

## Supporting Information

### Acetylene as an Essential Building Block for Prebiotic Formation of Pyrimidine Bases on Titan

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The supporting information includes: (1) coordinates for optimized geometries of all species, and (2) coordinates of geometries for all transition states.

#### Coordinates for optimized structures

##### Coordinates for 1

0 1

C	0.00000000	0.00000000	0.14633200
N	0.00000000	1.16210500	-0.61336800
H	0.20664700	1.98663400	-0.07038200
H	0.44978200	1.13290600	-1.51633700
N	0.00000000	-1.16210500	-0.61336800
H	-0.20664700	-1.98663400	-0.07038200
H	-0.44978200	-1.13290600	-1.51633700
O	0.00000000	0.00000000	1.36032500

##### Coordinates for 2

0 2

C	-0.05356900	0.07936500	-0.01555300
N	1.26937400	-0.23785300	-0.05611900
H	1.93991600	0.50713300	0.04273200
H	1.55394900	-1.18089800	0.15119300
N	-0.90474800	-1.02311000	0.06954200
H	-1.77175600	-0.75911900	-0.40707500
O	-0.49413500	1.22292900	0.02656200

##### Coordinates for 3

0 2

C	1.03687100	-0.14402100	0.06971700
N	-0.26993900	-0.75845000	-0.19979600

C	-1.51762500	-0.17193400	-0.06180200
N	-1.49594600	1.21747200	-0.03027700
H	-2.41725600	1.62129600	-0.10976000
H	-0.77096000	1.67740200	-0.56748600
O	-2.53804700	-0.82350100	0.04356800
H	-0.27913600	-1.76605900	-0.14133600
N	1.16835000	0.60014100	1.30593900
H	1.43378600	-0.04327300	2.04349800
H	0.29081200	1.04794900	1.55387400
N	1.34844700	0.78022500	-1.03986400
H	2.22939000	1.25284700	-0.86098900
H	1.34690400	0.29804400	-1.93438400
O	2.01237200	-1.06002300	-0.07893400

#### Coordinates for **4**

0 1

C	1.19536700	0.07345900	-0.01126900
N	0.01671100	-0.65851400	0.01007700
H	0.05056300	-1.66409400	-0.06943400
C	-1.32420600	-0.18757900	0.00451500
N	-1.46546700	1.15498700	0.06045500
H	-2.40236700	1.51548800	0.00911200
H	-0.64921100	1.75211300	0.01089600
O	1.24007000	1.29361400	-0.04362200
N	2.33098000	-0.70217200	-0.03122100
H	2.31169100	-1.64481900	0.32411000
H	3.18737600	-0.19062400	0.11151300
O	-2.22764300	-0.99904600	-0.03398600

#### Coordinates for **5a**

0 2

C	0.43011700	-0.28544200	-0.02840100
N	-0.89659200	-0.72868400	0.05699400
H	-1.10093600	-1.71528300	-0.02918000
C	-2.05081800	0.07198300	0.02437000
N	-1.90022500	1.42771100	0.26635300
H	-1.17018300	1.80734100	-0.34793400
O	0.70791300	0.90076200	-0.17958200
N	1.35896500	-1.26897000	0.03599100
H	1.11862100	-2.19102500	0.35949700
H	2.33976900	-0.96030400	0.06136000
O	-3.14255700	-0.43229600	-0.14591400
N	3.76502800	0.35658100	0.01531100
H	4.31164200	0.59432800	0.83702400
H	4.37844400	0.43206300	-0.79003600
H	3.03377000	1.05944400	-0.08511700

Coordinates for **6a**

0 2

C	-1.77714300	-0.41986600	-0.00817900
N	-1.03748500	0.75748800	-0.00100200
H	-1.51148200	1.64665700	-0.06254000
C	0.36829500	0.92736700	-0.00539000
N	1.09378000	-0.22629600	0.00685800
H	0.58066000	-1.10485900	-0.00827700
O	-1.27785500	-1.53372900	-0.03594000
N	-3.13507500	-0.22191300	-0.01812900
H	-3.53534600	0.64186400	0.31089600
H	-3.68394000	-1.05505700	0.12273900
O	0.82601600	2.05294700	-0.01563700
C	3.26519600	-1.26688300	0.01677200
C	2.49261500	-0.20446000	0.01327000
H	4.32185700	-1.47088200	0.02149900
H	2.90064900	0.80663500	0.01537100

Coordinates for **7a**

0 2

C	-1.43897400	-0.49920400	-0.01679700
C	-0.51742800	1.75804000	0.01522100
C	0.74553700	1.33852900	0.13717200
C	1.08259900	-0.12376900	0.10215300
N	-1.57403400	0.88066100	-0.14342900
O	-2.39761500	-1.24573200	0.00037000
N	-0.13689600	-0.91916400	0.10134400
H	-0.03123000	-1.89865800	0.32381100
H	-0.78494700	2.80713700	0.03759000
H	1.56075900	2.03010800	0.29297100
N	1.88614200	-0.44947800	-1.10999500
H	2.72803700	0.11881700	-1.15329800
H	2.14347000	-1.43460300	-1.11903700
O	1.95408700	-0.53667300	1.05407800
H	-2.52476100	1.21072500	-0.17955800

Coordinates for **8a**

0 2

C	1.40171000	-0.50119000	-0.02414900
C	0.47239900	1.76864800	0.00159800
C	-0.78640700	1.33637200	-0.02115400
C	-1.05518700	-0.14338100	-0.01361200
N	1.53927300	0.87926800	0.02747800
O	2.37156100	-1.23871200	0.01072300
N	0.10916300	-1.01421000	-0.13385500

H	-1.79477400	-1.36954600	-1.31395800
H	0.74154600	2.81696900	-0.00633900
H	-1.62523800	2.01603000	-0.06940600
N	-1.62090800	-0.54122600	1.24936500
H	-2.37245200	0.06140300	1.56085700
H	-1.89464600	-1.51667600	1.25781100
O	-1.86280600	-0.41825200	-1.15582800
H	2.48774700	1.21801600	0.07485400

Coordinates for **9a**

0 1

C	-1.18727700	-0.53189000	0.00006800
C	1.12920000	-0.25271400	-0.00270200
C	1.04916300	1.18527400	-0.00100600
C	-0.20022700	1.71225700	0.00139200
H	-0.39108200	2.77878700	0.00191200
N	2.35424400	-0.84327600	-0.03604900
H	3.18789500	-0.31521300	0.15390200
H	2.37919200	-1.84413500	0.07843500
N	0.08182600	-1.04931500	0.00289600
O	-2.21621000	-1.17448900	0.00101200
N	-1.27905300	0.89563100	0.00144700
H	-2.21877300	1.26418600	0.00314300
H	1.92816600	1.81343900	-0.01005700

Coordinates for **10a**

0 1

C	0.00257600	1.70638900	-0.00007500
C	1.22406900	-0.40695400	-0.00005900
C	-1.29320500	-0.34956200	-0.00015400
C	-1.20320700	1.10676400	-0.00038900
H	0.11973300	2.78281100	-0.00008000
N	-0.03201100	-0.98748300	-0.00052600
H	-0.04474600	-1.99943400	-0.00065300
N	1.17311500	0.98701300	0.00051100
H	2.07051900	1.44685500	0.00058800
O	-2.31347700	-1.00521700	0.00060000
O	2.26447400	-1.02457400	0.00002700
H	-2.12260500	1.67157600	-0.00070400

Coordinates for **5b**

0 2

C	1.55032400	0.10108500	-0.06488100
N	0.48360100	-0.58206600	0.52229300
H	0.47659200	-0.61607900	1.53396500
C	-0.84941100	-0.40112200	-0.05695000

N	-1.70028400	-1.43222600	0.56531000
H	-2.66047900	-1.32071400	0.25284700
H	-1.35150100	-2.34780500	0.28867200
O	1.46169700	0.70900500	-1.10963600
N	2.71694300	0.02487200	0.67939500
H	2.86700700	-0.80315200	1.23641000
H	3.52967600	0.34761700	0.17620100
O	-0.90567500	-0.74660400	-1.36446500
C	-1.41423400	0.93923300	0.22241900
C	-1.87594500	2.02359300	0.44916600
H	-2.27569800	2.99012900	0.63720700

Coordinates for **6b**

0 2

C	-1.77714300	-0.41986600	-0.00817900
N	-1.03748500	0.75748800	-0.00100200
H	-1.51148200	1.64665700	-0.06254000
C	0.36829500	0.92736700	-0.00539000
N	1.09378000	-0.22629600	0.00685800
H	0.58066000	-1.10485900	-0.00827700
O	-1.27785500	-1.53372900	-0.03594000
N	-3.13507500	-0.22191300	-0.01812900
H	-3.53534600	0.64186400	0.31089600
H	-3.68394000	-1.05505700	0.12273900
O	0.82601600	2.05294700	-0.01563700
C	3.26519600	-1.26688300	0.01677200
C	2.49261500	-0.20446000	0.01327000
H	4.32185700	-1.47088200	0.02149900
H	2.90064900	0.80663500	0.01537100

Coordinates for **7b**

0 1

C	-1.50773700	-0.13483700	-0.00002600
N	-0.20371700	-0.64279400	-0.00013200
C	0.79456800	0.19455900	-0.00029500
N	0.73180100	1.54266400	-0.00068100
H	1.57240100	2.09374300	-0.00178800
H	-0.20093000	1.94917800	-0.00072200
O	-1.84682400	1.05238600	0.00165200
N	-2.42504300	-1.13927100	-0.00439500
H	-2.11757900	-2.09568500	0.01052700
H	-3.40288500	-0.90792700	0.01139300
C	2.12721600	-0.36202500	0.00020000
C	3.24785200	-0.79492600	0.00065000
H	4.23090600	-1.19921900	0.00065900

