

Supporting information

-for-

The Conversion of Protonated Cytosine-SO₃⁻ to Uracil-SO₃⁻: Insights into the Novel Induced Hydrolytic Deamination through Bisulfite Catalysis

Lingxia Jin,^{a,b} Wenliang Wang^{*,a} Daodao Hu^a Jian Lü^{*,c}

^a*Key Laboratory for Macromolecular Science of Shaanxi Province, School of Chemistry and Chemical Engineering, Shaanxi Normal University, Xi'an 710062*

^b*School of Chemical & Environment Science, Shaanxi University of Technology, Hanzhong, Shaanxi 723001*

^c*Xi'an Modern Chemistry Research Institute, Xi'an 710065, People's Republic of China*

* Corresponding authors. Tel: +86-29-81530815 Fax: +86-29-81530727; e-mail: wlwang@snnu.edu.cn (W. L. Wang), lujian204@263.net (J. Lü).

Table and Figure from calculation

Contents:

Table S1 The energy information on the SO_3^{2-} -induced hydrolytic deamination

Fig.S1 Optimized stationary structures (bond distances in Å) in the gas phase for the SO_3^{2-} -induced hydrolytic deamination of protonated Cyt-SO_3^- (path E) are at B3LYP/6-311++G(d,p) level of theory.

Fig.S2 Optimized stationary structures (bond distances in Å) in the aqueous phase for the SO_3^{2-} -induced hydrolytic deamination of protonated Cyt-SO_3^- (path E) are at B3LYP/6-311++G(d,p) level of theory.

Fig. S3 Optimized stationary structures (bond distances in Å) in the aqueous phase for the direct hydrolytic deamination of protonated Cyt-SO_3^- (path A) are at B3LYP/6-311++G(d,p) level of theory.

Fig. S4 Optimized stationary structures (bond distances in Å) in the aqueous phase for the HSO_3^- -induced hydrolytic deamination of protonated Cyt-SO_3^- (path B—the HSO_3^- group toward the left side of protonated Cyt-SO_3^-) are at B3LYP/6-311++G(d,p) level of theory.

Fig. S5 Optimized stationary structures (bond distances in Å) in the aqueous phase for the HSO_3^- -induced hydrolytic deamination of protonated Cyt-SO_3^- (path C—the HSO_3^- group toward the above side of protonated Cyt-SO_3^-) are at B3LYP/6-311++G(d,p) level of theory.

Fig. S6 Optimized stationary structures (bond distances in Å) in the aqueous phase for the HSO_3^- -induced hydrolytic deamination of protonated Cyt-SO_3^- (path D—the HSO_3^- group toward the right side of protonated Cyt-SO_3^-) are at B3LYP/6-311++G(d,p) level of theory.

Section S1 The corresponding structure coordinates of all paths (paths A-E).

Table S1 Relative Energies ^a (in kcal·mol⁻¹) for the SO₃²⁻-induced Reaction (path E)

System	MP2//B3LYP method ^b		PCM ^c	
	ΔG^g	$\Delta G^{g\ddagger}$	ΔG^s	$\Delta G^{s\ddagger}$
R ^d +SO ₃ ²⁻	0.00	0.00	0.00	
E-RC	-163.42	-144.62	-28.81	
E-TS1	-136.08	-113.79	2.54	
E-IM1	-157.85	-137.79	-24.06	
E-TS2	-155.20	-135.70	-11.82	
E-IM2	-157.04	-137.50	-16.68	
E-TS3	-146.44	-124.37	-4.35	
E-IM3	-157.64	-137.45	-16.93	
E-TS4	-125.01	-103.57	--	
E-P	-167.31	-150.01	-25.08	
E-RC→E-IM1		22.29		31.35
E-IM1→E-IM2		2.09		12.24
E-IM2→E-IM3		13.13		12.33
E-IM3→E-P		33.88		--

^a ΔG^g , relative free energy in the gas phase; $\Delta G^{g\ddagger}$, activation free energy in the gas phase; ΔG^s , relative free energy in the aqueous phase; $\Delta G^{s\ddagger}$, activation free energy in the aqueous phase. ^b MP2/6-311++G(3df,3pd)//B3LYP/6-311++G(d,p) level. ^c MP2/6-311++G(3df,3pd)//B3LYP/6-311++G(d,p) with PCM model. ^d denotes protonated Cyt-SO₃⁻+H₂O.

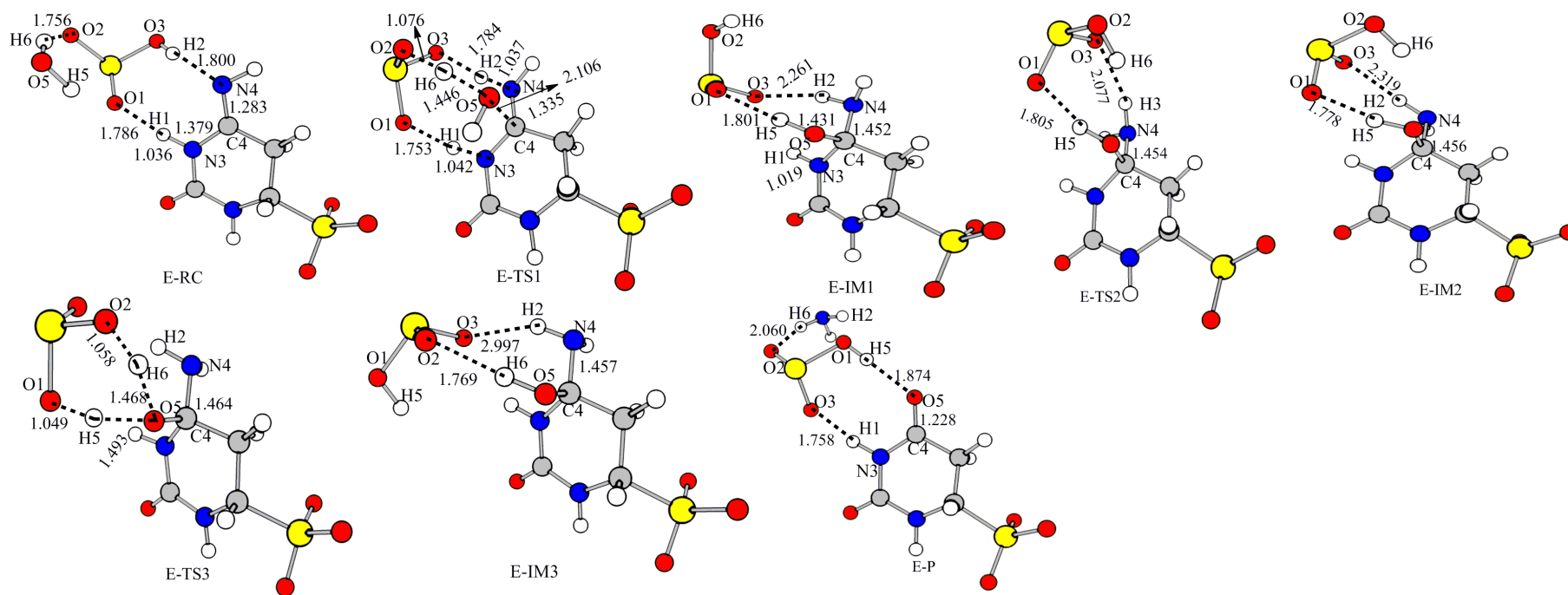


Fig.S1.

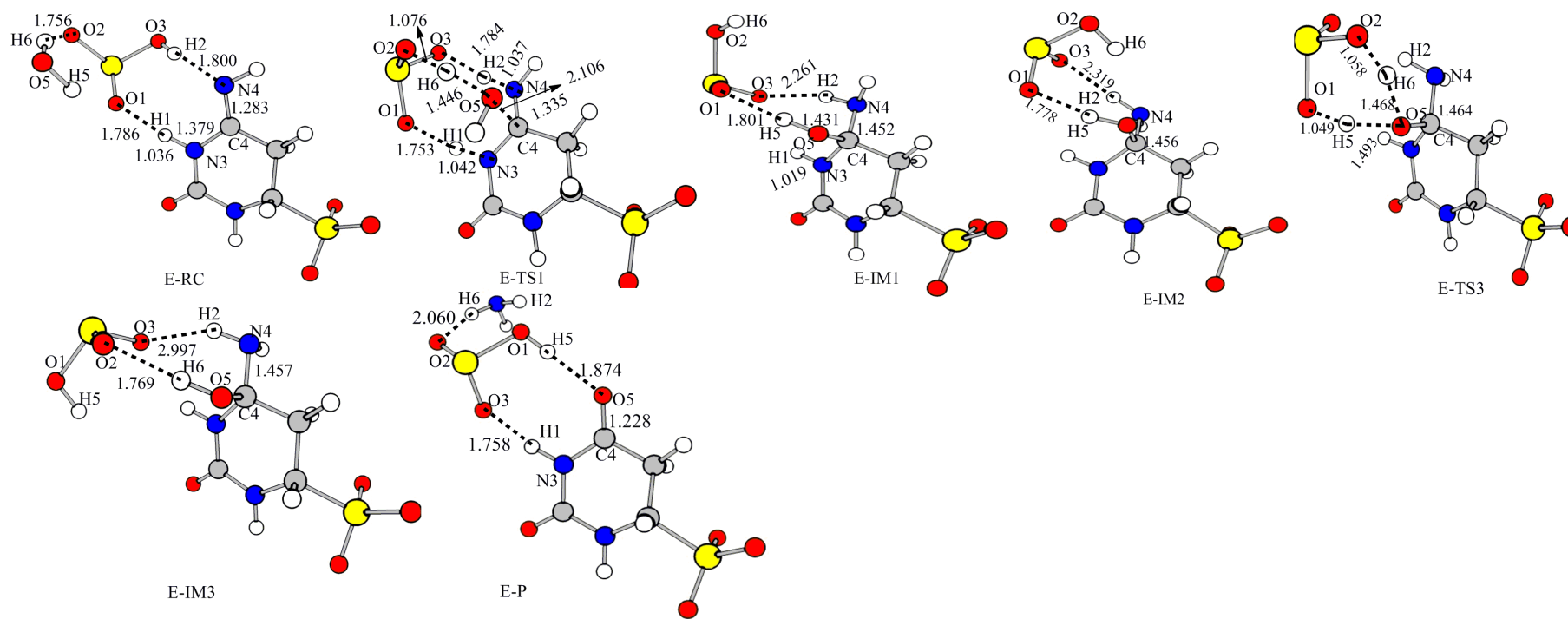


Fig.S2.

