

Supplementary Information

Free Radical Routes for Prebiotic Formation of DNA Nucleobases from Formamide

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The supporting information includes: (1) coordinates for optimized geometries of all species, (2) coordinates of geometries for all transition states, (3) Structure of two conformers of **3**, (3) structure of radical:neutral molecule complexes

List of Coordinates: From species 1 to 36

Coordinates of 1

FM

0 1

N	1.08421200	-0.15718500	-0.00011700
H	1.18222300	-1.16103000	0.00034000
H	1.90961500	0.41786200	0.00059000
C	-0.16375600	0.38544200	0.00001000
H	-0.13383100	1.49307900	-0.00003200
O	-1.19561900	-0.24528300	-0.00001800

Coordinates of 2

FM

0 2

N	1.12970100	-1.02793500	-0.08641100
H	1.07753000	-1.07267000	-1.10119700
H	2.10225500	-0.96690600	0.20103000
C	0.37741600	0.12871200	0.41306600
H	0.49002900	0.17211000	1.50472400
O	0.98032200	1.15545700	-0.24729800
C	-1.06333600	-0.03023000	0.09222700
N	-2.18639600	-0.11022000	-0.15043700

Coordinates of 3

FM

0 2
N -0.89084800 1.33292700 -0.07591200
H -1.20455200 1.18113500 -1.04460700
C -0.43644400 0.03548600 0.37760500
H -0.55323200 0.00010800 1.46930100
O -1.06580600 -1.07298400 -0.23858700
C 1.01167200 -0.04821000 0.08845400
N 2.13955400 -0.09039400 -0.14087100
H -1.90808100 -1.21875900 0.20512300

Coordinates of 4

FM

0 1
N 1.62953900 -0.32826900 0.00000300
H 1.30778900 -1.29990000 -0.00000200
C 0.65123200 0.48106200 -0.00000700
H 0.84753800 1.55307600 0.00001900
C -0.74520100 0.10278900 -0.00000200
N -1.85689900 -0.20834200 0.00000200

Coordinates of 5

FM

0 2
N -1.62814100 -0.46831700 -0.00030900
H -1.16189600 -1.38232700 0.00126700
C -0.61337800 0.56429100 0.00009300
H -0.78624800 1.21475900 -0.86956800
C 0.78659500 0.12297300 -0.00004300
N 1.87029200 -0.27022300 -0.00005700
H -0.78621800 1.21376700 0.87056400

Coordinates of 6

FM

0 2
N 0.22047600 -0.80663400 -0.44949700
H 0.66038000 -1.66514500 -0.75560000
C -1.06049500 -1.06449700 0.19534400
H -1.50972000 -1.95176800 -0.25748700
C -2.01506100 0.04220900 0.02809400
N -2.78303100 0.89314300 -0.08594200
H -0.97285700 -1.26507900 1.27595600
C 1.19111700 -0.04319900 0.32097500
H 1.02584400 -0.14424100 1.41083800
N 1.06713700 1.38125600 -0.02150800
H 1.71713500 1.96341900 0.49844000

H	1.18527900	1.50510600	-1.02366900
O	2.45856300	-0.29046500	-0.06454100

Coordinates of **7**

FM

0 2

N	-0.18292300	-0.11721300	0.92331700
H	-0.71624400	-0.71698400	1.54684400
C	1.03293800	-0.83581400	0.52029300
H	1.49310900	-1.26060500	1.41571600
C	2.00516800	0.07433500	-0.09580300
N	2.76249500	0.78351100	-0.59675800
H	0.83900800	-1.65870600	-0.18026400
C	-1.04245600	0.24968800	-0.18753300
H	-0.43209900	0.86457300	-0.87840100
N	-2.14712100	1.05216200	0.23410600
H	-1.75281900	1.78334100	0.83676500
O	-1.50562800	-0.90834200	-0.86167000
H	-2.38698500	-0.70335800	-1.19369700

Coordinates of **8**

FM

0 2

N	0.74359300	1.18960600	-0.30481800
H	0.70170500	1.59673900	-1.23312600
C	-0.59333300	1.20957900	0.31021900
H	-0.52136000	1.31054500	1.39413400
C	-1.18968200	-0.18085100	-0.00617300
N	-2.35466400	-0.55673000	0.26347400
H	-1.20711600	2.02086600	-0.07782500
C	1.09883100	-0.21377600	-0.42428900
H	1.76721400	-0.36643900	-1.27927100
N	-0.16218700	-0.90132900	-0.62462400
H	-0.17738600	-1.90789900	-0.53026600
O	1.69228400	-0.69594800	0.76594200
H	2.41658900	-0.09676300	0.98205800

Coordinates of **8-NH3**

FM

0 2

N	2.00875700	0.06712800	-0.32286200
H	2.31794700	0.30810600	-1.25881800
C	1.35946800	1.23424700	0.29556100
H	1.49812300	1.22944900	1.37783700
C	-0.14627700	1.04018900	-0.00096300
N	-1.05921700	1.85784500	0.28381800