Coordinates for **8b**

0 2

C	-0.57472300	1.39469000	-0.01942400
N	0.74569100	1.02598500	0.06170200
C	1.07776300	-0.23813700	0.01436500
N	0.25608600	-1.30585700	-0.00701100
H	0.64198300	-2.23498700	-0.03920000
H	-0.74760800	-1.15574500	-0.01305700
O	-1.56276700	0.65474800	-0.14363200
N	-0.78071100	2.75211900	0.14433800
H	-1.50179500	3.06219500	-0.51419200
C	2.48493700	-0.54895800	-0.00314900
C	3.65168800	-0.83381200	-0.01872700
H	4.69012500	-1.06215800	-0.03163500
N	-3.30285500	-1.99126600	0.05361200
H	-3.05004300	-1.00959000	-0.00102500
H	-2.90919500	-2.46649500	-0.75107400
H	-2.88678900	-2.38076800	0.89237300

Coordinates for **9b**

0 2

C	0.83802800	1.10694400	-0.00006700
C	-0.21900200	-1.01562700	-0.00011000
C	1.05360600	-1.65735400	-0.00010700
C	2.18340600	-0.93688000	0.00015300
H	3.17926400	-1.36524800	0.00038400
N	-1.36797200	-1.71941100	0.00001400
H	-1.35762200	-2.72380900	0.00017200
H	-2.24040000	-1.20776200	0.00022400
N	-0.28197800	0.30451900	-0.00029600
O	0.82649700	2.31910200	-0.00002500
N	2.08800800	0.42615400	0.00009800
H	2.90798500	1.01650000	0.00035400
N	-3.57638000	0.85466400	0.00005600
H	-3.85015400	0.34000300	-0.82812800
H	-3.84899400	0.34167700	0.82968300
H	-2.57004100	1.00184300	-0.00080200

Coordinates for **11**

0 1

C	1.56280600	0.07275300	-0.06851000
N	0.19539800	0.44061400	0.00778900
H	-0.03148300	1.41622500	-0.12094200
C	-0.88962300	-0.43146300	0.08880800
O	1.95830200	-1.03797100	-0.30267400
N	2.38490400	1.17468400	0.09474400

H	2.08953000	1.91766800	0.71027900
H	3.36432900	0.93878000	0.15113300
O	-0.82798600	-1.62104800	0.26178500
C	-2.16242800	0.27893400	-0.03987500
C	-3.23403600	0.81536500	-0.13256800
H	-4.18733200	1.27886700	-0.21822500

Coordinates for **12**

0 2

C	1.58120100	0.15978800	-0.00503200
N	0.22127200	0.47043800	-0.02451400
H	0.00292600	1.45724700	-0.05247700
C	-0.84763100	-0.43021800	0.02394800
O	2.05603000	-0.95535400	-0.12118700
N	2.36591300	1.30276600	0.02955300
H	3.27350200	1.02751000	0.41650700
O	-0.74092900	-1.62747700	0.09090000
C	-2.13549600	0.25415300	-0.00537400
C	-3.21900600	0.77311900	-0.03086200
H	-4.18193600	1.22440800	-0.05308100

Coordinates for **13**

0 2

C	0.12522800	1.74670800	0.00010800
C	1.14844900	-0.47167700	-0.00006100
C	-1.37789000	-0.20865000	-0.00016000
C	-1.09358800	1.21164100	-0.00072100
H	0.32118900	2.81248100	0.00008700
N	-0.15930200	-0.94135200	-0.00046300
H	-0.25294600	-1.95001000	-0.00076800
N	1.23477500	0.92043300	0.00037500
H	2.17135800	1.29572800	0.00076800
O	-2.44621500	-0.77260000	0.00063200
O	2.12357700	-1.18738700	0.00005900

Coordinates for **13-NH<sub>3</sub>**

0 2

C	-0.16736800	1.63541500	-0.00069200
C	0.38167500	-0.72103900	-0.00055400
C	-2.03898600	0.03398000	0.00042200
C	-1.47380200	1.36427400	0.00000100
H	0.23939700	2.64033400	-0.00091300
N	-0.99090700	-0.92810000	0.00020800
H	-1.28317200	-1.89781500	0.00034900
N	0.75597800	0.61254200	-0.00107200
H	1.77952400	0.77885100	-0.00100900

O	-3.19910800	-0.30931100	0.00088600
O	1.18714400	-1.63643200	-0.00094200
H	3.30630300	-0.67413900	0.00275000
N	3.59204000	0.30484600	0.00119100
H	4.17232300	0.46042600	0.81965700
H	4.17244200	0.45749300	-0.81774100

#### Coordinates for **14**

0 2

C	0.92609100	0.11496300	0.00649600
N	-0.33312300	-0.47383200	-0.02662400
H	-0.41948800	-1.46594900	0.13111200
N	1.96283100	-0.80240400	0.06635400
H	2.86844900	-0.38583500	-0.08700600
O	1.09801600	1.31641300	0.01555900
C	-1.50370600	0.30225500	-0.03972300
C	-2.73750400	-0.14212700	0.02186600
H	-3.30722000	-1.05317500	0.09615500
H	-1.28015100	1.36357600	-0.11189100
H	1.83703700	-1.70682100	-0.36278900

#### Coordinates for **15**

0 2

C	0.15133900	0.16318500	-0.05557500
N	-1.19813700	0.49823900	0.03346100
H	-1.47354700	1.46485800	-0.04441400
N	1.00253800	1.23287200	-0.09752700
H	1.99493000	0.99412700	-0.00163300
O	0.52232400	-1.00171300	-0.11762800
C	-2.20191600	-0.48083600	0.04184300
C	-3.49941200	-0.27552800	0.04838600
H	-4.22900800	0.51705200	0.04958500
H	-1.78181600	-1.48337900	0.04409400
H	0.69922900	2.12801300	0.25066800
N	3.48922200	-0.31310400	0.09094900
H	2.73101800	-0.99145700	0.00998400
H	4.01140000	-0.53050200	0.93379900
H	4.11377500	-0.45198700	-0.69715100

#### Coordinates for **16**

0 2

C	-0.29530600	0.18034500	-0.05942600
N	1.05420900	0.50553000	0.02044200
H	1.32897500	1.47395600	-0.04370000
N	-1.13640700	1.26224600	-0.09225800
H	-2.12575500	1.04588700	0.00316500



O	-0.67973300	-0.97915700	-0.12603500
C	2.05695500	-0.45991400	0.03865000
C	3.36600300	-0.20438500	0.05288500
H	3.76350600	0.80517600	0.04663800
H	4.07633000	-1.01863700	0.07058400
H	1.65736200	-1.46595800	0.04210300
H	-0.82724700	2.14914900	0.27163700
N	-3.61221700	-0.37692100	0.11051200
H	-2.85563700	-1.07144000	0.01379600
H	-4.48466700	-0.91713200	0.14053000

#### Coordinates for 17

0 2

C	0.99212500	0.00449700	-0.00000700
N	-0.10281600	-0.83974400	-0.00000200
H	0.18355100	-1.80810700	0.00000000
N	0.69326700	1.36676800	0.00000000
H	1.61079400	1.82563800	0.00001000
O	2.13410900	-0.44704900	0.00000400
C	-1.48887300	-0.61915300	0.00000100
C	-2.17408900	0.52550800	0.00000100
H	-1.69732200	1.49327200	-0.00000200
H	-3.25477400	0.47461600	0.00000300
H	-2.02326200	-1.56329900	0.00000500

#### Coordinates for 18

0 2

C	0.84830300	-0.02806000	0.00266100
N	0.04670100	1.11875700	-0.03927000
H	0.46406200	2.02603200	0.08763700
N	-0.03703500	-1.08119700	0.08529000
H	0.28905900	-2.01376600	-0.10311500
O	2.05852600	-0.06384600	-0.02264000
C	-1.30512000	0.82602000	0.10629200
C	-1.42954800	-0.66823600	-0.04567700
H	-1.85125200	-0.95842300	-1.02445600
H	-2.05650800	1.53612000	-0.20826300
H	-2.06303600	-1.12046300	0.72751400

#### Coordinates for 19

0 2

C	1.93209400	-0.26470000	0.01979200
N	0.86044400	-0.61079000	0.82609800
H	0.69738900	-1.57348500	1.07364400
N	1.64303400	0.99695700	-0.48475600
H	2.42066300	1.55941300	-0.79090500

O	2.91640900	-0.93188000	-0.21387000
C	-0.22094000	0.35380800	0.79068100
C	0.48399900	1.59067300	0.16858500
H	0.76864100	2.29902000	0.95503200
C	-1.46529500	-0.16680000	0.02108500
O	-1.84365700	-1.39784100	0.45028400
N	-2.54203500	0.79449500	0.11710000
H	-3.42330700	0.32309800	-0.05762300
H	-2.43198100	1.54972500	-0.55114500
H	-0.59216900	0.57975200	1.79212100
H	-0.15359500	2.11210700	-0.54853800
N	-1.11241400	-0.50041000	-1.38384200
H	-0.29239800	-1.09943100	-1.44098300
H	-1.89760600	-0.95206800	-1.84596900