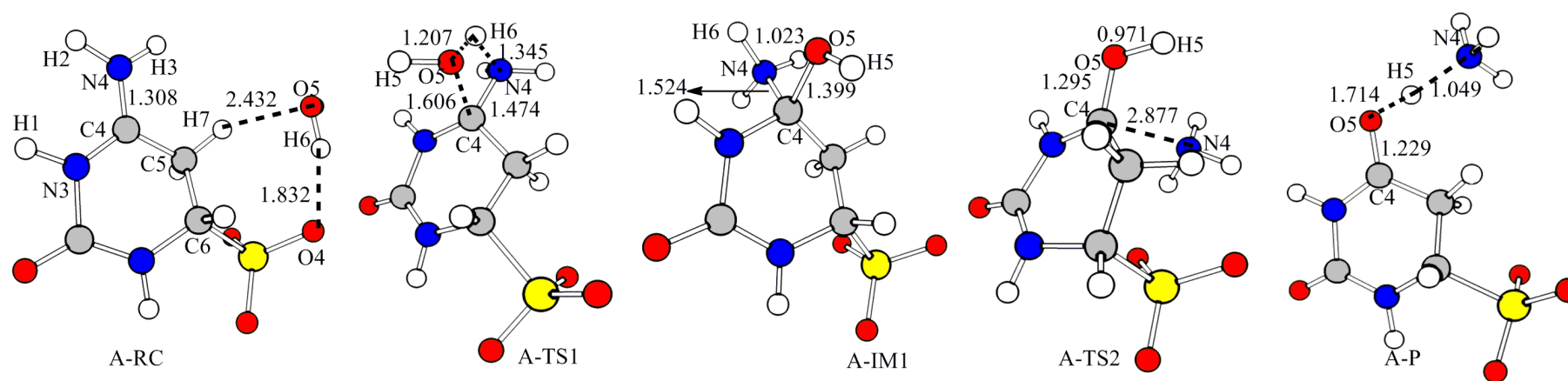


Fig.S3.

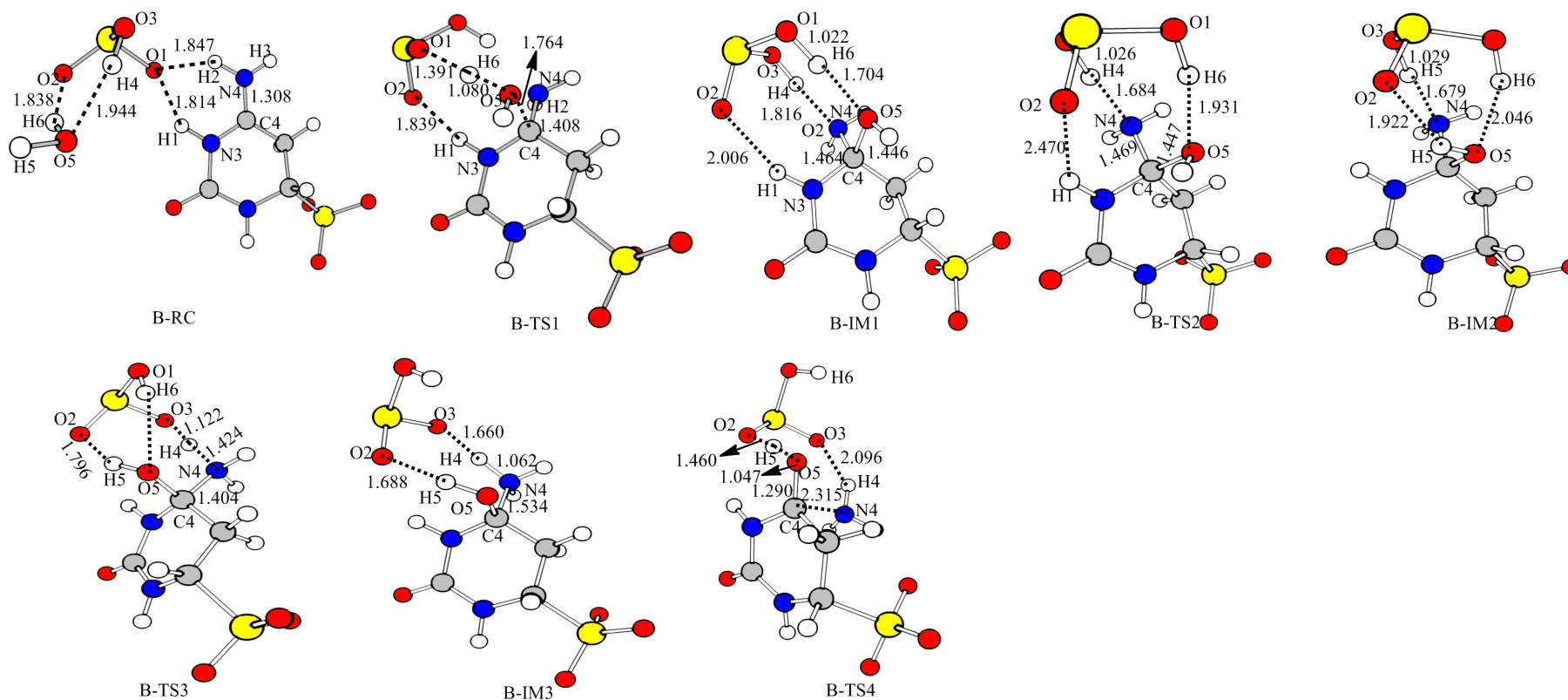


Fig.S4.

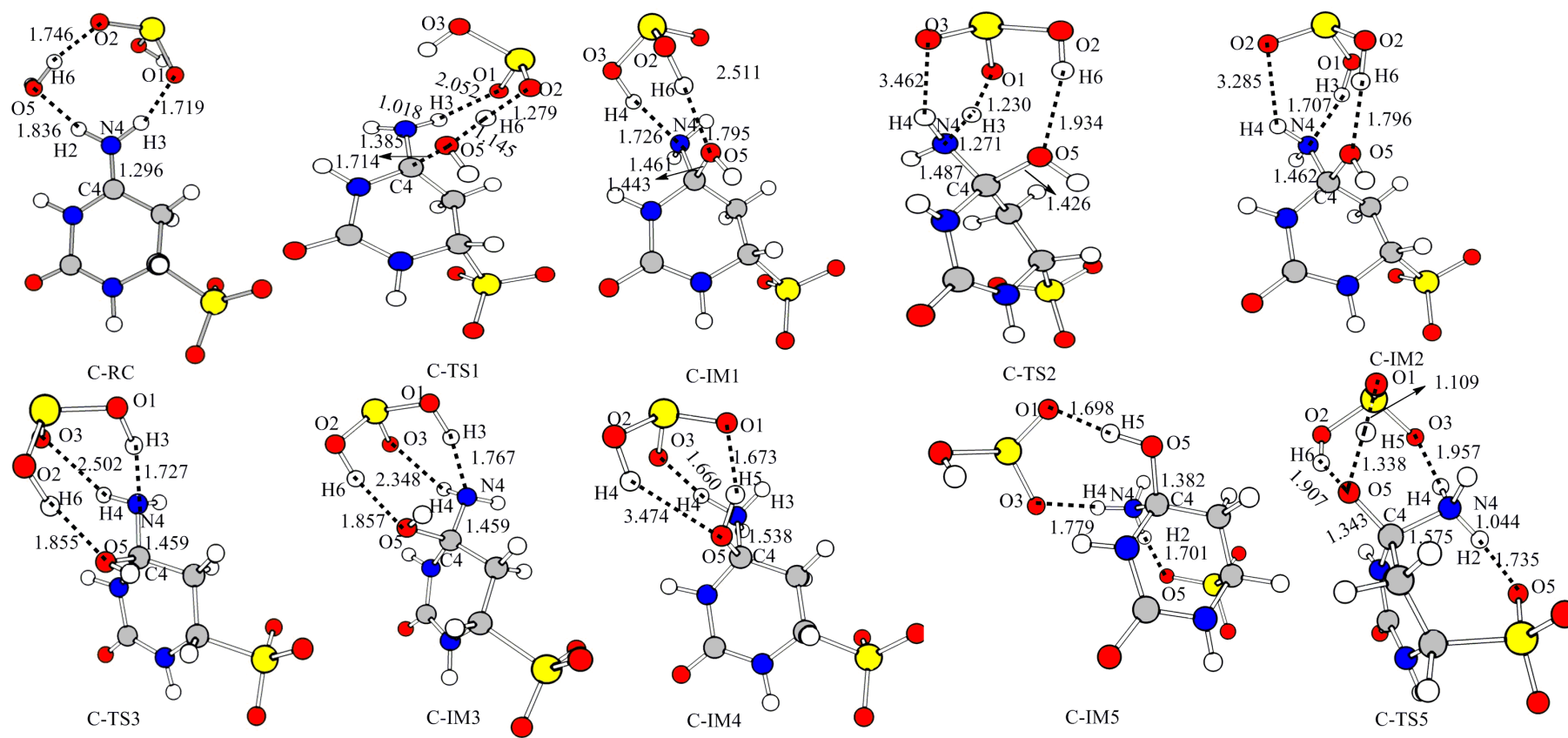


Fig.S5.