H	1.74300200	2.17271100	-0.10237300
C	0.96427300	-0.94398700	-0.42759100
H	1.15615400	-1.60012400	-1.28460600
N	-0.26292800	-0.20501400	-0.60201700
H	-1.18040400	-0.66123600	-0.53030700
O	0.88072700	-1.70370100	0.76717300
H	1.77358900	-2.01395900	0.95895900
H	-3.08107300	0.35446500	0.25838100
N	-3.12525700	-0.61735500	-0.04282800
H	-3.40149700	-1.17124600	0.76187400
H	-3.86591900	-0.68947500	-0.73315100

Coordinates of **9**

FM

0 2

N	-1.29801000	-1.34800200	0.12972600
H	-1.80810000	-1.63496000	0.95617200
C	-1.84850200	-0.08265200	-0.40017600
H	-1.90451900	-0.10134400	-1.49123100
C	-0.86605600	1.00126400	0.02793700
N	-1.03840300	2.23527400	-0.22399600
H	-2.85004600	0.11359100	-0.01684500
C	0.08138700	-1.07482100	0.48765600
H	0.36767600	-1.63299400	1.38548500
N	0.16027300	0.34788200	0.69798400
O	0.95812800	-1.43791400	-0.58753600
H	0.60174300	-2.25635600	-0.95250300
N	3.04926300	0.69815400	-0.00746400
H	3.96030200	1.00917900	-0.36557000
H	2.82589000	-0.15557700	-0.53828400
H	-0.25729400	2.79684700	0.11802800
H	1.08648900	0.76901400	0.73878900

Coordinates of **10-NH3**

FM

0 2

N	-2.00068100	0.33225700	0.43541400
H	-2.27459300	0.54828400	1.38596900
C	-1.17751500	1.41142900	-0.13063900
H	-1.44556000	1.62962100	-1.16853700
C	0.23506300	0.83844800	-0.07054300
N	1.30016900	1.53481100	-0.40527000
H	-1.26374700	2.33855800	0.43783200
C	-1.15962500	-0.86360400	0.41076900
H	-1.30041200	-1.45533300	1.32371700
N	0.23696800	-0.44603500	0.30322900
O	-1.43297000	-1.64549900	-0.73639400
H	-2.36912200	-1.50091100	-0.91731700

N	3.36427800	-0.65599400	0.12640600
H	3.82220000	-1.10788200	-0.65874100
H	3.96439500	-0.77134900	0.93674100
H	2.14517300	0.96151200	-0.22992100
H	2.49275900	-1.15142400	0.30543400

Coordinates of **10**

FM

0 2

N	0.84341500	1.15626400	-0.25764000
H	0.89262100	1.64490600	-1.14360500
C	-0.51041100	1.24145300	0.31208300
H	-0.48739500	1.38862700	1.39559400
C	-1.10119500	-0.12403900	-0.01631000
N	-2.35656800	-0.43625900	0.21502900
H	-1.09214900	2.05432300	-0.12413800
C	1.09795100	-0.27043100	-0.45126900
H	1.66368500	-0.44154500	-1.37483200
N	-0.19050000	-0.96279900	-0.52316700
O	1.77096200	-0.81503300	0.66500900
H	2.37449700	-0.12225600	0.95839000
H	-2.51145100	-1.38612900	-0.13806500

Coordinates of **11**

FM

0 1

N	-1.43175200	0.49624700	-0.07745800
H	-2.31440000	0.91143800	0.17039500
C	-0.14620800	1.18593500	0.02329300
H	0.03265800	1.85540100	-0.82002600
C	0.81608800	-0.01047500	0.00893000
N	2.07656000	0.11484300	-0.01456700
H	-0.05512700	1.75515500	0.95316900
C	-1.18261200	-0.84078800	0.00190000
H	-2.00922300	-1.54353800	0.02152200
N	0.05787400	-1.20723100	0.02008000
H	2.50370700	-0.81350200	-0.02618600

Coordinates of **12**

FM

0 2

N	1.37463400	0.57655500	-0.00006100
H	2.24778000	1.07910800	0.00012200
C	0.12434300	1.12749000	0.00003800
C	-0.77671000	0.03399600	0.00011100
N	-2.09213700	0.12937900	-0.00013900

H	-0.06072200	2.18764900	0.00012300
C	1.21992900	-0.79662900	-0.00005700
H	2.07496200	-1.45773600	-0.00015300
N	-0.02451300	-1.15995900	0.00007900
H	-2.47327800	-0.81999200	0.00019600

Coordinates of **14**

FM

0 2

N	-2.24621700	0.86643300	0.32630000
H	-2.87484800	1.59302500	0.62709300
C	-0.93115800	1.04704200	-0.07686400
C	-0.48987400	-0.21796500	-0.39604400
N	0.75305600	-0.62974900	-0.89669700
H	-0.45412400	2.00804300	-0.13076900
C	-2.53035000	-0.45700600	0.22140000
H	-3.49744800	-0.86851100	0.46607900
N	-1.48924900	-1.14302700	-0.20141500
C	1.96819600	-0.17164600	-0.22494300
N	2.08429200	1.26039200	-0.34586500
H	2.91084700	1.49233900	0.21718400
H	0.74380900	-1.63586700	-1.01251000
H	2.80606900	-0.62708800	-0.77755700
N	2.14760700	-0.54954300	1.18628700
H	1.33957400	-0.23475100	1.71781800
H	2.17881800	-1.56128500	1.27110600