Coordinates for **20**

0 2

C	1.41027000	0.73403200	-0.06697500
N	0.66051000	0.07155200	0.90014800
H	0.93234400	-0.89966900	1.07303800
N	0.58930100	1.71504700	-0.60852500
H	1.03207300	2.51225800	-1.03661200
O	2.55883700	0.50308600	-0.38094200
C	-0.73683500	0.41557500	0.77707600
C	-0.64958300	1.83198100	0.13994800
H	-0.59750100	2.59439400	0.92833400
C	-1.51410300	-0.57839500	-0.12178800
O	-0.96741900	-1.43051300	-0.79207400
N	-2.86764900	-0.40314300	-0.10724100
H	-3.43717900	-1.03907100	-0.64314600
H	-3.32229300	0.22466500	0.53414700
H	-1.22892200	0.46140600	1.75391300
H	-1.50239400	2.04961600	-0.50638100
N	1.71706200	-2.51229700	0.31837100
H	1.12529800	-2.90323400	-0.42451100
H	2.51416500	-2.09821100	-0.18349800

Coordinates for **21**

0 2

C	1.73855500	-0.28308800	-0.11352000
N	0.64676300	-0.81202500	0.54492200
H	0.39601800	-1.77842600	0.39684100
N	1.51106900	1.10242500	-0.14382900
H	2.19593300	1.72501600	-0.53941000
O	2.70371800	-0.85608100	-0.56089800
C	-0.41016800	0.16985800	0.74804200

C	0.25464600	1.45462900	0.31931800
H	0.10064800	2.40880900	0.80644000
C	-1.68614200	-0.26763700	-0.02735100
O	-2.00712300	-1.43931400	-0.05620100
N	-2.40685000	0.74151400	-0.57762800
H	-3.21608900	0.49697800	-1.12812800
H	-1.96834300	1.63791200	-0.72509900
H	-0.71914400	0.20689100	1.80296100

Coordinates for **22**

0 1

C	1.88686700	-0.24572100	0.02257400
N	0.62370300	-0.80892100	0.05895800
H	0.43777300	-1.79913600	0.07775800
N	1.60678700	1.12938900	-0.05085000
H	2.34071500	1.81541700	-0.10693200
O	2.97454500	-0.77893500	0.04885800
C	-0.37499200	0.15892400	0.00046800
C	0.24590100	1.36590900	-0.07222900
H	-0.16469300	2.35707200	-0.16297100
C	-1.78503300	-0.26677700	-0.01252800
O	-2.07356500	-1.44925600	-0.11069900
N	-2.72772400	0.72734700	0.05631900
H	-3.68192500	0.41760900	0.15935700
H	-2.49553200	1.62584700	0.44681600

Coordinates for **23**

0 2

C	1.84053300	-0.25858000	-0.00006700
N	0.57620500	-0.83083900	-0.00017500
H	0.39435000	-1.82345400	-0.00034400
N	1.55428300	1.12484800	0.00020800
H	2.28775000	1.81585400	0.00029000
O	2.92803700	-0.78292500	-0.00028500
C	-0.41348900	0.12716400	0.00007100
C	0.20738400	1.35336300	0.00036500
H	-0.24422100	2.32958200	0.00061700
C	-1.83569400	-0.21451600	0.00009000
O	-2.20457700	-1.39104900	0.00050300
N	-2.61974600	0.91154100	-0.00058500
H	-3.59316000	0.58637900	-0.00120000

Coordinates for **24**

0 2

C	-1.62630800	1.35727300	0.10697300
C	2.72360200	0.17437200	-0.09681000

C	0.27915500	-0.42232100	0.12760800
C	-1.09218300	0.10707600	0.06123600
N	1.29385900	0.50362500	0.16870700
N	3.56614000	1.28851800	0.26210900
H	3.75138900	1.87351300	-0.54259300
O	0.45381200	-1.63593400	0.17654500
N	-2.15649100	-0.78468600	-0.03556900
N	-2.99738900	1.22131800	0.03017800
C	-3.37495600	-0.13009400	-0.05877600
O	-4.49632600	-0.58072200	-0.13656300
H	-3.67960500	1.96092300	0.04496300
H	-1.15072600	2.31809700	0.20732800
H	1.05601400	1.44066700	-0.12289800
H	-2.04177200	-1.78511600	-0.07281400
H	3.21212100	1.82449800	1.04471100
N	3.08788900	-0.99123800	0.69994100
H	2.45863800	-1.77478400	0.52753400
H	4.07411400	-1.19843100	0.59090100
O	2.95575200	-0.26334100	-1.33949300

Coordinates for **25**

0 2

C	1.35969000	-1.20094100	-0.02361200
C	-2.01634700	-1.31836100	0.00119200
C	-0.44714800	0.71194000	-0.01869200
C	0.86178600	0.07111800	-0.00872200
N	-1.66229700	0.03102200	-0.03513500
N	-3.37749300	-1.48559400	-0.01864400
H	-4.01033400	-0.72050300	0.15213800
O	-0.49492600	1.94420800	-0.01585700
O	-1.24246900	-2.25640300	0.02173700
N	1.97079400	0.93024200	0.01270900
N	2.72764500	-1.10427700	-0.01143700
C	3.15936300	0.23609400	0.01087700
O	4.30173100	0.64244300	0.02480900
H	3.37954100	-1.87130600	-0.01718500
H	0.82062700	-2.12926700	-0.03959500
H	-2.43665700	0.69637600	-0.05592500
H	1.89074500	1.93387300	0.01950900
H	-3.70956900	-2.42294000	0.13355900
N	-3.52472200	2.33851400	0.02137900
H	-2.63192400	2.85096600	0.05978300
H	-4.25866800	3.05237500	-0.04615300

Coordinates for **26**

0 2

C	0.70065900	-1.14249100	-0.16884900
C	-2.59386300	-0.47762000	0.04357100
C	-0.60527200	1.14649800	-0.06094800
C	0.51254900	0.21008000	-0.03957700
N	-1.94693000	0.73878700	-0.11816100
N	-3.96565400	-0.29330000	0.08052900
H	-4.36116700	-1.15351300	0.47169200
O	-0.38306500	2.34852900	-0.03519900
O	-2.04961700	-1.57530100	0.07741200
N	1.78210800	0.77607800	0.08988700
N	2.04629400	-1.37341100	-0.10784900
C	2.77754300	-0.17788300	0.05322000
O	3.97812000	-0.05540500	0.13536600
H	2.50141100	-2.26971400	-0.17211400
H	-0.03492800	-1.91408700	-0.29255100
H	-2.56786400	1.53762400	-0.17457000
H	1.93862300	1.76853300	0.17156400

Coordinates for **27**

0 2

C	-0.26877100	-0.86498100	0.60181600
C	2.09758000	-0.71248200	-0.13267300
C	0.81391100	1.42256200	0.09462100
C	-0.33867800	0.61079200	0.33947000
N	1.99922400	0.66631300	0.09754700
N	0.89513500	-1.40186700	-0.09079600
H	1.03218100	-2.40295400	-0.07751700
O	0.79837800	2.62897200	-0.10311700
O	3.15798600	-1.24798000	-0.36661200
N	-1.62936900	0.92908900	0.04294700
N	-1.55778400	-1.29427000	0.08321600
C	-2.41955500	-0.22777200	-0.13774000
O	-3.58693200	-0.25757600	-0.42238600
H	-1.96790100	-2.18151600	0.33035800
H	-0.20548800	-1.08852600	1.68106000
H	2.85751500	1.17871400	-0.05700400
H	-1.92912100	1.84338600	-0.26334200

Coordinates for Uric acid (**28**)

0 1

C	-0.25935900	-0.76622700	0.00062000
C	2.15068000	-0.72646300	-0.00002900
C	0.80660500	1.43368600	-0.00031800
C	-0.35270400	0.59384900	0.00130600
N	1.99529900	0.65137900	-0.00098000
N	0.93685900	-1.42892300	-0.00072700

H	1.01183100	-2.43465300	0.00012100
O	0.84808300	2.64813700	-0.00016600
O	3.21963000	-1.29273900	0.00072800
N	-1.71527500	0.90981600	-0.00034100
N	-1.52512400	-1.28539700	-0.00036800
C	-2.48732700	-0.23299300	0.00001100
O	-3.68741100	-0.36370400	-0.00031000
H	-1.80329300	-2.25337000	0.00056100
H	2.86058900	1.17586400	0.00003300
H	-2.10121800	1.83937500	0.00464200

Coordinates for **29**

0 2

C	-1.61304200	1.33939100	0.13696100
C	2.70122000	0.17199100	-0.09041100
C	0.27607400	-0.46636200	0.13158500
C	-1.09207000	0.08544400	0.06276900
N	1.28870300	0.48948100	0.12440800
N	3.51462900	1.35155500	-0.06375500
H	3.51283300	0.06588000	-1.80701800
O	0.44606800	-1.66499200	0.22106500
N	-2.16498500	-0.79241000	-0.05834400
N	-2.98674800	1.21937100	0.05120400
C	-3.37706600	-0.12518800	-0.06734900
O	-4.50297900	-0.56375700	-0.15556800
H	-3.66212100	1.96440100	0.08652900
H	-1.12690100	2.29072100	0.27064500
H	1.03065500	1.35995700	-0.32096600
H	-2.06057700	-1.79377200	-0.10394800
H	3.15207700	1.96019800	0.67713900
N	3.17261500	-0.67412900	0.98739500
H	4.14504900	-0.92354800	0.85416300
H	2.99578600	-0.29247700	1.90886900
O	2.91603600	-0.49876100	-1.30213400

Coordinates for **30-OH**

0 2

C	1.74825300	-1.40777000	0.19501700
C	-2.65360200	-1.10045100	-0.03094300
C	-0.38515500	0.05817700	-0.02185800
C	1.04729800	-0.25594500	0.00217700
N	-1.22763700	-1.02195700	-0.10437200
N	-3.28667600	-2.18714800	-0.25804300
O	-0.74820500	1.23194500	0.01974200
N	1.98066000	0.76787200	-0.13659500
N	3.08566900	-1.08546900	0.16261600