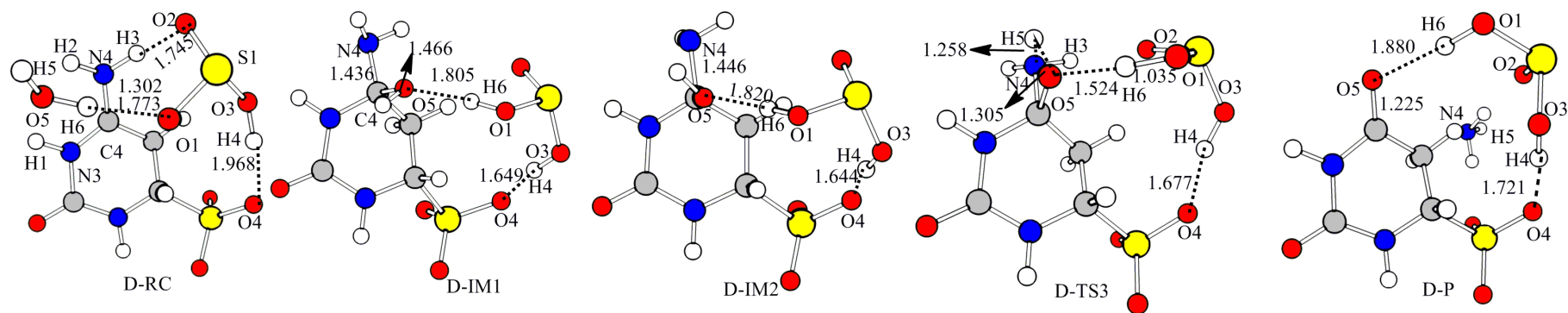


Fig.S6.

Section S1 The corresponding structure coordinates of all paths (paths A-E).

Path A

A-RC

N	0.82668200	-1.32289400	-0.31615900
C	2.15274700	-1.20703000	-0.20208800
O	3.00859600	-2.05773000	-0.19203400
N	2.60207500	0.19011400	-0.08570900
C	1.82045100	1.22699000	0.17880800
N	2.30586100	2.45433800	0.29098500
C	0.37225100	0.97505900	0.38669400
C	-0.09715900	-0.20407400	-0.44918600
H	3.28776500	2.67018800	0.19124800
H	-0.23734100	0.06419200	-1.49989900
H	1.66818900	3.22060200	0.45411100
H	0.42457600	-2.25347400	-0.40555800
H	-0.22011800	1.86801200	0.16783100
S	-1.78428600	-0.76082900	0.15222900
O	-1.85581700	-2.13386700	-0.38307300
O	-2.68696300	0.22554700	-0.49879600
O	-1.68994500	-0.63785400	1.62065500
H	0.21879500	0.72255500	1.44791300
H	3.61071000	0.27331100	-0.14904900
O	-1.89030100	2.86756800	-0.58892200
H	-2.58701400	3.51172300	-0.43642500
H	-2.33360800	1.99026500	-0.57765400

A-TS1

N	0.07510800	1.32863500	-0.33143900
C	-1.14836600	1.75877900	0.00105000
O	-1.53942900	2.89435200	0.15386700
N	-2.11941400	0.69156000	0.19032300
C	-1.85057700	-0.64102800	0.12068600
N	-2.82272700	-1.51168700	0.85543700
C	-0.40283600	-1.00140700	0.25774400
C	0.47611800	-0.05532400	-0.53846100
H	-3.43445100	-1.00761100	1.49345600
H	0.49869100	-0.30516300	-1.60224000
H	-2.36009200	-2.27108200	1.35300200
H	0.82358500	2.01501100	-0.39989400
H	-0.22906300	-2.02968600	-0.06075300
S	2.25261800	-0.24462100	0.05859800
O	2.85159300	1.01602100	-0.43430500
O	2.67786300	-1.48684900	-0.61207300
O	2.09870700	-0.33877900	1.52970100
H	-0.12307400	-0.90556700	1.31622500
H	-3.05803700	1.04745500	0.31852900
O	-2.42319700	-1.34607200	-1.27452500
H	-2.70559800	-0.70435000	-1.94324000
H	-3.15493900	-1.76014300	-0.36031900

A-IM1

N	-0.16352200	1.51072400	-0.72428000
C	0.46113600	0.27797200	-1.08842600
C	-0.55649300	-0.85557700	-1.20054800
N	-2.02351000	0.44206200	0.22959000
C	-1.30657700	1.62047700	0.04680600
O	-1.70232500	2.68214500	0.48184400
H	0.38848000	2.35704000	-0.75376500
C	-1.55773700	-0.89982400	-0.03596500
N	-0.93449400	-1.49087800	1.15264400
H	0.50375900	-0.60867800	1.57124400
H	-2.80346200	0.54597200	0.86533300

O	-2.67427800	-1.72147300	-0.34766600
H	-3.17035800	-1.31408000	-1.06914600
H	-0.69088400	-2.46123200	0.96084800
H	-1.61017500	-1.50046400	1.91402200
S	1.91128100	-0.13247100	0.03637100
O	2.27686500	-1.52315300	-0.22582200
O	2.87933000	0.94040300	-0.11781200
O	1.29471900	0.01250700	1.51465700
H	-1.12518100	-0.69212100	-2.11949100
H	-0.04480500	-1.81361500	-1.28950500
H	0.98636100	0.39162200	-2.03995200

A-TS2

N	-0.08479700	1.54053100	-0.22472700
C	-1.34684900	1.68303500	0.18137600
O	-1.85887200	2.56848900	0.81958700
N	-2.22353600	0.57745300	-0.23360100
C	-1.82592700	-0.56201100	-0.72543600
N	-1.20708000	-2.00091100	1.82691800
C	-0.41087800	-0.79809000	-1.08911600
C	0.51537900	0.41466200	-0.92941600
H	-1.72071000	-1.57876400	2.59623000
H	0.88795300	0.75432300	-1.89639700
H	-0.25191200	-1.63174800	1.86677500
H	0.59333900	2.19900000	0.15450900
H	-0.38472000	-1.17353800	-2.11621700
S	2.04247300	-0.10715900	0.03548900
O	2.76667500	-0.94350500	-0.93555000
O	1.46422900	-0.85566700	1.18673000
O	2.63277400	1.20215300	0.37934800
H	-0.06406700	-1.60625000	-0.43124000
H	-3.19011100	0.69153700	0.05803300
O	-2.75712500	-1.45476600	-0.94309500
H	-2.37118800	-2.32749600	-1.10916000
H	-1.14206400	-2.99124200	2.04891400

A-P

N	0.64263800	1.51466000	-0.17765700
C	-0.40263300	2.32813300	0.00726600
O	-0.42789300	3.51028200	0.24832200
N	-1.69541600	1.63718300	-0.09887900
C	-1.87586700	0.32982300	-0.07883800
N	-3.36523300	-2.68079600	0.09423400
C	-0.67635000	-0.54365500	-0.02019100
C	0.56137500	0.12385300	-0.59528900
H	-4.30836000	-2.87324500	0.42567800
H	0.60977200	0.03903800	-1.68408600
H	-2.72121500	-3.11882700	0.75078300
H	1.57968300	1.90182300	-0.09516600
H	-0.85955800	-1.49136800	-0.52587300
S	2.06408600	-0.79471700	0.05428200
O	3.14185900	0.18631300	-0.19195600
O	2.06151000	-2.00983100	-0.78363100
O	1.71914500	-1.01742400	1.48004900
H	-0.46702600	-0.76725400	1.04078400
H	-2.49897900	2.25512200	-0.04897900
O	-3.07768100	-0.12011600	-0.06789600
H	-3.15184500	-1.18705200	-0.01638200
H	-3.25643100	-3.16281200	-0.79595200

Path B

B-RC

N	-1.97179300	1.19029800	0.47598300
---	-------------	------------	------------

C	-0.74803800	1.71958900	0.26113000
O	-0.43904800	2.88548500	0.37894700
N	0.25284900	0.76336900	-0.13651200
C	-0.01276700	-0.47769100	-0.53238900
N	0.94594500	-1.30296100	-0.89682700
C	-1.44344400	-0.91624200	-0.59995300
C	-2.27761600	-0.22680200	0.46486400
H	0.67718500	-2.23183600	-1.18201300
H	-2.12925400	-0.67590700	1.45230500
H	4.12927400	-1.63845100	-0.28381500
H	-2.71189000	1.81221600	0.78242400
H	-1.52273700	-1.99970200	-0.50448600
S	-4.09862100	-0.45645300	0.10591100
O	-4.21180800	-0.25182700	-1.35846400
O	-4.70984300	0.61223400	0.93536000
O	-4.34477900	-1.84320100	0.56132900
H	-1.84755300	-0.63285400	-1.58114900
H	1.23481000	1.11406100	-0.19227500
O	4.92881000	-2.16017300	1.48232500
H	1.97156700	-1.09178700	-0.88096200
H	5.85955100	-2.37378800	1.59233900
S	4.22286700	0.67257400	-0.48983300
O	4.69773900	0.48136900	0.92609800
O	3.66969000	-1.03115300	-0.89460800
O	2.88083000	1.34380400	-0.56430800
H	4.88056900	-1.18026100	1.54655000

B-TS1

N	1.57915800	1.28673100	-0.36015400
C	0.44679100	1.86139200	0.12242100
O	0.25836700	3.06424800	0.20080900
N	-0.55335800	0.96295400	0.54553200
C	-0.46638200	-0.41558200	0.44333600
N	-1.38058500	-1.13145300	1.21359400
C	0.95316900	-0.93477800	0.45152200
C	1.86046300	-0.13374300	-0.46482500
H	-0.96823500	-1.85994500	1.77690500
H	1.79440100	-0.47254800	-1.50453900
H	-3.61284600	-1.87873000	0.40993400
H	2.34817400	1.90834200	-0.58397100
H	0.96910300	-1.98732800	0.17156500
S	3.65998400	-0.43596200	-0.03647100
O	3.71479900	-0.36616500	1.44383600
O	4.32939600	0.68970700	-0.73918600
O	3.91057800	-1.78014900	-0.60675500
H	1.33047500	-0.83403400	1.47551500
H	-1.46950900	1.36976600	0.72086600
O	-0.99377200	-0.82105700	-1.16776700
H	-2.07661500	-0.56019600	1.68206800
H	-0.45945600	-0.33508200	-1.81109500
S	-4.25836500	0.12508200	-0.25535600
O	-3.28022600	-0.07630000	-1.45350700
O	-4.49096500	-1.48763700	0.26156100
O	-3.50528100	0.77660000	0.87503700
H	-2.10531600	-0.46147600	-1.28777000

