

Supporting Information

Effectively improving the energy of monocyclic imidazoles to high level by the introduction of bridge-rings and nitro groups through different kinds of Diels-Alder reactions: a DFT study

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Table S1 The energy barrier for the normal Diels-Alder reaction

	DAE	TAE	DNE	TNE	DAA	DNA
DE1	8.45	8.47	3.40	1.58	8.76	2.91
DE2	8.70	8.72	3.65	1.83	9.01	3.16
DE3	9.62	9.64	4.57	2.75	9.93	4.08
DE4	9.76	9.78	4.71	2.89	10.07	4.22
DE5	9.85	9.87	4.80	2.98	10.16	4.31
DE6	9.97	9.99	4.92	3.10	10.28	4.43

Table S2 The energy barrier for the inverse Diels-Alder reaction

	DAE	TAE	DNE	TNE	DAA	DNA
DE1	2.16	2.20	6.24	7.02	3.05	6.84
DE2	0.54	0.58	4.62	5.40	1.43	5.22
DE3	1.07	1.11	5.15	5.93	1.96	5.75
DE4	0.51	0.55	4.59	5.37	1.40	5.19
DE5	1.14	1.18	5.22	6.00	2.03	5.82
DE6	0.29	0.33	4.37	5.15	1.18	4.97

Table S3 The energy barrier of LUMO→LUMO for the neutral Diels-Alder reaction

	DAE	TAE	DNE	TNE	DAA	DNA
DE1	4.06	4.08	0.99	2.81	4.37	1.48
DE2	5.68	5.70	0.63	1.19	5.99	0.14
DE3	5.15	5.17	0.10	1.72	5.46	0.39
DE4	5.71	5.73	0.66	1.16	6.02	0.17
DE5	5.08	5.10	0.03	1.79	5.39	0.46
DE6	5.93	5.95	0.88	0.94	6.24	0.39

Table S4 The energy barrier of HOMO→HOMO for the neutral Diels-Alder reaction

	DAE	TAE	DNE	TNE	DAA	DNA
DE1	2.23	2.19	1.85	2.63	1.34	2.45
DE2	2.48	2.44	1.60	2.38	1.59	2.20
DE3	3.40	3.36	0.68	1.46	2.51	1.28
DE4	3.54	3.50	0.54	1.32	2.65	1.14
DE5	3.63	3.59	0.45	1.23	2.74	1.05
DE6	3.75	3.71	0.33	1.11	2.86	0.93