C	3.27820900	0.29495700	-0.03673100
O	4.32708500	0.89252000	-0.10241900
H	3.86089700	-1.71439400	0.29299800
H	1.40499500	-2.41157300	0.38109300
H	-0.79311100	-1.90865700	-0.30858800
H	1.74049900	1.73955000	-0.24995300
H	-2.66851200	-2.96458000	-0.47329200
N	-3.29531900	0.03278900	0.36594700
H	-4.29868600	-0.03039000	0.29535700
H	-2.88812800	0.94390800	0.21567500
O	-2.76332800	3.19099000	-0.03927700
H	-1.88926800	2.74607000	-0.03049700

### Coordinates for **30**

0 1

C	-1.29532800	1.33348900	0.17821600
C	3.01651300	0.28007400	-0.02494400
C	0.59329400	-0.44952600	-0.01384200
C	-0.77327500	0.08792100	0.00805800
N	1.60490700	0.48599500	-0.04469000
N	3.86037700	1.21742400	-0.22922300
O	0.76996400	-1.66273700	-0.00948400
N	-1.84736800	-0.78757900	-0.12379300
N	-2.66742700	1.21180300	0.14235700
C	-3.06062900	-0.12689200	-0.04009700
O	-4.18702900	-0.56363400	-0.10573000
H	-3.34168200	1.95083800	0.25344100
H	-0.80933100	2.28008900	0.34471400
H	1.33556100	1.44571800	-0.19458800
H	-1.74657900	-1.78502800	-0.22550000
H	3.41286200	2.11445100	-0.39691100
N	3.40434300	-0.98992500	0.28337100
H	4.38387200	-1.17296100	0.13972700
H	2.73454600	-1.73656200	0.16031900

### Coordinates for **31**

0 2

C	-0.68360500	-1.11188200	-0.26813600
C	2.52524600	-0.29917600	0.10554000
C	0.62877100	1.12401800	-0.10233700
C	-0.53874400	0.23727200	-0.10517600
N	1.81977600	0.59944300	-0.60323500
N	2.10647300	-0.69713300	1.29798000
H	2.75515600	-1.37883600	1.69949800
O	0.51196700	2.30258000	0.17816700
N	-1.81360000	0.76600200	0.03974800

N	-2.02584900	-1.38957100	-0.20445100
C	-2.78445700	-0.21933700	-0.00235900
O	-3.98598300	-0.13082400	0.10695900
H	-2.46095300	-2.29457900	-0.27764400
H	0.06577300	-1.86799700	-0.41481300
N	3.70627100	-0.70207000	-0.48192600
H	3.84262900	-0.44756300	-1.44687700
H	4.15001400	-1.54776000	-0.16645700
H	-1.99525800	1.74061000	0.22328400

### Coordinates for **32**

0 2

C	0.26640400	-0.87633700	0.60543300
C	-2.03318100	-0.48214500	-0.09686600
C	-0.76140100	1.45322200	0.09443700
C	0.36975200	0.60197400	0.37933300
N	-2.00118500	0.81037500	0.03204700
N	-0.94579100	-1.33292700	-0.06069100
H	-1.11131400	-2.32639700	-0.11932100
O	-0.61700600	2.65555200	-0.10273600
N	1.67869200	0.88086500	0.09256300
N	1.51964400	-1.34096800	0.03282800
C	2.41929300	-0.28653400	-0.14801900
O	3.58351900	-0.35971600	-0.44529700
H	1.91989600	-2.22958600	0.29338700
H	0.22277100	-1.13759500	1.67866900
N	-3.23550700	-1.08456200	-0.37099000
H	-4.01612100	-0.44642000	-0.33221700
H	-3.41229900	-2.01201200	-0.01740100
H	1.98878100	1.79476700	-0.20506200

### Coordinates for **33**

0 2

C	0.16456400	-0.96461500	0.52360300
C	-2.07321300	-0.33062100	-0.10719000
C	-0.53513500	1.39571700	-0.01845300
C	0.38109500	0.48569500	0.85702300
N	-1.81071000	0.93809900	-0.25142800
N	-1.13776800	-1.31630200	0.11713500
H	-1.47349900	-2.24497300	0.32861300
O	-0.10675700	2.45696200	-0.41640000
N	1.79413900	0.66288700	0.57763200
N	1.29578700	-1.36679700	-0.18758600
C	2.31458600	-0.39650600	-0.14416600
O	3.41035600	-0.50513300	-0.63820900
H	1.50450400	-2.30457600	-0.49064400



H	0.14471300	0.70633800	1.90670300
N	-3.37788300	-0.74545300	-0.16206000
H	-4.00746200	-0.03047400	-0.49507200
H	-3.57667200	-1.67848500	-0.49060400
H	2.12328700	1.59247800	0.35713200

Coordinates for **34**

0 1

C	0.16165200	-0.86569800	0.15566900
C	-2.03442300	-0.49807000	-0.04273900
C	-0.74778800	1.42609000	-0.05133000
C	0.33036600	0.55045900	0.62406000
N	-1.97547700	0.81451600	-0.11939700
N	-0.97526200	-1.41950200	-0.07727000
O	-0.49781100	2.56198400	-0.38541300
N	1.72639500	0.79647400	0.36146000
N	1.40096500	-1.36669700	-0.05020800
C	2.39274000	-0.32643600	-0.04642000
O	3.54426700	-0.47591700	-0.35543000
H	1.59123000	-2.26419600	-0.47199100
H	0.10496300	0.59005800	1.70074700
N	-3.24174200	-1.08851300	-0.00839500
H	-4.06244600	-0.51273000	-0.09877100
H	-3.30116000	-2.08863600	-0.09750800
H	2.13633700	1.71494900	0.31549100

Coordinates for **34-NH<sub>2</sub>**

0 2

C	-0.76721000	0.90253500	0.15916300
C	1.46927100	0.84646600	0.03145900
C	0.45225200	-1.24666700	0.03031700
C	-0.75809700	-0.51636200	0.64810700
N	1.58086500	-0.47429900	-0.02849500
N	0.28893700	1.60449200	-0.04709500
O	0.37715800	-2.41963000	-0.26747200
N	-2.09670800	-0.95590000	0.34103700
N	-2.05678700	1.22660000	-0.09373700
C	-2.89553000	0.06036600	-0.10709300
O	-4.04508300	0.04568400	-0.45741600
H	-2.35223300	2.08322600	-0.53922900
H	-0.57227700	-0.50943100	1.73296900
N	2.57855000	1.58826800	0.08050100
H	3.49054500	1.13157800	0.03612100
H	2.48458700	2.58785000	0.01283700
H	-2.37485200	-1.92253100	0.29789700
N	4.62797800	-0.48444600	-0.21178500

H	3.77949700	-1.06847300	-0.27128000
H	5.42416400	-1.12167800	-0.32490300

Coordinates for **35**

0 2

C	0.49448100	-1.10980500	0.00014100
C	2.42340500	0.01153500	0.00002400
C	0.53335100	1.38136200	-0.00011100
C	-0.21634500	0.12389700	0.00066700
N	1.89603500	1.22197800	-0.00030200
N	1.79117300	-1.22852500	-0.00017500
O	-0.02970900	2.47969500	-0.00050600
N	-1.54062300	-0.14927200	0.00058800
N	-0.46097200	-2.09784800	-0.00002700
C	-1.75120800	-1.53926200	-0.00000500
O	-2.80332900	-2.12665200	-0.00042200
H	-0.29285100	-3.09140400	-0.00084900
H	-3.54232300	2.50053000	-0.81958000
N	3.77127800	-0.08608500	0.00246200
H	4.31891100	0.75723700	-0.00648700
H	4.20405300	-0.99292500	-0.00785900
H	-2.29377900	0.58962200	0.00110600
N	-3.02414600	2.20069500	0.00016900
H	-2.11795700	2.67576000	-0.00039400
H	-3.54307500	2.50388900	0.81817700

Coordinates for **36-NH<sub>2</sub>**

0 2

C	-0.35753400	-1.07553600	0.00122800
C	-2.40140800	-0.18510400	0.00261200
C	-0.44245400	1.35104100	-0.00341900
C	0.29895900	0.14385300	-0.00704600
N	-1.84285800	1.06205100	0.00340400
N	-1.69184600	-1.28716200	-0.00665500
O	-0.07357500	2.52304500	0.00108200
N	1.66850000	-0.10977900	-0.00888800
N	0.60762400	-2.04570400	0.00360700
C	1.90415200	-1.47102800	-0.00144400
O	2.95471900	-2.07193700	0.00017700
H	0.45087000	-3.04034500	0.01012400
H	-2.42697200	1.88514300	0.07236300
H	2.39630300	0.61008400	-0.00856500
N	-3.77263200	-0.26175600	0.06789000
H	-4.30602600	0.46530100	-0.38476200
H	-4.12324900	-1.19503100	-0.08985100
N	2.93413000	2.48639400	0.00108300

H	2.00491600	2.93356700	0.00771000
H	3.62430300	3.24474800	0.00822600

### Coordinates for **36**

0 1

C	-0.24422100	-0.76311800	0.00042800
C	1.98398800	-0.69156400	-0.00211600
C	0.73222100	1.46700100	0.00257000
C	-0.39690400	0.60780500	0.00786400
N	1.92956900	0.67427300	-0.00268700
N	0.91669200	-1.45451200	0.00795400
O	0.79833200	2.68438700	-0.00383900
N	-1.76505800	0.87685300	0.00752400
N	-1.50498100	-1.30840400	-0.00277200
C	-2.49472500	-0.30175300	0.00045800
O	-3.69454400	-0.45650300	-0.00188500
H	-1.72720100	-2.29057100	-0.00903900
H	2.77865300	1.22012900	-0.07163600
H	-2.19191500	1.78805400	0.00797500
N	3.22647500	-1.27282200	-0.06650600
H	3.99909700	-0.78949900	0.36567200
H	3.21003700	-2.26912900	0.09301100