Coordinates of **15**

FM

0 2

N	2.89672300	-1.15260900	0.60347100
H	3.34691800	-1.81293400	1.21565900
C	1.54293000	-0.84346600	0.59728000
C	1.40687100	0.09395400	-0.40331700
N	0.26050200	0.73759600	-0.88373300
H	0.82639800	-1.30735200	1.24951600
C	3.49050400	-0.41505000	-0.36833200
H	4.54724100	-0.46915800	-0.58031700
N	2.62313100	0.35559700	-0.99030600
C	-0.74530000	1.24758400	0.05751000
N	-1.43710200	0.11046100	0.64915900
H	-1.99717900	0.41264900	1.43924700
C	-2.19733400	-0.72830500	-0.23674600
H	-1.55066700	-1.04922100	-1.06151300
O	-2.84317100	-1.72825300	0.41377000
H	0.52279800	1.42543600	-1.57806800

H	-1.41006300	1.87145800	-0.55486600
N	-0.29022200	2.06859700	1.16945700
H	0.42612300	1.56754600	1.68889300
H	0.12591600	2.92564200	0.82075900
N	-3.36946700	-0.03572400	-0.84999000
H	-3.79245200	-0.60411400	-1.57923200
H	-4.07064500	0.15034100	-0.13501100

Coordinates of **16**

FM

0 2

N	-2.77904200	-0.75259400	0.90020600
H	-3.30468500	-0.96853100	1.73127300
C	-1.89854500	0.30815800	0.74956300
C	-1.40315600	0.16819700	-0.52670100
N	-0.50607000	0.97167000	-1.24613000
H	-1.71996400	1.03907200	1.51600200
C	-2.77881400	-1.45387500	-0.26213900
H	-3.38520700	-2.33323300	-0.41462700
N	-1.95629600	-0.92795500	-1.14396900
C	0.72300600	1.45989900	-0.63397100
H	1.29232700	1.88878900	-1.46961500
N	1.60975500	0.45186600	-0.05155300
N	0.36840300	2.42959200	0.39168700
H	1.19863900	2.90024400	0.73629800
H	2.21220600	-0.05586500	-0.69946700
C	1.52245700	-0.08515600	1.19781300
O	2.17502900	-1.04653100	1.57868800
H	-0.25601100	3.11886100	-0.01241000
H	-0.33379000	0.54581800	-2.14808700
H	0.82592100	0.44921200	1.85636600
N	3.50287100	-1.64637600	-1.05208100
H	3.34130500	-1.84791500	-0.05238400
H	4.06198400	-2.43097300	-1.40736700

Coordinates of **17**

FM

0 1

N	2.43675500	0.68399900	0.88208000
H	2.89055700	1.21867800	1.60454800
C	1.27790200	-0.06211800	1.03150900
C	1.02867000	-0.56769200	-0.22350500
N	0.01090200	-1.42346800	-0.67194000
H	0.76576200	-0.17368800	1.96908100
C	2.82377800	0.58599100	-0.41545000
H	3.70516700	1.07424700	-0.80127100
N	1.99343600	-0.15970000	-1.11226100
C	-1.37954400	-1.18868900	-0.30949700

H	-1.95005000	-1.86898100	-0.95732600
N	-1.91930700	0.14513000	-0.58646200
N	-1.53464100	-1.46241700	1.11007100
H	-2.51515200	-1.45336900	1.37056900
H	-2.16450600	0.34032300	-1.54889100
C	-1.81022000	1.26931300	0.19557300
H	-1.46928800	1.04878700	1.21635000
O	-2.09912600	2.38282700	-0.19008800
H	-1.14709300	-2.37736500	1.31131300
H	0.12408200	-1.57688200	-1.66586800

Coordinates of **18**

FM

0 2

N	-2.46044800	1.13802400	0.07230300
H	-2.86492000	2.06031000	0.11837800
C	-1.14215200	0.83992800	0.25771100
C	-1.03821100	-0.57021100	0.05936000
N	-0.03905900	-1.43285800	0.09174700
H	-0.41830400	1.61268100	0.44339700
C	-3.11888300	-0.03879400	-0.22312100
H	-4.18297200	-0.05915400	-0.40940000
N	-2.32653900	-1.06048500	-0.24150200
C	1.31225600	-1.10834800	0.47918600
H	1.42110400	-1.53426400	1.49235400
N	1.71374000	0.29615000	0.62339900
N	2.18776600	-1.73315000	-0.50240300
H	3.10329600	-1.91448100	-0.10486500
H	1.52915000	0.74069100	1.51309800
C	1.97175100	1.15705400	-0.40751700
H	2.14703300	0.63735300	-1.35967400
O	2.00745100	2.36663300	-0.27436200
H	1.76921400	-2.60773900	-0.79693700

Coordinates of **19**

FM

0 2

N	-2.19311400	0.43163400	0.25526700
H	-2.79990200	1.15510300	0.60438500
C	-0.77232700	0.42352900	0.44865800
C	-0.42633700	-0.99840700	-0.01970200
N	0.71927700	-1.41990500	-0.36008000
H	-0.48619900	0.63828500	1.47974400
C	-2.57433500	-0.85645200	-0.00638300
H	-3.62528200	-1.10408800	-0.10040700
N	-1.62630900	-1.72431800	-0.16209500
C	1.84533900	-0.47019300	-0.38551200
N	1.49599000	0.94336100	-0.20485600