B-IM1

N	1.61148200	1.34992700	-0.19425100
C	0.39405800	1.85123100	0.15786600
O	0.14585500	3.04641200	0.22493500
N	-0.59259900	0.90236100	0.46480200
C	-0.44781800	-0.51072900	0.32363700
N	-1.31534100	-1.16755700	1.31590500
C	1.02453100	-0.90588300	0.45376800

C	1.90600400	-0.04522000	-0.43004100
H	-1.11587200	-2.16561600	1.31419100
H	1.80745500	-0.30674900	-1.49390800
H	-3.06617500	-1.08293900	1.11830900
H	2.34621800	2.01608700	-0.39631700
H	1.14476300	-1.95962400	0.19625800
S	3.71568100	-0.37944400	-0.09238900
O	3.82757900	-0.43611900	1.38513300
O	4.37194400	0.79494600	-0.72327700
O	3.93577100	-1.67411100	-0.78192000
H	1.34557700	-0.76174500	1.48877700
H	-1.54126500	1.27195200	0.45111300
O	-0.98866800	-1.01131000	-0.93718700
H	-1.07242800	-0.80437600	2.23365300
H	-0.35220400	-0.81121200	-1.63491800
S	-4.41263900	0.01296900	-0.23023800
O	-3.70785400	-0.71553000	-1.53748800
O	-4.06106100	-1.07319600	0.94685500
O	-3.62345400	1.23476800	0.06685100
H	-2.73107400	-0.78857500	-1.40292800

B-TS2

N	1.71698700	1.35311500	-0.25521900
C	0.55604500	1.95769600	0.09757000
O	0.38993600	3.16863400	0.14877700
N	-0.50479900	1.09199100	0.42441800
C	-0.47532900	-0.33126500	0.35109300
N	-1.34087000	-0.86946300	1.42586600
C	0.96098800	-0.84439200	0.45060100
C	1.90026300	-0.07217300	-0.45470000
H	-0.95105800	-0.57372900	2.31801000
H	1.76947600	-0.34974500	-1.50584200
H	-3.03369600	-0.51340200	1.37209000
H	2.50944000	1.94844000	-0.46337400
H	0.97921200	-1.90318300	0.18818300
S	3.68084100	-0.51083300	-0.09205600
O	3.78073600	-0.52780400	1.38869800
O	4.41447600	0.60380200	-0.74886000
O	3.83310100	-1.83631600	-0.73819200
H	1.31607300	-0.73183600	1.47901200
H	-1.41341800	1.54087500	0.43657800
O	-1.08100300	-0.82178400	-0.88077400
H	-1.21058600	-0.05087700	-1.44711700
S	-4.42210300	-0.08621400	-0.28502100
O	-3.82570200	-1.44929700	-1.02990800
O	-4.03769600	-0.40617300	1.27001200
O	-3.56479600	1.04289000	-0.72929800
H	-2.83986100	-1.40729300	-1.02445500
H	-1.28883900	-1.88680200	1.40367800

B-IM2

N	1.82959300	1.33170100	-0.40450600
C	0.78686400	2.10417300	-0.01918800
O	0.76722600	3.32793000	-0.06764100
N	-0.32680800	1.40968000	0.48517200
C	-0.49419000	-0.01039800	0.46167400
N	-1.38727000	-0.36103300	1.59921400
C	0.86704000	-0.69446200	0.55108300
C	1.84848300	-0.11888100	-0.45254700
H	-1.00091600	0.04724000	2.44756700
H	1.64450900	-0.48188600	-1.46364800
H	-3.06287700	-0.09950800	1.37988600
H	2.66614200	1.80564500	-0.72238400
H	0.74657900	-1.76411300	0.37144600
S	3.58298500	-0.71104600	-0.09054400

O	3.74807100	-0.55528000	1.37673700
O	4.40586800	0.22125400	-0.90699900
O	3.55996900	-2.11621200	-0.56403800
H	1.27703900	-0.55070100	1.55453300
H	-1.15086100	1.98871700	0.57253500
O	-1.14855500	-0.47888500	-0.73020100
H	-1.73943300	0.22583200	-1.05388700
S	-4.42867100	-0.31421100	-0.36066500
O	-3.67557000	-1.76981400	-0.66083900
O	-4.06903400	-0.09862000	1.21120100
O	-3.66731600	0.70361300	-1.13897800
H	-2.70699800	-1.61196600	-0.74976200
H	-1.36527700	-1.37206100	1.72383800

B-TS3

N	1.78909500	1.35062600	-0.31392900
C	0.67289400	2.02959000	0.04204900
O	0.57140000	3.24881000	0.04994000
N	-0.41931600	1.23827000	0.45342500
C	-0.48420800	-0.18730800	0.32082900
N	-1.35157600	-0.67735500	1.46460500
C	0.91002800	-0.79452000	0.42582300
C	1.89521400	-0.08614500	-0.48317700
H	-1.30124600	-1.69503800	1.49268800
H	1.75552100	-0.37431200	-1.52889300
H	-2.62130800	-0.35950400	1.33645400
H	2.60317400	1.89786400	-0.56519400
H	0.86058800	-1.85141000	0.15913400
S	3.64179100	-0.61759600	-0.08456500
O	3.72676600	-0.58010900	1.39749600
O	4.44969200	0.42053000	-0.77733500
O	3.71555200	-1.97672600	-0.67249200
H	1.27457600	-0.70578800	1.45327900
H	-1.29340100	1.74859000	0.42291900
O	-1.10072400	-0.63722100	-0.86566400
H	-0.97261700	-0.32163300	2.34073700
H	-1.79862500	0.00416100	-1.12004800
S	-4.41347500	-0.06612000	-0.19976900
O	-4.21686000	-1.66860600	-0.73312700
O	-3.78597400	-0.12350200	1.24091600
O	-3.47957300	0.72108600	-1.07584900
H	-3.29293500	-1.78808700	-1.01466000

B-IM3

N	1.79106500	1.36423200	-0.15347900
C	0.58857200	1.91941800	0.13360100
O	0.38601600	3.11877400	0.24591600
N	-0.47517500	1.01168000	0.33821000
C	-0.39435900	-0.39618700	0.10922100
N	-1.19894900	-1.05432100	1.28604200
C	1.03486100	-0.91090100	0.21982900
C	2.01048200	-0.02013500	-0.52244700
H	-1.07968100	-2.06606700	1.23859800
H	1.95062900	-0.16451400	-1.60523600
H	-2.26182700	-0.83948300	1.22768500
H	2.57538900	1.99382100	-0.27213000
H	1.07648300	-1.92431700	-0.18186600
S	3.76491900	-0.49308600	-0.07982800
O	3.74537100	-0.67860100	1.39394900
O	4.53397500	0.68955800	-0.54586800
O	3.97817500	-1.73817400	-0.85463200
H	1.35004200	-0.93150500	1.26788400
H	-1.38233100	1.43282200	0.16078500
O	-0.99699000	-0.84724400	-1.05104900
H	-0.83496000	-0.71486300	2.17577100

H	-1.83337400	-0.33313400	-1.18128700
S	-4.40139500	0.21435300	0.03953400
O	-5.23486600	-0.97670800	-0.85945800
O	-3.78294500	-0.58430800	1.19440600
O	-3.26054800	0.61573800	-0.88520800
H	-4.57817300	-1.58962100	-1.22658600

B-TS4

N	-1.85850400	1.52273300	-0.00922900
C	-0.62985900	2.07451500	-0.12025700
O	-0.36236800	3.07153900	-0.76964100
N	0.39204400	1.39977200	0.59194500
C	0.27659300	0.09314300	0.97172700
N	0.29533800	-0.84133300	-1.00971200
C	-1.07973600	-0.37422200	1.41582600
C	-2.26121300	0.38060100	0.79313200
H	-0.54558400	-1.40469900	-1.16469800
H	-2.94211400	0.71496500	1.57928600
H	1.16360300	-1.37411100	-1.05472900
H	-2.58708100	1.92201000	-0.58924500
H	-1.07837000	-0.22937600	2.50119600
S	-3.37421300	-0.72961700	-0.22460800
O	-4.23902700	0.25919700	-0.91601900
O	-4.03605300	-1.55609600	0.80884000
O	-2.47858800	-1.49975900	-1.13473700
H	-1.16346800	-1.44600200	1.24238600
H	1.33344800	1.73382800	0.39545900
O	1.29082100	-0.49713200	1.50510700
H	0.33379900	-0.14668700	-1.75051700
H	2.21087300	-0.07306200	1.14989000
S	4.14965500	-0.03636400	-0.53316800
O	5.26542000	-0.95311700	0.40190100
O	3.34853400	-1.10048500	-1.22754000
O	3.26292200	0.61769200	0.56096800
H	4.81766300	-1.78830600	0.61074900

B-P

N	2.20718400	1.36426600	-0.10380600
C	1.29755800	2.34102400	0.04667900
O	1.46909300	3.41596700	0.59518900
N	0.02642500	2.05575300	-0.53230700
C	-0.43289800	0.83356700	-0.89481800
N	-0.38453400	0.06151200	2.21444900
C	0.55903400	-0.29301900	-0.92524700
C	2.02374100	0.12626000	-0.84158400
H	0.42155000	-0.56316500	2.18505400
H	2.47472900	0.20761400	-1.83501300
H	-1.23616200	-0.49164300	2.14661000
H	3.11771400	1.49463700	0.32320600
H	0.38083200	-0.88965300	-1.82040000
S	3.03590500	-1.19434100	0.01641600
O	4.29823600	-0.46782000	0.31602700
O	3.13905100	-2.26037600	-1.00395500
O	2.23738500	-1.55669200	1.21752700
H	0.31451000	-0.92146800	-0.06310300
H	-0.65968600	2.78305300	-0.37766300
O	-1.62762000	0.66788900	-1.18243300
H	-0.38653500	0.51773300	3.12085300
H	-3.27619700	1.11609100	-0.39761300
S	-4.26025000	-0.76222200	0.17497000
O	-3.49942500	-1.32798100	-1.18049300
O	-3.38974000	-1.03065200	1.33609500
O	-4.19438000	0.86901500	-0.14699800
H	-2.65017300	-0.84068300	-1.31031900