### Coordinates for optimized transition states (TS)

#### Coordinates for TS **1** → **2**

0 2

N	-0.06551400	-0.05173400	0.09400500
H	-0.04798200	-0.81743300	0.75098000
C	1.13580100	0.34653000	-0.47655800
N	2.26131500	0.04588900	0.29223100
H	2.09824700	0.18874800	1.28775300
O	1.18301700	0.89282800	-1.56544700
H	-0.83534300	-0.06996800	-0.55893100
H	3.34967400	0.66815800	-0.13032600
N	3.90013100	1.63166300	-0.52998100
H	3.31636500	1.91948000	-1.32019400
H	3.84439600	2.38157600	0.16120700

#### Coordinates for TS **2** → **3**

0 2

C	-0.06153000	-0.48592700	0.00753700
N	0.30136500	0.65281100	0.77171900
H	1.19126900	1.01022900	0.44785500
H	-0.40656600	1.37400100	0.72581500

N	-1.45574700	-0.57406800	-0.18118000
H	-1.70539300	-1.43531600	-0.65131400
H	-1.96217400	-0.50449300	0.69419900
O	0.72189100	-0.87184500	-0.94893200
N	0.45291300	-1.82498800	1.04950700
H	1.23507000	-1.57456000	1.64948400
C	0.43151700	-3.19696700	0.74920200
N	-0.06219300	-3.51659100	-0.48871000
H	0.15614300	-2.85538100	-1.22540100
H	-0.00928100	-4.49842500	-0.71384300
O	0.73635100	-4.00298900	1.61083600

Coordinates for TS 3 → 4

0 2

C	1.11465900	-0.18396800	-0.13337900
N	2.03153700	-1.27214300	-0.15585200
H	2.91855900	-0.94315200	-0.51749700
H	1.69420700	-2.03127600	-0.73642600
N	-0.22050300	-0.69636800	-0.10021300
H	-0.29075800	-1.62228700	0.30046800
C	-1.34096100	0.11243200	0.15385400
N	-2.51838200	-0.60754700	0.05817800
H	-3.34833200	-0.03763400	0.12104100
H	-2.56035400	-1.35932900	-0.61304300
O	1.38344200	0.91647700	-0.66727400
O	-1.30422800	1.28216100	0.46580200
N	1.33110500	0.57370100	1.57900600
H	2.26072600	1.00026600	1.61028900
H	0.65394900	1.34361200	1.58807900

Coordinates for TS 4 → 5a

0 2

C	1.15587000	-0.22775700	0.33519400
N	-0.06585000	-0.86014000	-0.02845500
H	0.07129000	-1.83567200	-0.25257900
C	-1.35916100	-0.36477300	0.09080500
N	-2.32606700	-1.24387600	-0.33831000
H	-3.25243900	-0.85010500	-0.38991800
H	-2.10229800	-1.94191800	-1.02996500
O	2.16653900	-0.91078700	0.34346100
N	1.09724900	1.11371700	0.56970100
H	2.18233000	1.60564300	1.19348200
H	0.17864000	1.42429500	0.89341000
O	-1.63066500	0.72523200	0.56723200
N	2.97605900	1.53431700	2.04111800
H	2.52609200	1.57906100	2.95606700

H	3.37179800	0.59666200	1.94334400
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Coordinates for TS **5a** → **6a**

0 2

C	0.96577400	0.14502400	0.19273900
N	-0.17575600	-0.65909200	0.14661500
H	-0.08898600	-1.61368600	-0.17387400
C	-1.53267100	-0.28094000	0.30353000
N	-1.77833600	0.94512500	0.87931900
H	-1.02239600	1.60458800	0.67122500
O	0.91517600	1.35728300	0.39001500
N	2.12920400	-0.51857500	-0.02929100
H	2.17022700	-1.52281600	0.02031700
H	2.98860200	0.02757900	0.10392100
O	-2.39520500	-1.08845300	0.00618600
C	-3.18662600	2.71757800	-0.79256100
C	-3.50492700	1.71315300	-0.18414500
H	-2.78674200	3.58456500	-1.26130600
H	-4.06276800	0.87905000	0.17422300
N	3.98972700	1.66757000	0.47414700
H	3.07292600	2.10682100	0.55172800
H	4.50298200	2.14869400	-0.25764600
H	4.48385000	1.82577700	1.34663100

Coordinates for TS **6a** → **7a**

0 2

C	-1.83027600	-0.41840400	0.07729600
N	-0.93349400	0.66344000	0.40626200
H	-1.39520600	1.53279200	0.64143800
C	0.33306400	0.86568700	-0.11498600
N	1.07216800	-0.28697400	-0.34804500
H	2.01646300	-0.09497000	-0.64393000
O	-2.00352800	-0.82686200	-1.08309000
N	-2.84020700	-0.48959500	1.03777600
H	-2.53174500	-0.48681000	1.99921100
H	-3.53577700	-1.19133700	0.82848300
O	0.81392700	1.97006100	-0.27485500
C	-0.48984700	-1.95451600	0.37158500
C	0.72781100	-1.58296700	0.01538300
H	-0.94146800	-2.91378600	0.55800000
H	1.56688200	-2.27724100	0.03853800

Coordinates for TS **7a** → **8a**

0 2

C	-1.36030100	-0.51699200	0.03473100
C	-0.49047000	1.77817800	0.00158200

C	0.78409500	1.39494400	-0.06664600
C	1.11048300	-0.06045400	-0.10759800
N	-1.52991100	0.85516500	0.02969900
O	-2.28012400	-1.29015700	0.19350400
N	-0.04696000	-0.97823700	-0.20981400
H	0.54131000	-1.48713700	0.78578800
H	-0.79599300	2.81579800	0.03099000
H	1.58615300	2.11855300	-0.09702600
N	2.07673400	-0.36055000	-1.11191700
H	2.92505900	0.17938600	-0.97762700
H	2.30762800	-1.34905400	-1.10117600
O	1.36057800	-0.63718700	1.19355000
H	-2.48361800	1.16624400	0.13367600

Coordinates for TS **8a** → **9a**

0 2

C	1.29692700	-0.53548900	-0.13085400
C	0.47407900	1.76555400	-0.02732000
C	-0.75628200	1.36287300	0.32280700
C	-0.98476000	-0.08085900	0.39715300
N	1.46556400	0.84887900	-0.27293600
O	2.21509500	-1.29505200	-0.36273900
N	0.05892200	-0.97391000	0.33080000
H	-1.32633000	-1.42933600	-1.38265300
H	0.75325900	2.80728100	-0.12106600
H	-1.55422500	2.06097500	0.52592200
N	-2.04480200	-0.50816400	1.16565100
H	-2.91222200	-0.01158200	1.02294700
H	-2.14949400	-1.51322900	1.19135600
O	-1.31448700	-0.45879700	-1.36616400
H	2.38628700	1.14301900	-0.56055000

Coordinates for TS **7a** → **10a**

0 2

C	-1.47357600	-0.48169600	0.10150500
C	-0.55938200	1.78133700	0.14069300
C	0.68789300	1.36498500	0.39231600
C	0.99107400	-0.08468100	0.40141000
N	-1.59249300	0.89234100	-0.08686300
O	-2.41719800	-1.23878600	0.01520500
N	-0.19309300	-0.87498300	0.42997000
H	-0.07407700	-1.86091600	0.61523200
H	-0.83140400	2.82867700	0.10547400
H	1.49907300	2.05129800	0.58228900
N	1.72115100	-0.39157200	-1.25207000
H	2.60557600	0.12379300	-1.27729700

H	1.98635300	-1.38168300	-1.25363200
O	2.02626200	-0.56384100	0.97229700
H	-2.52982100	1.21635600	-0.26410900

Coordinates for TS **4** → **5b**

0 2

C	1.59348900	-0.75017900	0.47835300
N	0.76298100	0.03695100	-0.31819000
H	0.99966100	1.01121700	-0.44127100
C	-0.61371700	-0.18627700	-0.54802300
N	-1.00782200	-1.48577800	-0.51580000
H	-2.00413100	-1.61629800	-0.59899100
H	-0.49884800	-2.08253700	0.12915300
O	1.26747200	-1.83142900	0.93770700
N	2.82207900	-0.18585400	0.71147900
H	3.18727000	0.52239400	0.09509000
H	3.49542200	-0.80103100	1.13950100
O	-1.23370200	0.68993000	-1.25690600
C	-1.53436600	0.85891100	0.85785700
C	-2.28174800	1.53884700	1.53971800
H	-2.87237500	2.07478400	2.24503900

Coordinates for TS **5b** → **6b**

0 2

C	1.68296800	-0.88406700	-0.52018600
N	0.46253800	-0.73005900	-1.28219700
H	0.27627700	0.42234700	-1.72765500
C	-0.77086800	-0.34073000	-0.52950700
N	-1.90215700	-1.02305500	-1.05304200
H	-2.76066800	-0.70438800	-0.61854200
H	-1.95428500	-0.90641600	-2.05931900
O	2.13708300	-1.99392900	-0.37978200
N	2.25172800	0.27599600	-0.10143400
H	1.69465000	1.11608900	-0.05557100
H	3.06246300	0.20005200	0.49275600
O	-0.54618000	1.00866600	-0.97027800
C	-0.73561000	-0.45356200	0.93011700
C	-0.73968800	-0.54081400	2.12642900
H	-0.73405800	-0.62387900	3.18610200