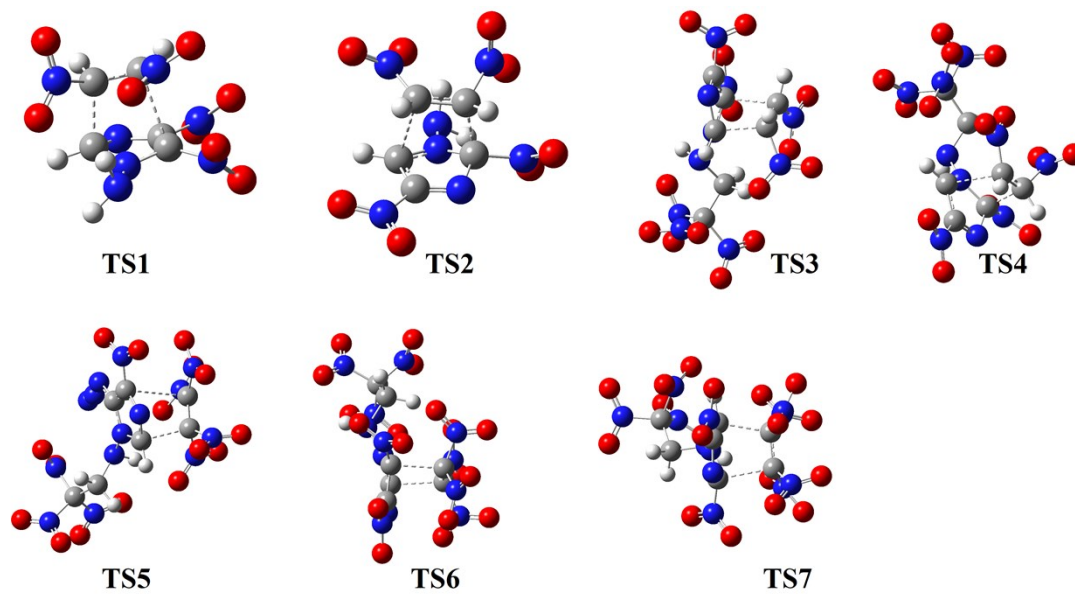


Fig. S1 The optimized structures of transition states (TS) to form the corresponding product (for example, from TS1 to P1, from TS2 to P2, and so forth)

The coordinates of all designed compounds

P1

C	1.49023000	-0.85808600	-0.24638600
N	0.95668000	-2.00119300	-0.11721300
C	-0.36014600	-1.66820300	0.53287700
C	-1.19747500	-1.05762300	-0.61366400
C	-0.56997400	0.37089900	-0.76871800
C	0.57132500	0.25511400	0.28827500
N	2.69775300	-0.63455600	-1.04635100
O	2.58066300	0.28734900	-1.85500300
O	3.65789700	-1.36086600	-0.87583700
N	1.27466900	1.49410800	0.75564900
O	0.60262400	2.50138500	0.89797300
O	2.46942000	1.35899500	0.98814400
N	-1.53620700	1.51932900	-0.47553400
O	-1.51706100	2.42257200	-1.29687000
O	-2.22893200	1.44612500	0.52555000
N	-2.69164900	-1.06918500	-0.34791500
O	-3.09245000	-1.64134600	0.65380500
O	-3.37257000	-0.55427500	-1.22393300
N	-0.12336300	-0.47068100	1.36120500
N	0.62824400	-0.59519500	2.54673300
H	-0.80486400	-2.50653000	1.06015500
H	-1.09200500	-1.61901900	-1.54244700
H	-0.18907800	0.57415000	-1.76578200
H	1.26950400	-1.38962500	2.53092400
H	-0.02692900	-0.68947900	3.31620300

P2

C	1.85179900	-0.11034300	-0.10128700
N	1.30436100	-1.12112200	-0.64274300

C	-0.08468500	-1.03176500	-0.08110100
C	-0.77747100	0.11162700	-0.86851300
C	-0.05483200	1.36032600	-0.27149500
C	0.87723200	0.68143700	0.77994500
N	3.20340800	0.33631700	-0.45464400
O	3.30450400	1.56064900	-0.55172600
O	4.07568000	-0.49887300	-0.61324700
N	-0.95287900	2.38389300	0.40742900
O	-1.74891700	1.98576600	1.24455700
O	-0.75484800	3.54537400	0.07760900
N	-2.28753700	0.15194500	-0.70442500
O	-2.82341400	-0.70053800	-0.01718600
O	-2.83386400	1.04521700	-1.33628800
N	0.02607700	-0.42286100	1.25251400
N	0.62470800	-1.13515500	2.32340600
N	-0.73917000	-2.38228500	-0.20755900
O	-1.04498200	-2.69451600	-1.34798600
O	-0.85403500	-3.06014400	0.80150800
H	-0.61947500	0.02220500	-1.94179200
H	0.49445600	1.93081000	-1.01547900
H	1.27989600	1.31427100	1.56632900
H	1.28768100	-1.83696700	1.98442600
H	-0.12858500	-1.63661900	2.78544800
P3			
C	-2.06345900	1.48678600	-0.91193700
N	-1.74813700	0.96095200	-2.01885400
C	-1.12382700	-0.33756000	-1.60061800
C	-2.31819400	-1.22954300	-1.18779700
C	-2.75400100	-0.59382700	0.18014800
C	-1.71868600	0.56206700	0.27001300

