-1.323
C	2.340	-2.463	-1.222
N	0.687	-0.928	-2.775
C	-0.161	-0.130	-3.496
O	-1.135	0.436	-3.033
N	0.110	0.075	-4.873
C	1.225	-0.353	-5.542
C	2.156	-1.163	-4.731
O	1.402	-0.079	-6.731
C	4.204	-2.126	-4.484
N	3.359	-1.379	-5.227
C	5.338	-2.679	-5.105
C	6.326	-3.315	-4.383
C	7.463	-3.973	-5.134
C	6.229	-3.285	-2.971
C	7.396	-3.668	-2.107
C	5.052	-2.856	-2.349
C	3.980	-2.368	-3.101
C	1.800	-1.371	-3.339
N	2.730	-2.006	-2.555
H	-0.530	0.700	-5.363
H	8.140	-3.232	-5.567
H	7.059	-4.562	-5.957
H	8.065	-4.629	-4.508
H	7.201	-3.377	-1.079
H	7.598	-4.739	-2.142
H	5.409	-2.569	-6.180
H	4.999	-2.879	-1.269
H	2.981	-3.282	-0.919
H	1.311	-2.795	-1.253
C	-3.851	0.190	-5.073
H	-4.193	-0.009	-6.086
H	-2.891	0.696	-5.107
N	-3.690	-1.133	-4.395
H	-4.594	-1.610	-4.220
H	-3.182	-1.773	-5.041
H	-3.205	-1.069	-3.485
N	-0.365	-2.416	-7.745
C	-1.504	-2.034	-8.551
C	-2.725	-1.884	-7.610
O	-2.714	-2.608	-6.562
O	-3.587	-1.063	-7.939
C	-0.525	-3.492	-6.981
H	-1.704	-2.780	-9.309
H	-1.327	-1.100	-9.061
H	-0.963	-4.366	-7.450
C	1.413	-3.461	-5.822
C	-0.060	-3.512	-5.595
H	0.134	-1.628	-7.340
H	2.013	-4.312	-5.568
H	1.835	-2.835	-6.590
H	-0.474	-2.658	-5.035
H	-0.364	-4.429	-5.095
O	-4.109	-5.322	-5.615
H	-3.694	-4.533	-5.984
H	-5.081	-5.107	-5.601
O	4.570	-0.789	-7.551
H	3.975	-0.919	-6.777
H	3.974	-0.645	-8.291
H_L	10.420	-3.584	-0.891
H_L	2.411	-1.639	-0.441
H_L	-4.567	0.805	-4.560

65

TS(2a, 3a)

C	9.893	-2.642	-1.126
S	8.904	-2.739	-2.653
H	9.299	-2.312	-0.273
H	10.642	-1.882	-1.329
C	2.332	-2.446	-1.217
N	0.694	-0.794	-2.705
C	-0.159	-0.013	-3.431
O	-1.192	0.470	-3.007
N	0.200	0.339	-4.763
C	1.175	-0.274	-5.480
C	1.790	-1.485	-4.798
O	1.446	0.064	-6.629
C	4.004	-2.377	-4.587
N	3.033	-1.832	-5.412
C	5.170	-2.899	-5.165
C	6.237	-3.378	-4.416
C	7.412	-3.995	-5.144
C	6.185	-3.249	-3.012
C	7.352	-3.614	-2.130
C	5.010	-2.778	-2.417
C	3.899	-2.412	-3.181
C	1.729	-1.354	-3.299
N	2.666	-1.991	-2.573
H	-0.397	1.028	-5.220
H	8.068	-3.226	-5.562
H	7.063	-4.608	-5.973
H	8.030	-4.616	-4.498
H	7.147	-3.316	-1.105
H	7.551	-4.687	-2.148
H	5.233	-2.887	-6.243
H	4.978	-2.695	-1.339
H	3.009	-3.243	-0.937
H	1.311	-2.806	-1.217
C	-3.844	0.196	-5.082
H	-4.190	-0.009	-6.093
H	-2.887	0.708	-5.125