Coordinates for TS **6b** → **7b**

0 2

C	-1.64093900	-0.37784100	-0.22877900
N	-0.27328200	-0.51160200	-0.59368500
H	0.84015600	1.38264100	-1.66696700
C	0.67375800	-0.02797500	0.23624100

N	0.43479200	0.32360800	1.53367400
H	1.20391000	0.75045300	2.02720600
H	-0.47257900	0.73018600	1.72023000
O	-2.31467100	-1.36600500	-0.03344200
N	-2.09061000	0.91239400	-0.14371600
H	-1.48928000	1.63535300	-0.52354300
H	-3.09016900	1.04339200	-0.11776500
O	0.56076200	1.63652600	-0.77417600
C	2.04119100	-0.40314700	-0.04624200
C	3.17804100	-0.73165700	-0.24552600
H	4.18070800	-1.02803600	-0.43754800

Coordinates for TS **7b** → **8b**

0 2

C	-0.29791000	-0.14751200	-3.31330400
C	1.56649200	1.34831100	-0.38831000
C	-0.29909000	-0.00053500	-2.12094800
H	-0.23959900	-0.26300500	-4.36842700
N	0.34836100	0.83264700	0.08784000
O	2.23541800	0.87234100	-1.29573900
N	-1.52709900	-0.45440000	-0.16983100
H	-2.24676400	-0.80473000	-0.77852500
H	-1.75049400	-0.26587400	0.79466500
N	1.94300700	2.49614600	0.27226500
H	1.51767600	2.69544900	1.47863700
H	2.93905600	2.66382900	0.14719600
N	1.38623900	2.37902900	2.63042600
H	0.90801700	1.47748600	2.57620600
H	2.30322200	2.19264800	3.04056400
C	-0.43216400	0.16454000	-0.69346800

Coordinates for TS **8b** → **9b**

0 2

C	-0.22018100	1.79998000	-1.51352300
C	1.53900700	-0.07763500	-0.01914400
C	-0.64533000	-0.58156600	-0.75679500
C	-0.74198400	0.69335700	-1.44245100
H	-0.02299400	2.81968000	-1.75298800
N	0.42909000	-0.91042700	-0.09495000
N	1.41247800	1.30605600	-0.11307400
H	2.27473800	1.67311600	-0.52081600
O	2.64444400	-0.52198900	0.27551600
N	-1.69271400	-1.41644500	-0.81905600
H	-2.49875900	-1.16405600	-1.36430900
H	-1.61863900	-2.33100700	-0.34618300
N	-0.72293800	-3.70354100	0.65372500



H	-0.97972700	-3.91409200	1.61327900
H	0.07455900	-3.06563500	0.67991600
H	-0.41177200	-4.57063300	0.22670100

Coordinates for TS **9b** → **9a**

0 2

C	0.26404500	0.47400800	-0.25009900
C	0.21695600	2.81919000	-0.11276200
C	-1.19326500	2.82055900	0.16335300
C	-1.83987200	1.64214800	0.22555000
H	-2.90023000	1.54222400	0.42823900
N	0.86756200	3.99881200	-0.17574900
H	0.36354400	4.86127300	-0.02875600
H	1.85513300	3.99542700	-0.36978800
N	0.88317200	1.69877400	-0.30446000
O	0.80645600	-0.59857800	-0.41447600
N	-1.13813000	0.49214600	0.02483000
H	-1.58311800	-0.41371700	0.06294500
H	-1.66871600	4.08588200	0.32610900
N	-1.93945700	5.26604400	0.44671600
H	-2.70236500	5.38521200	-0.22506500
H	-2.38551600	5.29499000	1.36743300

Coordinates for TS **5b** → **11**

0 2

C	1.52390400	-0.68093700	0.10521400
N	0.50476000	0.23710800	0.39597100
H	0.55177900	0.68951900	1.29756200
C	-0.78655900	0.19755800	-0.20006000
N	-1.45952200	-1.54770000	0.23446500
H	-2.33546700	-1.64758500	-0.28630900
H	-0.76389500	-2.13995200	-0.23480500
O	1.36995800	-1.69879200	-0.53561100
N	2.72389500	-0.32436700	0.68677900
H	2.93316600	0.65708700	0.78908300
H	3.49981700	-0.90700100	0.41116900
O	-0.93544200	-0.00439600	-1.42281900
C	-1.72497600	1.05171700	0.53918000
C	-2.49530800	1.79477900	1.08365100
H	-3.18608000	2.44214800	1.56710600

Coordinates for TS **11** → **12**

0 2

C	1.32534100	0.18232700	1.01467400
N	0.41233000	0.59539500	0.00398700
H	-0.34276300	-0.07139600	-0.10990800

C	0.24091600	1.73185900	-0.76709100
O	1.09159800	-0.87461900	1.57392800
N	2.35982400	1.01704300	1.33193500
H	3.28520300	0.44457800	2.12367300
H	2.71990900	1.57623300	0.56370800
O	-0.71250800	1.84531400	-1.50991400
C	1.23866200	2.78912700	-0.68763700
C	1.98221800	3.73346500	-0.72539100
H	2.63799400	4.57072300	-0.74933200
N	3.97101200	-0.45776400	2.39100400
H	3.34185400	-1.26270300	2.43564900
H	4.65503600	-0.64090700	1.65620300

Coordinates for TS **12** → **13**

0 2

C	0.11777200	1.38807400	-1.82232900
C	1.13661900	-0.49386900	0.29494100
C	-1.14293500	-0.61551600	-0.81289800
C	-0.70366900	0.50116200	-1.63866100
H	0.62215200	2.25121700	-2.19368700
N	-0.17190400	-0.97572600	0.11996800
H	-0.37776100	-1.81517700	0.64896900
N	1.43295700	0.77335200	-0.16445000
H	2.39201300	0.77894400	-0.51592200
O	-2.20485100	-1.18260000	-0.90220500
O	1.94331400	-1.13695700	0.94279400

Coordinates for TS **13-NH<sub>3</sub>** → **10a**

0 2

C	0.09248900	1.85792700	0.35740100
C	1.06385100	-0.35345200	-0.00903000
C	-1.38473800	0.08147000	-0.41387200
C	-1.12922600	1.45548100	-0.01689900
H	0.31977300	2.87113500	0.66924700
N	-0.22333700	-0.72008400	-0.37714400
H	-0.33555900	-1.68828300	-0.65155100
N	1.16344900	0.98485600	0.36269100
H	2.08776900	1.28748200	0.63148600
O	-2.45188900	-0.39361000	-0.75307600
O	2.00844900	-1.10999500	-0.00600500
H	-2.26453600	2.33228800	-0.12757000
N	-3.40122200	2.56348100	-0.06412600
H	-3.80202400	1.74328900	-0.53044600
H	-3.62644200	2.43060300	0.92559200

Coordinates for TS 2 → 14

0 2

C	0.18446700	-0.65964800	-1.31754600
N	0.69266600	-0.96471300	-0.04618700
H	0.55723300	-1.95296400	0.17423800
N	-1.04479100	-1.23770100	-1.59447300
H	-1.54839800	-0.79101400	-2.34739100
O	0.73957200	0.08784400	-2.10378700
H	-1.61440600	-1.55772600	-0.82565800
C	2.82615300	-0.90981400	-0.32319300
C	3.40877400	-1.76681500	0.31804700
H	3.80417600	-2.53570000	0.93770200
H	2.63916600	-0.11523800	-1.01608700

Coordinates for TS 15 → 16

0 2

C	-0.88096700	-0.13352400	0.79656800
N	0.37604500	-0.55623000	0.37743000
H	1.05367500	0.19347700	0.35241600
N	-1.86731000	-1.11340300	0.84759200
H	-1.54110000	-1.98306700	1.26464000
O	-1.07577000	1.04565000	1.04845200
C	0.72645800	-1.78742100	-0.17038700
C	1.96297800	-2.14534600	-0.52271600
H	2.81458000	-1.48646000	-0.39460800
H	2.14217900	-3.11556800	-0.96363000
H	-0.11133600	-2.45735100	-0.32355800
H	-2.98610900	-0.67606300	1.41250300
N	-3.55069700	-0.08524100	2.25988700
H	-3.37695200	-0.50944800	3.17241900
H	-3.08758700	0.82760200	2.26383900

Coordinates for TS 16 → 17

0 2

C	-1.10901600	0.32730600	0.20047000
N	0.18518500	-0.16509900	0.29087100
H	0.30928600	-1.10756900	0.63224900
N	-2.06173700	-0.63280500	0.51650200
H	-2.97797500	-0.27878600	0.25206700
O	-1.36633000	1.48679800	-0.07837500
C	1.30660700	0.61430800	0.03468100
C	2.56937600	0.19572200	0.14848600
H	2.82231200	-0.81007100	0.46625300
H	3.38496900	0.86847300	-0.07552200
H	1.05021500	1.62002100	-0.27409000

H	-1.82761500	-1.78667100	0.07240700
N	-1.70561300	-2.69948200	-0.75581800
H	-2.64075700	-3.03545600	-0.99731300
H	-1.32090200	-2.31149900	-1.61954200

Coordinates for TS **17** → **18**

0 2

C	0.39827100	-0.94201200	-1.53621100
N	1.02872900	-0.55615900	-0.30117500
H	1.99765900	-0.27741800	-0.34978700
N	-0.94915500	-0.78933200	-1.43628900
H	-1.46084300	-1.44584900	-2.02037100
O	1.06418900	-1.25801600	-2.50328900
C	0.19340800	-0.19773700	0.71248700
C	-1.03556100	-0.82336700	0.70736000
H	-1.11316200	-1.88526800	0.52021800
H	-1.87825800	-0.36619600	1.21188400
H	0.43252700	0.66818000	1.32113600