H	1.92389900	1.35870800	0.61377500
C	0.15810400	1.41612600	-0.43829200
H	-0.14852500	1.22849000	-1.48394100
O	-0.14714800	2.61394200	0.00711000
H	2.28845600	-0.60263400	-1.37803600
N	2.86705700	-0.80177400	0.59443600
H	2.42056600	-1.05664300	1.47194200
H	3.38120400	-1.61936100	0.28434200

Coordinates of **20**

FM

0 1

N	-2.10190400	0.43534300	0.46441700
H	-2.59031700	1.31633600	0.42588200
C	-0.66449100	0.33529800	0.57582400
C	-0.41041400	-1.01153800	-0.10463700
N	0.72773600	-1.41815700	-0.49600500
H	-0.36483700	0.27679700	1.63122500
C	-2.53768400	-0.74538900	-0.05931800
H	-3.59674500	-0.90620400	-0.22489100
N	-1.63881200	-1.64623900	-0.32552500
C	1.83513200	-0.47796800	-0.37900400
N	1.41605000	0.94173800	-0.36717500
H	2.08270500	1.61508100	-0.71863400
C	0.17951800	1.42063400	-0.07095400
O	-0.20781900	2.56004700	-0.24600500
H	2.42962400	-0.60422700	-1.28754700
N	2.73515400	-0.73086000	0.73954000
H	2.21740500	-0.70353900	1.61471300
H	3.10477200	-1.67360400	0.64906800

Coordinates of **21**

FM

0 2

N	-2.16411800	0.52438500	0.07184500
H	-2.68393300	1.38681100	0.14274600
C	-0.81597100	0.42836400	-0.06172800
C	-0.52203200	-0.95460400	-0.08643500
N	0.68510100	-1.47043300	-0.19405200
C	-2.64500300	-0.77256900	0.11961300
H	-3.70245100	-0.97226500	0.21543800
N	-1.71307800	-1.67708200	0.03270600
C	1.76916900	-0.51955800	-0.37127000
N	1.44695500	0.89840500	-0.11210300
H	2.23807200	1.52650700	-0.07860500
C	0.20181900	1.46772900	-0.03927100
O	-0.01993500	2.66414200	0.07315700

H	2.07751300	-0.61968400	-1.42420000
N	2.93902200	-0.82969400	0.43418600
H	2.65286500	-0.90843500	1.40763700
H	3.29235300	-1.74130100	0.15820500

Coordinates of **22**

FM

0 1

N	1.40692800	1.22935500	0.00000200
H	1.47181700	2.23573300	0.00000400
C	0.24467500	0.49811000	-0.00000900
C	0.64255600	-0.83716000	-0.00000300
N	-0.23103700	-1.89282600	0.00000200
C	2.42743100	0.31972500	0.00000500
H	3.46214500	0.62822800	0.00001100
N	2.01064000	-0.92756000	-0.00000100
C	-1.47573700	-1.54351500	0.00000600
H	-2.24783000	-2.30658800	0.00001800
N	-1.93749400	-0.24815400	-0.00000100
H	-2.93440400	-0.07455200	0.00000700
C	-1.12651300	0.91230200	-0.00002300
O	-1.59618200	2.03683800	0.00001200

Coordinates of **23**

FM

0 1

N	2.19614200	0.51049100	0.00000000
H	2.74291300	1.35709500	-0.00000100
C	0.81904000	0.43516900	0.00000000
C	0.51702200	-0.92634300	0.00000000
N	-0.74822000	-1.43362700	0.00000000
C	2.64295500	-0.77629000	0.00000000
H	3.69679500	-1.01220500	0.00000000
N	1.67204500	-1.66699800	0.00000000
C	-1.69091300	-0.53331700	0.00000000
N	-1.46075300	0.82954500	0.00000000
N	-2.99566500	-0.92927700	-0.00000100
H	-3.76528500	-0.28604400	0.00000300
H	-2.23298700	1.48270500	0.00000000
C	-0.18156600	1.44931900	0.00000100
O	-0.06901300	2.66434600	0.00000000
H	-3.17340000	-1.91848200	0.00000200

Coordinates of **24**

0 2

N	-2.73310400	-0.68309500	0.98304300
H	-3.19219000	-1.05607200	1.79762300

C	-1.62894800	0.16130000	0.98789400
C	-1.35186400	0.37701100	-0.34501000
N	-0.40602200	1.18862100	-0.98528100
H	-1.16754800	0.51596900	1.88957400
C	-3.06071600	-0.92155000	-0.31050000
H	-3.88732600	-1.55216300	-0.59925900
N	-2.24888500	-0.29951000	-1.13819700
C	0.93583700	1.43693200	-0.50320000
H	1.33417700	2.22875900	-1.15356800
N	1.87065600	0.33252200	-0.70667100
N	0.84829000	1.87044800	0.89924100
H	1.76796000	2.15190600	1.22344300
H	2.83812900	0.64428600	-0.68836100
C	1.74044300	-0.93903700	0.03060500
O	2.46574300	-1.94111000	-0.63531500
H	0.23399600	2.67860000	0.96173300
H	-0.42342900	1.00912300	-1.98062300
H	0.68318500	-1.21523800	0.02252500
N	2.30159100	-0.72939800	1.32965600
H	3.26410100	-2.06952800	-0.10865200
H	1.58681300	-0.25181000	1.88681700

