Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Reaction mechanism of sarcosine oxidase elucidated using FMO and QM/MM methods

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Takahide Kishimoto and Kazuo Kitaura

Model 2 Model 3

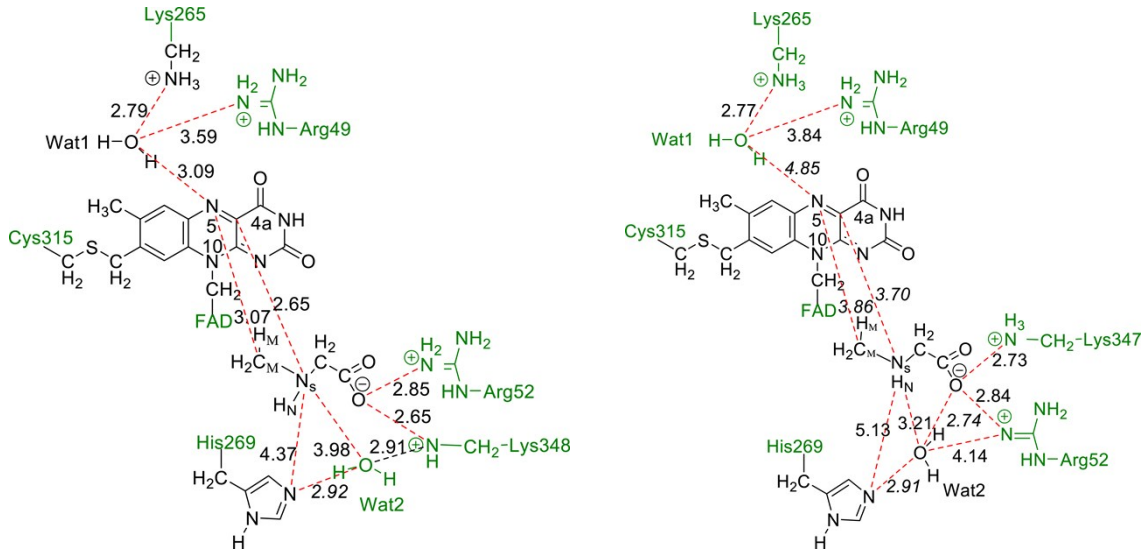


Figure S1. Arrangement of the active site of monomeric sarcosine oxidase (MSOX). The atoms corresponding to the QM and MM models are shown in black and green, respectively. The hydrogen bonds and important distances (Å) related to the initial state (state 1 of model 1) are denoted in red and black, respectively.

Computational details:

Cl^- anion

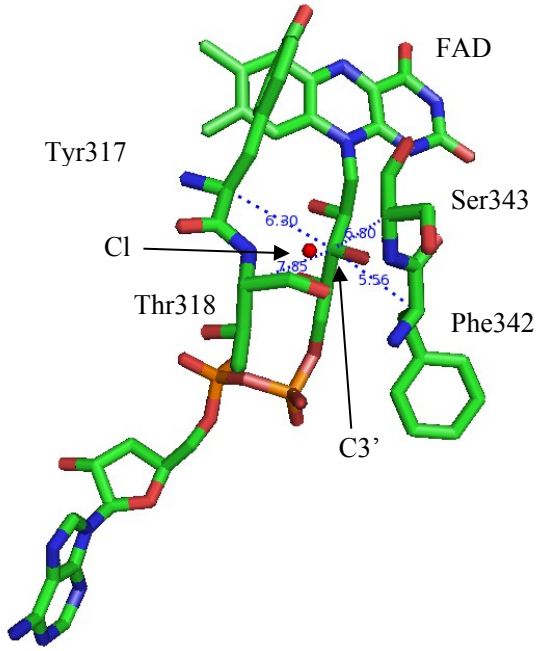
Crystal structure and model structures are compared especially around the Cl^- ion (Figure S2). In the X-ray structure (PDBID: 1EL5), the Cl^- anion closest to the FAD is coordinated by four hydrogen bonds with FAD O3' hydroxyl group, one water molecule and backbone amines of Thr318 and Gly344. Their hydrogen bonds are in 3.0 ~ 3.4 Å, therefore, the Cl^- anion is rigidly anchored to the protein framework, and Cl^- anion is expected to play important roles to stabilize the FAD and protein structures.

Experimentally, it was shown that Cl^- ions do not directly change the catalytic reactions [S1-S3]. Therefore, in the present study, we removed the closest Cl^- anion to construct a simplest model.

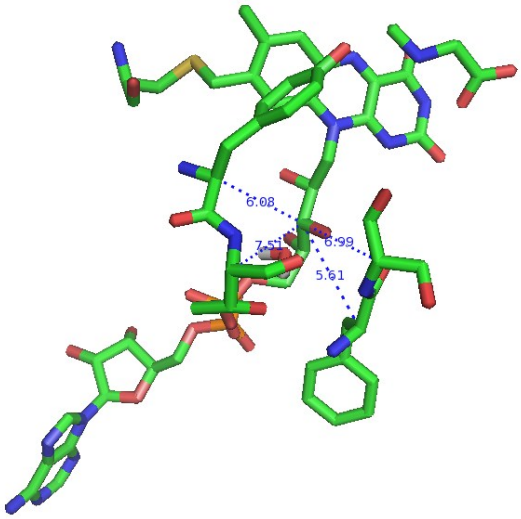
Our MD simulations, in which the Cl^- anion is deleted, showed that one water molecule comes to complement the space (Figure S2). During the equilibrated MD, no drastic structural changes are observed around the protein backbones (Figure S3). In facts, the distances between the Cα atoms for these backbones only fluctuate around the original x-ray distances. Protein structures used for the QM/MM calculations (models 1-3) are similar to the original X-ray structure (1EL5) as shown by their distances (Figure S3, Table S1).

For the following reasons, deletion of the Cl^- anion seems to be reasonable; (1) protein backbone structures are not changed and are still rigid without the Cl^- aniton, (2) the Cl^- anion is located far from the sarconsine reaction site (R >= 8.25 Å) and (3) by changing the water molecule to a Cl^- anion, only 1.2 kcal mol^{-1} is changed in energy for the QM/MM calculation with the 6-31G* basis set in the state 1 of the model 1 (still 2.1 kcal mol^{-1} for 6-311+G** basis set level). Therefore, the Cl^- anion has a small influence in energy via both direct and indirect interactions.

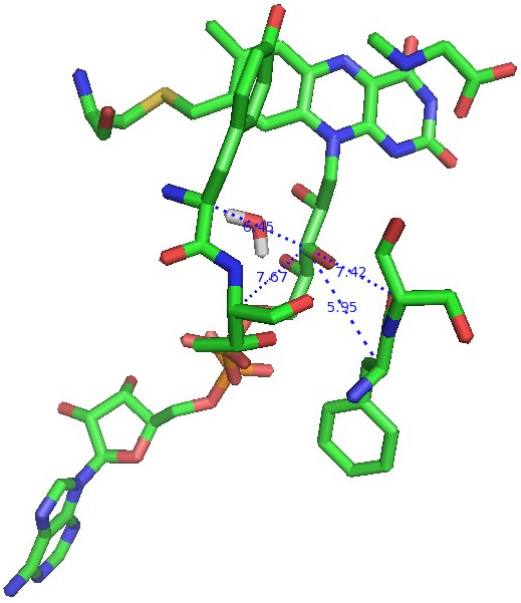
S1. Nishiya, Y. and Imanaka, T.: Analysis of interaction between the Arthrobacter sarcosine oxidase and the coenzyme flavin adenine dinucleotide by site-directed mutagenesis. Appl. Environ. Microbiol., 62, 2405-2410 (1996).
S2. Nishiya, Y., Kawamura, Y., and Imanaka, T.: Enzymatic assay for chloride ion with chloride-dependent sarcosine oxidase created by site-directed mutagenesis. Anal. Biochem., 245, 127-132 (1997).
S3. Nishiya, Y. and Kawamura, Y.: Effects of chloride ion on activity and stability of sarcosine oxidase. J. Anal. Bio-Sc., 20, 375-377 (1997).



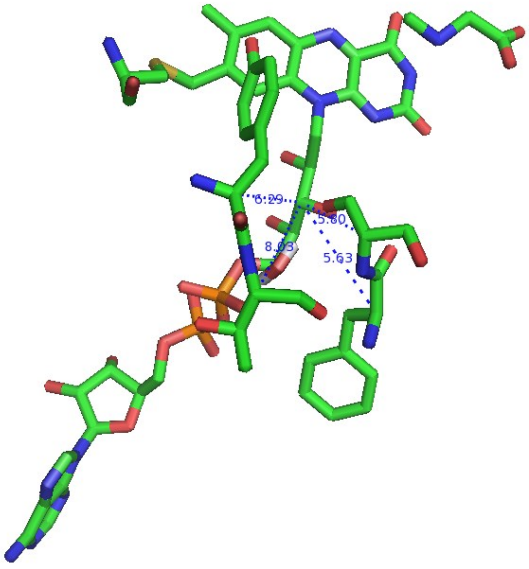
1EL5



Model 1



Model 2



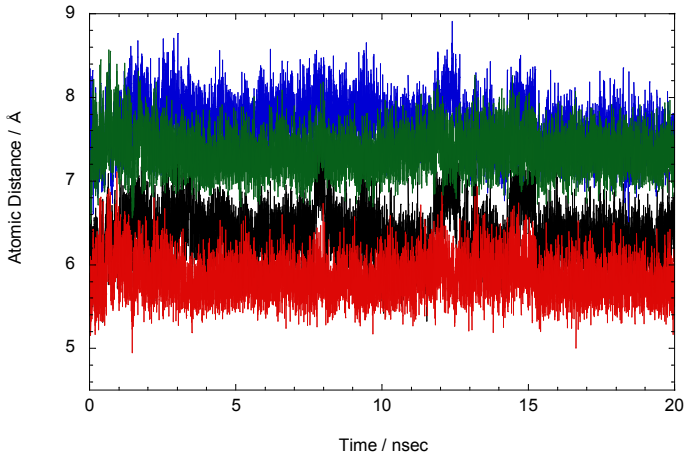
Model 3

Figure S2.

Table S1 Atomic distance between the C3’ atom of FAD and the Cα atoms of residues

	1EL5	model 1	model 2	model 3
Tyr317	6.30	6.08	6.45	6.29
Thr318	7.85	7.51	7.67	8.03
Phe342	5.56	5.61	5.95	5.63
Ser343	6.80	6.99	7.42	5.80

(A) model 1 and 2



(B) model 3

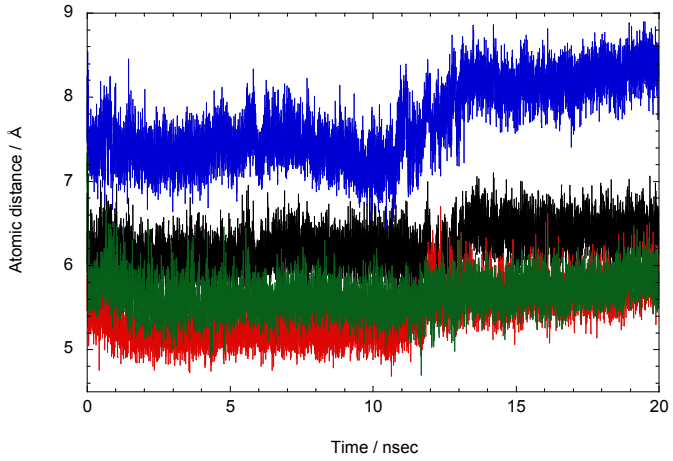


Figure S3. Atomic distances during the 20-nsec MD simulations for models 1 and 2 (A) and for model 3 (B). Black, blue, red and green lines show the distances between Cl^- and Tyr317Cα, Thr318Cα, Phe342Cα, and Ser343Cα, respectively.

Basis set

Results of the QM/MM calculations with diffuse functions (6-311+G*) are summarized in Table S2. For the relative energies, only the states ^{3}3 and 5 are destabilized by 4~5 kcal mol^{-1}, and energy changes for other key states are less than 2 kcal mol^{-1}. Similar small energy changes are calculated even for the relative energies at the optimized structures with the 6-311+G* basis sets (second entry of ΔE(B3LYP-D3//6-311+G*)).

We also checked the atomic charge densities with diffuse functions (Table S3). Qualitative changes are not observed. As shown by the Mulliken populations with the 6-311+G* tend to calculate the H charge more positive at H_M in $TS^{1,2}$(C(6-311+G*, Mulliken, H_M, $TS^{1,2}$)=0.46, C(6-31G*, Mulliken, H_M, $TS^{1,2}$)=0.26), it is clear that the transferring H atom (H_M) is far from the H^- state. On the otherhand, Löwdin population is more stable for the basis set increase (C(6-311+G*, Löwdin, H_M, $TS^{1,2}$)=0.27, C(6-31G*, Löwdin, H_M, $TS^{1,2}$)=0.23). Even at the optimized structure with the 6-311+G* basis sets, changes of the atomic charges are small and trends in the charge densities are maintained.

Therefore, QM/MM results for the 6-31G* basis set are reasonable enough to discuss on the relative energies and charge density analyses.

Table S2. QM/MM relative energies (ΔE / kcal mol^{-1}) of the model 1 states calculated with different QM basis sets.

[a] Molecular geometries are optimized at the B3LYP-D3/6-31G* of QM/MM.

	1	$TS^{1,2}$	2	$^{3}3$	$^{3}4$	$^{1}3$	$TS^{3,2}$	$TS^{1,5}$	5	$TS^{5,6}$	6
ΔE (B3LYP-D3 / 6-311+G*) [a]	0	11.3	-7.0	12.8	28.6	7.9	12.5	5.2	0.8	49.5	18.9
ΔE (B3LYP-D3 // 6-311+G*) [b]	0	10.1	-6.6	13.3	28.4	9.8	–	–	1.3	–	17.8
ΔE (B3LYP-D3 // 6-31G*) [a]	0	10.9	-5.3	8.9	30.0	4.6	12.7	4.3	0.3	44.9	16.3

[b] Molecular geometries are optimized at the B3LYP-D3/6-311+G* of QM/MM.

[c] Relative energies of $TS^{3,2}$, $TS^{1,5}$ and $TS^{5,6}$ are not converged by a simple saddle optimizer started from the TS structures obtained with 6-31G*.

Table S3. Atomic charges for the sarcosine, flavin and H_M moieties[a] calculated for model 1 key states with different basis sets.

	1			**TS^{1,2}**			**2**		
	Sarcosine	H_M	Flavin	Sarcosine	H_M	Flavin	Sarcosine	H_M	Flavin
Mulliken population analysis (B3LYP-D3/6-311+G*)									
Model 1	-0.87	0.27	-0.49	-0.72	0.46	-0.85	-0.14	0.31	-1.29
Model 2	-0.86	0.27	-0.48	-0.66	0.48	-0.92	-0.08	0.34	-1.41
Model 3	-1.01	0.26	-0.01	-0.80	0.51	-0.77	-0.14	0.31	-1.21
Mulliken population analysis (B3LYP-D3//6-311+G*)									
Model 1	-0.87	0.27	-0.50	-0.76	0.45	-0.84	-0.14	0.31	-1.29
Löwdin population analysis (B3LYP-D3/6-311+G*)									
Model 1	-0.88	0.20	-0.34	-0.53	0.27	-0.78	-0.12	0.33	-1.33
Model 2	-0.83	0.21	-0.35	-0.46	0.28	-0.81	-0.04	0.32	-1.27
Model 3	-1.10	0.21	-0.10	-0.56	0.29	-0.77	-0.12	0.31	-1.27
Löwdin population analysis (B3LYP-D3//6-311+G*)									
Model 1	-0.88	0.20	-0.32	-0.54	0.26	-0.75	-0.11	0.33	-1.30

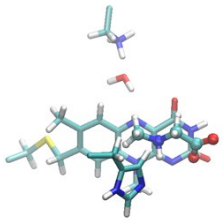
[a] H_M is not included in the sarcosine and flavin moieties.

Table S4. Atomic charges for the sarcosine, flavin and H_M moieties[a] calculated with 6-31G* basis sets.

	1			**TS^{1,2}**			**2**		
	Sarcosine	H_M	Flavin	Sarcosine	H_M	Flavin	Sarcosine	H_M	Flavin
Mulliken population analysis (B3LYP-D3//6-31G*)									
Model 1	-0.93	0.16	-0.20	-0.60	0.26	-0.69	-0.14	0.32	-1.21
Model 2	-0.92	0.14	-0.17	-0.57	0.28	-0.67	-0.10	0.33	-1.20
Model 3	-1.10	0.16	0.01	-0.60	0.28	-0.68	-0.20	0.31	-1.16
Löwdin population analysis (B3LYP-D3//6-31G*)									
Model 1	-0.93	0.14	-0.23	-0.55	0.23	-0.68	-0.15	0.28	-1.16
Model 2	-0.90	0.15	-0.19	-0.56	0.24	-0.67	-0.09	0.27	-1.15
Model 3	-1.09	0.15	0.00	-0.56	0.24	-0.65	-0.18	0.27	-1.13

[a] H_M is not included in the sarcosine and flavin moieties.

Model 2



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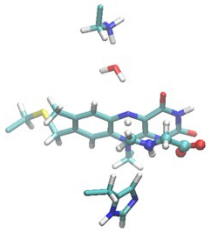
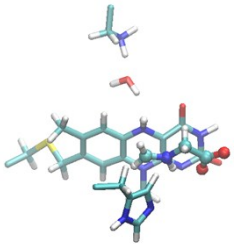


TS^{1,2}



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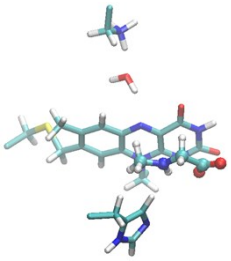
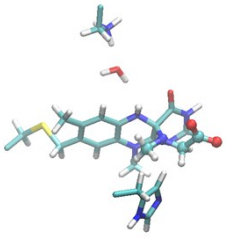


^{3}3



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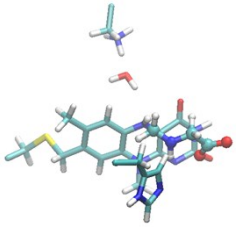
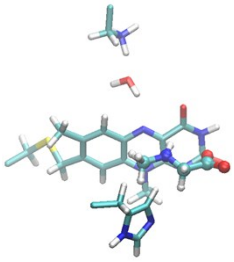


TS^{1,5}



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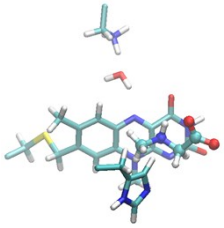

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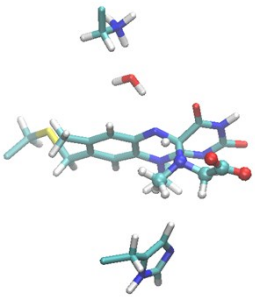
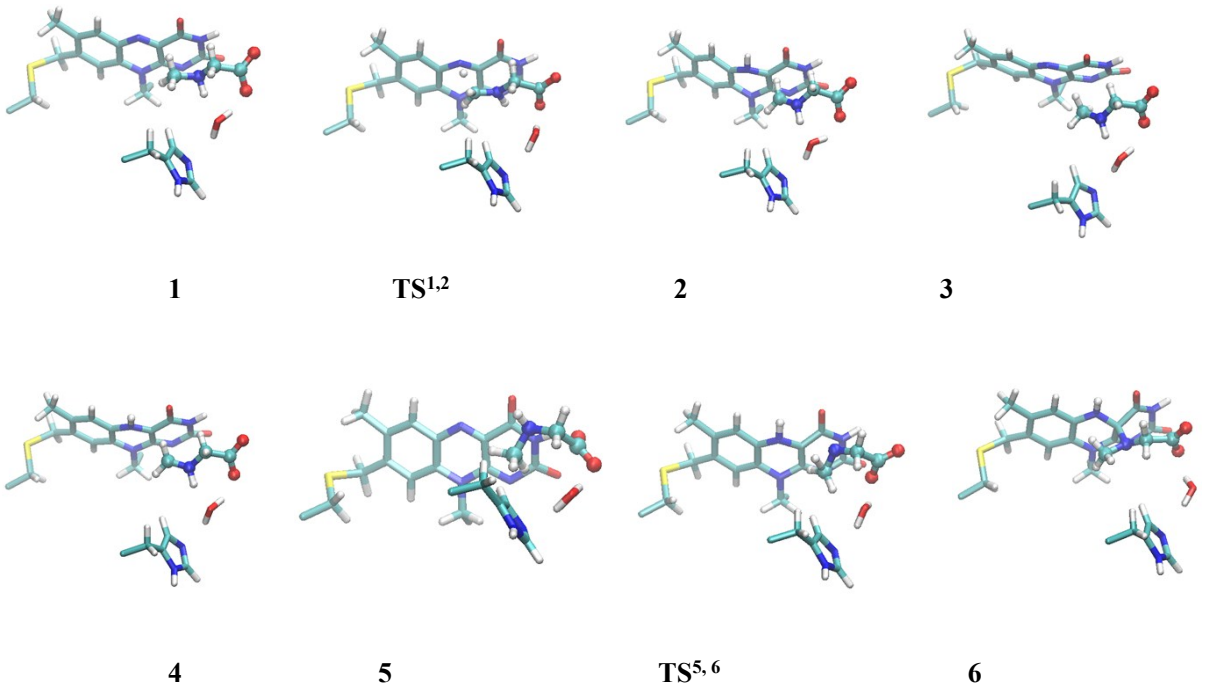