N	-2.88073800	2.69984600	-0.79003900
O	-3.67279100	2.66058500	0.15473300
O	-2.72805700	3.59234500	-1.60108800
N	-0.51278000	-0.10919700	-0.27932900
N	0.71842100	0.55562000	-0.29946400
C	1.63535200	0.04917200	0.71658300
N	-2.68020600	-1.56203700	1.36241900
O	-1.57993300	-1.98617400	1.68494000
O	-3.75191900	-1.82889000	1.87572900
N	-1.94048400	-2.69981000	-1.08903700
O	-0.82495900	-3.03269200	-1.45486200
O	-2.83721900	-3.43260400	-0.69335200
C	3.06071200	0.02533500	0.16304800
N	3.99701300	-0.79160400	1.05749300
O	3.86017900	-0.56660200	2.25201700
O	4.78029700	-1.54847300	0.51973700
N	3.68473600	1.42532700	0.07100500
O	4.89751200	1.48959400	0.12060500
O	2.89149500	2.34820800	-0.05613700
N	3.07902200	-0.58526800	-1.24252500
O	2.57071200	-1.69037000	-1.31229800
O	3.56500200	0.08081700	-2.13772600
N	-1.53555000	1.25647300	1.57819000
O	-2.13880200	0.84215800	2.55144900
O	-0.76452800	2.21576100	1.53690400
H	-0.43852500	-0.74592900	-2.33562000
H	-3.13717600	-1.20632500	-1.90671300
H	-3.77953700	-0.23431300	0.18391200
H	0.64818000	1.57057500	-0.27883200
H	1.35109200	-0.98126900	0.93676000

H	1.64360700	0.62126700	1.64963400
P4			
C	-1.82920200	1.83138900	-0.26917800
N	-2.31071800	1.21726100	-1.27051900
C	-1.72023500	-0.14360600	-1.09438900
C	-2.55750600	-0.77458400	0.05468100
C	-1.99615600	-0.00391000	1.28960500
C	-0.94769700	0.92624600	0.60736100
N	-2.24963200	3.18520100	0.10966900
O	-2.37113500	3.33466500	1.32690700
O	-2.43606600	4.00931800	-0.76677300
N	-0.40626300	0.03939800	-0.45256500
N	0.53376700	0.67712100	-1.31730400
C	1.80073700	0.00057400	-1.42998000
N	-1.32890700	-0.85877900	2.35772700
O	-0.58432100	-1.75573900	1.99262600
O	-1.57415900	-0.52738200	3.50831500
N	-2.47716200	-2.28489500	0.18586000
O	-1.80970700	-2.90666300	-0.62151500
O	-3.16061900	-2.73828100	1.09279800
C	2.76879500	0.03249700	-0.21580900
N	4.11611000	-0.63348700	-0.57168600
O	4.47408300	-0.48870300	-1.73046000
O	4.70333200	-1.20182800	0.32723000
N	2.20221600	-0.74477900	0.97571700
O	2.04629900	-1.92927500	0.75812400
O	1.95321200	-0.11874400	1.99432700
N	3.12043800	1.45417800	0.23611700
O	4.29423600	1.71147400	0.41838100
O	2.17336800	2.22486300	0.36384000

N	-1.76267700	-0.89901900	-2.40102100
O	-2.89150700	-1.03471100	-2.85119600
O	-0.71769400	-1.29127800	-2.88588800
H	-3.61815100	-0.57642400	-0.09161600
H	-2.75352900	0.56164700	1.82592800
H	-0.20792900	1.38350800	1.26027700
H	0.64319100	1.66297500	-1.10034500
H	2.34656700	0.44171800	-2.26715000
H	1.62266400	-1.05220200	-1.65852600