Path C

C-RC

N	2.65887500	1.28557200	-0.14029200
C	1.83004100	2.32064400	0.06231900
O	2.12828800	3.48021900	0.27810200
N	0.43920600	1.97369200	-0.00439100
C	-0.07073900	0.72319700	-0.01116400
N	-1.35293300	0.53439700	-0.04862100
C	0.90527000	-0.40821800	0.08154600
C	2.24763200	-0.05180600	-0.54011200
H	-2.02515800	1.32214100	-0.05284800
H	2.22979300	-0.14488800	-1.63009100
H	-1.81198600	-0.40846200	-0.08636700
H	3.66084400	1.44739000	-0.09906500
H	0.48705700	-1.30573000	-0.37360800
S	3.58145200	-1.24213000	0.02551800
O	4.81185200	-0.46126000	-0.27080700
O	3.35761200	-2.42867200	-0.82523900
O	3.30400700	-1.43499400	1.46861300
H	1.07113700	-0.62377400	1.14620800
H	-0.18019800	2.77420000	0.02677800
O	-3.51067000	2.31577500	-0.15346000
H	-4.28760200	-1.46720400	1.96241000
H	-3.95028800	2.55911100	0.66732000
S	-4.45708300	-1.28565100	-0.26020800
O	-4.70788300	0.05196900	-0.90959300
O	-2.97210300	-1.61156700	-0.19895600
O	-4.76581400	-0.82445600	1.42118200
H	-4.03507300	1.53707400	-0.48685100

C-TS1

N	2.23840100	1.16167700	-0.47404100
C	1.64729300	2.31895400	-0.11025600
O	2.15234200	3.42891800	-0.17412700
N	0.32421600	2.19169700	0.37763100
C	-0.40477200	1.02315000	0.43190800
N	-1.53521600	1.12263200	1.22896700
C	0.46580900	-0.21622700	0.51562900
C	1.64543400	-0.16529000	-0.44183400
H	-1.43715400	1.74888800	2.01321400
H	1.37592300	-0.49312500	-1.45294000
H	-2.03093600	0.24720100	1.42578600
H	3.21709600	1.19864500	-0.73991700
H	-0.13219700	-1.11214400	0.35426600
S	2.98397900	-1.38386500	0.05474400
O	4.14344500	-0.87444800	-0.72670600
O	2.43822100	-2.68276300	-0.39501900
O	3.11079500	-1.22429000	1.52254400
H	0.85599000	-0.25264800	1.53912100
H	-0.17472300	3.06968100	0.41341200
O	-1.16369700	0.86926300	-1.15919400
H	-4.48160700	1.03710400	0.26187500
H	-0.52425500	0.52836100	-1.79984300
S	-4.02012200	-1.08593300	-0.18033200
O	-3.06225500	-0.62724000	-1.31477400
O	-3.24811600	-1.14109100	1.10851500
O	-5.03743800	0.28672900	-0.00223300
H	-2.07060800	0.16860900	-1.17818700

C-IM1

N	2.03904200	1.32700600	-0.37583800
C	1.03963500	2.18131500	-0.03353500
O	1.13650800	3.40140300	-0.05510600

N	-0.15852900	1.57649100	0.37259000
C	-0.45325600	0.17879800	0.28241900
N	-1.50621800	-0.11720100	1.25508600
C	0.84114600	-0.61580900	0.47726300
C	1.93771400	-0.11637200	-0.44731900
H	-1.14594500	0.04436500	2.19116400
H	1.78975500	-0.45309500	-1.48315700
H	-1.78418400	-1.09590700	1.18010800
H	2.93722700	1.73100800	-0.61236700
H	0.65329300	-1.67544000	0.29961200
S	3.59182400	-0.87463100	-0.00276500
O	4.53723100	0.01380200	-0.72895400
O	3.47390400	-2.24978400	-0.54230200
O	3.66865400	-0.78734800	1.47495400
H	1.18491300	-0.49052100	1.50762800
H	-0.94166900	2.21486900	0.39156300
O	-1.08134200	-0.18346000	-0.97845800
H	-3.13349600	0.57563200	1.01901200
H	-0.40107700	-0.23341400	-1.66049400
S	-4.64567400	-0.48705000	-0.15038100
O	-3.82702200	-0.20332700	-1.55863400
O	-4.09793800	-1.73335900	0.44039700
O	-4.09216800	0.75834400	0.77250700
H	-2.85132900	-0.23242700	-1.41378700

C-TS2

N	-2.18552700	1.31464000	0.33121900
C	-1.30431300	2.29963300	0.03429300
O	-1.57054400	3.49226300	0.00644500
N	0.00466200	1.86915300	-0.26651100
C	0.48829600	0.53024500	-0.09802800
N	1.58681200	0.29048000	-1.07074800
C	-0.64926000	-0.46143100	-0.33449200
C	-1.87040400	-0.09193500	0.48792900
H	1.22750000	0.36209300	-2.02020200
H	-1.75071200	-0.35716300	1.54652800
H	2.21045600	-0.69093200	-0.90771900
H	-3.15311000	1.57772600	0.47994200
H	-0.31102100	-1.46690600	-0.08284300
S	-3.36075600	-1.10133400	-0.03978600
O	-4.47416100	-0.31822300	0.55721600
O	-3.10399100	-2.41840300	0.58389000
O	-3.31578300	-1.08690400	-1.52123100
H	-0.93934600	-0.44348600	-1.38950700
H	0.67926400	2.61798500	-0.17741700
O	1.14946500	0.33246900	1.15646900
H	2.36948300	0.96097400	-0.94932600
H	0.48101200	0.31897800	1.85163900
S	4.46191000	-0.69949200	-0.10342400
O	4.09299900	-0.67599100	1.55477000
O	3.27030900	-1.52219000	-0.68602800
O	4.27181400	0.73519600	-0.55226200
H	3.17959400	-0.35077700	1.65018100

C-IM2

N	2.18883500	1.29305200	-0.38985200
C	1.34781800	2.29939900	-0.04412900
O	1.64945600	3.48678700	-0.03408500
N	0.05296600	1.89972600	0.31647800
C	-0.47615800	0.56349700	0.23190500
N	-1.53989300	0.32850700	1.20145500
C	0.66344600	-0.43538500	0.42983700
C	1.84752300	-0.11568400	-0.46498900
H	1.66809400	-0.42376600	-1.50245500
H	-1.15704600	0.41176200	2.13842800

H	3.15340900	1.53348700	-0.58647000
H	0.29811100	-1.44083700	0.22379400
S	3.35149700	-1.12180400	0.02110800
O	3.40015700	-1.04745800	1.50124900
O	4.44167600	-0.38435400	-0.67267800
O	3.04694700	-2.46300200	-0.52862500
H	1.00181800	-0.39234300	1.46936500
H	-0.60006300	2.66898600	0.36632200
O	-1.15143700	0.35847600	-1.04079300
S	-4.52573200	-0.66473700	-0.10535000
O	-3.51657600	-1.58411400	0.80801900
O	-4.46854300	0.71579200	0.44488500
O	-3.71041300	-0.65309200	-1.54105800
H	-0.53991700	0.58757700	-1.74968900
H	-2.28508200	1.02034800	1.09711200
H	-2.68538700	-1.05718200	1.01102500
H	-2.80543900	-0.27560400	-1.42719000

C-TS3

N	2.05841500	1.34294200	-0.36907100
C	1.10801700	2.25048100	-0.02719500
O	1.26429900	3.46416200	-0.06990900
N	-0.10284000	1.711171000	0.43518500
C	-0.47862000	0.33297300	0.30680600
N	-1.50639700	-0.03462700	1.28480200
C	0.76262700	-0.53902600	0.47785100
C	1.87881200	-0.09127900	-0.44886000
H	1.70353400	-0.40745800	-1.48419200
H	-1.08815400	-0.06283200	2.21092900
H	2.96363300	1.70230000	-0.64548500
H	0.51467700	-1.58629000	0.29288100
S	3.48013600	-0.95122500	-0.01142600
O	3.57570100	-0.86546800	1.46597000
O	4.47933100	-0.13533300	-0.74957100
O	3.26256700	-2.31925900	-0.54197100
H	1.11960400	-0.45504100	1.50803100
H	-0.84444900	2.39844900	0.45069700
O	-1.07958400	0.12174700	-1.00658800
S	-4.54001900	-0.57635800	-0.14769700
O	-3.55279900	-1.72010200	0.49949900
O	-4.38208800	0.64717800	0.68381700
O	-3.77798500	-0.28335400	-1.58264700
H	-0.69277000	-0.67123300	-1.39736500
H	-2.24991800	0.66744300	1.30827300
H	-2.70753900	-1.28507700	0.83270700
H	-2.84525700	0.00542500	-1.42733000

C-IM3

N	2.00169100	1.35551900	-0.35338000
C	1.00911300	2.21393600	-0.00751400
O	1.10428300	3.43411400	-0.04481700
N	-0.17346800	1.61514700	0.45668300
C	-0.47977500	0.22214900	0.32932700
N	-1.48336500	-0.20313100	1.31162000
C	0.80255600	-0.59114400	0.48509600
C	1.88798700	-0.08538600	-0.44706800
H	1.71255400	-0.39839400	-1.48196200
H	-1.03996200	-0.30586000	2.22046000
H	2.88520200	1.76003700	-0.63715200
H	0.60559600	-1.64825400	0.29250600
S	3.52881700	-0.87403900	-0.02876600
O	3.63476200	-0.79303000	1.44862300
O	4.48571000	-0.01159600	-0.77019500
O	3.36780700	-2.24837200	-0.56422700

H	1.16324700	-0.49844500	1.51342900
H	-0.94648200	2.26585500	0.48625200
O	-1.06690800	0.00102800	-0.98905400
S	-4.53774900	-0.52036300	-0.16286000
O	-3.58925400	-1.74776800	0.38821900
O	-4.32182300	0.63043100	0.75464600
O	-3.78159600	-0.15385200	-1.58272000
H	-0.84787800	-0.89710100	-1.26939200
H	-2.21505300	0.50479200	1.40770600
H	-2.73717200	-1.37140800	0.76991800
H	-2.83427300	0.08150700	-1.42302800