TS^{5,6}

Model 3



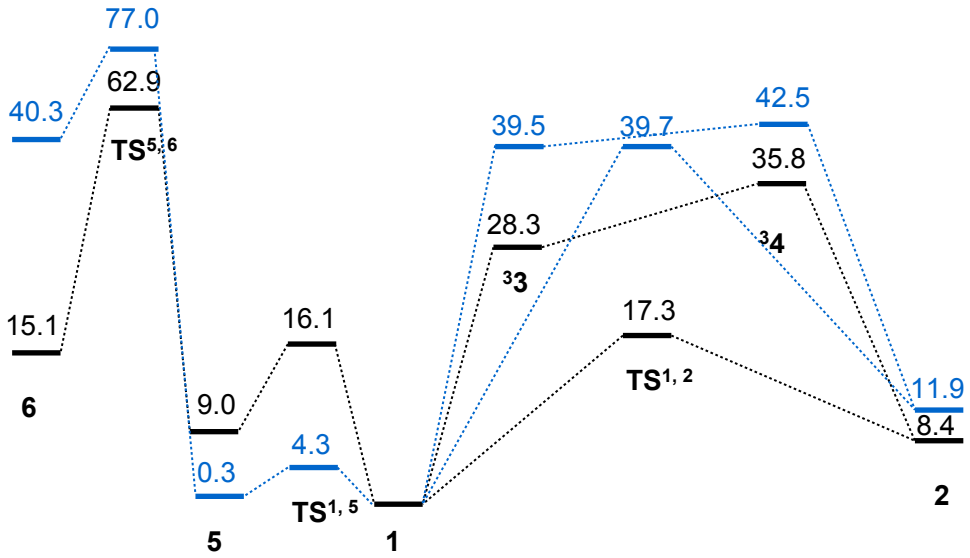


Figure S4. Key states and energy profiles of model 1 for the three reaction pathways: hydride-transfer mechanism: **1** → **2**, single-electron transfer (SET) mechanism: **1** → ^{3}**3** → ^{3}**4** → **2**, and polar mechanism: **1** → **5** → **6**. Energy profiles in two different conformations (models 2 - 3) are shown in black and blue, respectively.

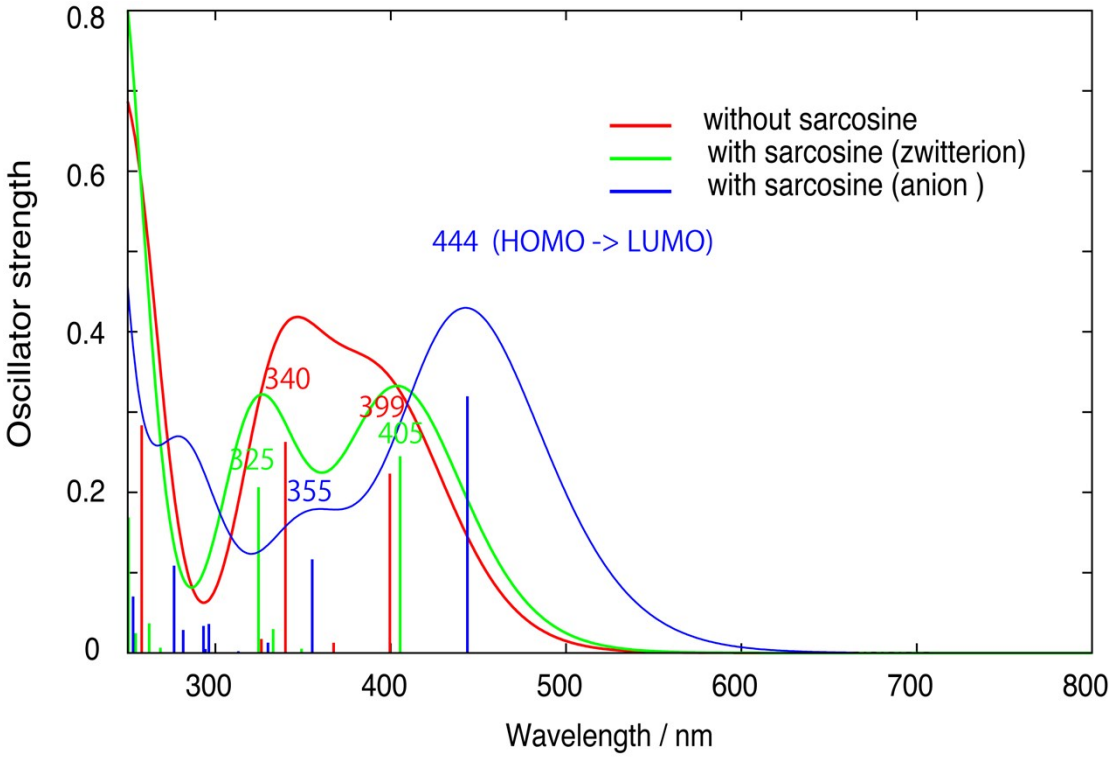


Figure S5. Calculated UV-VIS spectrum of MSOX without sarcosine in state 1 of model 2

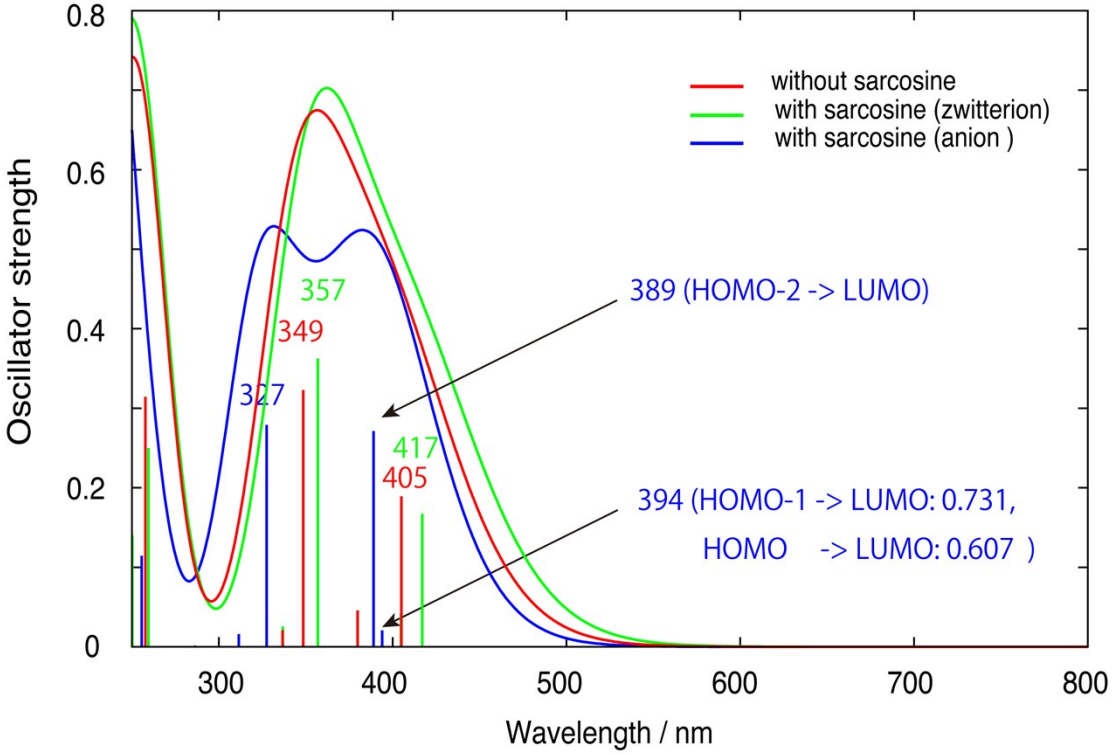


Figure S6. UV-VIS spectrum of MSOX in model 3

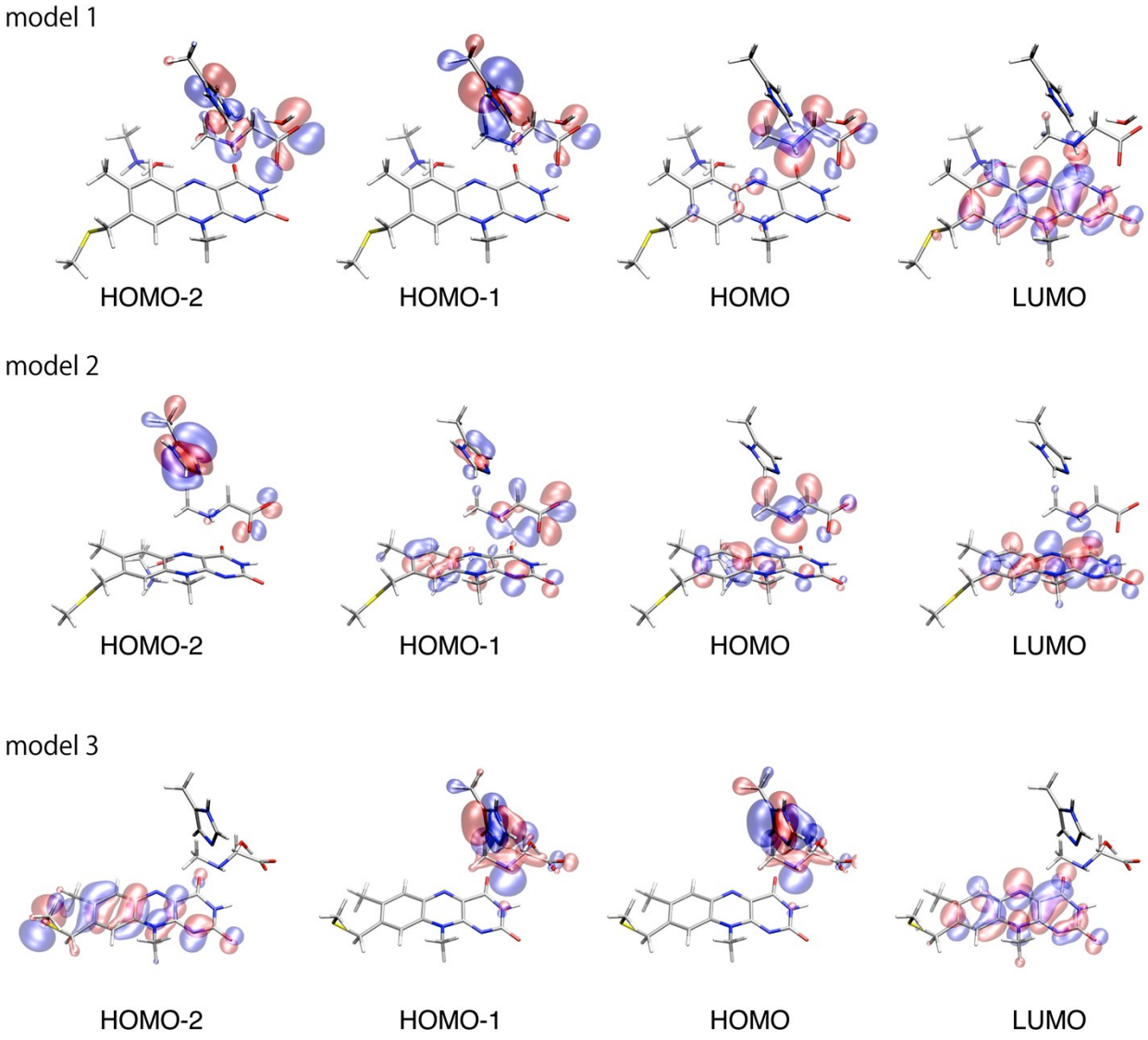
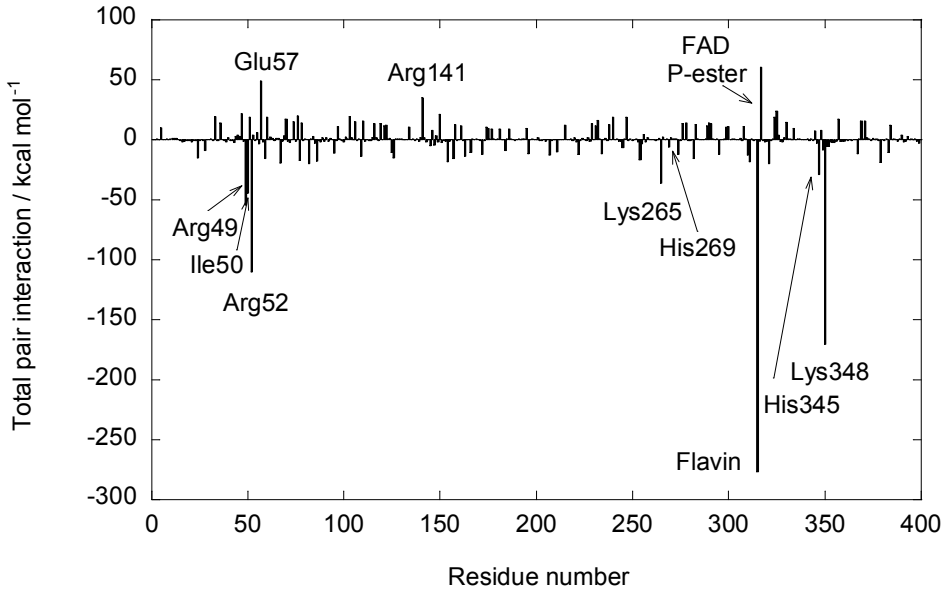


Figure S7. Frontier molecular orbitals in state 1 of models 1, 2 and 3.

Model 2



Model 3

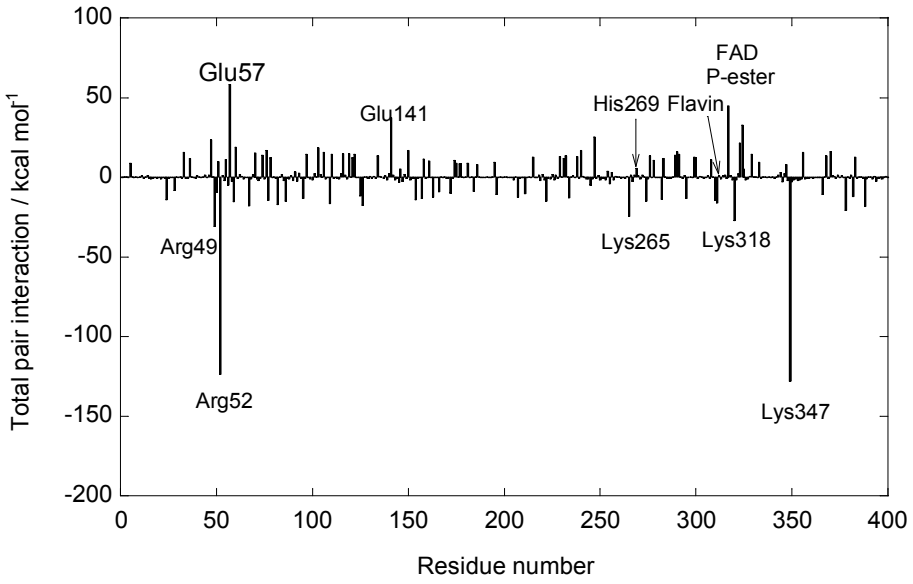


Figure S8. Total pair interaction energies for sarcosine in models 2 and 3 calculated at the FMO level.

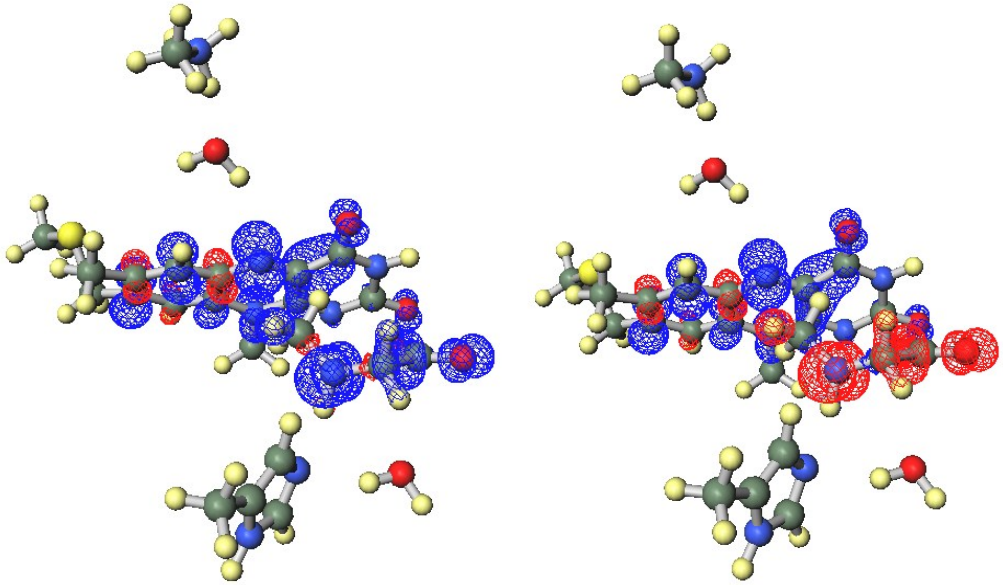
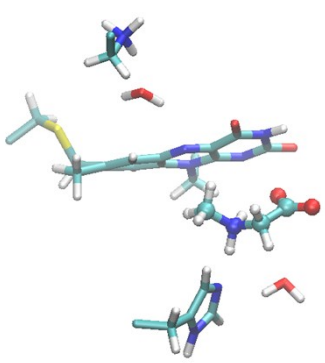
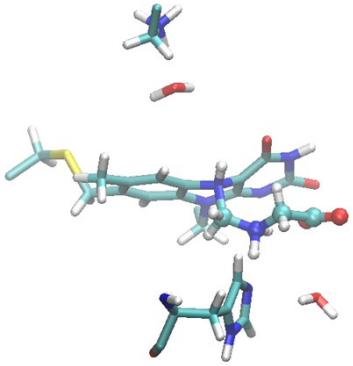


Figure S9. Spin density of state 3 (triplet and singlet) of model 1.