Coordinates of **25**

FM

0 1

N	2.44463500	0.59946300	0.89626000
H	2.91485900	1.09352100	1.63688200
C	1.29523000	-0.16236200	1.03223300
C	1.00710000	-0.58523100	-0.24436900
N	-0.02478400	-1.41376200	-0.71307600
H	0.80596500	-0.32738600	1.97413400
C	2.79187300	0.58857100	-0.41615800
H	3.65996200	1.10489100	-0.79556700
N	1.94298600	-0.11537500	-1.13426400
C	-1.41341600	-1.17203100	-0.33459600
H	-1.99217200	-1.82630600	-1.00237400
N	-1.95493600	0.17041300	-0.56037200
N	-1.56293100	-1.49421600	1.07448700
H	-2.54070300	-1.46685300	1.34339500
H	-2.13954400	0.38369900	-1.53182100
C	-1.74392500	1.26982100	0.25739700
H	-1.19738900	-2.42494000	1.24052300
H	0.07743900	-1.52877500	-1.71342000
H	-1.43109700	0.99582000	1.26100300
N	-1.92553300	2.50178300	-0.01823800
H	-2.21454600	2.62558000	-0.99337800

Coordinates of **26**

FM

0 2

N	2.55495700	0.67956900	0.90879500
H	3.04711400	1.09384900	1.68287800
C	1.44827200	-0.15292600	1.00161500
C	1.12064900	-0.44191400	-0.30385000
N	0.13169800	-1.27994900	-0.83509500
H	0.99951300	-0.43649600	1.93487600
C	2.84396600	0.83224400	-0.40859300
H	3.67143900	1.42866000	-0.76080900
N	1.99788500	0.17042600	-1.16849500
C	-1.24343900	-1.30425600	-0.34040700
H	-1.74829200	-2.02889700	-0.99572400
N	-2.05507300	-0.09611400	-0.44599800
N	-1.21053600	-1.70853000	1.05823700
H	-2.15818900	-1.80162600	1.40698400
H	-2.34074700	0.09019700	-1.40087100
C	-1.72209100	1.09357000	0.22148000
H	-0.73858500	-2.60279200	1.13760400
H	0.17064100	-1.23873300	-1.84537900
H	-1.29278500	0.96566300	1.21158100
N	-2.61752000	2.14669000	-0.07803800
H	-3.58375200	1.96150400	0.20372800
H	-2.32037400	3.02372200	0.32780900

Coordinates of 27

FM

0 2

N	1.97659700	0.25312800	0.88073100
H	2.37530300	0.33986200	1.80492600
C	0.51588600	0.12599100	0.80161800
C	0.40873800	-0.93352400	-0.26115500
N	-0.83304900	-1.23658200	-0.77844000
H	0.05520100	-0.17425500	1.75054000
C	2.51258000	-0.74734000	0.03665200
H	3.57527400	-0.88040800	-0.08695600
N	1.57992100	-1.38036300	-0.68367700
C	-1.91320900	-0.34132000	-0.33041600
H	-2.69667300	-0.39619300	-1.09817200
N	-1.56060700	1.06358200	-0.19594800
N	-2.33493800	-0.81673100	0.98255300
H	-3.09242100	-0.23791000	1.32771100
H	-1.72950400	1.57634600	-1.05262900
C	-0.20930400	1.41740400	0.28095700
H	-2.63339300	-1.78488500	0.93403900
H	-0.84345300	-1.51128700	-1.75151200
H	-0.28731300	2.13416900	1.10696900
N	0.49416900	2.10097700	-0.79974500
H	1.35564800	2.49835600	-0.43549100
H	0.77853000	1.42086700	-1.50368300

Coordinates of **28**

FM

0 1

N	1.95256900	0.22351300	0.86401200
H	2.42539200	0.47243300	1.71945100
C	0.49970000	0.12354200	0.78067300
C	0.35579800	-0.87524800	-0.36153900
N	-0.73862400	-1.09973200	-0.97037200
H	0.04852200	-0.26555300	1.69651300
C	2.45951800	-0.74081300	0.02737800
H	3.52897000	-0.91994000	-0.00037500
N	1.61908100	-1.37460100	-0.72475300
C	-1.86388100	-0.37671900	-0.35851400
H	-2.66567900	-0.35431600	-1.10600100
N	-1.61148900	1.02745000	0.00044300
N	-2.24339800	-1.09461900	0.86398700
H	-3.06975000	-0.65717500	1.25990000
H	-1.92916800	1.64366600	-0.73759300
C	-0.24429500	1.41861700	0.34564100
H	-2.46466100	-2.05983200	0.63721300
H	-0.26075500	2.11697100	1.19022400
N	0.36138400	2.13477500	-0.77377000
H	1.27206700	2.50201400	-0.51413900
H	0.49736000	1.50795600	-1.56385300