N	-3.662	-1.124	-4.407
H	-4.556	-1.620	-4.241
H	-3.106	-1.747	-5.049
H	-3.188	-1.046	-3.492
N	-0.068	-2.099	-7.893
C	-1.374	-1.986	-8.517
C	-2.512	-1.958	-7.464
O	-2.292	-2.516	-6.349
O	-3.548	-1.375	-7.823
C	0.399	-3.250	-7.468
H	-1.522	-2.835	-9.177
H	-1.450	-1.092	-9.125
H	0.023	-4.115	-8.008
C	1.264	-3.414	-6.354
C	0.769	-2.723	-5.093
H	0.328	-1.251	-7.494
H	1.503	-4.462	-6.210
H	2.420	-2.751	-6.291
H	-0.270	-2.400	-5.152
H	0.883	-3.413	-4.263
O	-4.129	-5.394	-5.617
H	-3.616	-4.622	-5.879
H	-5.078	-5.105	-5.616
O	4.527	-0.674	-7.376
H	3.909	-0.942	-6.658
H	3.972	-0.663	-8.161
C_MM	10.629	-3.966	-0.803
C_MM	2.432	-1.287	-0.118
C_MM	-4.857	1.058	-4.354

65

TS(2b, 3b)

C	9.889	-2.653	-1.133
S	8.912	-2.757	-2.664
H	9.287	-2.327	-0.284
H	10.637	-1.890	-1.329
C	2.372	-2.504	-1.184
N	0.735	-0.798	-2.636
C	-0.114	-0.009	-3.370
O	-1.171	0.432	-2.958
N	0.276	0.402	-4.671
C	1.307	-0.155	-5.371
C	1.830	-1.443	-4.725
O	1.704	0.282	-6.437
C	4.007	-2.440	-4.562
N	3.032	-1.881	-5.367
C	5.163	-2.970	-5.152
C	6.240	-3.440	-4.411
C	7.417	-4.042	-5.146
C	6.203	-3.301	-3.009
C	7.378	-3.652	-2.135
C	5.038	-2.825	-2.401
C	3.921	-2.460	-3.155
C	1.772	-1.357	-3.229
N	2.698	-2.034	-2.532
H	-0.303	1.116	-5.112
H	8.061	-3.263	-5.564
H	7.074	-4.657	-5.976
H	8.047	-4.656	-4.505
H	7.175	-3.351	-1.111
H	7.589	-4.722	-2.152
H	5.213	-2.968	-6.231
H	5.019	-2.735	-1.324
H	3.033	-3.320	-0.921
H	1.341	-2.833	-1.175
C	-3.835	0.174	-5.075
H	-4.185	-0.032	-6.085
H	-2.880	0.691	-5.126
N	-3.646	-1.144	-4.399
H	-4.542	-1.631	-4.219
H	-3.104	-1.785	-5.037
H	-3.166	-1.061	-3.488
N	-0.556	-3.713	-8.075
C	-1.256	-2.465	-8.381
C	-2.447	-2.208	-7.409
O	-2.367	-2.722	-6.253
O	-3.356	-1.487	-7.850
C	0.313	-3.858	-7.096
H	-1.621	-2.503	-9.400
H	-0.582	-1.615	-8.322
H	0.442	-4.872	-6.724
C	1.005	-2.775	-6.539
C	0.729	-2.544	-5.074
H	-1.019	-4.535	-8.433
H	2.340	-2.660	-6.290
H	0.832	-1.865	-7.105
H	-0.291	-2.212	-4.883
H	0.938	-3.433	-4.473
O	-4.038	-5.309	-5.650
H	-3.538	-4.497	-5.794
H	-4.998	-5.060	-5.656
O	4.557	-0.784	-7.393
H	3.949	-0.996	-6.652
H	3.960	-0.596	-8.123
C_MM	10.625	-3.976	-0.811
C_MM	2.517	-1.356	-0.084
C_MM	-4.849	1.026	-4.334

65

TS(3a, 5a)

C	9.909	-2.644	-1.114
S	8.925	-2.730	-2.636
H	9.317	-2.316	-0.260
H	10.664	-1.890	-1.312
C	2.367	-2.482	-1.229
N	0.734	-0.822	-2.711
C	-0.138	-0.044	-3.422
O	-1.166	0.435	-2.973
N	0.176	0.268	-4.765
C	1.239	-0.245	-5.448
C	2.002	-1.243	-4.740
O	1.442	0.088	-6.640
C	4.157	-2.290	-4.530
N	3.227	-1.614	-5.280
C	5.281	-2.853	-5.130
C	6.322	-3.400	-4.383
C	7.475	-4.047	-5.119
C	6.249	-3.300	-2.986
C	7.415	-3.663	-2.110
C	5.076	-2.821	-2.380