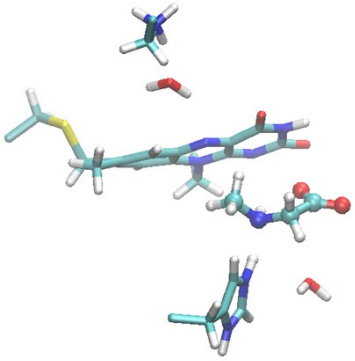
Model 1



state **11**

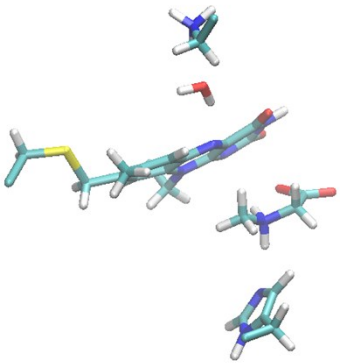


state **12**

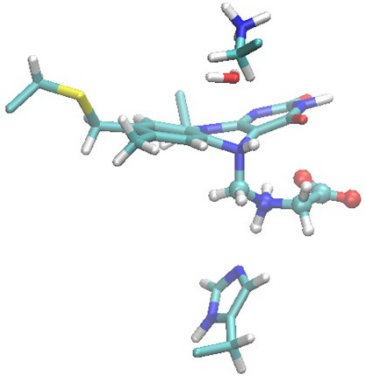


state **13**

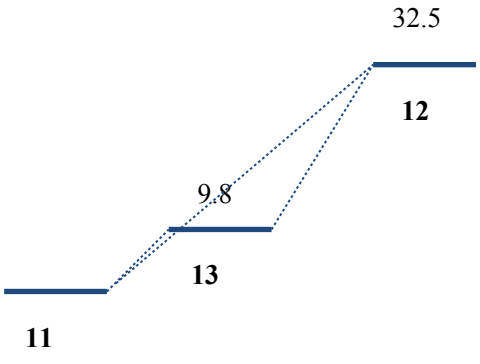
Model 2



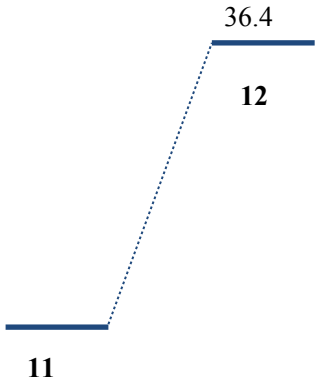
state **11**



state **12**



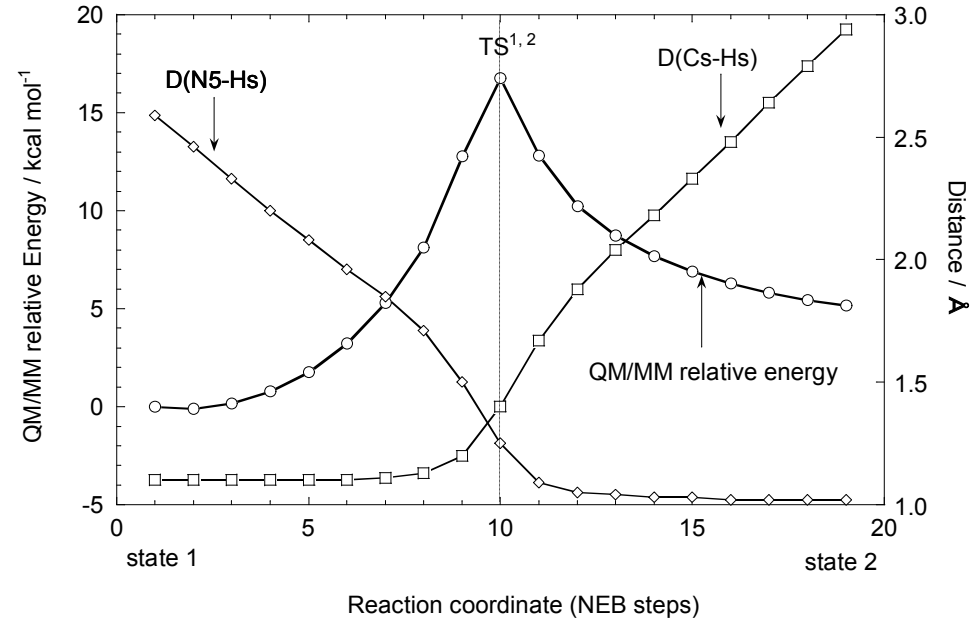
Model 1 zitterion



Model 2 zitterion

Figure S10. Key states and energy profiles for the hydrido transfer reactions (11 -> 12) and the proton transfer to His269 (11 -> 13) in the zwitterion state.

(A)



(B)

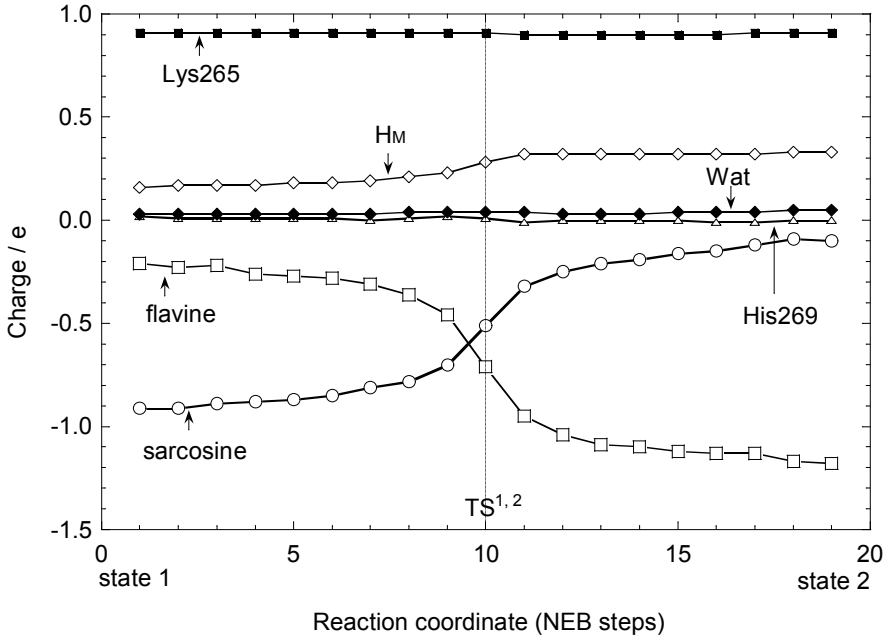
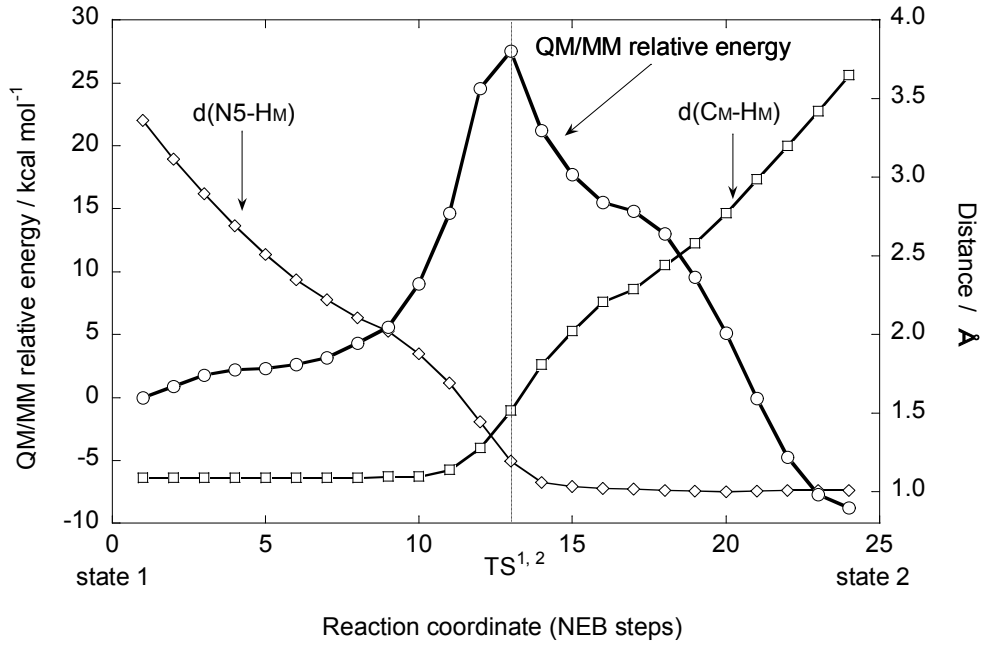


Figure S11 (A) Relative energies (left y axis) and atomic distances (right y axis) and (B) atomic charges along the NEB steps in the hydride transfer pathway (1 → 2) of model 2

(A)



(B)

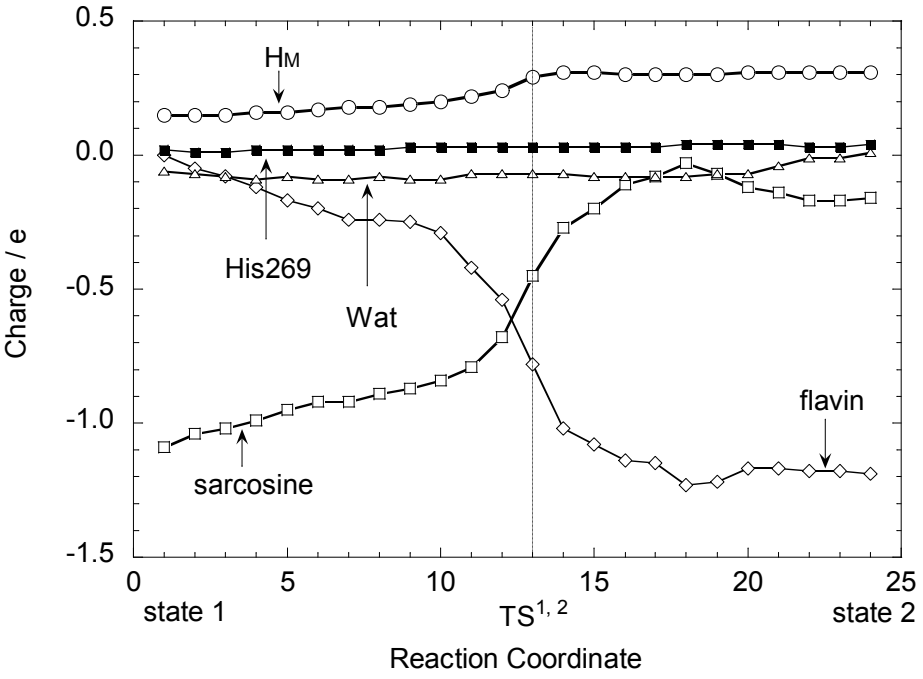


Figure S12. (A) Relative energies (left y axis) and atomic distances (right y axis) and (B) atomic charges along the NEB steps in the hydride transfer pathway (1 → 2) of model 3

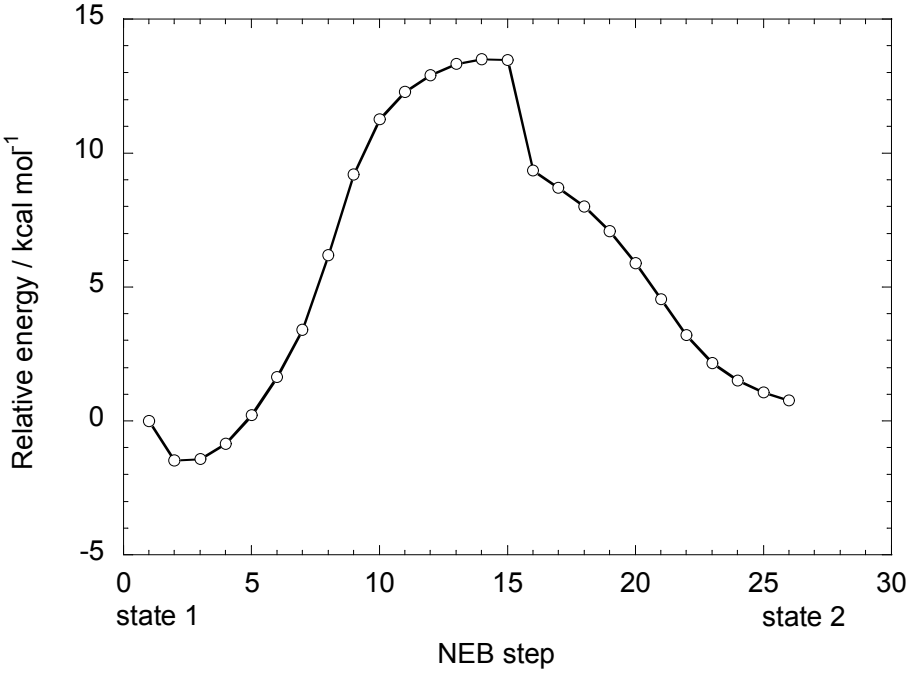


Figure S13. Relative energies along the NEB steps connecting states state1 and 5 in model 1

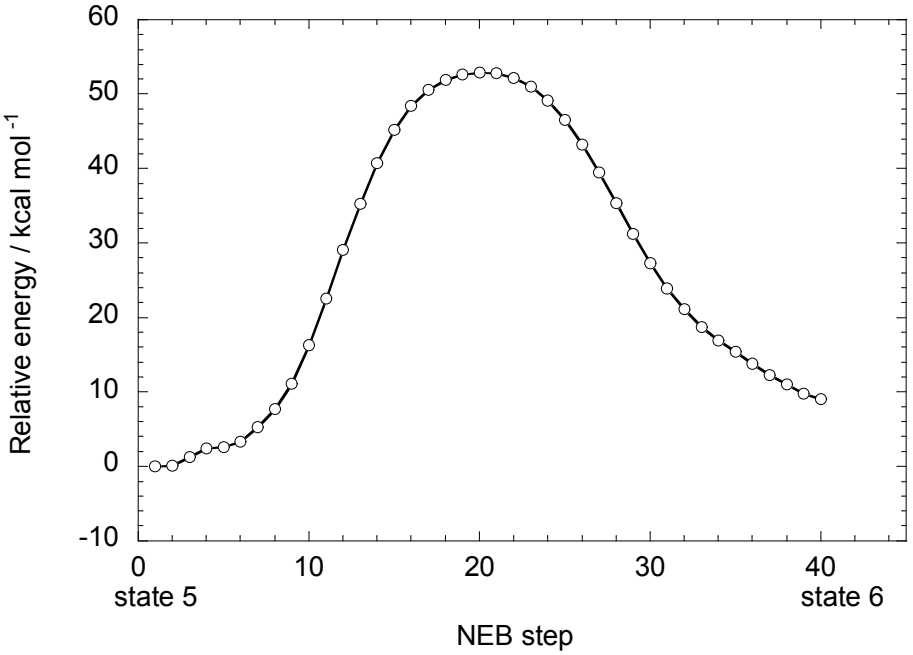


Figure S14. Relative energies along the NEB steps connecting states 5 and 6 in model 1.

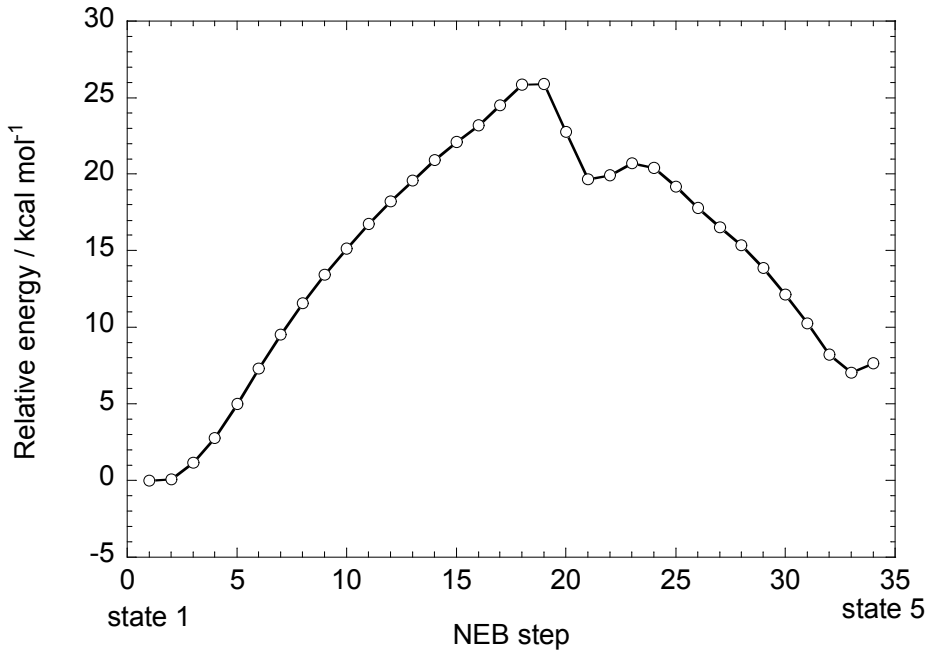


Figure S15. Relative energies along the NEB steps connecting the states 1 and 5 in model 2.

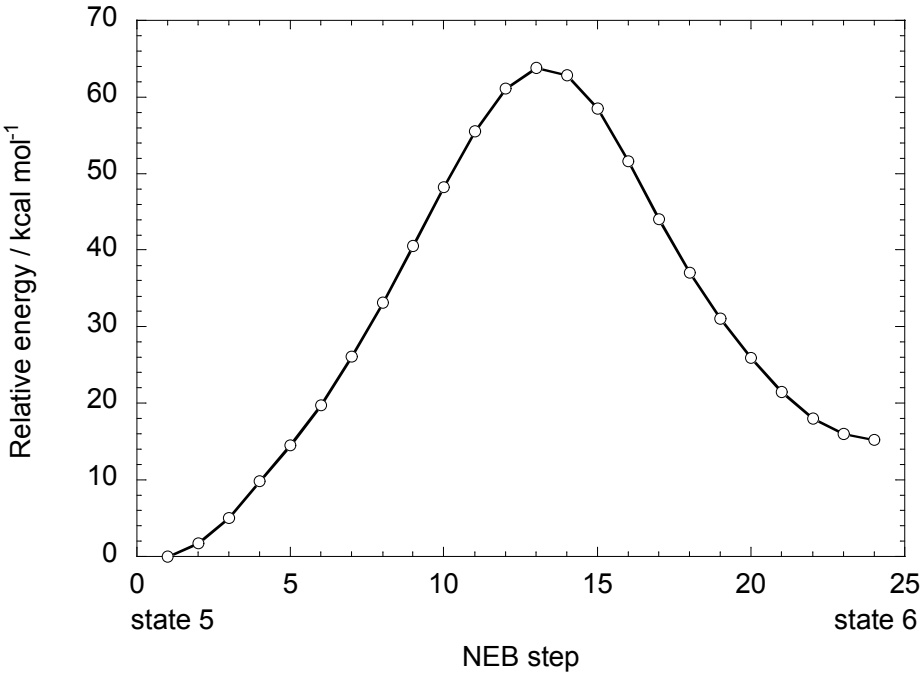


Figure S16. Relative energies along the NEB steps connecting the states 5 and 6 in model 2.

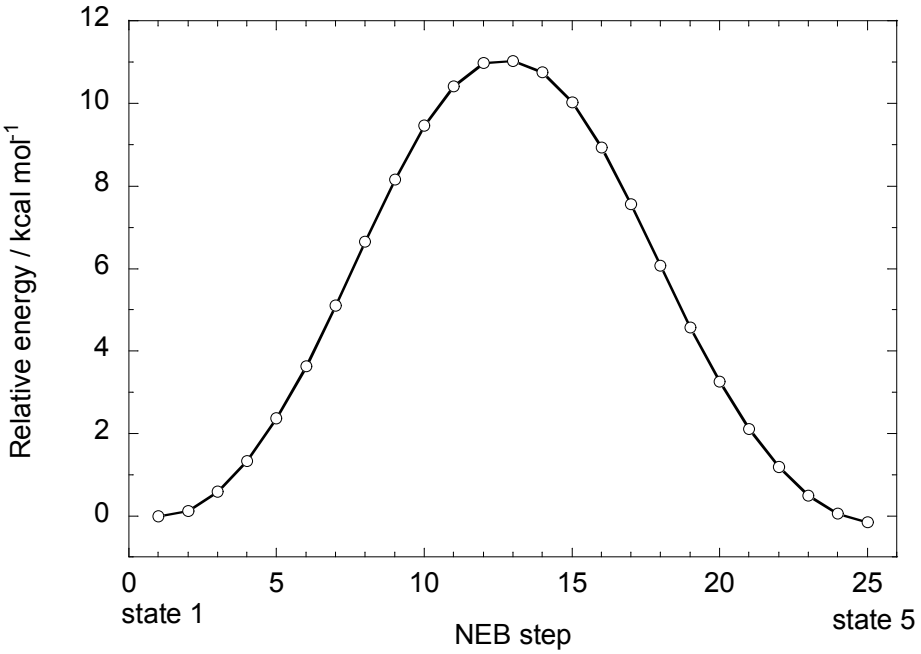


Figure S17. Relative energies along the NEB steps connecting the states 1and 5 in model 3.