C-TS4

N	2.11994000	1.33902300	-0.34299500
C	1.19758000	2.28283400	-0.04377300
O	1.39664100	3.48913100	-0.06541600
N	-0.06697000	1.79532500	0.35430800
C	-0.48525800	0.44073600	0.20024700
N	-1.53186000	0.12574900	1.22966500
C	0.70253100	-0.49925900	0.39144000
C	1.87017900	-0.08251500	-0.48241700
H	-2.25418300	-0.82106000	0.88193400
H	1.70924800	-0.35357500	-1.53018300
H	-1.10769700	0.03396900	2.15025600
H	3.05487900	1.65648800	-0.56927200
H	0.41058500	-1.52602000	0.16003900
S	3.41266000	-1.02142600	0.00132700
O	4.47713900	-0.22303000	-0.66069000
O	3.17173400	-2.36435000	-0.57698600
O	3.43564200	-0.97809600	1.48442900
H	1.03382600	-0.46711700	1.43401100
H	-0.78085800	2.50628500	0.26168800
O	-1.11688000	0.28453600	-1.06897500
H	-1.26559800	-0.65882300	-1.22858300
S	-4.43675700	-0.74142600	0.01949700
O	-4.12912500	-0.32723900	-1.59892900
O	-3.14968300	-1.56986600	0.39831100
O	-4.35249500	0.56478200	0.76033200
H	-3.38429400	0.29979900	-1.61677400
H	-2.25211200	0.85729000	1.26725600

C-IM4

N	2.03423500	1.35982700	-0.34178600
C	1.04099400	2.22905900	-0.05044700
O	1.14232600	3.44656500	-0.07679100
N	-0.19000400	1.64716700	0.33785100
C	-0.49745500	0.26029200	0.22152800
N	-1.41278500	-0.07665600	1.42587500
C	0.76405700	-0.59024300	0.36733700
C	1.88670900	-0.07345800	-0.51061600
H	-1.55176500	-1.08976600	1.47628700
H	1.73492100	-0.33710500	-1.56115500
H	-0.97651800	0.26534200	2.28040600
H	2.94238200	1.74809300	-0.56756700
H	0.53449800	-1.62426100	0.10296600
S	3.49998000	-0.89717400	-0.04220900
O	4.49846900	-0.00553200	-0.68770600
O	3.37024100	-2.24656600	-0.63849400
O	3.51688200	-0.87372900	1.44248900
H	1.11952300	-0.56409100	1.40291700
H	-0.96242900	2.28084200	0.17421000
O	-1.23887500	0.01502300	-0.93252800
H	-1.79419300	-0.79704200	-0.81952800
S	-4.39267000	-0.71434900	0.02831000
O	-4.50328000	0.11867000	-1.45233600

O	-3.19679200	-1.64711700	-0.16842200
O	-3.94741600	0.38777000	1.00497700
H	-3.65816400	0.57189000	-1.61294300
H	-2.42359400	0.30352600	1.29688600

C-IM5

N	-1.82333300	1.73693400	0.27005300
C	-0.50183500	2.00453000	-0.01726600
O	-0.15426000	3.01480100	-0.61042000
N	0.42159400	1.08992400	0.45551500
C	0.14860800	-0.16856100	1.08582000
N	0.28610100	-1.27806900	0.02340200
C	-1.26303800	-0.18324700	1.67368000
C	-2.31691500	0.48896700	0.79638100
H	0.15200200	-2.18151300	0.47684900
H	-3.20684400	0.67914900	1.40055200
H	-0.46886900	-1.16341900	-0.71766600
H	-2.47075500	2.28802100	-0.27602600
H	-1.18554500	0.36407400	2.61551300
S	-3.00507200	-0.61499400	-0.54870300
O	-4.09111500	0.18920400	-1.14236400
O	-3.40928300	-1.84556000	0.17234500
O	-1.84865500	-0.83967300	-1.49329900
H	-1.57241000	-1.20368200	1.90186100
H	1.40147300	1.32424900	0.32522700
O	1.05395900	-0.46263300	2.09205200
H	1.96076800	-0.22117400	1.76895400
S	3.95502400	-0.57512100	-0.20503000
O	4.40456800	0.51277900	-1.44398400
O	3.26263300	0.33560200	0.81268500
O	2.87511400	-1.42966200	-0.85501400
H	3.59827900	0.93991700	-1.77589700
H	1.25753700	-1.27430900	-0.39014600

C-TS5

N	-2.22812700	1.57320700	0.42907000
C	-1.17302100	2.19531400	-0.20004200
O	-1.29626600	3.26223800	-0.78677700
N	0.05694000	1.57457300	-0.08278300
C	0.37699400	0.32417400	0.56910800
N	0.46593700	-0.76206200	-0.57712500
C	-0.78065100	-0.07735100	1.50083700
C	-2.18150500	0.24111900	0.97975300
H	0.63819700	-1.67677400	-0.15853100
H	-2.89218200	0.17082000	1.80631900
H	-0.45106300	-0.81573200	-1.10974200
H	-3.13075900	1.91136400	0.12624000
H	-0.60822000	0.49536900	2.41500200
S	-2.87240000	-1.01991900	-0.21873500
O	-4.27342000	-0.59308700	-0.40885900
O	-2.66290800	-2.32088300	0.46117900
O	-2.03509200	-0.86808700	-1.46675800
H	-0.71367800	-1.13620500	1.75310500
H	0.83417800	2.11521900	-0.43338800
O	1.57063000	0.37831400	1.18145700
H	2.41517800	-0.65753500	1.10991100
S	4.07577700	-0.57785700	-0.33428400
O	4.07861500	0.98993100	0.24675300
O	3.28093400	-1.30572400	0.85799200
O	3.17269000	-0.57393600	-1.53157500
H	3.17189300	1.16240500	0.60069700
H	1.28680200	-0.55418400	-1.17068400

C-P

N	2.20718400	1.36426500	-0.10380600
C	1.29755800	2.34102400	0.04667900
O	1.46909300	3.41596700	0.59518900
N	0.02642500	2.05575300	-0.53230700
C	-0.43289800	0.83356700	-0.89481700
N	-0.38453300	0.06151200	2.21445000
C	0.55903400	-0.29302000	-0.92524600
C	2.02374100	0.12626000	-0.84158400
H	0.42155100	-0.56316300	2.18505400
H	2.47472800	0.20761400	-1.83501300
H	-1.23616000	-0.49164300	2.14660900
H	3.11771400	1.49463700	0.32320600
H	0.38083200	-0.88965300	-1.82039900
S	3.03590500	-1.19434100	0.01641500
O	4.29823600	-0.46782000	0.31602700
O	3.13905100	-2.26037600	-1.00395500
O	2.23738500	-1.55669200	1.21752700
H	0.31451000	-0.92146800	-0.06310200
H	-0.65968600	2.78305300	-0.37766300
O	-1.62762000	0.66788900	-1.18243300
H	-0.38653500	0.51773200	3.12085500
H	-3.27619700	1.11609100	-0.39761300
S	-4.26025000	-0.76222200	0.17497000
O	-3.49942600	-1.32798000	-1.18049400
O	-3.38973900	-1.03065300	1.33609500
O	-4.19438000	0.86901600	-0.14699700
H	-2.65017400	-0.84068300	-1.31032000

Path D

D-RC

N	1.84626200	1.36355100	-0.25951500
C	1.25890700	2.55811600	-0.07783700
O	1.69581400	3.65678900	-0.36366000
N	-0.05389300	2.47050500	0.51287000
C	-0.60867600	1.35548400	1.02124500
N	-1.87073100	1.31227100	1.36203900
C	0.28815700	0.16937300	1.16174800
C	1.12317700	0.10416700	-0.10923400
H	-2.46766800	2.06001700	1.02059300
H	0.48347400	-0.08427800	-0.97607600
H	-0.54392100	-2.49053200	-0.30967800
H	2.73476200	1.32491500	-0.74825300
H	-0.29689800	-0.73867600	1.29959600
S	2.32389700	-1.31103000	-0.10008200
O	3.32765500	-0.87072800	-1.10296900
O	1.46430200	-2.44588600	-0.53073700
O	2.82773900	-1.40059700	1.28750200
H	0.95366400	0.30062600	2.02204400
H	-0.63743900	3.27189300	0.30759600
O	-2.63135100	2.15174200	-1.24130900
H	-2.35705100	0.36504100	1.38714900
S	-2.66494400	-1.58966200	-0.38255800
O	-2.02405000	-0.51111900	-1.25763300
O	-1.32210000	-2.42066600	0.28265000
O	-3.18116300	-0.94960100	0.90381200
H	-2.45256000	1.17951800	-1.30769500
H	-3.03523000	2.39594000	-2.07757600

D-TS1

N	-2.34127500	-0.30397700	-0.45355300
C	-2.56499400	-1.62645500	-0.26311700
O	-3.60386600	-2.21501900	-0.52032500
N	-1.47589900	-2.35634800	0.27979900

C	-0.24146400	-1.82288800	0.56487900
N	0.62883600	-2.53754500	1.32604700
C	-0.28475400	-0.34423700	0.81915800
C	-1.05680900	0.35743200	-0.27148500
H	0.71820000	-3.51506100	1.08045800
H	-0.49527000	0.38396000	-1.20798800
H	1.87679900	1.82940800	-0.05742200
H	-3.09397600	0.23233400	-0.86614300
H	0.72238600	0.04074000	0.92911600
S	-1.23823100	2.15298900	0.13197500
O	-2.16874000	2.63805800	-0.91460600
O	0.17853300	2.60357600	-0.02632900
O	-1.75192700	2.22667100	1.51574200
H	-0.80375600	-0.19631900	1.77264800
H	-1.61676600	-3.35597200	0.27028500
O	0.64941800	-1.92887600	-1.12422500
H	1.53490000	-2.06134300	1.39691000
S	3.36839500	0.08349300	-0.19408200
O	2.55440200	-0.46762200	-1.43252800
O	2.85196200	1.65073800	-0.06871700
O	2.86610800	-0.66012700	1.02283800
H	1.62623800	-1.17578100	-1.24649500
H	0.04798400	-1.74289300	-1.85511600