Coordinates of **29**

FM

0 2

N	1.97050200	0.63269000	0.42048600
H	2.37431800	1.49613500	0.74804500
C	0.65063700	0.40156400	0.14925100
C	0.58285100	-0.94799600	-0.26576700
N	-0.52145800	-1.60731000	-0.56900700
C	2.65088300	-0.54454200	0.13949100
H	3.72250500	-0.61125100	0.26101300
N	1.87364500	-1.49766500	-0.27248900
C	-1.73428800	-0.79766500	-0.35601000
H	-2.44839500	-1.12318200	-1.12420000
N	-1.64483200	0.65648300	-0.49183100
N	-2.17773600	-1.07670100	1.01225500
H	-3.14456100	-0.78407200	1.11736100
H	-1.55869300	0.91617300	-1.46948500
C	-0.54216300	1.29943600	0.25169000
H	-2.12085700	-2.07517000	1.18503100
H	-0.85580500	1.36562500	1.30002700
N	-0.32971300	2.64723300	-0.26022100
H	-0.28334200	3.34743900	0.46560000

H 0.47444900 2.72040800 -0.86967300

Coordinates of **30**

FM

0 1

N	2.09441800	0.83823000	0.30185500
H	2.61612500	1.65284600	0.57569100
C	0.71617200	0.73885000	0.07927600
C	0.48428600	-0.66925800	-0.21615400
N	-0.65476200	-1.19616200	-0.51010400
C	2.59011200	-0.43189900	0.14537400
H	3.64706000	-0.62388700	0.27977700
N	1.71784300	-1.34443500	-0.16269600
C	-1.82058300	-0.34110000	-0.35108300
H	-2.52429500	-0.56968500	-1.15620300
N	-1.51590500	1.10713500	-0.45008500
N	-2.54738000	-0.57788300	0.89847100
H	-2.96983700	-1.50199700	0.86060600
H	-2.32423800	1.69979600	-0.33434200
C	-0.30237200	1.61385300	-0.06910300
H	-1.88609200	-0.59805200	1.67195600
H	-0.22390800	2.69009700	0.03057900

Coordinates of **31**

Coordinates of **32**

0 1

C	-0.23437600	0.70133600	0.00000000
C	-0.21695400	-0.71461300	0.00000000
C	2.01794100	-0.66554700	0.00000000
C	0.97610600	1.37969300	0.00000000
C	-2.26577300	-0.14987000	0.00000000
H	2.96313100	-1.19880000	0.00000000
H	-3.34643000	-0.16324200	0.00000000
N	-1.50604000	-1.21242400	0.00000000
N	-1.57229200	1.03865800	0.00000000
H	-1.97059800	1.96398600	0.00000000
N	0.91775300	-1.41489100	0.00000000
N	2.10886800	0.67840000	0.00000000
H	1.05421500	2.46387300	0.00000000

Coordinates of **33**

FM

0 1

N	1.42489200	-1.22709000	-0.25810800
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H	1.48897700	-2.21296400	-0.45533000
C	0.28074300	-0.45729400	-0.21043400
C	0.70982100	0.81753400	0.08733800
N	-0.12695300	1.91566500	0.22082700
C	2.47230200	-0.38113500	0.00871100
H	3.49372900	-0.72989000	0.03208300
N	2.07938100	0.85102400	0.22277400
C	-1.36250700	1.63200500	-0.00141600
H	-2.11054000	2.41754700	0.07753900
N	-1.87707800	0.41128500	-0.36967200
H	-2.88132800	0.31685500	-0.39077900
C	-1.14590500	-0.85924800	-0.38253900
H	-1.31768700	-1.36301700	-1.34600800
N	-1.71992200	-1.76066400	0.62720700
H	-1.50600600	-2.73115400	0.42111800
H	-1.35611500	-1.54009000	1.55022800

Coordinates of **34**

FM

0 2

N	1.31578200	-1.35061700	0.00000000
H	1.31671800	-2.35566200	0.00000100
C	0.21757200	-0.50707800	0.00000000
C	0.78641400	0.80294400	0.00000000
N	0.01325800	1.94778000	0.00000000
C	2.45263500	-0.52987400	0.00000100
H	3.44771100	-0.94398400	0.00000100
N	2.14101400	0.74660100	-0.00000200
C	-1.25551300	1.75548900	0.00000000
H	-1.93499100	2.60299200	0.00000200
N	-1.88762100	0.51690500	-0.00000100
H	-2.89294200	0.48571400	0.00000800
C	-1.14363100	-0.69305600	0.00000000
N	-1.86881900	-1.87724400	0.00000000
H	-2.87108400	-1.87845100	-0.00001200
H	-1.40556600	-2.76513300	0.00000300

Coordinates of **35**

FM

0 1

N	1.27089800	-1.34467800	0.00000000
H	1.27006400	-2.35108500	0.00000100
C	0.18327400	-0.48447800	0.00000000
C	0.73720900	0.80773100	0.00000000
N	-0.00437400	1.92725200	0.00000000
C	2.38596200	-0.54262200	0.00000000
H	3.37929800	-0.96828400	0.00000000
N	2.11787000	0.73585100	-0.00000100

C	-1.30750000	1.68819800	0.00000000
H	-1.95857700	2.55751400	0.00000000
N	-1.94514700	0.50230700	0.00000000
C	-1.21489200	-0.61537700	0.00000000
N	-1.88097700	-1.80510300	-0.00000100
H	-1.41636100	-2.69355100	0.00000200
H	-2.88663500	-1.77471000	0.00000100