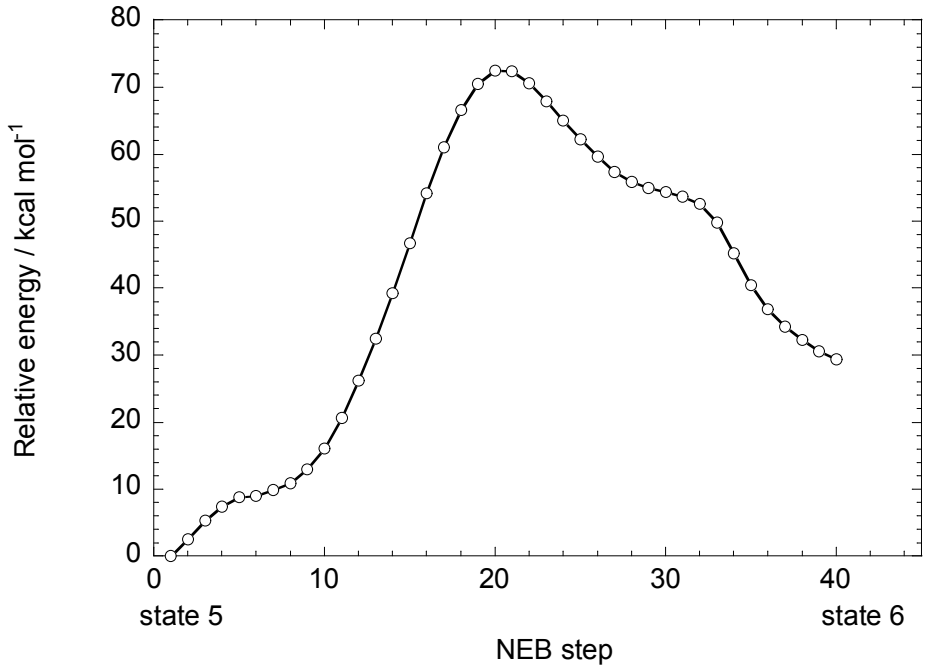
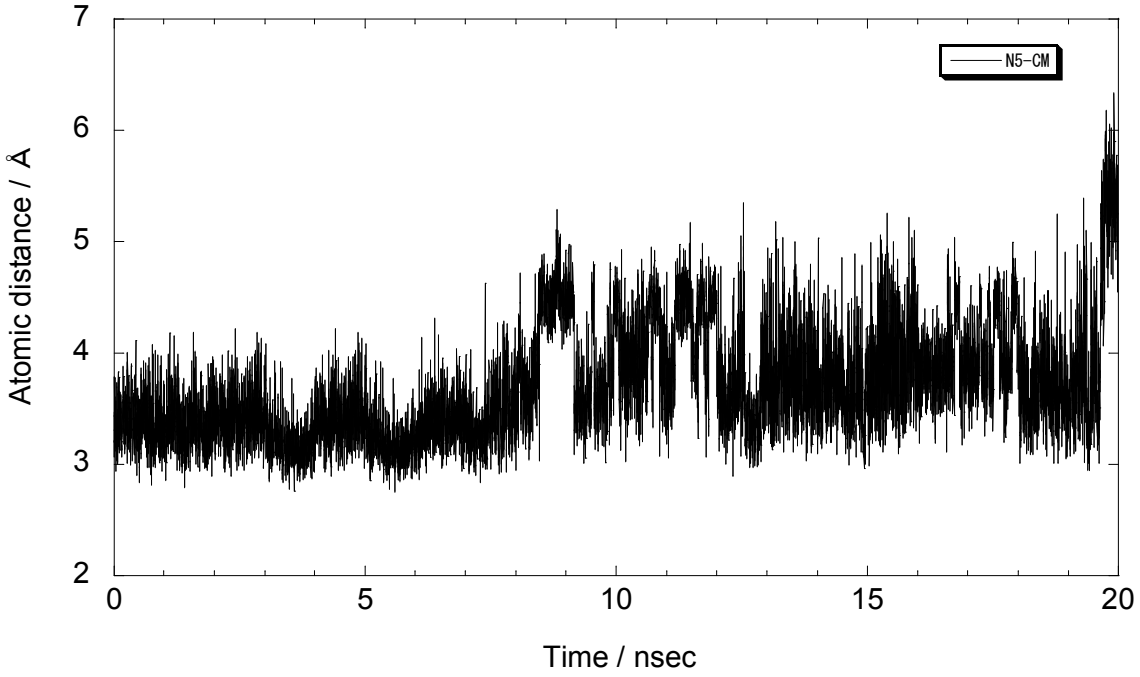


Figure S18. Relative energies along the NEB steps connecting states 5 and 6 in model 3.

(A) Atomic distance between atoms N5 and C_M



(B) Atomic distance between atoms Ns and C4a

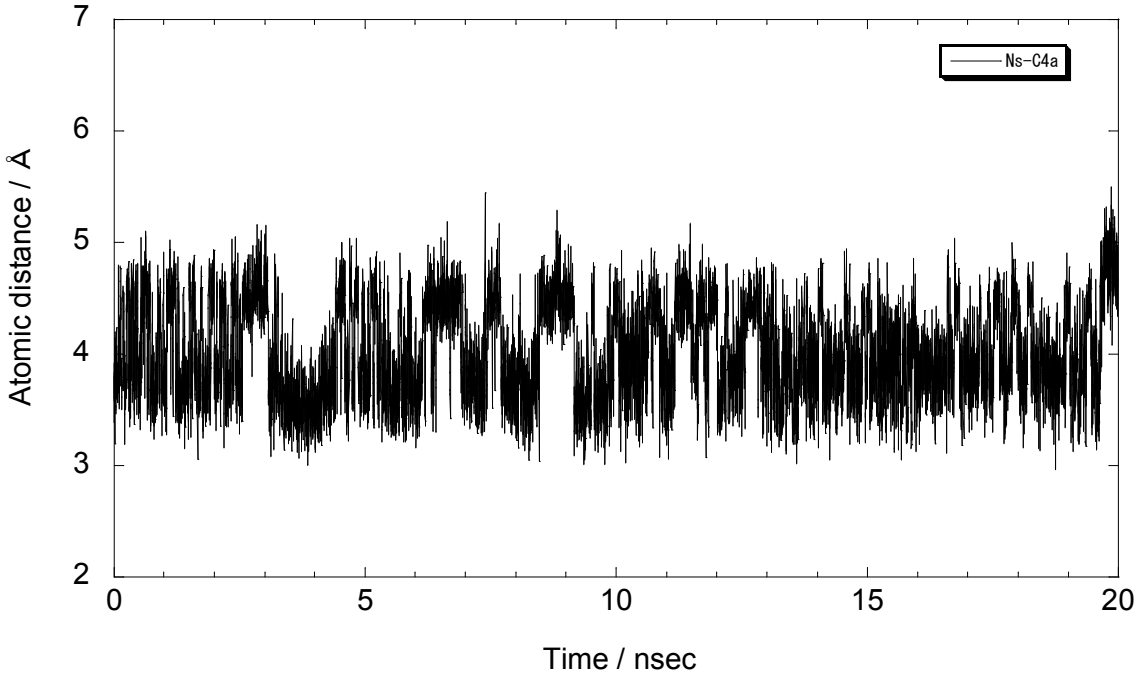
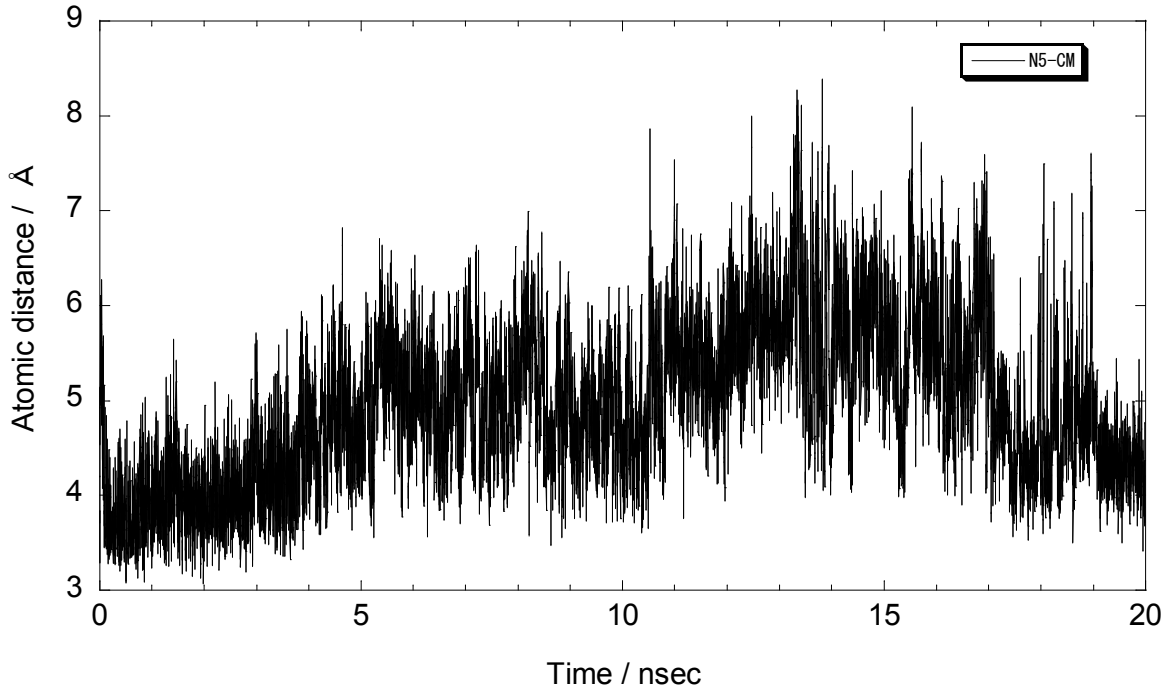


Figure S19. Atomic distances during the 20-nsec MD simulations for models 1 and 2

(A) Atomic distance between atoms N5 and C_M



(B) Atomic distance between atoms Ns and C4a

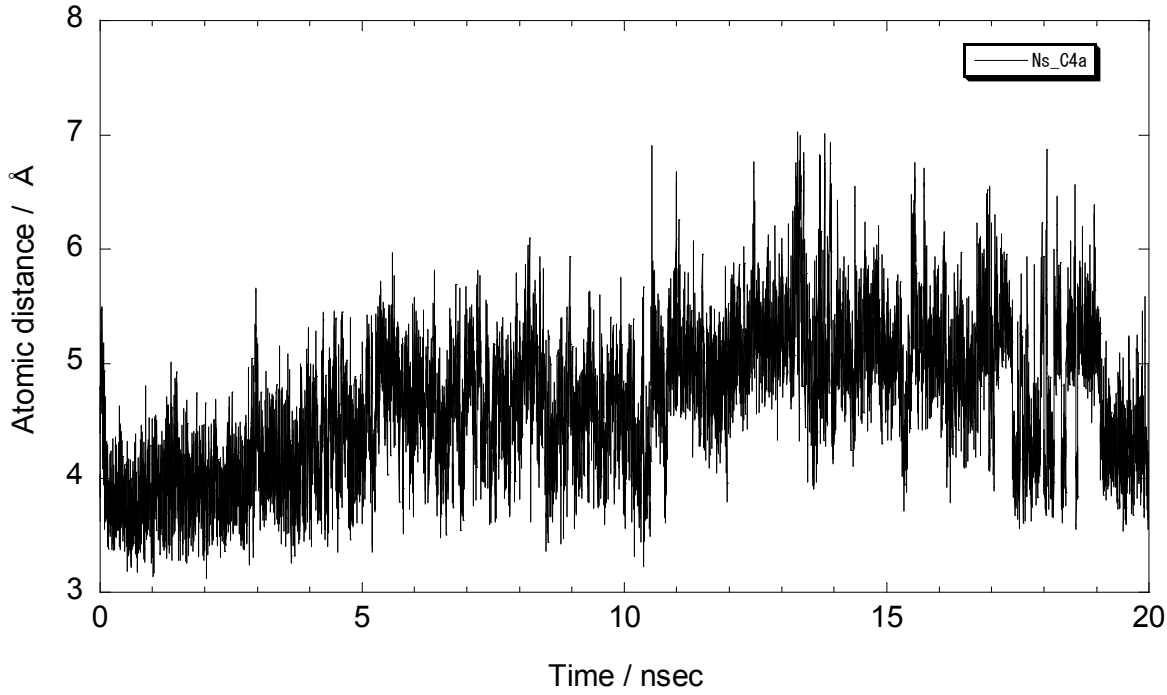


Figure S20. Atomic distances during the 20-nsec MD simulations of model 3

RESP charge of Cys-FAD

"N" -0.415700
"CA" 0.021300
"C" 0.597300
"O" -0.567900
"CB" -0.123100
"SG" -0.400000
"H" 0.271900
"HA" 0.112400
"HB2" 0.111200
"HB3" 0.111200
"P" 1.210100
"PA" 1.210100
"O1P" -0.824000
"O2P" -0.824000
"O3P" -0.510000
"C5'" 0.015700
"O5'" -0.511300
"C4'" 0.178300
"O4'" -0.620100
"C3'" 0.005400
"O3'" -0.675100
"C2'" 0.267600
"O2'" -0.635900
"C1'" -0.059900
"C1B" 0.050900
"N1" -0.566500
"N1A" -0.759400
"O1A" -0.824000
"C2" 0.696700
"C2A" 0.576700
"C2B" 0.185300
"O2" -0.385942
"O2A" -0.824000

"O2B" -0.630800
"C3B" 0.164300
"N3" -0.265803
"N3A" -0.733600
"O3B" -0.626200
"C4" 0.413800
"C4A" 0.420100
"C4B" 0.170400
"C4X" 0.058723
"O4" -0.334054
"O4B" -0.398100
"C5A" 0.022600
"C5B" 0.127100
"C5X" 0.050990
"N5" -0.524800
"O5B" -0.511300
"C6" -0.004515
"C6A" 0.685600
"N6A" -0.891100
"C7" -0.037198
"C7M" 0.016811
"N7A" -0.583200
"C8" -0.062780
"C8A" 0.154100
"C8M" 0.052430
"C9" -0.186325
"C9A" -0.006246
"N9A" 0.008500
"C10" 0.296439
"N10" -0.050000
"HN3" 0.043920
"HM71" 0.031149
"HM72" 0.031149
"HM73" 0.031149

"HM81" 0.168268
"HM83" 0.168268
"HO2'" 0.389800
"HO2A" 0.426600
"HO3'" 0.428900
"HO3A" 0.422000
"HO4'" 0.412200
"H6" 0.110588
"H9" 0.348270
"H01" 0.040600
"H02" 0.040600
"H2'" 1 0.032900
"H3'" 0.126200
"H1B" 0.174100
"H4'" 0.119100
"H2A" 0.049500
"H2B" 0.030900
"H3B" 0.036700
"H4B" 0.078000
"H8A" 0.169600
"H1'1" 0.127800
"H1'2" 0.127800
"H5'1" 0.075200
"H5'2" 0.075200
"H61A" 0.396200
"H62A" 0.396200

Resp charge of sarcosine ion

"N1" -0.650079
"C1" 0.083755
"C2" 0.619188
"O1" -0.702534
"O2" -0.702534
"H1" 0.310739

"C3" 0.091823

"H2" -0.014741

"H3" -0.014741

"H4" -0.006959

"H5" -0.006959

"H6" -0.006959

Resp charge of sarcosine (twitter ion)

"N1" -0.031397

"C1" -0.122934

"C2" 0.633220

"O1" -0.616774

"O2" -0.616774

"C3" -0.184666

"H1" 0.215369

"H2" 0.082143

"H3" 0.082143

"H4" 0.114767

"H5" 0.114767

"H6" 0.114767

"H7" 0.215369

Coordinates of all models

model 1

state 1 -2147.820603985 H

C	39.346788	50.300121	47.939236
H	39.720423	49.287508	48.076705
H	40.123000	51.015389	48.227685
N	38.174806	50.478070	48.855108
H	37.287376	50.170681	48.417113
H	38.327396	49.892140	49.713005
H	38.070401	51.472935	49.103734
C	47.226989	42.077772	51.945812
H	46.738162	42.073286	50.966830

H	47.961276	41.265847	51.940705
C	46.158262	41.870222	52.972926
N	46.371882	41.577024	54.307131
H	47.265273	41.407173	54.770327
C	45.158326	41.467443	54.907981
H	45.047915	41.192037	55.946311
N	44.171578	41.688845	54.055439
C	44.789618	41.936060	52.846580
H	44.217151	42.121911	51.948337
C	41.665187	53.245481	56.502675
S	41.811993	51.984315	55.200352
H	41.118562	52.871235	57.369516
H	41.081959	54.057976	56.062366
C	39.953980	46.138959	57.606975
N	38.276081	44.568752	56.042633
C	37.473447	43.715823	55.295876
O	36.730725	42.894431	55.818365
N	37.386458	43.910228	53.910496
C	38.206983	44.713792	53.157351
C	39.168014	45.511782	53.958995
O	38.055892	44.868807	51.947991
C	40.651074	47.245621	54.081668
N	39.869625	46.413551	53.326688
C	41.568644	48.066370	53.407299
C	42.313142	49.030352	54.068219
C	43.413021	49.756394	53.322651
C	42.002182	49.268245	55.432095
C	42.498030	50.513729	56.114578
C	41.171048	48.395284	56.141906
C	40.547283	47.316322	55.496089
C	39.060018	45.414330	55.419213
N	39.765858	46.356173	56.161466
H	36.849248	43.202231	53.414977
H	43.124313	49.932955	52.283826

H	44.306250	49.122088	53.303816
H	43.685884	50.716324	53.765309
H	42.124812	50.554543	57.137875
H	43.589367	50.584850	56.123651
H	41.694044	47.889664	52.344649
H	40.995092	48.585223	57.193569
H	40.928657	46.507293	57.901417
H	39.880319	45.069444	57.784861
N	41.032831	43.353094	53.220891
C	40.732332	42.163484	52.428476
C	39.647072	41.303628	53.110413
O	39.173603	41.817120	54.166170
O	39.313146	40.216104	52.574731
C	41.886279	44.341154	52.597130
H	41.621563	41.530055	52.274390
H	40.388229	42.476521	51.434737
H	41.295627	44.939289	51.888156
H	42.732368	43.910419	52.041835
H	42.294287	45.010033	53.358215
H	41.357333	43.074024	54.143500
O	42.100956	39.658598	54.363037
H	42.819068	40.309745	54.251609
H	42.532067	38.809814	54.597959
O	39.364768	48.747085	50.650764
H	39.232084	47.917289	51.143497
H	39.784568	49.371823	51.302168
H_	39.058379	50.448438	46.905574
H_	47.750983	43.035108	52.052892
H_	42.635353	53.655749	56.809711
H_	39.181704	46.651890	58.264204

state 2 -2147.829091873 Hl

C	39.343399	50.313958	47.938914
H	39.684809	49.289863	48.083469

H	40.134901	51.007768	48.222445
N	38.171984	50.534724	48.844870
H	37.280308	50.216092	48.422697
H	38.333605	49.972889	49.719252
H	38.078119	51.538629	49.060555
C	47.232653	42.077466	51.946142
H	46.742221	42.074099	50.967488
H	47.968214	41.266782	51.937710
C	46.168366	41.866256	52.974851
N	46.385024	41.552630	54.302995
H	47.279289	41.377937	54.762014
C	45.175413	41.446652	54.909296
H	45.065936	41.159047	55.944414
N	44.186833	41.691804	54.065425
C	44.800942	41.950156	52.856381
H	44.230552	42.154213	51.959432
C	41.654650	53.255440	56.508864
S	41.765057	52.002207	55.193786
H	41.115150	52.877964	57.378301
H	41.075276	54.079850	56.086124
C	39.941649	46.132967	57.595855
N	38.121814	44.582078	56.091330
C	37.344158	43.725656	55.347434
O	36.645024	42.831225	55.838378
N	37.258209	43.940929	53.961393
C	38.143619	44.722465	53.237650
C	39.112052	45.365787	54.043977
O	38.054077	44.884382	51.993011
C	40.747656	47.115173	54.063606
N	40.143188	46.071877	53.385813
C	41.647050	47.950954	53.404758
C	42.296680	49.010665	54.046028
C	43.383609	49.756466	53.299524
C	41.943912	49.274674	55.376840

C	42.428419	50.507268	56.086978
C	41.067186	48.407834	56.058476
C	40.498794	47.285032	55.455369
C	38.965149	45.382526	55.428678
N	39.711709	46.337436	56.169781
H	36.682834	43.277357	53.448294
H	43.086513	49.947337	52.264652
H	44.288717	49.139043	53.262111
H	43.646348	50.713738	53.755492
H	42.041177	50.533370	57.106880
H	43.519914	50.577772	56.118944
H	41.861096	47.737152	52.363071
H	40.849298	48.632504	57.093483
H	40.930581	46.501221	57.864174
H	39.868275	45.068137	57.798516
N	41.369177	42.905053	53.264298
C	40.966269	41.844584	52.331697
C	39.746765	41.132798	52.983655
O	39.359083	41.696382	54.050439
O	39.292795	40.127635	52.414110
C	42.018217	43.982740	53.056629
H	41.786860	41.128895	52.235036
H	40.713628	42.271122	51.357578
H	39.997149	46.157836	52.385718
H	42.384060	44.215477	52.060211
H	42.235657	44.633385	53.892075
H	40.948048	42.709766	54.187519
O	42.132432	39.679097	54.305154
H	42.880881	40.304078	54.269795
H	42.513927	38.812078	54.567312
O	39.306253	48.782961	50.619497
H	38.828369	48.134320	51.159444
H	39.751758	49.397215	51.278377
H_	39.068305	50.466242	46.910521