D-IM1

N	-2.15320600	0.41666700	-0.72136700
C	-2.96292600	-0.66309300	-0.55565800
O	-4.15614500	-0.67924400	-0.83188500
N	-2.33024900	-1.82383400	-0.07940100
C	-0.97816400	-1.84794700	0.44914500
N	-0.90799000	-2.78206100	1.54475200
C	-0.53929500	-0.45418800	0.88187900
C	-0.78025100	0.51717300	-0.25834700
H	-0.89044800	-3.73056800	1.18000900
H	-0.08006900	0.34854100	-1.08200800
H	2.28037600	1.38848700	-0.17296300
H	-2.57097800	1.24562700	-1.12446300
H	0.51613800	-0.46939300	1.15786100
S	-0.42012700	2.26326500	0.25131600
O	-0.96379700	3.06064400	-0.87191400
O	1.08181400	2.26039700	0.33030500
O	-1.06770600	2.47901200	1.55826900
H	-1.12917600	-0.14773500	1.74842000
H	-2.98276800	-2.45825300	0.35776100
O	-0.09072200	-2.28513100	-0.63942300
H	-0.03606000	-2.64268900	2.04617300
S	3.40523500	-0.59996100	-0.22870300
O	2.45446800	-1.32256600	-1.40109300
O	3.14836700	0.96427000	-0.50421500
O	2.78123800	-0.98622500	1.06601900
H	1.58824400	-1.60728000	-1.02753400
H	-0.65320200	-2.45592700	-1.40358200

D-TS2

N	-2.15234800	0.44977900	-0.72116200
C	-2.96948500	-0.63006200	-0.58620400
O	-4.15656300	-0.63602000	-0.88945100
N	-2.35081300	-1.79208000	-0.10615800
C	-1.01195300	-1.84784800	0.45731600
N	-0.98916600	-2.79944100	1.55323300
C	-0.55501300	-0.45541500	0.88041000
C	-0.77924100	0.52257600	-0.25812900
H	-0.48892700	-3.63009400	1.25768300
H	-0.07893000	0.34470200	-1.08061000
H	2.28710000	1.37304400	-0.20659700

H	-2.55451900	1.28482500	-1.12697300
H	0.49940300	-0.48774200	1.15974500
S	-0.39333300	2.26140100	0.26171500
O	-0.93378800	3.07443800	-0.85135500
O	1.10865300	2.24258800	0.33363300
O	-1.03133000	2.47186000	1.57454200
H	-1.14250600	-0.13207300	1.74432500
H	-3.00284700	-2.46351100	0.27184700
O	-0.11370000	-2.33817000	-0.58551800
H	-0.49604000	-2.41263900	2.34981100
S	3.41051500	-0.61328400	-0.24460500
O	2.44100800	-1.37525000	-1.37998300
O	3.14108000	0.94041200	-0.56383900
O	2.80909500	-0.96207200	1.07008600
H	1.58480600	-1.65116000	-0.98089700
H	-0.65765200	-2.48082600	-1.36875300

D-IM2

N	-2.18556300	0.46171800	-0.65392500
C	-2.95159700	-0.66317300	-0.59417000
O	-4.07144500	-0.75411200	-1.08463000
N	-2.39433300	-1.73657900	0.10704600
C	-1.00821400	-1.82146800	0.48396300
N	-0.89547700	-2.86073700	1.49692300
C	-0.53023400	-0.42924900	0.88961300
C	-0.79776500	0.54881700	-0.24028600
H	0.06315500	-2.88899000	1.83450400
H	-0.12897400	0.37234000	-1.08897800
H	2.27706500	1.36153700	-0.18328000
H	-2.56238200	1.23426400	-1.18653900
H	0.53075300	-0.46486300	1.13743300
S	-0.39460900	2.28477600	0.26262200
O	-0.91954300	3.09794300	-0.85748800
O	1.10913400	2.24288600	0.33515300
O	-1.02475500	2.51903000	1.57550500
H	-1.08792900	-0.10914300	1.77272600
H	-2.89591100	-2.60389000	-0.02286600
O	-0.15928000	-2.23359700	-0.61253500
H	-1.50022500	-2.64194300	2.28271900
S	3.39041500	-0.63894100	-0.26613400
O	2.42254500	-1.35456300	-1.43095700
O	3.13819700	0.92628700	-0.52726800
O	2.78237900	-1.03151800	1.03477500
H	1.53935900	-1.58175600	-1.06291500
H	-0.33120000	-3.17016400	-0.77208000

D-TS3

N	-2.44603300	-0.16929100	-0.33149300
C	-2.67907300	-1.51290100	-0.26179100
O	-3.74974700	-2.03240300	-0.54627600
N	-1.60714100	-2.31557400	0.19433000
C	-0.24952300	-1.81447600	0.24287700
N	0.60454700	-2.69124900	1.17643700
C	-0.29273500	-0.37141000	0.70127400
C	-1.11302900	0.40593700	-0.29811400
H	1.35220900	-2.11664800	1.58156400
H	-0.64752900	0.39245300	-1.28903200
H	1.81672200	1.80099700	-0.08134000
H	-3.19137300	0.38309300	-0.73335400
H	0.71335200	0.01752700	0.79052200
S	-1.10004500	2.19688300	0.14787500
O	-2.05244500	2.81758900	-0.79782500
O	0.34115300	2.53025400	-0.13222800
O	-1.46302700	2.29151300	1.57640600

H	-0.77187800	-0.29977800	1.68097800
H	-1.69643900	-3.24433000	-0.20076800
O	0.51253500	-2.10884400	-0.88711600
H	0.11976900	-3.25826900	1.86886600
S	3.33440900	0.04753000	-0.20496600
O	2.50699700	-0.52716000	-1.49100400
O	2.80363200	1.57311800	-0.09346300
O	2.85361200	-0.73432500	0.98561600
H	1.70069100	-1.10370200	-1.24379800
H	0.97951500	-2.97000200	0.04655800
D-P			
N	2.54739200	0.17705600	-0.25497100
C	2.94750100	1.45019100	-0.00580200
O	4.08787300	1.87076000	-0.09534500
N	1.89411500	2.32832800	0.36627800
C	0.58307700	1.98331300	0.62418300
N	-1.36558200	-1.71948800	3.04294500
C	0.36402600	0.49874600	0.73090700
C	1.14066400	-0.16881700	-0.39095700
H	-2.01303700	-1.27400600	2.39573800
H	0.75741600	0.14037800	-1.36979000
H	-1.50965800	-0.86154300	-1.30284500
H	3.22917400	-0.45173300	-0.66088700
H	-0.69736400	0.27597400	0.69533900
S	0.89444500	-2.00080700	-0.40561400
O	1.96303400	-2.48671100	-1.30415800
O	-0.49075300	-2.09915400	-0.97892100
O	0.98395600	-2.45759400	0.99665500
H	0.74390000	0.14385500	1.69494000
H	2.13700200	3.30997500	0.36820900
O	-0.29264700	2.83013100	0.73972700
H	-0.61864200	-2.11877100	2.47407700
S	-3.22338600	0.50340200	-0.69976000
O	-2.79299500	2.09670900	-0.59860400
O	-1.97714200	-0.02637300	-1.63091300
O	-3.06373300	-0.10899200	0.64035300
H	-1.98663000	2.25945000	-0.05520000
H	-1.86293700	-2.49718500	3.46629300
Path E			
E-RC			
N	-1.86085400	1.21007000	-0.21360300
C	-0.52256800	1.42277800	-0.41672800
O	-0.06887300	2.50513200	-0.76030500
N	0.30386300	0.31353000	-0.20686400
C	-0.13239900	-0.97120500	0.03031600
N	0.72228600	-1.90916000	0.24350600
C	-1.63238700	-1.18060000	-0.03839700
C	-2.39136000	0.04037300	0.45041200
H	2.67044500	-1.91205300	0.34988100
H	-2.33565500	0.13052300	1.54256800
H	0.23915600	-2.79103300	0.39775100
H	-2.45608200	2.02634600	-0.25210200
H	-1.91156800	-2.05981900	0.54312700
S	-4.22109900	-0.09471200	0.12171000
O	-4.69268600	1.30657300	0.31262800
O	-4.68232700	-1.04875500	1.16552900
O	-4.35623200	-0.60055600	-1.26853500
H	-1.91632800	-1.35781100	-1.08181900
H	1.32899600	0.47352800	-0.25345300
O	5.19528200	2.06352900	1.37940600
H	4.28824800	1.95265900	1.05309700
H	5.58679800	1.25705700	0.99276400

S	4.12781200	-0.58603800	-0.66428400
O	5.52476500	-0.32350300	-0.15366900
O	3.65431400	-1.91583100	0.34402000
O	3.16498100	0.51384300	-0.20976300

E-TS1

N	-1.46969100	1.28948900	0.22387100
C	-0.24397900	1.78738200	-0.10007100
O	0.02667500	2.97974000	-0.04395400
N	0.71067600	0.85389100	-0.53744700
C	0.45658600	-0.46568600	-0.67911600
N	1.32876200	-1.23647100	-1.33358900
C	-0.97250500	-0.93322600	-0.60444200
C	-1.80444800	-0.11293700	0.36198400
H	2.35961200	-1.01341900	-1.31189200
H	-1.66764800	-0.46185500	1.38879300
H	1.15721500	-2.22243200	-1.19450900
H	-2.15815000	1.95565200	0.54737400
H	-0.98861200	-1.98286500	-0.31880100
S	-3.63642200	-0.31733900	0.06024500
O	-4.21747100	0.81896800	0.83586800
O	-3.94191300	-1.66110000	0.61776800
O	-3.83506100	-0.20872900	-1.40977800
H	-1.40268900	-0.82830600	-1.60838300
H	1.72349900	1.14823300	-0.45943000
O	1.06147000	-1.27418500	1.33127900
H	0.69362500	-0.83316000	2.10506800
H	2.45232600	-0.97103200	1.35915700
S	4.22407700	0.01888900	0.17834800
O	3.52010500	-0.76289900	1.43753400
O	4.00907700	-0.91227000	-1.03821400
O	3.35539500	1.26832700	-0.06360800