P5

C	-0.63679700	1.44388600	-0.75289800
N	-0.69816400	0.76899700	-1.82273000
C	-0.85542000	-0.62317100	-1.32983500
C	-2.28650000	-0.85102100	-0.78610500
C	-2.32877200	0.08820100	0.46536500
C	-0.77383400	0.56739800	0.51283400
N	-0.42163000	2.89532200	-0.73373600
O	-1.23262300	3.54420900	-0.08779100
O	0.56165100	3.30451100	-1.33640400
N	-0.18612600	-0.68925200	-0.00612300
N	1.19089200	-0.86610600	0.14012200
C	2.10643200	-0.21143700	-0.80596500
N	-2.77604100	-0.63217400	1.75317100
O	-1.89019400	-1.19095500	2.38476300
O	-3.96080800	-0.60698900	2.00242100
N	-2.42102500	-2.38376100	-0.43332900
O	-1.56322200	-3.11581900	-0.89869000
O	-3.39419400	-2.70812000	0.21512900
N	-3.19723300	1.35193100	0.35274500
O	-3.47441400	1.72912900	-0.77728100

O	-3.41849500	1.92410000	1.39997900
N	-3.41265200	-0.67114100	-1.82139600
O	-3.04080500	-0.58782000	-2.98035100
O	-4.54883300	-0.71384600	-1.39178300
C	3.53307700	-0.27662400	-0.26646700
N	4.47008000	0.64213100	-1.06822900
O	4.31335400	0.57391400	-2.27837700
O	5.27222800	1.30764000	-0.44649200
N	4.15721500	-1.67733100	-0.35028600
O	3.36677800	-2.61209900	-0.29976700
O	5.36596200	-1.73442000	-0.44584300
N	3.57314800	0.16524700	1.20317100
O	3.08597300	1.26415000	1.40364500
O	4.05814200	-0.60758300	2.00675400
N	-0.27368400	1.19084500	1.67617700
N	0.22278700	0.47239500	2.57349600
N	0.72144400	0.00828200	3.47549000
H	-0.53833900	-1.36638200	-2.05214600
H	1.37261100	-1.86332100	0.20123600
H	1.86446100	0.85021700	-0.88062900
H	2.10507800	-0.63159800	-1.81913400
P6			
C	-1.47815000	1.50295600	-0.98875000
N	-1.22241200	0.72665000	-1.95351700
C	-0.63077500	-0.46504000	-1.28425000
C	-1.80437500	-1.21836700	-0.58500300
C	-2.06260100	-0.29397300	0.65517800
C	-1.05137800	0.87154300	0.36395600
N	-1.98611900	2.87418500	-1.18940700
O	-1.48587200	3.69616700	-0.42190000

O	-2.77945300	3.07028600	-2.08596000
N	0.07221100	0.02461500	-0.08310800
N	1.34394500	0.55616800	-0.33776800
C	2.31535100	0.18019500	0.68558300
N	-1.74772700	-1.03086000	1.97358500
O	-0.93821100	-0.51758000	2.72472200
O	-2.37105400	-2.06272100	2.13487500
N	-1.32677400	-2.68379100	-0.22879500
O	-0.25237200	-2.76421800	0.33583400
O	-2.04387100	-3.58701500	-0.60226100
N	-3.51609800	0.26828000	0.80174400
O	-3.82690300	1.05391800	-0.08274900
O	-4.16246200	-0.06098800	1.76400700
N	-3.00535800	-1.45709900	-1.50037900
O	-2.73657900	-1.56901200	-2.68345800
O	-4.08808300	-1.58765700	-0.95689300
C	3.67655800	-0.06372100	0.03428700
N	4.63218100	-0.78875900	0.98552600
O	4.61884700	-0.35401400	2.12819900
O	5.30991000	-1.68820600	0.52955000
N	4.38047400	1.24066100	-0.36598000
O	5.59510300	1.22747900	-0.38833100
O	3.63636200	2.17333200	-0.63897600
N	3.52497300	-0.91436000	-1.23206800
O	3.99881300	-0.47694300	-2.26325700
O	2.91254300	-1.95550900	-1.06372400
N	-0.85013600	1.82595900	1.51025400
O	0.27914800	2.23814800	1.70738000
O	-1.87153900	2.13727300	2.10053900
H	-0.00906100	-1.06509200	-1.94158200