H_	47.753944	43.036389	52.056168
H_	42.633289	53.652139	56.809286
H_	39.180542	46.656102	58.273761

state 3 triplet -2147.806357812 H

C	39.366904	50.283351	47.943535
H	39.759057	49.274053	48.058076
H	40.128633	51.004552	48.241410
N	38.198766	50.419180	48.873387
H	37.309082	50.113229	48.438653
H	38.367295	49.809406	49.716577
H	38.080734	51.402834	49.152708
C	47.272045	42.060756	51.939369
H	46.781271	42.050392	50.961657
H	48.023910	41.264849	51.927807
C	46.213193	41.834686	52.964546
N	46.411101	41.541035	54.300163
H	47.299906	41.376111	54.774815
C	45.198109	41.454627	54.897523
H	45.070474	41.191384	55.936577
N	44.224437	41.691196	54.031088
C	44.853298	41.925620	52.824212
H	44.295318	42.140523	51.923250
C	41.660936	53.248530	56.507657
S	41.787641	51.990614	55.198971
H	41.119799	52.873225	57.377528
H	41.078213	54.068282	56.080909
C	39.940541	46.150985	57.593760
N	38.193637	44.599047	56.085122
C	37.400416	43.746735	55.357452
O	36.701142	42.860282	55.863721
N	37.313818	43.934700	53.972678
C	38.126694	44.758928	53.217087
C	39.053910	45.553729	54.000797

O	38.015965	44.828923	51.983597
C	40.625582	47.230337	54.063225
N	39.870374	46.393174	53.314363
C	41.585143	48.031438	53.406516
C	42.303323	49.023908	54.057385
C	43.410884	49.744965	53.315441
C	41.996268	49.272811	55.414864
C	42.491901	50.511689	56.097496
C	41.126396	48.419058	56.114061
C	40.496543	47.344838	55.484153
C	38.961501	45.465765	55.420664
N	39.710486	46.388574	56.169834
H	36.743913	43.259128	53.469267
H	43.133396	49.907012	52.270810
H	44.313346	49.122408	53.313906
H	43.669532	50.714153	53.749120
H	42.127784	50.550332	57.124857
H	43.582621	50.595252	56.097000
H	41.725618	47.848471	52.346616
H	40.949988	48.624365	57.162480
H	40.928611	46.516443	57.864429
H	39.864969	45.082721	57.770975
N	41.801706	42.422525	52.809058
C	41.103079	41.407315	52.184942
C	39.699595	41.015194	53.031818
O	39.368231	41.797057	53.923811
O	39.209870	39.969197	52.586379
C	41.533494	43.826454	52.617181
H	41.667418	40.476843	52.189570
H	40.737562	41.693304	51.195445
H	40.526137	43.976421	52.225175
H	42.254062	44.241839	51.896895
H	41.654837	44.354116	53.564605
H	42.463396	42.153336	53.555678

O	42.243249	39.538832	54.423254
H	43.074777	40.034726	54.348665
H	42.512010	38.611908	54.658352
O	39.406406	48.664001	50.668628
H	39.312795	47.848438	51.199173
H	39.811840	49.322962	51.301437
H_	39.078505	50.452400	46.918054
H_	47.770709	43.029095	52.053048
H_	42.635926	53.650967	56.809082
H_	39.177834	46.663727	58.273058

state 3 singlet -2147.813220624 H

C	39.359798	50.266277	47.946514
H	39.749442	49.255773	48.064218
H	40.127456	50.986161	48.240513
N	38.194653	50.407011	48.878078
H	37.305658	50.100701	48.444933
H	38.363689	49.803825	49.727612
H	38.081002	51.392465	49.152149
C	47.286474	42.050339	51.935667
H	46.799313	42.035081	50.956227
H	48.044088	41.260140	51.930309
C	46.222811	41.822884	52.959860
N	46.421142	41.531943	54.295953
H	47.309064	41.360373	54.770394
C	45.208048	41.451639	54.894994
H	45.078613	41.188435	55.933330
N	44.234169	41.688798	54.028461
C	44.863191	41.919266	52.820851
H	44.302373	42.134623	51.919987
C	41.665134	53.255594	56.506071
S	41.800910	52.000866	55.197049
H	41.123719	52.877332	57.373628
H	41.084514	54.074778	56.076843

C	39.928866	46.155416	57.584350
N	38.181310	44.613312	56.081062
C	37.395071	43.756268	55.352350
O	36.699666	42.866935	55.862007
N	37.308544	43.936879	53.966152
C	38.112644	44.770582	53.210020
C	39.031908	45.573861	53.996194
O	38.002372	44.841678	51.977471
C	40.619992	47.233962	54.059559
N	39.852488	46.407907	53.309510
C	41.576959	48.037686	53.404378
C	42.303589	49.022215	54.058457
C	43.411444	49.742827	53.316801
C	41.991860	49.276087	55.415824
C	42.492016	50.515109	56.097484
C	41.115067	48.424390	56.112329
C	40.487023	47.351986	55.478951
C	38.946927	45.480721	55.414412
N	39.694844	46.402653	56.164490
H	36.748167	43.254469	53.459391
H	43.132730	49.906881	52.272326
H	44.313839	49.120275	53.314761
H	43.671329	50.712652	53.749181
H	42.125244	50.556010	57.124138
H	43.582722	50.595669	56.100325
H	41.726572	47.848488	52.347065
H	40.939412	48.621681	57.161275
H	40.912221	46.524729	57.861397
H	39.857047	45.087436	57.763031
N	41.806191	42.424048	52.801082
C	41.105504	41.406888	52.182195
C	39.699670	41.019732	53.030407
O	39.347947	41.828727	53.893159
O	39.227718	39.949752	52.621259

C	41.542286	43.829943	52.611789
H	41.664593	40.474301	52.197115
H	40.740317	41.687219	51.190579
H	40.541009	43.982148	52.208704
H	42.273199	44.253124	51.905550
H	41.652479	44.351149	53.564677
H	42.466419	42.152877	53.548201
O	42.240527	39.515316	54.420812
H	43.074678	40.008133	54.345482
H	42.510962	38.583885	54.645617
O	39.405858	48.695558	50.691948
H	39.314202	47.870362	51.204754
H	39.817144	49.341477	51.333766
H_	39.064461	50.431636	46.917664
H_	47.777512	43.023191	52.048633
H_	42.638247	53.657785	56.810719
H_	39.168485	46.664021	58.259776

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C	39.334678	50.320251	47.933537
H	39.680974	49.299004	48.089255
H	40.125498	51.019047	48.211203
N	38.164951	50.547664	48.838704
H	37.277349	50.215343	48.419919
H	38.336142	50.003149	49.723185
H	38.064717	51.553307	49.042238
C	47.270660	42.055450	51.935294
H	46.780772	42.043901	50.956727
H	48.020903	41.258775	51.926251
C	46.208783	41.835669	52.963237
N	46.415050	41.496771	54.286971
H	47.305002	41.293802	54.744304
C	45.208215	41.441310	54.901467
H	45.085291	41.148187	55.933296

N	44.231434	41.738923	54.057733
C	44.849602	41.981416	52.847149
H	44.281201	42.241803	51.964829
C	41.662549	53.259680	56.506286
S	41.786146	52.030584	55.171500
H	41.130112	52.866186	57.373342
H	41.075274	54.087416	56.102885
C	39.951702	46.166177	57.608543
N	38.172307	44.588009	56.114228
C	37.398192	43.744319	55.376667
O	36.680375	42.856682	55.854908
N	37.292289	43.944986	53.965554
C	38.147379	44.723353	53.236542
C	39.080536	45.463328	54.045914
O	38.091428	44.866327	51.995208
C	40.687012	47.239263	54.072893
N	39.910435	46.323082	53.398659
C	41.592802	48.048727	53.393537
C	42.301841	49.061999	54.036600
C	43.433585	49.760785	53.317332
C	41.995448	49.287661	55.426620
C	42.485536	50.527196	56.091727
C	41.137445	48.439287	56.121181
C	40.508321	47.343680	55.502679
C	38.972361	45.454353	55.469064
N	39.735738	46.385283	56.180147
H	36.793736	43.209697	53.468706
H	43.199908	49.874919	52.254824
H	44.360671	49.171423	53.376977
H	43.649294	50.757057	53.714836
H	42.131070	50.585093	57.121009
H	43.574763	50.627034	56.070460
H	41.734847	47.880189	52.328879
H	40.944786	48.651154	57.165808

H	40.927523	46.550549	57.892695
H	39.888839	45.098953	57.794054
N	41.715326	42.425324	53.010065
C	41.009906	41.368529	52.310355
C	39.679832	40.993583	53.033541
O	39.194575	41.852474	53.807931
O	39.217475	39.866702	52.733773
C	41.432297	43.687722	52.907693
H	41.652291	40.490261	52.278142
H	40.775486	41.699716	51.292236
H	39.962354	46.231170	52.388739
H	40.702551	44.000810	52.171026
H	41.961618	44.400124	53.529679
H	42.425379	42.128139	53.704450
O	42.305273	39.511411	54.471931
H	43.170933	39.929038	54.347366
H	42.516771	38.558213	54.667778
O	39.316911	48.851472	50.663050
H	38.799729	48.241451	51.209848
H	39.759784	49.471573	51.324163
H_	39.056809	50.461939	46.900165
H_	47.772159	43.024542	52.045956
H_	42.638106	53.661359	56.809711
H_	39.171538	46.668614	58.266646

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C	39.346620	50.292093	47.930730
H	39.726765	49.280379	48.063796
H	40.116142	51.010031	48.216582
N	38.176503	50.462209	48.852083
H	37.287411	50.149815	48.420044
H	38.338606	49.876711	49.709243
H	38.066313	51.455153	49.103491
C	47.238381	42.071738	51.939061

H	46.748406	42.068237	50.960504
H	47.978701	41.265102	51.928659
C	46.172107	41.851172	52.964265
N	46.386504	41.542956	54.295334
H	47.279270	41.373273	54.757855
C	45.172462	41.417339	54.892305
H	45.058501	41.121814	55.924675
N	44.187171	41.642874	54.040500
C	44.804235	41.911722	52.836933
H	44.230546	42.117214	51.943492
C	41.674809	53.242473	56.500003
S	41.837217	51.989305	55.190269
H	41.129598	52.859621	57.363814
H	41.085607	54.052346	56.063507
C	39.980339	46.163950	57.610105
N	38.280038	44.624731	56.067271
C	37.448771	43.791210	55.321525
O	36.733276	42.954741	55.853270
N	37.304550	44.030003	53.946508
C	38.159359	44.787490	53.185021
C	39.154138	45.558743	53.973457
O	38.015722	44.936005	51.972078
C	40.680979	47.259052	54.084638
N	39.896295	46.422639	53.338675
C	41.599581	48.073582	53.402835
C	42.343562	49.042305	54.055375
C	43.443108	49.764547	53.306080
C	42.045187	49.279185	55.421679
C	42.547209	50.524334	56.096034
C	41.206392	48.420151	56.135307
C	40.579379	47.339301	55.497669
C	39.063774	45.460534	55.435425
N	39.800482	46.383106	56.167418
H	36.849377	43.260386	53.455192

H	43.161168	49.918154	52.262354
H	44.342210	49.138057	53.306946
H	43.705136	50.734962	53.733445
H	42.190294	50.566121	57.124611
H	43.638393	50.596547	56.087503
H	41.708881	47.907500	52.336758
H	41.035159	48.617372	57.186316
H	40.954764	46.540469	57.907821
H	39.913760	45.094992	57.783203
N	40.681869	43.369461	52.534690
C	40.803142	41.913238	52.524875
C	39.526778	41.203362	53.008613
O	39.346498	40.010056	52.673081
O	38.779890	41.898136	53.760621
C	41.942592	44.084422	52.518750
H	41.601610	41.623534	53.214959
H	41.083929	41.526331	51.531567
H	42.538674	43.890090	51.612153
H	42.531519	43.782468	53.387809
H	41.757813	45.162869	52.557043
H	40.055189	43.693294	51.802027
O	42.170391	39.553144	54.507622
H	42.941012	40.116106	54.320249
H	42.524086	38.646086	54.676338
O	39.409455	48.751884	50.658493
H	39.301184	47.922421	51.158677
H	39.811280	49.394048	51.309647
H_	39.060405	50.446322	46.903603
H_	47.755920	43.032804	52.049646
H_	42.641802	53.658678	56.809883
H_	39.188021	46.667203	58.262140

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C	39.337390	50.292919	47.930192

H	39.688342	49.271230	48.067634
H	40.125867	50.990626	48.215122
N	38.169621	50.502529	48.844159
H	37.280379	50.172759	48.426088
H	38.339361	49.949876	49.724294
H	38.063322	51.505742	49.056920
C	47.234261	42.071880	51.935103
H	46.753348	42.067363	50.952065
H	47.970453	41.261259	51.934356
C	46.158038	41.861935	52.952680
N	46.357680	41.515076	54.276306
H	47.245551	41.319288	54.739148
C	45.139254	41.415624	54.868376
H	45.015206	41.103601	55.894766
N	44.162612	41.691314	54.018990
C	44.792762	41.970300	52.823553
H	44.229812	42.217512	51.933430
C	41.667601	53.262099	56.510629
S	41.806139	52.001460	55.206888
H	41.123235	52.888034	57.378409
H	41.085128	54.077403	56.075262
C	39.942001	46.143112	57.542491
N	38.252635	44.593253	55.972523
C	37.422509	43.754583	55.245031
O	36.637201	42.974920	55.756574
N	37.238664	44.060117	53.860056
C	38.111547	44.778053	53.116014
C	39.416672	45.176660	53.828127
O	37.915791	45.108759	51.947187
C	40.623040	47.304199	54.007647
N	39.784965	46.482837	53.264075
C	41.565536	48.107125	53.364989
C	42.305351	49.071131	54.044646
C	43.419823	49.788872	53.311603

C	41.997640	49.290112	55.402089
C	42.488390	50.520083	56.110950
C	41.137215	48.412333	56.075240
C	40.510872	47.349543	55.415323
C	39.094659	45.370198	55.352978
N	39.750055	46.347152	56.085217
H	36.533115	43.497298	53.386819
H	43.133052	50.004823	52.279245
H	44.297931	49.134761	53.269562
H	43.717936	50.728282	53.782279
H	42.103186	50.549658	57.130315
H	43.579306	50.595146	56.135988
H	41.721409	47.958789	52.301229
H	40.970490	48.573256	57.132926
H	40.925111	46.512626	57.819367
H	39.877162	45.075383	57.722891
N	40.393861	44.156841	53.598086
C	40.173767	42.993266	52.728603
C	39.396914	41.842911	53.404975
O	39.199183	40.791363	52.753378
O	39.009205	42.100404	54.581124
C	41.794991	44.482441	53.829466
H	41.159172	42.603361	52.461305
H	39.699839	43.267263	51.777345
H	42.279651	44.900742	52.932102
H	42.326805	43.577908	54.130868
H	41.908695	45.193512	54.643806
H	40.092745	46.350494	52.304415
O	42.053390	39.652940	54.366028
H	42.736376	40.330587	54.201606
H	42.532479	38.832514	54.603071
O	39.323324	48.810885	50.691229
H	38.908347	48.149259	51.268011
H	39.766035	49.450229	51.328373

H_	39.058701	50.449763	46.901635
H_	47.754153	43.031441	52.047381
H_	42.640124	53.669466	56.815196
H_	39.169535	46.652627	58.220935

$TS^{1,2}$ -2147.803294246 H -1223.399 cm^{-1}

C	39.343648	50.293672	47.930950
H	39.720343	49.280877	48.066329
H	40.116047	51.009006	48.214538
N	38.175166	50.469839	48.853575
H	37.284749	50.151112	48.429194
H	38.343065	49.893681	49.715821
H	38.064155	51.465379	49.095642
C	47.226804	42.080397	51.938573
H	46.740933	42.079913	50.957911
H	47.958359	41.265569	51.933056
C	46.156599	41.872798	52.963747
N	46.370104	41.531831	54.286166
H	47.262916	41.342202	54.742598
C	45.159312	41.431489	54.891785
H	45.048677	41.122077	55.920395
N	44.172313	41.702775	54.052696
C	44.789185	41.976287	52.848452
H	44.216288	42.213362	51.961536
C	41.673417	53.234112	56.491976
S	41.833090	51.978750	55.180187
H	41.126702	52.850735	57.354200
H	41.085067	54.043863	56.054023
C	39.944830	46.133468	57.584262
N	38.191211	44.588509	56.068508
C	37.393832	43.730096	55.335097
O	36.687577	42.864555	55.850659
N	37.285688	43.936904	53.952816
C	38.141622	44.716778	53.198966

C	39.114378	45.448150	53.987829
O	38.031484	44.820199	51.970210
C	40.718442	47.139092	54.058565
N	40.006164	46.209975	53.291883
C	41.631754	47.964463	53.396009
C	42.320490	48.987284	54.042947
C	43.414027	49.725836	53.300111
C	41.980590	49.246599	55.388679
C	42.475740	50.485090	56.089426
C	41.115734	48.389485	56.078748
C	40.527767	47.279210	55.454244
C	39.005480	45.400044	55.412616
N	39.737617	46.339951	56.149556
H	36.726379	43.249840	53.452710
H	43.112086	49.935704	52.270748
H	44.305848	49.091302	53.251006
H	43.697645	50.671287	53.767489
H	42.083617	50.522956	57.106193
H	43.567871	50.537426	56.126516
H	41.784340	47.786680	52.336729
H	40.914026	48.600834	57.120637
H	40.928252	46.504427	57.864427
H	39.872618	45.067808	57.776746
N	41.244701	43.246290	53.235069
C	40.813588	42.121985	52.413578
C	39.694860	41.314734	53.121047
O	39.273350	41.843885	54.187819
O	39.315960	40.251955	52.575726
C	41.809674	44.392982	52.788285
H	41.663481	41.447209	52.246973
H	40.464622	42.493397	51.443758
H	40.911008	45.352430	52.790080
H	42.124650	44.379840	51.743282
H	42.506887	44.858014	53.485601

H	41.196605	43.068231	54.235100
O	42.108147	39.677657	54.325554
H	42.827679	40.332551	54.243796
H	42.535235	38.831128	54.575797
O	39.423931	48.761619	50.652880
H	39.289899	47.941319	51.160076
H	39.825999	49.402680	51.307978
H_	39.058304	50.446891	46.903579
H_	47.753456	43.036271	52.050118
H_	42.639709	53.651737	56.804918
H_	39.170072	46.650388	58.249033

$TS^{3,2}$ -2147.800358681 H -1537.593 cm^{-1}

C	39.339138	50.256552	47.943997
H	39.714684	49.237908	48.052380
H	40.121515	50.958250	48.241021
N	38.171402	50.421767	48.866048
H	37.279691	50.122667	48.427255
H	38.334163	49.831014	49.721778
H	38.076725	51.413601	49.124530
C	47.248070	42.059284	51.947281
H	46.765822	42.043220	50.973873
H	47.998840	41.253110	51.941884
C	46.187760	41.851395	52.974455
N	46.400917	41.538467	54.305229
H	47.296888	41.346129	54.750715
C	45.193558	41.460622	54.920536
H	45.082403	41.160965	55.946473
N	44.209469	41.723705	54.078318
C	44.823141	41.962390	52.859729
H	44.238857	42.176900	51.972567
C	41.679764	53.226392	56.479890
S	41.832624	51.971212	55.176510
H	41.120408	52.858574	57.349771