E-IM1

N	1.69556100	1.27609700	-0.27139700
C	0.49420500	1.80661700	0.11042000
O	0.27793800	3.02348600	0.09307200
N	-0.45236700	0.90770300	0.54651400
C	-0.34532600	-0.53586900	0.40405700
N	-1.15376000	-1.13304900	1.46311000
C	1.12727800	-0.93472000	0.55708900
C	1.99779000	-0.13593700	-0.39760300
H	-2.07895500	-0.69708100	1.45929000
H	1.85984100	-0.48055000	-1.42693500
H	-1.28764800	-2.11115900	1.22314200
H	2.39013000	1.92796500	-0.60646300
H	1.23368800	-1.99993800	0.34866600
S	3.82217800	-0.39822800	-0.10634200
O	4.44274000	0.69940000	-0.91074200
O	4.07432100	-1.76286100	-0.64889900
O	4.05792100	-0.27589700	1.35695400
H	1.43492300	-0.73847200	1.58456600
H	-1.37835300	1.29019200	0.69546900
O	-0.74704400	-0.97637100	-0.89880400
H	-1.68875000	-0.74697900	-1.03975600
H	-5.05411000	-1.81679600	-0.06187500
S	-4.44207400	0.29460300	-0.36202300
O	-5.58187000	-1.01436100	0.06651000
O	-3.69850600	0.55778700	0.92227100
O	-3.54826800	-0.44180600	-1.34206500

E-TS2

N	2.01638400	1.27795000	-0.37402900
C	0.97648500	2.07728100	-0.01206900

O	0.98743800	3.30225500	-0.17319900
N	-0.10101000	1.44631300	0.59371900
C	-0.32580400	-0.00140900	0.55567200
N	-1.17445700	-0.34713200	1.70071300
C	1.04132300	-0.69266800	0.66475500
C	2.00510800	-0.17360400	-0.38742900
H	-1.89017600	-1.00711600	1.40758900
H	1.74305000	-0.55372000	-1.37948000
H	-1.67515000	0.47092000	2.02813000
H	2.81048300	1.73176800	-0.80385500
H	0.89861400	-1.76658300	0.54691900
S	3.75475900	-0.77856900	-0.14956800
O	4.52951200	0.11407100	-1.06704600
O	3.70423500	-2.20021200	-0.58754000
O	4.08979400	-0.59483500	1.28717400
H	1.44528500	-0.49831100	1.65878700
H	-0.93852700	2.01277500	0.54767000
O	-0.91182300	-0.41693000	-0.66815000
H	-1.82672900	-0.05803400	-0.71117600
H	-4.51834000	-1.52117200	-1.66151100
S	-4.77903600	-0.01223100	-0.03620800
O	-5.32714500	-1.08847300	-1.34723200
O	-4.42757500	-0.95639300	1.07940300
O	-3.52308100	0.58361200	-0.65204000

E-IM2

N	1.86235300	1.29397900	-0.30721800
C	0.72252100	1.94292100	0.06807300
O	0.61309200	3.17298600	0.01522500
N	-0.29261900	1.14516300	0.56214000
C	-0.35452800	-0.32463600	0.41591500
N	-1.18149700	-0.90735400	1.46907000
C	1.07729600	-0.86063600	0.52616100
C	2.02073800	-0.14236900	-0.42345300
H	-2.16787100	-0.66997300	1.33866100
H	1.85886400	-0.47467500	-1.45365300
H	-0.89716800	-0.52025300	2.36400300
H	2.61518400	1.86761800	-0.66009600
H	1.05925300	-1.92580700	0.30211200
S	3.81201200	-0.57107300	-0.11620100
O	4.53595800	0.46346000	-0.91773400
O	3.94653200	-1.95430300	-0.64981100
O	4.03939200	-0.46048600	1.34990000
H	1.43089700	-0.72369300	1.55099400
H	-1.18548500	1.61889300	0.59893800
O	-0.86752700	-0.69489900	-0.84276200
H	-1.76822700	-0.31621100	-0.94629900
H	-4.52992500	-1.99301200	-0.72036200
S	-4.68316700	0.17238600	-0.18966900
O	-5.29036900	-1.39319400	-0.77312200
O	-4.27690300	-0.12242700	1.23217400
O	-3.44903400	0.37660000	-1.04743200

E-TS3

N	1.76586100	1.29597900	-0.41375900
C	0.75050500	2.12338800	-0.03647400
O	0.76860800	3.34082500	-0.26506000
N	-0.28265700	1.53358900	0.66526600
C	-0.54783100	0.06426200	0.69906200
N	-1.29718900	-0.26134100	1.92608600
C	0.83326200	-0.62001800	0.77670100
C	1.74819700	-0.15289200	-0.34150800
H	-2.28569200	-0.05131300	1.79649100
H	1.44098400	-0.58970800	-1.29704300

H	-0.94605400	0.28972800	2.70311800
H	2.53287800	1.71843100	-0.91727200
H	0.67857900	-1.69580600	0.70717400
S	3.50788900	-0.74840900	-0.14688600
O	4.24603200	0.08433400	-1.14853600
O	3.44497600	-2.19488400	-0.49478600
O	3.90931100	-0.47990700	1.26102500
H	1.30276900	-0.39515600	1.73842100
H	-1.11159100	2.11292400	0.67703900
O	-1.26961700	-0.33130800	-0.40495100
H	-2.42293300	0.43476700	-0.93356100
H	-2.30220900	-1.33793400	-0.34513200
S	-4.34623600	-0.53017400	-0.52485800
O	-3.27847600	-1.75934000	-0.48794200
O	-4.58989900	-0.08500400	0.88416700
O	-3.41594600	0.61345200	-1.24531100

E-IM3

N	1.45526900	1.26825700	-0.13157600
C	0.21505500	1.58073600	0.35369900
O	-0.15574500	2.75133500	0.50261800
N	-0.57684400	0.51204500	0.70486600
C	-0.30829100	-0.88695000	0.33197700
N	-0.97772300	-1.78592100	1.27514700
C	1.20642300	-1.10673100	0.37988000
C	1.93848900	-0.06128700	-0.44557300
H	-1.97427000	-1.55966000	1.26951800
H	1.83748100	-0.27590300	-1.51393900
H	-0.64847900	-1.55692500	2.20984500
H	2.04933400	2.04388100	-0.38675700
H	1.42506100	-2.10283800	-0.00149800
S	3.78602100	-0.11176600	-0.17534300
O	4.24605100	1.16292900	-0.80745800
O	4.22094300	-1.33821900	-0.89991800
O	4.00863900	-0.16638300	1.29519900
H	1.54681000	-1.04136800	1.41641000
H	-1.54225000	0.73141200	0.92753000
O	-0.74105500	-1.16716900	-0.98036900
H	-3.95769300	1.80179600	-0.61830500
H	-1.70588500	-1.00804100	-1.05964800
S	-4.47056100	-0.32628000	-0.16623000
O	-3.56124300	-0.81785100	-1.27133700
O	-3.66699100	-0.15845000	1.10817600
O	-4.81215500	1.34144700	-0.62653000

E-TS4

N	-1.70488600	1.32862300	0.18468700
C	-0.47098600	1.84025000	-0.12132300
O	-0.26953200	3.05433600	-0.20265400
N	0.52479000	0.91785600	-0.36238600
C	0.40647700	-0.50288100	-0.11552300
N	1.34291200	-1.29803700	-1.03544500
C	-1.04697800	-0.93755200	-0.35313000
C	-1.99165100	-0.06481700	0.45128800
H	2.18213200	-0.71935300	-1.26996200
H	-1.92155900	-0.29880200	1.51905000
H	0.92692400	-1.75784500	-1.84174800
H	-2.43363300	1.99763700	0.38722300
H	-1.15664200	-1.97898800	-0.04930800
S	-3.78133300	-0.41140700	0.04341600
O	-4.48929400	0.76517500	0.63118000
O	-4.05974900	-1.69933600	0.73602100
O	-3.87225200	-0.49053800	-1.43979500
H	-1.30902500	-0.83583200	-1.41100100
H	1.47166500	1.28438300	-0.41520800

O	0.98026100	-0.97470900	1.05857600
H	2.76993000	-0.24178400	1.41234200
H	1.52605500	-1.74250100	0.09114300
S	4.54270600	0.14525000	0.04591900
O	5.01021800	-1.27031300	-0.17239300
O	3.42684200	0.48087000	-0.96469200
O	3.67867000	0.12233000	1.53778700
E-P			
N	2.06787400	1.20447700	0.24611200
C	0.76636300	1.59603000	0.37481400
O	0.43442700	2.71794600	0.72622400
N	-0.19101300	0.60871000	0.07294300
C	0.07749400	-0.71949000	-0.15174500
N	-6.17165900	-1.49193600	1.69229300
C	1.53337700	-1.13594200	-0.03410800
C	2.48039100	-0.01390500	-0.41905200
H	-5.42485800	-2.02116100	1.24190600
H	2.51736500	0.11634900	-1.50786700
H	-5.78245400	-1.20230100	2.58735200
H	2.77250200	1.92085100	0.36261400
H	1.69085100	-2.01971900	-0.65028000
S	4.25343500	-0.38349000	0.02764500
O	4.89440500	0.96097200	-0.06251100
O	4.68050500	-1.34008500	-1.02663000
O	4.22508100	-0.95363400	1.39835500
H	1.72433100	-1.41173300	1.00959100
H	-1.19076500	0.89876000	0.06442800
O	-0.80604000	-1.53102300	-0.40092900
H	-2.81546200	-1.35184400	-0.46643000
H	-6.18075400	-0.64039900	1.12118900
S	-4.03953900	0.47749200	-0.91104700
O	-5.41298300	0.68163800	-0.33218700
O	-2.96014200	1.14642100	-0.07613800
O	-3.78215800	-1.23245500	-0.51705300