H	1.34732000	1.55755700	-0.51443900
H	1.98846600	-0.76363600	1.12394700
H	2.43676800	0.91614100	1.48465800
P7			
C	-0.40742400	1.26817300	-0.94123700
N	-0.66216200	0.33702200	-1.76854300
C	-0.95183600	-0.79815100	-0.87631000
C	-2.34644700	-0.58661400	-0.18199200
C	-1.99088000	0.56828700	0.81718000
C	-0.48067700	0.80476100	0.50861500
N	-0.01970900	2.63063400	-1.35461300
O	-0.07694700	3.46901800	-0.45915500
O	0.33487500	2.78930000	-2.50922000
N	-0.10899800	-0.61852500	0.34220700
N	1.19988500	-1.01569000	0.48656200
C	2.23875900	-0.80824600	-0.52350700
N	-2.79671200	1.88573500	0.61606800
O	-2.73822100	2.35009700	-0.51359500
O	-3.33047000	2.36964400	1.58853500
N	-3.48296900	-0.26964000	-1.14838500
O	-3.30257000	-0.59396900	-2.30936100
O	-4.47897400	0.22289300	-0.64810300
N	-0.74040800	-2.10073400	-1.61028200
O	-1.61391700	-2.94856400	-1.54973400
O	0.32795600	-2.18299900	-2.19840500
N	-2.21246000	0.19664300	2.29567800
O	-3.31049100	-0.26246700	2.55271000
O	-1.30160500	0.44267300	3.06518700
N	-2.82036900	-1.93063900	0.54668700
O	-2.00527200	-2.43335500	1.29391600

O	-3.92516800	-2.32645700	0.26327300
C	3.50476900	-0.24587300	0.13305200
N	4.49946000	0.26316800	-0.91651500
O	4.69732200	-0.52897800	-1.82591800
O	4.98910800	1.36241600	-0.75046400
N	4.26379800	-1.30349800	0.94884300
O	5.45255400	-1.11464000	1.11226200
O	3.58794500	-2.23551200	1.36345800
N	3.16426500	0.91249700	1.07004900
O	3.61083300	0.88800900	2.19763900
O	2.44180800	1.76353600	0.56597100
H	0.06284200	1.35045000	1.27212300
H	1.25655300	-1.90248400	0.97097200
H	1.91039500	-0.09247400	-1.27504900
H	2.51716300	-1.72349400	-1.04911900
TS1			
C	1.50566000	-0.97657300	0.18211300
N	0.81727700	-2.02670800	0.46983900
C	-0.34956500	-1.51665700	1.03500700
C	-1.25035600	-1.14873300	-0.61295700
C	-0.56552200	-0.05830200	-1.19043900
C	0.84672900	0.22287700	0.59849000
N	2.68736500	-1.01968600	-0.67612800
O	3.40648200	-1.98372200	-0.58288300
O	2.80396900	-0.06956100	-1.42837400
N	1.43604100	1.55769600	0.70110300
O	2.62286700	1.57780000	0.95048100
O	0.69088900	2.49561700	0.54463700
N	-1.14576800	1.26685100	-1.14005800
O	-0.77880300	2.05883100	-1.97836700

O	-1.94966300	1.50084800	-0.24314300
N	-2.69171800	-0.97411300	-0.22314800
O	-2.98624400	-0.94858200	0.95782400
O	-3.46472100	-0.92685900	-1.14867600
N	-0.09988300	-0.20483000	1.46190100
N	-0.86277200	0.63632500	2.26584700
H	-0.99479400	-2.14926400	1.63191900
H	-1.16637700	-2.09319300	-1.14150300
H	0.10136200	-0.17550800	-2.03390600
H	-1.08342100	0.12304700	3.11465900
H	-1.72044500	0.87554100	1.76806300