H	41.090830	54.041012	56.037371
C	39.926833	46.129038	57.606610
N	38.115914	44.595912	56.104360
C	37.340660	43.730523	55.356676
O	36.664026	42.844495	55.875369
N	37.205759	43.967036	53.985747
C	38.083609	44.731884	53.234629
C	39.076853	45.420899	54.030839
O	37.976933	44.858027	52.007310
C	40.769135	47.016812	54.081736
N	40.082378	46.045434	53.345338
C	41.683686	47.833970	53.413652
C	42.317960	48.917535	54.029366
C	43.386227	49.680463	53.275901
C	41.941480	49.216750	55.355383
C	42.452821	50.454494	56.058675
C	41.071803	48.370464	56.060377
C	40.519690	47.233110	55.466865
C	38.953661	45.387696	55.445259
N	39.710756	46.331442	56.169917
H	36.684467	43.255517	53.480292
H	43.068256	49.867931	52.244867
H	44.301305	49.073500	53.217218
H	43.633843	50.641071	53.724852
H	42.063923	50.491825	57.079799
H	43.544395	50.492016	56.092113
H	41.883157	47.593177	52.379962
H	40.845002	48.611405	57.086424
H	40.913630	46.494054	57.879192
H	39.855355	45.062942	57.805894
N	41.643845	42.883736	53.080417
C	40.997011	41.778691	52.405231
C	39.724435	41.211723	53.128006
O	39.181071	41.954133	53.986176

O	39.367326	40.070084	52.749934
C	41.823017	44.136819	52.609656
H	41.699724	40.947591	52.361691
H	40.733665	42.085931	51.391871
H	40.932507	45.062006	52.976598
H	41.687912	44.228603	51.528635
H	42.704839	44.632647	53.021188
H	42.113572	42.631977	53.948619
O	42.214743	39.552025	54.425863
H	43.029075	40.060730	54.322441
H	42.506617	38.634514	54.621390
O	39.411946	48.737742	50.641213
H	39.290701	47.892121	51.115851
H	39.815315	49.368269	51.310260
H_L	39.062229	50.433980	46.916489
H_L	47.762299	43.024801	52.051613
H_L	42.642870	53.649613	56.804720
H_L	39.154723	46.654327	58.264592

$TS^{1,5}$ -2147.813737915 -89.17 cm^{-1}

C	39.347154	50.287556	47.930784
H	39.713465	49.270691	48.062178
H	40.128861	50.992355	48.215987
N	38.178214	50.469892	48.851791
H	37.290819	50.143048	48.427701
H	38.345245	49.899360	49.718121
H	38.062389	51.467284	49.084877
C	47.239197	42.070587	51.932066
H	46.737719	42.077796	50.959535
H	47.978667	41.263005	51.907126
C	46.181254	41.842850	52.962705
N	46.395022	41.559653	54.298979
H	47.286678	41.398981	54.766648

C	45.179301	41.416992	54.890429
H	45.064761	41.135531	55.926698
N	44.195747	41.606940	54.029775
C	44.814567	41.867985	52.825552
H	44.244972	42.040317	51.922646
C	41.679447	53.244962	56.485765
S	41.851016	51.977523	55.188793
H	41.116093	52.878972	57.345484
H	41.104744	54.051971	56.025781
C	39.977706	46.149369	57.618943
N	38.266248	44.611673	56.091720
C	37.435971	43.778706	55.347862
O	36.742460	42.917209	55.867523
N	37.266267	44.037675	53.976176
C	38.105319	44.812326	53.222239
C	39.112260	45.570737	54.005141
O	37.987782	44.946904	52.005183
C	40.674417	47.236782	54.094448
N	39.872969	46.410492	53.355136
C	41.590732	48.052070	53.409326
C	42.331920	49.025225	54.059850
C	43.432872	49.745620	53.310917
C	42.039200	49.261454	55.428039
C	42.538495	50.507430	56.105215
C	41.205469	48.398990	56.144021
C	40.574415	47.319807	55.508301
C	39.042450	45.455787	55.457660
N	39.796726	46.367631	56.182711
H	36.801374	43.280107	53.475285
H	43.148619	49.911004	52.269751
H	44.326436	49.110468	53.301358
H	43.705560	50.708242	53.748316
H	42.168185	50.552472	57.128938
H	43.629961	50.574636	56.113382

H	41.696468	47.887252	52.342563
H	41.039393	48.593382	57.196230
H	40.950783	46.525805	57.921984
H	39.907705	45.081109	57.795706
N	40.842485	43.335234	52.831886
C	40.833440	41.917181	52.493489
C	39.569838	41.211818	53.028869
O	38.796034	41.926698	53.736253
O	39.392387	40.009933	52.723455
C	42.029865	44.086609	52.477756
H	41.712495	41.413586	52.904309
H	40.863121	41.766613	51.398507
H	42.184624	44.146126	51.388735
H	42.907740	43.634515	52.935466
H	41.941848	45.112790	52.850970
H	40.020906	43.762870	52.428939
O	42.129569	39.588602	54.501371
H	42.868452	40.207035	54.359153
H	42.525273	38.699770	54.648830
O	39.402444	48.770696	50.659265
H	39.287195	47.939559	51.153507
H	39.809131	49.406438	51.314633
H_	39.062182	50.447046	46.903976
H_	47.756852	43.030662	52.046546
H_	42.641850	53.659235	56.805283
H_	39.181078	46.655388	58.260447

TS[5,6] -2147.749036211 H -1706.21cm-1

C	39.349156	50.280257	47.931009
H	39.721456	49.264958	48.059251
H	40.126618	50.989941	48.216680
N	38.184132	50.457668	48.859086
H	37.291226	50.143006	48.437300
H	38.353385	49.880019	49.723482

H	38.076852	51.453346	49.102425
C	47.233930	42.072890	51.937505
H	46.752142	42.066181	50.954894
H	47.971184	41.262731	51.935433
C	46.160260	41.861392	52.957507
N	46.363961	41.535729	54.285441
H	47.254062	41.356595	54.751308
C	45.146604	41.415330	54.876367
H	45.027982	41.112291	55.906084
N	44.166189	41.659845	54.022724
C	44.792892	41.936986	52.824432
H	44.228242	42.154289	51.927023
C	41.667434	53.261816	56.513252
S	41.793652	51.985422	55.218941
H	41.123254	52.899796	57.385067
H	41.083883	54.073949	56.070778
C	39.934025	46.106493	57.543004
N	38.267000	44.532197	55.993696
C	37.399056	43.731897	55.280612
O	36.636598	42.928823	55.795736
N	37.193541	44.045308	53.911030
C	38.056882	44.773806	53.153980
C	39.351580	45.190535	53.847382
O	37.859272	45.063124	51.979766
C	40.626345	47.227013	53.993810
N	39.883201	46.373628	53.207263
C	41.544362	48.078016	53.355608
C	42.274124	49.042879	54.037272
C	43.378838	49.776044	53.303571
C	41.977815	49.255857	55.403031
C	42.460542	50.488347	56.117358
C	41.139231	48.356259	56.072278
C	40.529233	47.284764	55.406132
C	39.119239	45.298093	55.360737

N	39.765296	46.282773	56.080188
H	36.489471	43.482462	53.436225
H	43.103643	49.960682	52.262912
H	44.269227	49.135203	53.288285
H	43.654116	50.728752	53.760826
H	42.067871	50.516822	57.134251
H	43.551934	50.563332	56.151978
H	41.686404	47.937561	52.289382
H	40.963140	48.519059	57.127954
H	40.917360	46.476705	57.820102
H	39.863208	45.043632	57.746556
N	40.448532	44.226062	53.182688
C	40.121642	42.969777	52.445259
C	39.416148	41.841032	53.256219
O	39.149774	40.790302	52.637050
O	39.170317	42.117764	54.463925
C	41.683260	44.034166	53.965207
H	41.081055	42.581838	52.092448
H	39.552472	43.242346	51.559402
H	42.497550	43.903090	53.249690
H	41.609622	43.145600	54.589190
H	41.895075	44.916921	54.565787
H	40.536659	45.435288	52.594318
O	42.047968	39.675624	54.324981
H	42.736888	40.352767	54.176238
H	42.524799	38.866677	54.602874
O	39.384685	48.762685	50.701460
H	39.229452	47.966977	51.243879
H	39.800791	49.415320	51.336982
H_	38.945705	50.508158	46.484585
H_	47.967901	43.426530	52.093199
H_	43.041519	53.840092	56.937266
H_	38.842890	46.845922	58.484362

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C	39.447009	50.231234	47.909775
H	40.125371	49.367994	47.885182
H	40.031761	51.092097	48.246451
N	38.372965	49.946653	48.883324
H	37.558061	49.555036	48.406844
H	38.954427	48.735752	50.307796
H	38.028380	50.822918	49.272257
C	47.237661	42.071403	51.939960
H	46.763474	42.058651	50.953612
H	47.973706	41.261032	51.950113
C	46.154028	41.869617	52.950954
N	46.340776	41.573455	54.288380
H	47.225667	41.390780	54.764138
C	45.115627	41.471299	54.867210
H	44.984505	41.189035	55.901567
N	44.144391	41.703552	53.996120
C	44.789284	41.947437	52.799322
H	44.239337	42.133339	51.885670
C	41.674759	53.243122	56.502329
S	41.836702	51.984709	55.200162
H	41.125947	52.868949	57.367790
H	41.088214	54.049537	56.056278
C	39.966383	46.155218	57.579698
N	38.295078	44.593775	55.992627
C	37.462564	43.755613	55.258580
O	36.695295	42.969842	55.781700
N	37.345901	43.983687	53.864669
C	38.211018	44.720244	53.115351
C	39.264733	45.418269	53.908769
O	38.120786	44.885419	51.904153
C	40.638310	47.343439	54.047501
N	39.820385	46.481885	53.327712
C	41.547352	48.148906	53.363245

C	42.319262	49.082794	54.041104
C	43.415476	49.806769	53.290826
C	42.042934	49.285683	55.415516
C	42.541933	50.523037	56.108629
C	41.217325	48.402355	56.116724
C	40.559839	47.355327	55.456204
C	39.109987	45.410520	55.386425
N	39.794466	46.365605	56.120733
H	36.732020	43.332540	53.376315
H	43.104634	50.019326	52.265823
H	44.290807	49.149182	53.234473
H	43.723941	50.743122	53.758020
H	42.175609	50.554013	57.134298
H	43.634055	50.588408	56.113274
H	41.610992	48.050883	52.284196
H	41.059887	48.568986	57.174883
H	40.945380	46.525974	57.868108
H	39.899135	45.086827	57.754755
N	40.863453	43.773111	53.562932
C	40.588177	42.580427	52.733029
C	39.560037	41.644777	53.383002
O	39.157274	42.038825	54.519489
O	39.218059	40.615347	52.765943
C	41.932573	44.602565	53.016882
H	41.522156	42.012520	52.616550
H	40.262422	42.906352	51.739705
H	41.568080	45.138239	52.132566
H	42.782977	43.983540	52.710302
H	42.278973	45.309809	53.767646
H	41.046196	43.477269	54.524237
O	42.073347	39.679764	54.337623
H	42.794059	40.323577	54.199755
H	42.510179	38.839509	54.593198
O	39.416316	48.350418	51.106850

H	39.629566	46.725449	52.335181
H	39.740993	49.181499	51.536307
H_	39.093123	50.415643	46.902272
H_	47.755856	43.032019	52.049173
H_	42.642053	53.659596	56.810568
H_	39.181355	46.662492	58.244335

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C	36.998672	48.078186	53.544511
H	37.372605	47.152516	53.969263
H	37.373465	48.159015	52.520402
N	37.530580	49.163725	54.376447
H	38.170153	48.890703	55.113677
C	37.591211	50.458129	54.010177
N	36.938201	50.905431	52.934652
H	36.608945	50.276693	52.204022
H	36.978290	51.892327	52.701711
N	38.287182	51.322074	54.756341
H	38.737952	51.065838	55.634232
H	38.207033	52.312466	54.539927
C	47.236824	42.071932	51.940736
H	46.753379	42.064400	50.959101
H	47.975218	41.263371	51.939071
C	46.163455	41.861567	52.961302
N	46.366382	41.574697	54.298451
H	47.256056	41.401361	54.767741
C	45.147241	41.460011	54.887775
H	45.027115	41.180123	55.923942
N	44.167711	41.675652	54.025004
C	44.796711	41.922032	52.821937
H	44.234043	42.099846	51.915539
C	41.674813	53.246640	56.499641
S	41.843440	51.989922	55.195963
H	41.126125	52.867423	57.362625

H	41.089829	54.056384	56.057485
C	39.962123	46.153570	57.592887
N	38.289001	44.591640	56.021137
C	37.478153	43.744060	55.274043
O	36.725220	42.933947	55.795354
N	37.389226	43.948836	53.887191
C	38.213575	44.748174	53.134430
C	39.177079	45.543965	53.937794
O	38.068479	44.898700	51.924114
C	40.659139	47.279026	54.071033
N	39.875717	46.451628	53.312358
C	41.589302	48.090486	53.403519
C	42.336076	49.050621	54.066763
C	43.446087	49.765826	53.326631
C	42.027302	49.283280	55.430655
C	42.527781	50.522777	56.115864
C	41.179781	48.421527	56.133433
C	40.551421	47.347318	55.484960
C	39.073136	45.436404	55.401108
N	39.778138	46.376455	56.147134
H	36.848310	43.244169	53.390612
H	43.160304	49.949337	52.288292
H	44.331560	49.120985	53.306153
H	43.730310	50.720342	53.773988
H	42.151885	50.566555	57.137720
H	43.619595	50.585002	56.129101
H	41.714510	47.923015	52.339732
H	41.011435	48.607871	57.186792
H	40.941526	46.520620	57.885242
H	39.888656	45.084880	57.763917
N	40.977641	43.435794	53.261213
C	40.671863	42.235261	52.484604
C	39.618448	41.368020	53.193728
O	39.176279	41.870319	54.269968

O	39.276769	40.278522	52.667757
C	41.894180	44.360334	52.624703
H	41.568666	41.617250	52.319007
H	40.298541	42.537875	51.497604
H	41.364107	44.922394	51.843721
H	42.752179	43.859063	52.153290
H	42.285612	45.064104	53.361632
H	41.279186	43.168643	54.195735
O	42.099793	39.656060	54.365255
H	42.815615	40.306297	54.233870
H	42.536049	38.809323	54.598850
O	39.139445	48.589047	50.990419
H	39.362663	47.734073	51.405832
H	39.633175	49.262707	51.527787
H_	35.899362	48.036534	53.547405
H_	47.755019	43.032533	52.050144
H_	42.641808	53.661108	56.811113
H_	39.178453	46.661221	58.253420

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C	36.984784	47.995954	53.784886
H	37.250477	47.079962	54.317207
H	37.455794	47.981297	52.800345
N	37.461068	49.111521	54.607090
H	38.222035	48.853711	55.225024
C	37.619535	50.382731	54.036237
N	37.069217	50.644922	52.911531
H	37.887251	49.212771	51.456456
H	37.176201	51.624153	52.650827
N	38.429615	51.249353	54.748860
H	38.587583	51.080836	55.739517
H	38.240009	52.224831	54.528981
C	47.240270	42.070551	51.939653
H	46.765449	42.057216	50.954338

H	47.977393	41.260702	51.949273
C	46.158878	41.867995	52.952588
N	46.346285	41.578497	54.290993
H	47.232684	41.398611	54.767427
C	45.122255	41.476711	54.871304
H	44.992138	41.198795	55.906935
N	44.150935	41.701398	53.999127
C	44.793727	41.940975	52.800513
H	44.243297	42.118057	51.885604
C	41.700806	53.208355	56.471149
S	41.954298	51.972184	55.163120
H	41.142378	52.805435	57.317593
H	41.097557	53.999038	56.018559
C	39.956145	46.138760	57.595784
N	38.272728	44.555462	56.024420
C	37.442539	43.720979	55.283930
O	36.680109	42.925752	55.798578
N	37.321653	43.951323	53.889010
C	38.187909	44.685560	53.146531
C	39.232992	45.378003	53.949490
O	38.113235	44.861383	51.933757
C	40.600314	47.313820	54.062949
N	39.796629	46.429155	53.363085
C	41.503500	48.118147	53.370931
C	42.285278	49.046612	54.042831
C	43.402293	49.740771	53.296414
C	42.015326	49.257169	55.418098
C	42.542035	50.485085	56.110839
C	41.180319	48.386017	56.122282
C	40.526766	47.329952	55.471023
C	39.083960	45.376914	55.418532
N	39.776057	46.335084	56.140495
H	36.698252	43.309569	53.400671
H	43.099068	49.970208	52.272087

H	44.261623	49.063933	53.239942
H	43.732056	50.667858	53.768066
H	42.132954	50.543097	57.119353
H	43.635166	50.490684	56.170069
H	41.596657	47.992955	52.297791
H	41.031025	48.554572	57.180471
H	40.936015	46.509175	57.879268
H	39.885873	45.072023	57.782539
N	40.879912	43.722020	53.580597
C	40.629694	42.526704	52.751363
C	39.577458	41.606368	53.382089
O	39.155483	42.018671	54.505026
O	39.234824	40.575416	52.767397
C	41.941470	44.563762	53.044302
H	41.562980	41.950395	52.672369
H	40.337095	42.843276	51.744774
H	41.581461	45.084920	52.148554
H	42.807234	43.957949	52.753111
H	42.265428	45.286202	53.790743
H	41.055799	43.433080	54.544067
O	42.085479	39.672329	54.339563
H	42.813798	40.309022	54.210409
H	42.510039	38.825380	54.594051
O	38.757051	48.862825	51.138695
H	39.609264	46.590381	52.370235
H	39.384155	49.484316	51.608364
H_	35.893471	47.996687	53.654176
H_	47.757123	43.031501	52.049527
H_	42.649148	53.648251	56.802178
H_	39.173963	46.654633	58.252879

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state 1 -2071.385572309 H

C	45.023348	54.758348	49.632321
H	45.375048	53.734085	49.750502
H	45.826805	55.449373	49.893182
N	43.887411	54.949126	50.581604
H	44.043844	54.387365	51.447507
H	43.727933	55.944216	50.803153
H	42.994889	54.614566	50.174199
C	52.508308	45.633986	53.888490
H	51.882514	45.856531	53.018734
H	52.831870	44.591173	53.786172
C	51.655789	45.811387	55.113539
N	52.137818	45.879421	56.405865
H	53.126602	45.832192	56.642697
C	51.072078	45.923021	57.250109
H	51.181136	45.986103	58.324599
N	49.926224	45.874934	56.588535
C	50.288518	45.825800	55.253472
H	49.536261	45.784530	54.477255
C	49.361741	57.680962	57.579367
S	48.794680	56.404682	56.424293
H	48.907473	57.592166	58.563510
H	49.004724	58.612570	57.142041
C	46.052200	50.871840	58.835211
N	44.102826	49.572846	57.427635
C	43.071965	48.916305	56.786928
O	42.145209	48.380953	57.375002
N	42.995875	49.006159	55.372883
C	43.905066	49.600434	54.538509
C	45.024323	50.282399	55.249201
O	43.747246	49.668369	53.321316
C	46.676087	51.871180	55.245646
N	45.749805	51.122799	54.559026
C	47.605268	52.626790	54.508032
C	48.501248	53.492302	55.115011

C	49.578676	54.169748	54.290998
C	48.374258	53.689236	56.517314
C	49.159223	54.767096	57.224764
C	47.523143	52.880883	57.273092
C	46.722257	51.900665	56.661837
C	44.995081	50.220993	56.722164
N	45.910461	51.012612	57.380456
H	42.222676	48.489891	54.957761
H	50.514409	54.254581	54.852223
H	49.314090	55.190907	53.990588
H	49.788376	53.597113	53.385319
H	48.857285	54.830136	58.271595
H	50.236525	54.578323	57.173632
H	47.625943	52.460405	53.434388
H	47.472069	53.024892	58.345285
H	47.056850	51.152484	59.128038
H	45.870195	49.834912	59.093662
N	46.543013	48.128641	54.993278
C	46.004311	46.987479	54.254861
C	44.948528	46.269994	55.105788
O	44.696074	46.807995	56.216582
O	44.406748	45.223300	54.650580
C	47.708770	48.759124	54.405396
H	46.782691	46.258709	53.978727
H	45.546925	47.341360	53.320684
H	48.446404	48.033020	54.029601
H	48.202733	49.387611	55.151610
H	47.398589	49.392395	53.563494
H	46.687030	47.857318	55.962806
O	45.079046	53.070847	52.258820
H	45.141144	52.309254	52.876451
H	45.674074	53.766276	52.619013
H_	44.697890	54.921576	48.620011
H_	53.396706	46.282815	53.852169