C	3.993	-2.383	-3.134
C	1.813	-1.309	-3.305
N	2.735	-1.991	-2.559
H	-0.451	0.910	-5.247
H	8.130	-3.296	-5.570
H	7.102	-4.681	-5.923
H	8.103	-4.654	-4.470
H	7.208	-3.377	-1.083
H	7.639	-4.729	-2.145
H	5.340	-2.852	-6.211
H	5.034	-2.786	-1.300
H	3.005	-3.319	-0.969
H	1.331	-2.793	-1.242
C	-3.835	0.182	-5.067
H	-4.179	-0.013	-6.081
H	-2.881	0.699	-5.102
N	-3.651	-1.145	-4.405
H	-4.547	-1.631	-4.226
H	-3.120	-1.768	-5.067
H	-3.162	-1.074	-3.497
N	-0.156	-2.095	-7.904
C	-1.441	-1.947	-8.551
C	-2.584	-1.895	-7.517
O	-2.418	-2.523	-6.429
O	-3.570	-1.215	-7.848
C	0.282	-3.297	-7.529
H	-1.594	-2.793	-9.214
H	-1.492	-1.053	-9.162
H	0.035	-4.102	-8.215
C	0.945	-3.569	-6.346
C	0.652	-2.871	-5.163
H	0.178	-1.292	-7.380
H	1.519	-4.483	-6.305
H	3.379	-1.518	-6.281
H	-0.280	-2.318	-5.134
H	0.933	-3.372	-4.250
O	-4.044	-5.295	-5.601
H	-3.558	-4.537	-5.946
H	-5.006	-5.051	-5.632
O	3.620	-0.960	-7.980
H	2.813	-0.461	-7.755
H	3.301	-1.749	-8.436
C_MM	10.631	-3.977	-0.805
C_MM	2.517	-1.361	-0.093
C_MM	-4.854	1.027	-4.330

65

TS(3b, 5b)

C	9.911	-2.647	-1.117
S	8.937	-2.745	-2.641
H	9.312	-2.320	-0.266
H	10.666	-1.890	-1.311
C	2.404	-2.490	-1.214
N	0.763	-0.867	-2.698
C	-0.124	-0.109	-3.416
O	-1.129	0.406	-2.955
N	0.149	0.140	-4.782
C	1.274	-0.267	-5.429
C	2.066	-1.273	-4.712
O	1.551	0.160	-6.563
C	4.229	-2.239	-4.500
N	3.346	-1.471	-5.221
C	5.333	-2.820	-5.114
C	6.355	-3.411	-4.377
C	7.497	-4.066	-5.122
C	6.276	-3.334	-2.978
C	7.443	-3.695	-2.109
C	5.109	-2.859	-2.363
C	4.039	-2.384	-3.111
C	1.862	-1.327	-3.277
N	2.791	-1.988	-2.530
H	-0.476	0.787	-5.261
H	8.154	-3.319	-5.577
H	7.110	-4.693	-5.926
H	8.124	-4.682	-4.481
H	7.237	-3.409	-1.082
H	7.672	-4.759	-2.145
H	5.396	-2.785	-6.194
H	5.065	-2.843	-1.283
H	3.046	-3.318	-0.941
H	1.371	-2.812	-1.247
C	-3.828	0.183	-5.068
H	-4.165	-0.015	-6.083
H	-2.876	0.706	-5.102
N	-3.638	-1.139	-4.401
H	-4.531	-1.634	-4.236
H	-3.080	-1.763	-5.048
H	-3.167	-1.059	-3.485
N	-0.574	-3.452	-8.347
C	-1.245	-2.160	-8.406
C	-2.450	-2.042	-7.429
O	-2.343	-2.607	-6.299
O	-3.417	-1.368	-7.834
C	0.162	-3.835	-7.288
H	-1.588	-1.984	-9.420
H	-0.543	-1.357	-8.178
H	0.217	-4.905	-7.099
C	0.679	-2.889	-6.465
C	0.855	-3.002	-5.069
H	-1.053	-4.181	-8.852
H	3.482	-1.395	-6.229
H	0.521	-1.886	-6.810
H	0.079	-2.534	-4.479
H	1.204	-3.948	-4.648
O	-4.035	-5.285	-5.644
H	-3.547	-4.472	-5.825
H	-4.998	-5.045	-5.655
O	3.616	-0.966	-7.976
H	2.819	-0.458	-7.737
H	3.276	-1.778	-8.374
C_MM	10.633	-3.978	-0.804
C_MM	2.521	-1.361	-0.087
C_MM	-4.851	1.027	-4.332