List of coordinates files for transition states

Coordinates for TS 1→2

FM

0 2

N	1.22960500	-0.15198000	-0.25730900
H	1.29172400	-1.14778400	-0.09976400
H	1.95906800	0.42723700	0.12800000
C	0.00906400	0.37371700	-0.49379700
H	0.00927000	1.46550800	-0.60010300
O	-0.94649000	-0.33283000	-0.95291600
C	-1.13304600	0.46900800	1.20089900
N	-1.59012400	0.55475900	2.26580600

Coordinates for TS 2→3

FM

0 2

N	1.15991000	-1.10930900	0.05145400
H	1.96440200	-1.01390200	0.67945800
C	0.30832400	0.07780400	0.24225100
H	0.44271800	0.60900700	1.18766800
O	0.95855300	0.69943900	-0.84304000
C	-1.11880500	-0.20224900	0.01834100
N	-2.24336800	-0.39195400	-0.14186300
H	1.41255600	-0.44043800	-1.02041900

Coordinates for TS 3→4

FM

0 2

N	-1.03749300	1.00181100	-0.34915100
H	-1.98573600	1.03733500	0.02992100
C	-0.27194100	0.35751700	0.47735600
H	-0.55388500	0.05247600	1.48475600
O	-0.95201300	-1.44224000	-0.24520900
C	1.14355200	0.26361700	0.19523900
N	2.27964200	0.19404000	0.01226000

H	-0.74457800	-1.30609600	-1.18712700
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Coordinates for TS 4→5

FM

0 2

N	1.50548900	-0.72917700	0.02192700
C	0.63800800	0.09478200	-0.44753900
H	0.84286500	0.87060700	-1.19079500
C	-0.77139200	-0.13372800	-0.19936400
N	-1.90327300	-0.29451200	-0.04925100
H	2.44008600	-0.46801100	-0.29926700
H	0.69691500	1.61049600	0.76352400

Coordinates for TS 5→6

FM

0 2

N	-0.06860500	-0.47710900	-0.56087900
H	-0.39141900	-0.29121900	-1.51362500
C	-0.53486900	0.61389100	0.29422100
H	-0.23872600	1.57254700	-0.14707000
C	0.05394200	0.52401100	1.63446800
N	0.50747900	0.45761000	2.69124200
H	-1.62733800	0.62059900	0.38632900
C	-0.80408200	-2.06451000	-0.18264100
H	-0.62102100	-2.05448900	0.90214100
N	-0.10525200	-3.09157800	-0.81012500
H	0.86320100	-3.18732200	-0.53706900
H	-0.24838500	-3.13233100	-1.81079900
O	-1.95221900	-1.72233300	-0.63751300

Coordinates for TS 6→7

FM

0 2

N	-0.22989500	-0.28691800	-0.64204000
H	0.22081500	-0.81694700	-1.38125900
C	-1.01962900	-1.17879800	0.20907700
H	-1.57133800	-1.86875000	-0.43360100
C	-1.99968100	-0.43009100	1.00686400
N	-2.75616200	0.15492100	1.64916300
H	-0.41167800	-1.78434200	0.89651700
C	0.74814200	0.48881900	0.05385600
H	0.26034500	1.15769400	0.76620700
N	1.69701900	1.10537900	-0.87317400
H	1.97504300	2.01665500	-0.50011100
O	1.83210000	-0.21645600	0.65781300

H 2.43968500 0.21293900 -0.33790800

Coordinates for TS 7→8

FM

0 2

N -0.24193900 -0.39205100 0.87491900
H -0.62965400 -1.12540700 1.45141500
C 1.16711600 -0.55555200 0.56626700
H 1.76486700 -0.45903300 1.47571400
C 1.52488200 0.53741400 -0.36881000
N 2.19357600 1.41396200 -0.77643200
H 1.42658700 -1.50379800 0.07121900
C -1.05836700 -0.03729600 -0.26503400
H -1.66600500 -0.89867500 -0.60527200
N -0.17723400 0.26704000 -1.36751800
H -0.36645800 1.22087200 -1.68447700
O -1.93419700 1.00177100 0.14138600
H -2.68954600 1.00348300 -0.45682000

Coordinates for TS 8-NH₃→9

FM

0 2

N 0.70569200 0.93059700 -0.84123500
H 0.62825700 0.81933400 -1.84625400
C -0.59824900 1.33690600 -0.28448800
H -0.46990700 2.00866900 0.56672500
C -1.23355900 0.03571900 0.21632900
N -2.40661700 -0.05152200 0.70098100
H -1.21952000 1.83745900 -1.02635900
C 1.00508200 -0.36699300 -0.24853100
H 1.56625800 -0.98800700 -0.95656700
N -0.28279800 -0.94376400 0.04885600
H -0.40533200 -1.81083700 0.56312400
O 1.72740300 -0.22233100 0.96084000
H 2.46561200 0.36857800 0.77119400
H -2.54565100 -1.13443600 1.07823300
N -2.35608300 -2.45778100 1.48104700
H -2.66048600 -2.34856100 2.45420800
H -3.16921000 -2.87115100 1.01216200