H_	50.451289	57.756531	57.675988
H_	45.302168	51.513011	59.410955

state 2 -2071.372220588 H

C	45.022169	54.755696	49.634375
H	45.365894	53.728633	49.756454
H	45.827827	55.442417	49.896924
N	43.885085	54.954323	50.580553
H	44.046864	54.398064	51.451537
H	43.728920	55.951181	50.797491
H	42.991480	54.618924	50.177542
C	52.536961	45.603800	53.865948
H	51.919584	45.814052	52.986492
H	52.889076	44.571970	53.758377
C	51.664722	45.763995	55.075442
N	52.114203	45.837130	56.380079
H	53.095962	45.788251	56.645149
C	51.028252	45.898390	57.197119
H	51.105695	45.959073	58.274175
N	49.899251	45.857322	56.505556
C	50.294677	45.790146	55.180650
H	49.567057	45.720439	54.382868
C	49.363861	57.694623	57.591945
S	48.771050	56.435693	56.426180
H	48.915657	57.598439	58.577721
H	49.009605	58.632676	57.165601
C	46.025277	50.869375	58.815948
N	43.994386	49.595157	57.468071
C	42.963915	48.932697	56.848752
O	42.058768	48.341964	57.442804
N	42.895308	48.993167	55.440795
C	43.837470	49.589929	54.614339
C	44.919746	50.177596	55.310258
O	43.723114	49.605760	53.361543

C	46.738654	51.772986	55.212789
N	45.857916	50.920973	54.541248
C	47.657083	52.534041	54.488774
C	48.500290	53.470926	55.094673
C	49.552990	54.173855	54.261594
C	48.332651	53.705729	56.470973
C	49.128195	54.771153	57.185932
C	47.430411	52.916809	57.209910
C	46.672580	51.893798	56.623718
C	44.903506	50.213168	56.714296
N	45.870980	50.991129	57.371845
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H	50.502290	54.257911	54.802818
H	49.274862	55.200149	53.991214
H	49.749869	53.624256	53.338792
H	48.848517	54.821117	58.240027
H	50.204907	54.588247	57.111306
H	47.719455	52.363567	53.416191
H	47.344849	53.096617	58.274815
H	47.027803	51.165819	59.103565
H	45.857071	49.836185	59.100727
N	46.814010	47.828513	55.143211
C	46.110215	46.949148	54.194151
C	45.037649	46.211418	55.046288
O	44.834558	46.739458	56.170142
O	44.463021	45.217327	54.555050
C	47.930829	48.438665	55.025236
H	46.806063	46.254506	53.720130
H	45.606767	47.566090	53.439598
H	48.489627	48.384609	54.095450
H	48.313703	48.997482	55.873363
H	46.213890	50.442217	53.718581
H	46.253625	47.834899	56.022833
O	45.079081	53.085127	52.267144

H	44.986242	52.412656	52.972039
H	45.671873	53.782498	52.631970
H_	44.703041	54.918689	48.618740
H_	53.404399	46.277037	53.846961
H_	50.455089	57.762613	57.682483
H_	45.278309	51.507150	59.398704

state 3 triplet -2071.340405931 H

C	45.030073	54.744620	49.636249
H	45.387007	53.721366	49.746359
H	45.828340	55.438695	49.900708
N	43.897912	54.920437	50.593510
H	44.066129	54.348076	51.452359
H	43.740060	55.911404	50.832076
H	43.002809	54.590210	50.189130
C	52.530534	45.613709	53.872715
H	51.909135	45.831571	52.998882
H	52.874335	44.580175	53.761047
C	51.668804	45.775613	55.088535
N	52.125185	45.858467	56.389540
H	53.109056	45.821996	56.648716
C	51.042978	45.903929	57.213057
H	51.127139	45.964318	58.289309
N	49.910822	45.844527	56.529275
C	50.299462	45.779745	55.203192
H	49.568992	45.691690	54.409938
C	49.360052	57.678722	57.579156
S	48.780939	56.417579	56.410014
H	48.907242	57.578817	58.562707
H	49.002966	58.615453	57.152146
C	46.038384	50.869960	58.830907
N	44.038962	49.588749	57.464605
C	43.001914	48.936085	56.842608
O	42.093731	48.356655	57.436509

N	42.931103	49.005294	55.436595
C	43.856996	49.602289	54.596948
C	44.944263	50.266460	55.288737
O	43.713888	49.596350	53.361274
C	46.686322	51.785074	55.218718
N	45.813665	51.007443	54.534303
C	47.635685	52.542987	54.486279
C	48.494232	53.453752	55.080951
C	49.548501	54.154847	54.246164
C	48.357031	53.684157	56.475168
C	49.159116	54.756400	57.169197
C	47.480781	52.891881	57.234960
C	46.694299	51.891399	56.649174
C	44.923390	50.240033	56.719771
N	45.886136	51.005091	57.383805
H	42.153208	48.502759	55.014301
H	50.504881	54.216609	54.778497
H	49.280945	55.188448	53.995114
H	49.727591	53.615843	53.314287
H	48.898620	54.808849	58.228020
H	50.235844	54.580220	57.075737
H	47.678349	52.356872	53.416863
H	47.412225	53.077648	58.300124
H	47.040920	51.159681	59.119171
H	45.861273	49.836376	59.107421
N	46.779854	47.843168	54.913187
C	46.056260	46.902860	54.104690
C	45.019116	46.208207	55.028265
O	44.855302	46.773405	56.137470
O	44.423911	45.198591	54.588574
C	47.935641	48.595339	54.517537
H	46.742330	46.192541	53.624729
H	45.512825	47.441537	53.309005
H	48.723890	47.914461	54.170707

H	48.296733	49.173653	55.367382
H	47.662335	49.263878	53.690119
H	46.385811	47.878734	55.866816
O	45.099263	53.012845	52.270547
H	45.154981	52.239387	52.877503
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H_	50.450496	57.753873	57.675818
H_	45.294474	51.512300	59.409612

state 4 -2071.328520936 H

C	45.017781	54.764770	49.631980
H	45.352765	53.736417	49.759371
H	45.825717	55.449426	49.891931
N	43.876903	54.981103	50.570123
H	44.023916	54.434586	51.445372
H	43.722565	55.980804	50.774114
H	42.985336	54.643832	50.162939
C	52.522611	45.620501	53.872523
H	51.894590	45.854813	53.007717
H	52.863220	44.587371	53.742397
C	51.670221	45.769547	55.098913
N	52.149824	45.778098	56.395736
H	53.135953	45.708729	56.636677
C	51.083507	45.832220	57.236569
H	51.188370	45.843153	58.313028
N	49.939382	45.845635	56.569373
C	50.303356	45.829066	55.234210
H	49.551815	45.852656	54.456765
C	49.365194	57.665545	57.579166
S	48.799163	56.407826	56.392761
H	48.911280	57.549190	58.559778
H	48.997711	58.601672	57.159599

C	46.021699	50.856663	58.866938
N	43.966277	49.605193	57.525710
C	42.952920	48.924940	56.885253
O	42.049514	48.339039	57.469498
N	42.871660	49.011964	55.476205
C	43.836946	49.542633	54.653430
C	44.940013	50.140073	55.375678
O	43.719144	49.616294	53.419587
C	46.766804	51.653166	55.283193
N	45.951935	50.723471	54.659227
C	47.671416	52.403108	54.520484
C	48.476524	53.385189	55.092003
C	49.507848	54.096108	54.241746
C	48.315854	53.658938	56.472554
C	49.128326	54.737710	57.156976
C	47.433688	52.887106	57.243653
C	46.679164	51.843933	56.679841
C	44.884581	50.209225	56.796013
N	45.863329	50.971185	57.424724
H	42.103077	48.492292	55.055891
H	50.492011	54.084892	54.725172
H	49.270977	55.152389	54.072095
H	49.617930	53.610690	53.271137
H	48.865462	54.801703	58.214657
H	50.200243	54.532027	57.071911
H	47.736388	52.182615	53.459646
H	47.344548	53.101966	58.301650
H	47.022474	51.155561	59.152451
H	45.848440	49.825729	59.157248
N	47.037164	47.523432	54.652683
C	46.115530	46.578691	54.051566
C	44.994803	46.186183	55.024284
O	44.816738	46.924497	56.026846
O	44.316818	45.161587	54.721567

C	47.625050	48.540831	53.950823
H	46.638920	45.673057	53.731945
H	45.652154	47.033716	53.165264
H	47.742076	48.343837	52.893693
H	48.451955	49.037108	54.457626
H	46.443011	50.048636	53.978285
H	46.981796	47.577781	55.664423
O	45.076817	53.094416	52.220368
H	45.032909	52.370498	52.868934
H	45.681803	53.775752	52.594415
H_	44.701753	54.924467	48.616550
H_	53.398196	46.283954	53.849634
H_	50.454425	57.750396	57.676979
H_	45.269560	51.505433	59.421697

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C	45.022782	54.746483	49.634116
H	45.376513	53.722512	49.746733
H	45.821232	55.439667	49.899954
N	43.885329	54.926133	50.583214
H	44.046360	54.353017	51.444449
H	43.723988	55.917919	50.814902
H	42.994835	54.592781	50.171929
C	52.521524	45.620688	53.873752
H	51.895093	45.851927	53.006919
H	52.856761	44.585270	53.748209
C	51.667090	45.774454	55.097531
N	52.140305	45.834584	56.395106
H	53.126779	45.786276	56.640699
C	51.069273	45.877594	57.231678
H	51.168801	45.923073	58.307763
N	49.927951	45.837169	56.560429
C	50.298198	45.788999	55.227012

H	49.552243	45.733693	54.445012
C	49.363080	57.695103	57.591984
S	48.772312	56.433023	56.435119
H	48.915962	57.603018	58.578617
H	49.010705	58.631923	57.162528
C	46.062979	50.898489	58.818004
N	44.135786	49.589700	57.405223
C	43.098556	48.944477	56.768502
O	42.192634	48.369100	57.359259
N	43.036475	48.990424	55.355112
C	43.885229	49.691154	54.524762
C	45.029641	50.339290	55.225874
O	43.678438	49.835517	53.327467
C	46.668732	51.938851	55.227417
N	45.728432	51.211239	54.541252
C	47.599103	52.682420	54.482551
C	48.519082	53.526931	55.082046
C	49.588251	54.193971	54.241034
C	48.418828	53.716160	56.484493
C	49.228766	54.785224	57.167732
C	47.559291	52.920992	57.249083
C	46.736946	51.959008	56.642990
C	45.012713	50.274925	56.699055
N	45.922102	51.057320	57.360504
H	42.238094	48.511204	54.939766
H	50.556796	54.190093	54.753285
H	49.367031	55.243614	54.015268
H	49.717821	53.659884	53.297789
H	49.004267	54.818802	58.234909
H	50.301971	54.625435	57.028132
H	47.604115	52.516384	53.408706
H	47.528128	53.067619	58.322206
H	47.062311	51.188720	59.113931
H	45.895946	49.856290	59.065020

N	46.170301	48.318347	54.905220
C	45.720566	47.097442	55.568375
C	45.180417	46.106823	54.483317
O	45.500260	46.379074	53.313932
O	44.461774	45.150547	54.908015
C	47.567631	48.710046	55.097028
H	44.921574	47.308702	56.289924
H	46.542336	46.633411	56.119132
H	47.736013	49.054510	56.118134
H	47.808179	49.511772	54.393696
H	48.247710	47.869219	54.907915
H	46.012914	48.112769	53.903889
O	45.069260	53.073296	52.252823
H	45.119918	52.312657	52.874449
H	45.668946	53.763420	52.614666
H_	44.699265	54.915107	48.620882
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H_	50.453416	57.761559	57.681716
H_	45.307161	51.523124	59.403782

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C	45.012939	54.759427	49.634037
H	45.340432	53.727964	49.760728
H	45.826743	55.437605	49.892910
N	43.873811	54.984708	50.571634
H	44.024949	54.447638	51.454634
H	43.720297	55.987030	50.764625
H	42.981881	54.643541	50.169287
C	52.527616	45.609531	53.868569
H	51.904723	45.832329	52.996748
H	52.873325	44.576670	53.750151
C	51.664596	45.763866	55.086636
N	52.130061	45.821062	56.387405
H	53.114396	45.773791	56.640124

C	51.054157	45.869332	57.217199
H	51.146230	45.914998	58.293993
N	49.917116	45.833462	56.538293
C	50.295373	45.785611	55.206966
H	49.553694	45.745685	54.420008
C	49.363068	57.668617	57.577742
S	48.792925	56.410545	56.395682
H	48.908270	57.562170	58.559415
H	48.999480	58.603954	57.152762
C	46.033104	50.860233	58.846305
N	44.033880	49.550554	57.491019
C	43.000492	48.894967	56.866007
O	42.073687	48.357317	57.456593
N	42.926881	48.916714	55.443197
C	43.874290	49.451641	54.618520
C	45.226936	49.736402	55.301951
O	43.675686	49.733419	53.444792
C	46.697561	51.708429	55.218104
N	45.793036	50.859759	54.579847
C	47.583217	52.491526	54.469979
C	48.420271	53.442435	55.056213
C	49.442399	54.162178	54.199556
C	48.303833	53.670284	56.444340
C	49.118714	54.735170	57.148756
C	47.450762	52.855683	57.202727
C	46.686778	51.832045	56.622484
C	44.975987	50.127398	56.771013
N	45.874126	50.945560	57.387942
H	42.068215	48.535875	55.044282
H	50.406570	54.238763	54.714036
H	49.156564	55.193236	53.956888
H	49.614889	53.626220	53.264723
H	48.847049	54.787808	58.205138
H	50.192030	54.533476	57.071870

H	47.636581	52.314426	53.398830
H	47.391838	53.026735	58.270747
H	47.034827	51.168476	59.119610
H	45.876427	49.831167	59.148282
N	46.062833	48.552540	55.281248
C	45.552616	47.231244	55.655507
C	45.116966	46.282672	54.478789
O	45.500253	46.590875	53.348472
O	44.429105	45.274955	54.868217
C	47.514528	48.720999	55.213221
H	44.728584	47.310588	56.374385
H	46.355114	46.709457	56.182674
H	47.934378	49.239258	56.083340
H	47.815333	49.242169	54.298376
H	47.956832	47.726892	55.170339
H	46.027685	50.593951	53.626943
O	45.044346	53.154083	52.301458
H	44.881700	52.585204	53.073800
H	45.657011	53.866622	52.613094
H_	44.697316	54.920996	48.618009
H_	53.400960	46.276785	53.846327
H_	50.452836	57.750721	57.676037
H_	45.282269	51.505778	59.411674

$TS^{1,2}$ -2071.357323169 H

C	45.023465	54.751635	49.633126
H	45.364824	53.724349	49.753361
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H	44.037737	54.393286	51.446331
H	43.727344	55.946848	50.798908
H	42.992065	54.617206	50.169983
C	52.533172	45.609542	53.870550

H	51.912959	45.825906	52.994752
H	52.883682	44.578347	53.757385
C	51.667611	45.766870	55.085383
N	52.130175	45.830093	56.386756
H	53.114210	45.784204	56.642276
C	51.051723	45.877810	57.213847
H	51.140357	45.927766	58.290645
N	49.916834	45.838265	56.532813
C	50.298815	45.789343	55.204119
H	49.561220	45.746609	54.413721
C	49.368536	57.696570	57.594979
S	48.780557	56.438821	56.426340
H	48.919575	57.598193	58.579901
H	49.013050	58.633889	57.168239
C	46.030720	50.870965	58.840017
N	44.036944	49.612393	57.457274
C	43.008907	48.952511	56.822725
O	42.093809	48.382148	57.407306
N	42.941141	49.037971	55.413912
C	43.893238	49.598215	54.583689
C	45.005971	50.201472	55.292619
O	43.751619	49.629740	53.350450
C	46.759386	51.760996	55.254760
N	45.972327	50.828530	54.550671
C	47.659435	52.534465	54.515343
C	48.491762	53.479861	55.105456
C	49.543890	54.181209	54.270071
C	48.333960	53.709430	56.493933
C	49.132237	54.783551	57.197381
C	47.460228	52.918108	57.247606
C	46.706061	51.883664	56.658335
C	44.954007	50.218909	56.726329
N	45.898313	50.996136	57.390052
H	42.172429	48.524250	54.987929

H	50.493309	54.260978	54.810930
H	49.269490	55.207384	53.996780
H	49.738081	53.625887	53.350217
H	48.858313	54.839250	58.252449
H	50.206304	54.586090	57.119688
H	47.714949	52.337329	53.447840
H	47.380396	53.102675	58.312057
H	47.028090	51.166692	59.140541
H	45.859167	49.835945	59.114107
N	46.716280	47.909058	54.955285
C	46.024111	46.896660	54.170049
C	44.971144	46.226100	55.074403
O	44.783114	46.788227	56.183181
O	44.380207	45.206475	54.634912
C	47.581056	48.818987	54.472825
H	46.732953	46.143118	53.807630
H	45.529470	47.360289	53.306297
H	47.993459	48.608164	53.486911
H	48.265369	49.248092	55.207882
H	46.807936	49.928059	54.201804
H	46.480300	47.855727	55.946692
O	45.083489	53.035647	52.250265
H	45.128505	52.247506	52.827950
H	45.684990	53.704563	52.642170
H_	44.705012	54.918577	48.617960
H_	53.402190	46.281237	53.850251
H_	50.459752	57.765621	57.685035
H_	45.272825	51.508415	59.405515

TS[5,6] -2071.270957441 H

C	45.026253	54.747063	49.633589
H	45.373342	53.719728	49.748566
H	45.828343	55.435228	49.898138
N	43.890334	54.934276	50.584109

H	44.048187	54.372828	51.451365
H	43.735685	55.930033	50.809832
H	42.997017	54.605331	50.176992
C	52.529471	45.605899	53.863625
H	51.911621	45.822966	52.986943
H	52.878307	44.573852	53.751353
C	51.659382	45.761965	55.075516
N	52.118231	45.820200	56.378352
H	53.101447	45.770001	56.635879
C	51.038562	45.874643	57.202537
H	51.125820	45.922358	58.279465
N	49.904650	45.841964	56.517773
C	50.289628	45.790493	55.188057
H	49.551930	45.747695	54.397425
C	49.364773	57.655218	57.571853
S	48.811244	56.415509	56.361942
H	48.910190	57.520142	58.549782
H	48.991729	58.595740	57.166537
C	46.053560	50.893620	58.836128
N	44.066382	49.543596	57.523080
C	43.008417	48.906980	56.920425
O	42.103566	48.355100	57.531922
N	42.887759	48.969578	55.507791
C	43.820377	49.499535	54.663365
C	45.169786	49.859127	55.318524
O	43.626088	49.698070	53.476649
C	46.653311	51.706679	55.154820
N	45.787411	50.854876	54.483675
C	47.544947	52.507986	54.412869
C	48.396852	53.442424	54.994664
C	49.424119	54.152870	54.137858
C	48.302879	53.673415	56.387725
C	49.136406	54.725184	57.087066
C	47.456145	52.860939	57.148778

C	46.686896	51.840895	56.570460
C	44.995557	50.131080	56.790477
N	45.883371	50.966245	57.373188
H	42.029540	48.576700	55.118707
H	50.407373	54.157364	54.622743
H	49.180095	55.206590	53.956813
H	49.540798	53.654453	53.174491
H	48.881337	54.769432	58.148373
H	50.208172	54.521759	56.991805
H	47.590926	52.321337	53.343516
H	47.405044	53.031747	58.217694
H	47.048452	51.228087	59.098012
H	45.924309	49.861248	59.140902
N	46.102898	48.684178	54.976972
C	45.632571	47.308195	55.412526
C	45.175341	46.273635	54.326008
O	45.587064	46.449278	53.180962
O	44.459470	45.339796	54.828951
C	47.560766	48.876252	55.312650
H	44.829974	47.442816	56.137634
H	46.458454	46.837968	55.949185
H	47.707101	49.211124	56.330706
H	48.018643	49.590319	54.629273
H	48.045113	47.912115	55.166912
H	46.154255	49.575729	53.938651
O	45.041587	53.050266	52.310725
H	45.063540	52.288944	52.929961
H	45.658457	53.720596	52.678688
H_L	44.704027	54.914243	48.619195
H_L	53.400800	46.275766	53.845097
H_L	50.453589	57.746047	57.673124
H_L	45.291983	51.519741	59.408572

model 3

state 1 -1975.028173127 H

C	34.008327	38.666919	38.838615
H	33.832052	39.692750	39.177404
H	33.081441	38.330341	38.369915
C	34.340721	37.840596	40.045421
N	34.119864	36.480735	40.152383
H	33.771777	35.836989	39.439707
C	34.522233	36.084743	41.381749
H	34.441416	35.060206	41.718903
N	35.006724	37.099787	42.087151
C	34.864130	38.203264	41.263386
H	35.108998	39.195510	41.610924
C	44.106342	43.246376	40.823688
S	44.223495	44.937162	41.513529
H	43.154179	43.061368	40.325659
H	44.229638	42.542736	41.649624
C	40.490539	41.308863	45.638425
N	38.184903	41.913253	46.990818
C	37.016675	42.169510	47.696318
O	36.772852	41.639231	48.766459
N	36.119506	43.127690	47.191341
C	36.253843	43.843824	46.026139
C	37.593956	43.670677	45.382036
O	35.425274	44.651377	45.638091
C	39.264112	44.494729	44.051245
N	37.955842	44.520016	44.468361
C	39.731586	45.560766	43.257555
C	41.065872	45.701318	42.919328
C	41.525399	46.913499	42.152888
C	41.983126	44.718316	43.380385
C	43.478620	44.876684	43.209574
C	41.535208	43.652129	44.156588
C	40.179803	43.507408	44.495492
C	38.467737	42.644968	45.947386