Coordinates for TS **18** → **19**

0 2

C	1.73274600	-0.40568700	0.33850100
N	0.57777100	-0.58324400	1.10357200
H	0.36544800	-1.51257200	1.42944600
N	1.55395200	0.79266800	-0.32437300
H	2.35534500	1.25180700	-0.72458000
O	2.68424700	-1.15027200	0.28409800
C	-0.45367600	0.35782100	0.75671500
C	0.38116100	1.50687600	0.14897800
H	0.63048200	2.24431700	0.92300800
C	-1.57584800	-0.22213300	-0.23573600
N	-2.73115800	0.69824500	-0.13446800
H	-3.46644100	0.31237800	-0.72257300
H	-2.48379300	1.61023600	-0.51037200
H	-1.03149400	0.67903000	1.62975900
H	-0.13871100	2.00440800	-0.66981900
O	-1.10811200	-0.22064000	-1.49048700
N	-2.07483800	-1.52900400	0.16419500
H	-1.41703800	-2.25578500	-0.08931400
H	-2.30996800	-1.58152700	1.14898500

Coordinates for TS **19** → **20**

0 2

C	1.78637800	-0.68402700	0.22388600
N	0.44539600	-1.08966200	0.22197500
H	0.25391400	-1.98486700	0.64799700

N	1.77113400	0.69790100	0.20847500
H	2.59405900	1.17193700	-0.12833300
O	2.75432100	-1.40985200	0.23277300
C	-0.44513800	0.04186500	0.47310000
C	0.42848600	1.22209300	-0.01258800
H	0.23707300	2.12501500	0.56489500
C	-1.79388000	-0.13838300	-0.24897300
O	-2.78670100	-0.61987700	0.38222900
N	-2.47966700	1.60038500	-0.03905100
H	-3.27672200	1.59082900	-0.68091800
H	-2.88426400	1.65855900	0.89981000
H	-0.68098500	0.14625600	1.53789600
H	0.22971900	1.44105900	-1.06795400
N	-1.69042900	-0.33777800	-1.62740900
H	-0.77459000	-0.63396300	-1.93627900
H	-2.43339500	-0.92574500	-1.97975000

Coordinates for TS **20** → **21**

0 2

C	1.83078100	-0.51118300	-0.10837500
N	0.54286000	-0.92060200	0.15370900
H	0.35686000	-1.85063800	0.49450600
N	1.76952100	0.89035200	-0.15142600
H	2.54311300	1.39723300	-0.55183400
O	2.81967000	-1.18531000	-0.27721600
C	-0.32661500	0.19291100	0.51061600
C	0.43293100	1.37446700	-0.11820100
H	0.30923200	2.32295800	0.40818800
C	-1.78840000	-0.15399500	0.15600400
O	-2.27143400	-1.12902200	0.70681300
N	-2.45995800	0.65935800	-0.68939200
H	-3.39749400	0.35854100	-0.91598300
H	-1.98277600	1.27130900	-1.35641900
H	-0.34179100	0.33885000	1.60192100
H	-0.00346500	1.61760400	-1.25033700
N	-0.62236000	1.99213900	-2.49978200
H	-0.20008300	2.91550100	-2.63297600
H	-0.10892700	1.37178400	-3.13320900

Coordinates for TS **21** → **22**

0 2

C	1.98971700	-0.33616300	-0.02546500
N	0.70602800	-0.84671700	-0.02353700
H	0.48545500	-1.82676700	0.05162200
N	1.77316500	1.04569700	-0.20904200
H	2.53893700	1.69654200	-0.26917100

O	3.05145800	-0.90182900	0.09427200
C	-0.25410500	0.15442600	-0.13972800
C	0.43793300	1.33159600	-0.32766800
H	0.06466500	2.32311800	-0.51649800
C	-1.64686100	-0.22370900	-0.50346300
O	-1.91096300	-1.37053000	-0.81272500
N	-2.55979800	0.79950500	-0.51109000
H	-3.51751600	0.51062300	-0.64725700
H	-2.41964300	1.56895000	0.12595500
H	-0.80128500	0.48638900	1.71624100

Coordinates for TS **22** → **23**

0 2

C	2.11164100	-0.07897800	0.23385300
N	0.83354100	-0.60800600	0.23323100
H	0.60583800	-1.56865000	0.43651500
N	1.88478000	1.26885000	-0.09913300
H	2.64074200	1.92880300	-0.17663800
O	3.17339300	-0.61343900	0.46535500
C	-0.12364100	0.35098500	-0.07739100
C	0.54312900	1.51999000	-0.29069200
H	0.17389900	2.48993200	-0.57688500
C	-1.54334800	-0.04502300	-0.15464400
O	-1.84958300	-1.20546900	0.10918500
N	-2.43387100	0.89581400	-0.60357600
H	-3.70336900	0.58457100	-0.38231400
H	-2.17200700	1.85530100	-0.39139400
N	-4.57349900	0.13526300	0.28042700
H	-4.23801600	-0.79617300	0.53920200
H	-4.69117700	0.66179600	1.14733800

Coordinates for TS **23** → **24**

0 2

C	-0.34782900	-0.92629400	-0.17285500
C	2.80362500	-0.56152100	1.69721200
C	0.43390300	0.97743100	1.40467600
C	-0.23188800	0.36447200	0.26292700
N	1.26886000	0.15359100	2.18132400
N	3.25379000	-1.33036800	2.79126000
H	3.54113100	-0.74792700	3.56583600
O	0.18330300	2.13376400	1.71807200
N	-1.06168100	1.13916000	-0.54291900
N	-1.21911600	-0.92230700	-1.23113800
C	-1.70794600	0.37492500	-1.49519300
O	-2.49652900	0.70150900	-2.35278200
H	-1.51972800	-1.71936400	-1.76804900

H	0.15159600	-1.80482700	0.19420200
H	1.52001800	0.70832600	3.00082900
H	-1.21388400	2.12536500	-0.40068800
H	2.60483800	-2.05158900	3.07876300
N	2.55160800	-1.40863600	0.57258400
H	2.58192900	-0.85197700	-0.27430200
H	3.27793100	-2.11517200	0.53376200
O	3.34704200	0.59905000	1.52317100

Coordinates for TS **24** → **25**

0 2

C	-1.94871300	1.05367200	1.08259500
C	1.06196000	1.77041500	-0.27890800
C	0.23653200	-0.36389200	0.92653300
C	-1.20583300	-0.08297300	0.96490200
N	1.13428800	0.64625000	0.61636100
N	0.18191500	1.62238100	-1.34820200
H	0.17626400	2.42510700	-1.96077400
O	0.63904400	-1.47586700	1.23358200
N	-2.08931500	-1.15742200	1.07134700
N	-3.26110300	0.66835200	1.24772200
C	-3.39077900	-0.73280700	1.26515300
O	-4.40490200	-1.37857200	1.40878800
H	-4.05350400	1.27380100	1.38407700
H	-1.61756900	2.07888800	1.09781400
H	2.09452100	0.35823000	0.75703600
H	-1.79155300	-2.11909500	1.11664200
H	-0.73801000	1.26545200	-1.13220900
N	0.48950400	3.12417100	0.79467700
H	1.12887100	3.14846400	1.59224000
H	0.63912500	3.99729800	0.28270000
O	2.16597900	2.38026900	-0.47497100

Coordinates for TS **25** → **26**

0 2

C	0.85119500	-0.97042900	-0.63011600
C	-2.62675800	-0.67504100	-0.24436900
C	-0.70110100	1.04540600	-0.15419300
C	0.47866200	0.18508500	-0.00968100
N	-1.88731400	0.47917800	-0.63704700
N	-2.09333000	-1.48228700	0.72308200
H	-1.07948000	-1.52749100	0.75922600
O	-0.61524300	2.24226300	0.05055900
O	-3.73542700	-0.82486200	-0.72599400
N	1.58554300	0.63492600	0.70611700
N	2.15822500	-1.22269300	-0.28020300

C	2.67158000	-0.21099200	0.55484600
O	3.78623600	-0.13033700	1.01568100
H	2.73191800	-1.98641200	-0.59826900
H	0.30042700	-1.58901800	-1.31786500
H	-2.51800200	1.18413000	-1.00264800
H	1.62731200	1.52411400	1.17854000
H	-2.76489100	-2.64229600	0.89303000
N	-3.29661800	-3.57436700	0.45013700
H	-3.96598300	-3.19742700	-0.22486100
H	-2.64895300	-4.17815200	-0.05656300

Coordinates for TS **26** → **27**

0 2

C	0.42592900	2.20826000	-0.64621700
C	1.17924800	-0.48105400	0.18377800
C	-1.01187400	0.08057300	-0.94419900
C	-0.78011300	1.51224200	-0.70277900
N	0.09268600	-0.71362100	-0.72292600
N	1.10777300	0.68238800	0.88214900
H	2.03372000	0.92209900	1.23464600
O	-2.09271600	-0.33663400	-1.31907400
O	2.01795100	-1.35644800	0.31467000
N	-1.76506700	2.36343800	-0.28479400
N	0.12264500	3.47401200	-0.22438300
C	-1.24963200	3.61666300	0.05267900
O	-1.82718300	4.58799600	0.46762200
H	0.76706100	4.23873900	-0.10349100
H	1.35174900	1.97900700	-1.14231200
H	-0.00339900	-1.68207600	-1.00214200
H	-2.73351000	2.10536300	-0.16579200