TS2

C	-1.77013600	0.68745000	0.10805900
N	-0.96552500	1.49173600	-0.49766100
C	0.26338400	1.11552600	0.03359100
C	0.61616700	-0.32176500	-1.04652600
C	-0.35422900	-1.30938800	-0.73405400
C	-1.14537900	-0.07914300	1.14442100
N	-3.18146800	0.53980200	-0.25792600
O	-3.74993600	-0.39137700	0.28259500
O	-3.63966200	1.32923000	-1.04626000
N	0.00245400	-2.43296200	0.08918900
O	0.93066500	-2.28744800	0.88478700
O	-0.65856500	-3.44350000	-0.02702300
N	2.06342200	-0.68254500	-0.83465300
O	2.69567700	-0.08262100	0.01477300
O	2.49043600	-1.52761200	-1.57971300
N	0.04947800	0.50401100	1.29614900
N	0.95076400	0.16950100	2.30534300
N	1.32676700	2.14114700	-0.08820500

O	1.63909600	2.42426600	-1.21953300
O	1.76171000	2.61065600	0.94176100
H	0.54014300	0.11646700	-2.03856800
H	-1.17294600	-1.53774400	-1.40151300
H	-1.56484800	-0.76584800	1.86707800
H	1.48518600	1.01537000	2.49520600
H	1.57701800	-0.55192100	1.94810300

TS3

C	-2.86931100	0.74351900	-1.00856100
N	-2.50282400	0.05566200	-2.03424600
C	-1.21893600	-0.39057200	-1.70986100
C	-1.84206400	-1.90934000	-0.64635100
C	-2.38760800	-1.32520000	0.51452000
C	-1.84109600	0.77246800	-0.00714300
N	-4.26193100	1.16651700	-0.83847200
O	-4.70866500	1.91272400	-1.67385600
O	-4.83707100	0.68438900	0.11730500
N	-0.71217100	0.38653600	-0.67695300
N	0.61104000	0.79860600	-0.56340800
C	1.45904500	0.09123400	0.39838300
N	-1.64693000	-1.29139700	1.75818600
O	-0.44312600	-1.50924500	1.70620100
O	-2.26830800	-0.99293300	2.75639200
N	-0.65995900	-2.82266600	-0.51880100
O	0.40511000	-2.47344600	-0.98979300
O	-0.89765200	-3.88499800	0.00233800
C	2.89877200	0.35757900	-0.00225000
N	3.86049300	-0.59178700	0.68663200
O	3.59990100	-0.79976800	1.84957400
O	4.78625100	-1.00299200	0.03636800

N	3.36634300	1.75925000	0.35751300
O	4.53506200	1.90013900	0.60219600
O	2.50018000	2.60944000	0.34303900
N	3.07258000	0.19612600	-1.50274800
O	2.73999100	-0.88424600	-1.92131900
O	3.48913400	1.14968000	-2.11305700
N	-1.79406900	1.60948500	1.17530700
O	-2.78765400	2.25633600	1.41573200
O	-0.76323600	1.56574500	1.82171100
H	-0.53418200	-0.75104000	-2.46753900
H	-2.55461500	-2.37806900	-1.31788500
H	-3.45322500	-1.21804800	0.67244800
H	0.61965600	1.79823700	-0.37417100
H	1.29574900	-0.98017200	0.28962300
H	1.30648600	0.38004200	1.44137900
TS4			
C	2.71071800	1.07373400	0.78135700
N	3.06646200	-0.14103900	1.03220400
C	1.89261300	-0.84146700	0.80688000
C	2.09311400	-0.95102100	-1.08835400
C	1.86365300	0.36655700	-1.54461700
C	1.30977500	1.22227200	0.53449700
N	3.67305900	2.17023400	0.66241300
O	3.25358300	3.14990600	0.07314200
O	4.76808800	2.00574400	1.14053800
N	0.79315800	0.03752600	0.93557700
N	-0.49881500	-0.14513400	1.41019800
C	-1.49324600	-0.80568000	0.57333600
N	0.60416000	0.73127700	-2.14554000
O	-0.33781400	-0.04764100	-2.00509500