N	39.698199	42.497224	45.330200
H	35.221250	43.181997	47.666067
H	41.969706	46.631769	41.194062
H	42.286325	47.476448	42.707728
H	40.682053	47.584282	41.970651
H	43.802289	45.848501	43.596319
H	44.011056	44.118975	43.783278
H	39.004686	46.316379	42.973208
H	42.272151	42.978782	44.576154
H	41.192540	41.122408	44.829690
H	39.810087	40.474142	45.759760
N	34.719767	41.390952	44.867228
C	33.284184	41.701181	44.970698
C	32.625989	40.964442	46.144295
O	32.917722	39.717575	46.257548
O	31.861125	41.598631	46.896806
C	35.253122	41.915656	43.614347
H	33.155862	42.780246	45.103228
H	32.744551	41.401014	44.053736
H	35.090582	42.997422	43.588276
H	36.334618	41.749096	43.566144
H	34.786348	41.474281	42.717019
H	34.774753	40.372563	44.824468
O	33.239111	38.731172	43.721961
H	33.136834	38.925797	44.681344
H	33.903445	38.026910	43.641688
H_	34.793401	38.700115	38.068836
H_	44.925578	43.094828	40.109510
H_	41.071106	41.416230	46.611170

state 2 -1975.009150416 H

C	33.990669	38.648559	38.813454
H	33.791835	39.672697	39.146903
H	33.076898	38.288806	38.336045

C	34.320161	37.836173	40.030916
N	34.083487	36.483728	40.178933
H	33.754643	35.817856	39.475207
C	34.448028	36.124555	41.431193
H	34.347903	35.111374	41.798269
N	34.924311	37.160924	42.115418
C	34.824392	38.232434	41.243720
H	35.098326	39.232796	41.544867
C	44.109148	43.265998	40.829125
S	44.285085	44.938372	41.555322
H	43.150061	43.121404	40.328160
H	44.207318	42.545459	41.645631
C	40.525829	41.261709	45.625935
N	38.252362	41.881978	47.077933
C	37.120152	42.150399	47.798773
O	36.839516	41.623776	48.877359
N	36.219761	43.104845	47.273048
C	36.402293	43.825652	46.100025
C	37.580231	43.491319	45.403897
O	35.544923	44.665567	45.700719
C	39.267754	44.389121	43.965142
N	37.907095	44.164935	44.194028
C	39.728510	45.488997	43.239861
C	41.083212	45.672362	42.945202
C	41.528610	46.900885	42.195314
C	42.004413	44.721219	43.408267
C	43.492201	44.895997	43.249855
C	41.546014	43.653875	44.202302
C	40.193816	43.458310	44.486475
C	38.471469	42.567694	45.955751
N	39.695655	42.392508	45.288079
H	35.404405	43.314635	47.840451
H	42.003893	46.636255	41.243529
H	42.268963	47.473788	42.771224

H	40.672994	47.555986	41.998199
H	43.811639	45.883507	43.601352
H	44.028275	44.151214	43.837728
H	39.008252	46.237172	42.910756
H	42.288040	42.988826	44.627666
H	41.252171	41.100225	44.828739
H	39.891100	40.388781	45.747224
N	34.182822	41.347540	44.206631
C	33.099221	41.959367	44.979676
C	32.565711	41.072650	46.145260
O	32.936049	39.854917	46.207876
O	31.797767	41.670310	46.910033
C	35.239443	41.980815	43.863354
H	33.450591	42.920983	45.361241
H	32.268694	42.144542	44.291290
H	37.315798	44.973386	44.062971
H	36.006013	41.460610	43.305357
H	35.339728	43.032548	44.115556
H	34.021088	40.327985	43.937500
O	33.334586	38.852590	43.765171
H	33.176215	38.860616	44.738099
H	33.946256	38.120273	43.536921
H_	34.784687	38.693215	38.056289
H_	44.924768	43.102806	40.113095
H_	41.090341	41.394495	46.606987

state 3 triplet -1975.024622342 H

C	34.001483	38.673358	38.830361
H	33.828281	39.699920	39.166212
H	33.072424	38.338737	38.365277
C	34.337740	37.846257	40.035968
N	34.137741	36.485345	40.144204
H	33.800566	35.834528	39.431043
C	34.543338	36.091131	41.370730

H	34.471141	35.066106	41.708701
N	35.014351	37.112712	42.078580
C	34.856416	38.212299	41.254097
H	35.117422	39.208177	41.580069
C	44.126377	43.265138	40.835108
S	44.327806	44.927240	41.572032
H	43.162756	43.133754	40.341929
H	44.227335	42.533538	41.638512
C	40.539348	41.254488	45.597762
N	38.263438	41.894647	47.062443
C	37.142103	42.188268	47.793788
O	36.854793	41.653512	48.864647
N	36.269530	43.181549	47.290982
C	36.440875	43.880046	46.103160
C	37.591754	43.489976	45.379621
O	35.628748	44.765799	45.721736
C	39.285778	44.391613	43.951638
N	37.921699	44.161963	44.175588
C	39.745178	45.492778	43.228679
C	41.098764	45.682398	42.935143
C	41.531077	46.914922	42.182531
C	42.022862	44.734207	43.405626
C	43.514699	44.900808	43.255880
C	41.561876	43.661341	44.189850
C	40.208797	43.460242	44.468468
C	38.486490	42.568444	45.936315
N	39.707885	42.389052	45.264888
H	35.462654	43.400789	47.867397
H	42.023934	46.657349	41.239381
H	42.243834	47.517225	42.760780
H	40.665832	47.548696	41.964970
H	43.843262	45.883029	43.610508
H	44.041748	44.157696	43.851680
H	39.023113	46.237737	42.897527

H	42.306358	43.000694	44.617234
H	41.259106	41.085233	44.799525
H	39.907197	40.382246	45.722766
N	34.465966	41.167899	44.236916
C	33.069447	41.435628	44.584922
C	32.661412	40.806017	45.954412
O	33.116447	39.641015	46.170981
O	31.905106	41.481795	46.665535
C	35.370439	42.060847	44.013605
H	32.899777	42.512152	44.570663
H	32.474633	40.935888	43.814669
H	37.328269	44.971425	44.054911
H	36.374338	41.778012	43.733264
H	35.101867	43.110661	44.091954
H	34.683395	40.171570	44.180902
O	33.030078	38.058508	43.856088
H	33.112143	38.298587	44.797955
H	33.837759	37.572017	43.602523
H_	34.782647	38.704071	38.057049
H_	44.931784	43.100875	40.107607
H_	41.112727	41.385473	46.573171

state 4 -1974960523992 H

C	33.997746	38.654287	38.826879
H	33.805637	39.678271	39.161999
H	33.079025	38.303570	38.352799
C	34.328331	37.836197	40.041438
N	34.095223	36.479498	40.169167
H	33.755256	35.825713	39.461093
C	34.477498	36.100291	41.409717
H	34.382195	35.082305	41.762975
N	34.961665	37.123574	42.105082
C	34.841895	38.213624	41.258457
H	35.108020	39.208971	41.581023

C	44.106485	43.260109	40.826783
S	44.272192	44.935885	41.542898
H	43.150454	43.106617	40.324932
H	44.209860	42.540955	41.641988
C	40.527881	41.273147	45.637801
N	38.235063	41.880973	47.075876
C	37.074898	42.123132	47.754641
O	36.796375	41.632841	48.844987
N	36.131320	43.040158	47.194796
C	36.324912	43.786397	46.058784
C	37.581002	43.497659	45.402416
O	35.563047	44.698425	45.683782
C	39.288892	44.419218	43.997756
N	37.958206	44.286771	44.362847
C	39.733441	45.500691	43.231950
C	41.077861	45.675916	42.921044
C	41.520630	46.900477	42.166514
C	42.006742	44.714956	43.395052
C	43.497040	44.890539	43.237093
C	41.560713	43.651145	44.183562
C	40.207071	43.463894	44.500476
C	38.493002	42.584579	45.975387
N	39.723576	42.434264	45.320223
H	35.292559	43.206632	47.742399
H	41.991348	46.635121	41.215215
H	42.257144	47.483174	42.736261
H	40.666671	47.554154	41.969389
H	43.817373	45.872295	43.601008
H	44.034113	44.147277	43.823883
H	39.007401	46.249759	42.920821
H	42.303639	42.989557	44.611877
H	41.247228	41.093974	44.841360
H	39.869175	40.419926	45.756589
N	34.219689	41.302452	44.287690

C	33.117772	41.899833	45.011420
C	32.563301	41.044853	46.172952
O	32.897663	39.813683	46.240015
O	31.814476	41.651974	46.960757
C	35.203511	42.048542	43.760521
H	33.449744	42.860411	45.412179
H	32.282804	42.125170	44.331279
H	37.258059	44.938961	44.041327
H	35.911754	41.573298	43.099774
H	35.126477	43.125502	43.819777
H	34.087778	40.317406	44.015911
O	33.224743	38.685058	43.786552
H	33.129821	38.823420	44.756551
H	33.894839	37.992283	43.636689
H_	34.787927	38.696631	38.062944
H_	44.923378	43.100224	40.111546
H_	41.092316	41.397972	46.617144

state 5 -1975.027869863 H

C	33.999095	38.657312	38.830039
H	33.809370	39.682455	39.163723
H	33.079048	38.308962	38.356304
C	34.329464	37.838722	40.043622
N	34.106642	36.481697	40.172059
H	33.764821	35.826557	39.465698
C	34.507210	36.104165	41.408333
H	34.422919	35.085693	41.762694
N	34.995791	37.129745	42.097201
C	34.852095	38.218335	41.256269
H	35.127215	39.213828	41.569886
C	44.123886	43.266106	40.831787
S	44.351032	44.927925	41.557834
H	43.160751	43.140229	40.335350
H	44.220698	42.536441	41.637896

C	40.506866	41.339651	45.618290
N	38.166447	41.972113	46.897913
C	36.909256	42.159969	47.481445
O	36.623210	41.628646	48.542126
N	35.981456	42.995897	46.842735
C	36.281380	43.911088	45.870964
C	37.656786	43.756831	45.297306
O	35.531292	44.817680	45.541157
C	39.367332	44.551832	44.008322
N	38.052064	44.600884	44.394565
C	39.853421	45.604744	43.212519
C	41.192492	45.732348	42.896109
C	41.667683	46.937685	42.130052
C	42.090149	44.744641	43.381289
C	43.586373	44.890770	43.239064
C	41.622018	43.683790	44.154436
C	40.261478	43.555144	44.475895
C	38.500167	42.712113	45.878235
N	39.748965	42.549752	45.299239
H	34.970712	42.803067	47.019210
H	42.101219	46.655862	41.166643
H	42.438406	47.487933	42.682600
H	40.831942	47.620341	41.956563
H	43.910285	45.864921	43.617727
H	44.101454	44.136701	43.831005
H	39.134423	46.360411	42.909863
H	42.349012	43.006131	44.585851
H	41.216947	41.139345	44.819084
H	39.803941	40.521327	45.724259
N	34.172586	42.349113	44.168961
C	33.002472	41.574446	44.564924
C	33.133249	41.045203	46.002956
O	33.576403	41.826858	46.882604
O	32.753364	39.856562	46.237828

C	35.311643	41.496282	43.885248
H	32.147139	42.261865	44.563079
H	32.782354	40.726113	43.896270
H	35.670889	41.057110	44.821072
H	35.095383	40.662452	43.194245
H	36.126926	42.097259	43.466811
H	33.952307	42.899780	43.343359
O	32.899784	38.053793	43.892314
H	32.961926	38.552342	44.729876
H	33.797518	37.760135	43.661685
H_	34.788958	38.696748	38.065223
H_	44.932885	43.100585	40.110929
H_	41.077612	41.426444	46.600889

state 6 -1974.963971468 H

C	33.994325	38.644020	38.826127
H	33.787809	39.667977	39.152717
H	33.084449	38.280946	38.344253
C	34.318577	37.840046	40.050730
N	34.113034	36.480097	40.189880
H	33.795437	35.812595	39.483275
C	34.462068	36.131271	41.451488
H	34.379960	35.115575	41.815531
N	34.899478	37.176374	42.146157
C	34.788998	38.247210	41.276274
H	35.023785	39.252843	41.592338
C	44.026494	43.202229	40.793485
S	43.922532	44.917179	41.445934
H	43.114526	42.918964	40.267392
H	44.172679	42.534541	41.644713
C	40.317993	41.223453	45.727722
N	37.987738	41.829526	47.079466
C	36.888666	42.158968	47.848494
O	36.609152	41.612208	48.894485

N	36.178246	43.357334	47.506743
C	36.295463	43.973686	46.305023
C	37.013005	43.178340	45.232852
O	35.747342	45.007718	45.949034
C	38.942735	44.301261	44.038734
N	37.597472	44.097404	44.263727
C	39.412092	45.428296	43.340319
C	40.755864	45.608320	43.010940
C	41.190494	46.847286	42.269818
C	41.693400	44.634202	43.407132
C	43.181317	44.802590	43.183572
C	41.238750	43.553796	44.177960
C	39.889270	43.365032	44.497781
C	38.170382	42.395224	45.923531
N	39.424909	42.322752	45.355582
H	35.448453	43.637790	48.161792
H	41.674529	46.585634	41.323599
H	41.916720	47.432500	42.850230
H	40.336296	47.494221	42.059888
H	43.530009	45.765088	43.574250
H	43.740714	44.028553	43.711473
H	38.693601	46.196541	43.058780
H	41.981032	42.872249	44.572343
H	40.978438	41.012014	44.888354
H	39.700092	40.360996	45.946041
N	35.908023	42.389987	44.717167
C	34.475067	42.538020	45.088261
C	33.903431	41.555456	46.138847
O	32.772786	41.809808	46.600409
O	34.616379	40.538758	46.387826
C	36.051054	41.811062	43.403524
H	34.197134	43.557382	45.354650
H	33.910705	42.322969	44.176029
H	35.756912	40.758681	43.423596

H	35.406147	42.303812	42.681897
H	37.086815	41.945332	43.083354
H	36.961837	44.844267	44.019539
O	33.646192	39.310352	43.988381
H	34.107576	39.565875	44.813485
H	34.084653	38.494071	43.689947
H_	34.792075	38.690676	38.070728
H_	44.882577	43.086433	40.112114
H_	40.961566	41.403212	46.657547

$TS^{1,2}$ -1974.964853697 H -1472.31 cm^{-1}

C	33.999801	38.657773	38.831649
H	33.810838	39.683011	39.163906
H	33.080085	38.306945	38.360309
C	34.326352	37.846780	40.052426
N	34.120069	36.485736	40.182973
H	33.803686	35.821931	39.471921
C	34.463750	36.127619	41.442972
H	34.377558	35.110721	41.802598
N	34.896440	37.168539	42.146626
C	34.788865	38.245663	41.284269
H	35.018606	39.249580	41.611165
C	44.036002	43.210703	40.790500
S	43.943405	44.940691	41.394354
H	43.121685	42.913546	40.278147
H	44.190343	42.562432	41.655546
C	40.398042	41.262345	45.734794
N	38.153878	41.892675	47.209451
C	37.008897	42.153451	47.944127
O	36.741843	41.559747	48.978835
N	36.139496	43.169696	47.505297
C	36.279400	43.880309	46.324955
C	37.528722	43.645108	45.651421
O	35.426846	44.659721	45.888401

C	39.055141	44.327962	44.042101
N	37.703486	44.287687	44.462452
C	39.485897	45.414372	43.269038
C	40.821419	45.612101	42.928231
C	41.240533	46.855728	42.187735
C	41.771894	44.660346	43.361161
C	43.258828	44.850878	43.132957
C	41.359218	43.599535	44.172267
C	40.013815	43.418879	44.535032
C	38.394077	42.625103	46.137878
N	39.584222	42.426405	45.438426
H	35.265551	43.260599	48.017024
H	41.711339	46.610552	41.231606
H	41.969483	47.438863	42.767268
H	40.377075	47.499981	42.005664
H	43.585909	45.823991	43.517111
H	43.833748	44.095134	43.670198
H	38.740864	46.160252	43.004371
H	42.119611	42.949306	44.587881
H	41.057329	41.056210	44.893331
H	39.739081	40.420755	45.920307
N	35.646749	41.964987	44.537668
C	34.201312	42.169704	44.675723
C	33.660094	41.385121	45.901061
O	34.451844	40.475761	46.318661
O	32.524379	41.649888	46.320499
C	36.364293	42.337899	43.461211
H	33.991212	43.238720	44.782305
H	33.697697	41.779127	43.783639
H	36.928619	43.631588	43.686317
H	37.352497	41.901537	43.389063
H	35.807451	42.406000	42.539456
H	36.000069	41.270644	45.198285
O	33.306557	38.905637	44.074730

H	33.834688	39.232144	44.825948
H	33.862568	38.216928	43.666224
H_	34.789519	38.696688	38.067455
H_	44.886684	43.087666	40.106930
H_	41.034906	41.395380	46.670315

TS[5,6] -1974.905407749 H -1764.77cm-1

C	33.995580	38.648173	38.828010
H	33.791924	39.674332	39.147792
H	33.083856	38.284233	38.349445
C	34.315338	37.848963	40.058176
N	34.112114	36.488302	40.198322
H	33.803552	35.818086	39.489651
C	34.443003	36.143228	41.465561
H	34.357745	35.127938	41.829723
N	34.866056	37.191647	42.164803
C	34.766450	38.260015	41.290696
H	35.005485	39.266159	41.604845
C	44.026781	43.201766	40.794530
S	43.891291	44.929785	41.398523
H	43.118527	42.894142	40.276194
H	44.184204	42.555711	41.661608
C	40.368315	41.239782	45.715911
N	38.113144	41.835342	47.202380
C	36.975851	42.113341	47.941810
O	36.710013	41.533003	48.984403
N	36.131744	43.162339	47.530802
C	36.280979	43.866875	46.360359
C	37.408675	43.459312	45.559453
O	35.571845	44.808113	46.006921
C	38.928968	44.269539	43.993509
N	37.599067	44.170106	44.420935
C	39.377220	45.378131	43.250279
C	40.718368	45.588337	42.928547

C	41.145277	46.841658	42.206636
C	41.678282	44.643791	43.353153
C	43.165921	44.834387	43.134404
C	41.257621	43.576610	44.151848
C	39.913590	43.377712	44.494752
C	38.328911	42.518352	46.096335
N	39.513198	42.362912	45.397644
H	35.310582	43.335623	48.105336
H	41.642391	46.598694	41.262798
H	41.859551	47.426565	42.802242
H	40.286492	47.483798	41.998374
H	43.495857	45.805609	43.520873
H	43.732926	44.073611	43.674551
H	38.643532	46.136582	42.987721
H	42.014833	42.925539	44.570639
H	41.041926	41.041696	44.884805
H	39.736640	40.379955	45.908760
N	35.453435	42.829300	44.223439
C	34.105077	42.753677	44.638958
C	33.754919	41.655089	45.873904
O	32.629069	41.836278	46.348490
O	34.610142	40.776221	46.125711
C	35.822548	41.712388	43.412926
H	33.740553	43.709639	44.992454
H	33.441106	42.346832	43.863287
H	35.597120	40.771302	43.926431
H	35.272198	41.700524	42.460909
H	36.893167	41.804970	43.210329
H	36.470321	43.878710	43.958717
O	33.317651	38.933949	44.189791
H	33.904452	39.349712	44.847033
H	33.874093	38.271605	43.737944
H_	34.791909	38.687133	38.071078
H_	44.883820	43.087120	40.110464

H_ 40.987354 41.406753 46.659534