Coordinates for TS **27** → **28**

0 2

C	-0.27686600	-0.74250900	-0.14822700
C	2.12755900	-0.70133800	-0.33878300
C	0.81248700	1.46629600	-0.25078300
C	-0.35752800	0.63574000	-0.17351000
N	1.98817000	0.68173600	-0.28793000
N	0.91258800	-1.39712000	-0.36950700
H	0.99745700	-2.39596700	-0.25144700
O	0.84413400	2.68033800	-0.28611300
O	3.19498000	-1.26689900	-0.36627900
N	-1.69630200	0.96917700	-0.26744000
N	-1.54821600	-1.23351000	-0.35304500
C	-2.48762000	-0.17070000	-0.32851000
O	-3.68803400	-0.26699900	-0.35081800



H	-1.85439900	-2.18278100	-0.20798400
H	-0.25793800	-0.68130200	1.80565800
H	2.85991900	1.19540200	-0.30743100
H	-2.07403000	1.90034300	-0.19481300

Coordinates for TS **24** → **29**

0 2

C	-1.64678300	1.26166400	0.42534400
C	2.66392200	0.16982700	0.14926700
C	0.23391900	-0.49746200	0.06866400
C	-1.12777700	0.05670100	0.06557200
N	1.23927500	0.43628700	0.24682300
N	3.51090900	1.21406800	0.75876400
H	3.94235200	1.23291600	-0.43559000
O	0.40298400	-1.70089900	-0.06770500
N	-2.19721900	-0.75121100	-0.31014800
N	-3.01354700	1.18615900	0.25741700
C	-3.40559000	-0.08516500	-0.19860100
O	-4.52828000	-0.47359200	-0.43075500
H	-3.68722000	1.90660800	0.45731300
H	-1.16022800	2.13943500	0.81483600
H	1.00748200	1.35329600	-0.11044900
H	-2.10281900	-1.71786300	-0.57821300
H	2.94368800	2.04739800	0.93770900
N	2.99358700	-1.11174300	0.63735800
H	2.41064700	-1.83466800	0.22875400
H	3.97975500	-1.29216500	0.49917300
O	3.16863700	0.56846700	-1.13577900

Coordinates for TS **29** → **30-OH**

0 2

C	-1.60298100	1.33609200	0.00162200
C	2.69976300	0.33811500	0.27345000
C	0.31273200	-0.37406200	0.39892000
C	-1.05537700	0.10115000	0.16948300
N	1.30211200	0.58682300	0.27005900
N	3.58986900	1.34352400	0.16337900
H	3.80947000	-0.02099400	-1.75469700
O	0.51254700	-1.54183000	0.70581800
N	-2.10358800	-0.81466000	0.14654500
N	-2.96326600	1.16671100	-0.13139300
C	-3.32455600	-0.19037400	-0.03869700
O	-4.43527000	-0.66526800	-0.10846100
H	-3.65177400	1.88978700	-0.25878000
H	-1.14085600	2.30862800	-0.00511500
H	1.06023900	1.36370100	-0.32788300

H	-1.98501300	-1.80699200	0.27441600
H	3.12742300	2.18322800	-0.18018600
N	3.09886800	-0.76993300	0.94615400
H	4.09569500	-0.91285900	0.96375500
H	2.48463500	-1.57297600	0.91319600
O	2.86592400	0.14508100	-1.61920000

Coordinates for TS **30** → **31**

0 2

C	-1.41616700	1.52408500	0.16035400
C	1.55585400	2.17786900	-0.22690200
C	0.65161500	-0.08738300	0.16789800
C	-0.75566700	0.33384500	0.06869400
N	1.63402900	0.87035600	0.31665600
N	1.45234500	3.23599700	0.48416000
O	0.90458300	-1.29099700	0.17269500
N	-1.72724700	-0.65256300	-0.10809800
N	-2.75991300	1.25650500	0.02848800
C	-3.00156000	-0.12027900	-0.13177600
O	-4.07224900	-0.67198600	-0.26175000
H	-3.51120800	1.92567500	0.06171700
H	-1.03009300	2.51630500	0.31663800
H	2.78103800	0.36277400	0.33389300
H	-1.51386400	-1.63618800	-0.15389000
H	1.49753100	2.98899300	1.47063400
N	1.69466600	2.25269500	-1.59637900
H	1.53014600	3.16817600	-1.98957800
H	1.35081500	1.47835600	-2.14242000
N	3.70939300	-0.37352700	-0.05068900
H	3.30323600	-1.31254800	-0.08784400
H	3.99918000	-0.13289800	-1.00120800

Coordinates for TS **31** → **32**

0 2

C	0.70439600	2.34266800	0.19451100
C	1.44873800	0.46705000	-1.67175300
C	-0.71020100	0.37050800	-0.77795500
C	-0.50288800	1.69533700	-0.12667500
N	0.38779200	-0.24230700	-1.30568600
N	1.51818800	1.81762400	-1.73280200
H	2.48450100	2.13957600	-1.77760600
O	-1.85073600	-0.06941700	-0.81504000
N	-1.48264000	2.64481500	-0.10202600
N	0.38459500	3.65018500	0.44661900
C	-0.98395600	3.90337400	0.23095800
O	-1.56525300	4.95430900	0.32632600

H	1.01329600	4.37852700	0.74425500
H	1.58728300	1.89598400	0.61864500
N	2.54923500	-0.28153100	-2.03486400
H	2.33755500	-1.25433800	-2.20590900
H	3.20450600	0.13385000	-2.67931900
H	-2.43597100	2.46121400	-0.38134000

Coordinates for TS **32** → **33**

0 2

C	0.28040300	-0.96422800	0.47322400
C	-2.05104500	-0.54699900	-0.03053600
C	-0.76419600	1.38277500	0.19158500
C	0.37815300	0.52207600	0.55624100
N	-1.99825400	0.74712100	0.03289100
N	-0.98582500	-1.43960000	0.03916300
H	-1.23512300	-2.37278700	0.33612000
O	-0.61355200	2.57907000	0.03363400
N	1.70502500	0.81784100	0.20250000
N	1.49575900	-1.37603100	-0.12332500
C	2.41261600	-0.30038300	-0.19856500
O	3.57067100	-0.37606600	-0.52188500
H	1.89229400	-2.29264600	0.02086300
H	0.30145300	-0.24790700	1.63086300
N	-3.27638700	-1.15038700	-0.14828000
H	-4.01923800	-0.49837900	-0.35378700
H	-3.32797400	-2.03022500	-0.64002700
H	2.08382700	1.75038200	0.18212000

Coordinates for TS **33** → **34**

0 2

C	0.21669700	-0.92349100	0.09829900
C	-2.00600500	-0.58502800	-0.12264600
C	-0.72791000	1.34753100	0.02712600
C	0.33966900	0.44414900	0.68894300
N	-1.94326500	0.72539400	-0.13780400
N	-0.92127600	-1.48906500	-0.17296100
H	-1.31704700	-2.83332400	0.64520700
O	-0.48627500	2.50541700	-0.22315400
N	1.73789500	0.73397400	0.48780400
N	1.46475400	-1.38549100	-0.14020400
C	2.43376600	-0.33074500	-0.01998700
O	3.59161500	-0.42464600	-0.32595300
H	1.68094100	-2.23254000	-0.64532700
H	0.07763300	0.40667400	1.75858900
N	-3.20637900	-1.18134700	-0.16430900
H	-4.02871600	-0.60253500	-0.19439200

H	-3.27310700	-2.18517400	-0.19203100
H	2.12304900	1.66426500	0.50914600

Coordinates for TS **34-NH<sub>2</sub>** → **35**

0 2

C	0.25036800	-0.94603900	0.05730100
C	-1.89768400	-0.33462500	0.12672900
C	-0.40710800	1.42660700	0.39018300
C	0.61673600	0.34039600	0.70047500
N	-1.69750600	0.95335100	0.32038600
N	-0.95935000	-1.33486000	-0.15863800
O	-0.07827500	2.59198300	0.32116100
N	1.99696000	0.47729700	0.37239700
N	1.40742800	-1.55527000	-0.29900300
C	2.52147000	-0.66930100	-0.17556600
O	3.65004800	-0.91410200	-0.50929100
H	1.47359500	-2.42233100	-0.81116900
H	0.48618000	0.15139300	1.87883800
N	-3.16385800	-0.79251800	0.13430000
H	-3.91522200	-0.12691500	0.20797700
H	-3.34216600	-1.74144400	-0.14756500
H	2.55381900	1.29646800	0.55217500
N	0.22975100	0.14628500	3.37857100
H	0.58940600	1.07514900	3.63493300
H	-0.78991200	0.27717300	3.40892400

Coordinates for TS **35** → **36-NH<sub>2</sub>**

0 2

C	0.11839400	-0.74716100	-0.04434400
C	-2.08031800	-0.42020700	-0.14388500
C	-0.71162300	1.57331900	0.12065200
C	0.37113500	0.62431900	0.09797600
N	-1.94030100	0.92395400	-0.03223200
N	-1.07210500	-1.31734300	-0.14213600
O	-0.59695700	2.78507600	0.23147500
N	1.73174200	0.79659700	0.12851400
N	1.34406000	-1.37047900	-0.05933300
C	2.38902000	-0.43620700	0.04534600
O	3.57538600	-0.65163300	0.06582500
H	1.50537000	-2.36109100	-0.15031700
N	-3.33783700	-0.87513300	-0.28463400
H	-4.09394700	-0.19665500	-0.11246400
H	-3.47930400	-1.86783200	-0.19087500
H	2.21384500	1.67282400	0.25880400
H	-2.96221900	1.46707100	0.09215400
N	-4.37340500	1.70850500	0.29889100

H	-4.61295300	2.07903800	1.21843900
H	-4.84788500	2.30852900	-0.37575000