O	0.54788500	1.79318900	-2.72266800
N	1.19561600	-2.05822600	-1.55509300
O	0.44613300	-2.58167300	-0.75151800
O	1.34721000	-2.37792800	-2.70610400
C	-2.65879600	0.14495400	0.31656600
N	-3.85054300	-0.61157200	-0.24196900
O	-3.56656600	-1.49323000	-1.01728800
O	-4.94232000	-0.25502400	0.12633900
N	-2.34134300	1.25704200	-0.66711700
O	-3.04918600	1.35523800	-1.63153400
O	-1.38823500	1.94195100	-0.36599300
N	-3.12708300	0.80501900	1.60217000
O	-3.11172200	0.07469200	2.56866300
O	-3.49139900	1.94964800	1.53762000
N	1.84140700	-2.18833700	1.41445600
O	2.71338400	-2.94296300	1.06388700
O	0.95190800	-2.40263200	2.21346100
H	3.11409700	-1.31397600	-1.16186300
H	2.66420100	1.01493000	-1.87256000
H	0.71133700	2.11545500	0.41661200
H	-0.41640100	-0.60945300	2.30902700
H	-1.89980000	-1.67600700	1.09402400
H	-1.10055600	-1.13877500	-0.38191600
TS5			
C	-1.73076100	1.48728900	-1.16367800
N	-1.77369700	0.42545400	-1.93461500
C	-0.79159600	-0.37938500	-1.49863900
C	-2.00610600	-1.42311400	-0.06561500
C	-2.57024900	-0.47051200	0.74433500
C	-0.61071800	1.48282500	-0.28164300

N	-2.73037100	2.54503500	-1.25396800
O	-2.45507700	3.57982100	-0.67703600
O	-3.73157800	2.29377500	-1.88209600
N	0.02315100	0.32995700	-0.59401900
N	1.20711200	-0.05945600	0.01007400
C	2.22459200	-0.43198900	-0.96672500
N	-1.95716700	-0.13683800	2.01553900
O	-0.72477400	-0.21612500	2.05531400
O	-2.66301600	0.16911000	2.93788300
N	-1.02893200	-2.39248400	0.56572000
O	-0.00282300	-2.62456500	-0.05023500
O	-1.38621700	-2.90718200	1.59013400
N	-3.81278500	0.19199700	0.37841400
O	-4.41128400	-0.31422200	-0.55231300
O	-4.11006900	1.21080600	0.96296800
N	-2.85314800	-2.30258700	-0.98968300
O	-2.65572000	-2.24892800	-2.17396900
O	-3.58235700	-3.04519700	-0.38106200
C	3.59284000	-0.15511500	-0.36678000
N	4.67762000	-0.14379700	-1.42401800
O	4.57362000	-1.03235500	-2.23972800
O	5.52203500	0.70828600	-1.33663600
N	3.99634500	-1.20193800	0.65723600
O	3.07241900	-1.69209100	1.26941800
O	5.17247900	-1.42481900	0.76992400
N	3.60832700	1.19482600	0.32783700
O	3.14718000	2.09537500	-0.33510600
O	4.05386500	1.23508600	1.44497300
N	-0.28147700	2.41734800	0.63542900
N	0.64403600	2.16868300	1.45690000

N	1.40504000	2.15528100	2.27437000
H	-0.40235600	-1.21835500	-2.05891300
H	1.02816000	-0.80819800	0.67746700
H	2.12206500	0.21281300	-1.84265400
H	2.18630800	-1.48081100	-1.27940100
TS6			
C	2.18228500	-1.11958900	-1.21305300
N	1.78200100	-0.23375500	-2.05716100
C	0.51813900	0.11961100	-1.63136200
C	1.30629600	1.44809000	-0.15267100
C	1.72954700	0.51467700	0.81819200
C	1.21098400	-1.31084500	-0.16115900
N	3.49087200	-1.77677200	-1.33395200
O	3.67428000	-2.68188800	-0.54238700
O	4.22086500	-1.38654000	-2.20531300
N	0.04988900	-0.79928200	-0.72482200
N	-1.27020000	-1.20906000	-0.61789600
C	-2.06651800	-0.74740000	0.51216700
N	0.99437600	0.45154500	2.13333900
O	0.21867900	-0.46496600	2.31018900
O	1.25894300	1.34450300	2.89047000
N	0.08133800	2.26199400	0.07282500
O	-0.68431200	1.88569800	0.93959000
O	-0.06982600	3.21045300	-0.65448800
N	3.19662000	0.35443100	1.06373400
O	3.89912400	0.46105300	0.07594400
O	3.54363700	0.08818300	2.18226000
N	2.31316900	2.37652500	-0.79722600
O	2.35872700	2.41858600	-1.99679200
O	2.91399900	3.05684000	0.00361600

C	-3.39108000	-0.23013100	-0.03613900
N	-4.08834300	0.68698800	0.94337500
O	-4.09786200	0.26293200	2.07673100
O	-4.56758900	1.70185600	0.50944400
N	-4.36003900	-1.35945300	-0.34386200
O	-5.53297500	-1.11875900	-0.22972900
O	-3.83299900	-2.39227200	-0.69695100
N	-3.18098600	0.53654000	-1.32958200
O	-3.88623300	0.25628000	-2.26137300
O	-2.29534200	1.36268800	-1.28254200
N	1.16462600	-2.42030500	0.80023500
O	0.25502600	-3.21199500	0.63730400
O	2.01823800	-2.43782100	1.64578100
H	-0.16378400	0.70816600	-2.23596400
H	-1.29971500	-2.21946300	-0.72198100
H	-1.57360400	0.07423200	1.02189800
H	-2.26909900	-1.53383400	1.24311200

TS7

C	-1.33412100	1.47461000	-1.22651900
N	-1.62157000	0.44489700	-1.95917000
C	-0.85379000	-0.53815400	-1.40611700
C	-2.26659000	-0.83198700	0.25807600
C	-1.79427500	0.24342700	1.03320100
C	-0.40218500	1.17236200	-0.17701500
N	-1.95944900	2.78595300	-1.40137000
O	-1.68736200	3.58494600	-0.52343100
O	-2.64892000	2.94984700	-2.37384600
N	0.14445600	-0.01752900	-0.62202600
N	1.26349500	-0.59774600	-0.05600900
C	2.44019300	-0.57498600	-0.91348200

N	-2.74096200	1.35609000	1.34818100
O	-3.51149800	1.65565100	0.46069400
O	-2.61597200	1.87584500	2.42723700
N	-3.71895900	-0.86599100	-0.15054100
O	-3.98140600	-0.88668000	-1.32210700
O	-4.47432900	-0.92181200	0.79330200
N	-0.67230100	-1.83461100	-2.07664700
O	-1.67114200	-2.46551100	-2.31131400
O	0.48010300	-2.14159300	-2.31728800
N	-0.99994500	-0.07555900	2.28366200
O	-1.58148800	-0.79198200	3.06070300
O	0.08874200	0.43137900	2.41221100
N	-1.84703300	-2.20606700	0.59130700
O	-0.66230100	-2.34723800	0.86893800
O	-2.66768300	-3.07776800	0.51251800
C	3.58620200	0.01888600	-0.10311300
N	4.73882400	0.45507600	-0.97782500
O	5.02794600	-0.35329500	-1.83279900
O	5.25297600	1.51623100	-0.73864700
N	4.15782100	-0.97254700	0.89569000
O	5.29608400	-0.78689000	1.24034400
O	3.39410900	-1.84148400	1.25245900
N	3.09199100	1.22315600	0.67301500
O	3.28704500	1.24908600	1.85666400
O	2.51117000	2.03670200	-0.01601600
H	0.15404500	1.84972400	0.45881600
H	1.05481000	-1.49750700	0.36597400
H	2.26337500	0.07501400	-1.77210200
H	2.73201100	-1.56149700	-1.27772400