Coordinates for TS 9→10-NH₃

FM

0 2

N -0.17332800 1.31735400 -0.59186700
H -0.78649200 1.75409700 -1.27064400
C -0.78089100 1.36617200 0.75281900

H	-0.01910900	1.51944800	1.52157700
C	-1.42394500	-0.00306600	0.93148200
N	-2.17906700	-0.29648600	1.91974400
H	-1.51389300	2.16768800	0.83936600
C	-0.03089900	-0.09483400	-0.90550600
H	-0.15963800	-0.26400300	-1.98014600
N	-1.05914400	-0.79607700	-0.14973700
O	1.24517100	-0.57262900	-0.48778800
H	1.88406200	0.08984100	-0.77687800
N	-0.19164500	-2.97742800	0.52995400
H	-0.09851100	-2.84882700	1.54065500
H	0.75875100	-2.88202800	0.16387100
H	-2.51295400	-1.25960600	1.84537200
H	-0.83942900	-1.99973700	0.06981500

Coordinates for TS 10→11

FM

0 2

N	-0.90106500	1.31161800	-0.95047100
H	-0.63955200	2.06613700	-1.56633000
C	-1.32970300	1.56391200	0.42789300
H	-0.72257200	2.33914600	0.90413400
C	-1.04322500	0.20415000	1.05930100
N	-1.43487600	-0.13343300	2.22163800
H	-2.38425400	1.83310700	0.49212200
C	-0.18649800	0.16089900	-0.94663200
H	0.24414200	-0.21929200	-1.86086900
N	-0.31993400	-0.58573700	0.15022800
O	1.66639300	0.68447600	-0.18329100
H	2.01893100	-0.14301900	0.17952600
H	-1.11266600	-1.08335600	2.41973900

Coordinates for TS 11→12

FM

0 2

N	-0.97862000	0.86319300	-0.07314500
H	-1.70652600	1.44874800	-0.47713800
C	0.31283900	1.40409600	0.22980300
C	1.13093000	0.14285500	0.35103900
N	2.34921700	0.11895700	0.74758100
H	0.33179600	2.06406800	1.09870900
C	-0.84427300	-0.46569900	-0.27218600
H	-1.68021400	-1.06537000	-0.61020400
N	0.34635400	-0.95312900	-0.02971600
H	2.67689600	-0.85053100	0.76691800
C	-0.31858800	3.22529000	-1.84066900
N	-1.48621200	3.22513200	-1.84076600
H	0.61652500	2.06819400	-0.64965600

Coordinates for TS 12→14

FM

0 2

N	-2.68203600	0.74383200	-0.97475300
H	-3.26889000	1.32463000	-1.55159700
C	-1.37321300	0.40727500	-1.23170700
C	-0.98502500	-0.38566100	-0.15929400
N	0.23410400	-0.98549800	0.02786200
H	-0.85185500	0.73537600	-2.11420600
C	-3.03364300	0.14840000	0.20613000
H	-4.02131100	0.24995000	0.62998400
N	-2.04280300	-0.52925200	0.72391700
C	1.70655100	0.08215900	0.22952700
N	1.51510800	0.54620600	1.47696400
H	2.01831800	-0.05446500	2.13903600
H	0.18791300	-1.51553700	0.89923100
H	1.45124400	0.78426800	-0.56291000
N	2.83033800	-0.69986100	-0.11074700
H	3.05132200	-1.38927300	0.59977100
H	2.71353800	-1.16513300	-1.00375800

Coordinates for TS 14→15

FM

0 2

N	3.11254600	-0.91330000	0.50171900
H	3.64684300	-1.60120500	1.00642600
C	1.73561800	-0.74117100	0.57081300
C	1.47202100	0.30362100	-0.28939600
N	0.25543400	0.88900900	-0.63955000
H	1.09502300	-1.37349900	1.15787400
C	3.59514800	0.00049600	-0.37698600
H	4.64319800	0.07859200	-0.62218000
N	2.63610800	0.75830800	-0.86551200
C	-0.74489300	1.18018700	0.38757300
N	-1.28894000	-0.08120400	0.87784800
H	-1.57727100	0.06331900	1.84720900
C	-2.78415800	-0.63017600	0.05501000
H	-2.68011600	-1.69822700	0.29112200
O	-3.53832700	0.11840200	0.77098700
H	0.40869000	1.66498300	-1.26949600
H	-1.53954000	1.73643800	-0.11751000
N	-0.30923000	1.97745700	1.53471400
H	0.55915600	1.59625700	1.90321900
H	-0.11090300	2.92758900	1.23742900
N	-2.69029300	-0.35695800	-1.31127700
H	-2.47541500	-1.11920400	-1.93283300
H	-3.36264200	0.31357400	-1.64858200

Coordinates for TS 15→16

FM

0 2

N	2.77107600	-1.12362300	1.02025100
H	3.19515300	-1.73473100	1.69872200
C	1.40874100	-0.90452900	0.86420700
C	1.31981700	-0.01022800	-0.18033000
N	0.19282200	0.54123800	-0.80059900
H	0.66264000	-1.40247800	1.45572600
C	3.41556500	-0.37920800	0.08713700
H	4.48988900	-0.37005700	-0.01383700
N	2.57156400	0.31317800	-0.64848500
C	-0.93916500	1.00646700	0.00475100
N	-1.65364800	-0.15419900	0.52191800
H	-2.27757000	0.08419800	1.28338800
C	-2.19294500	-1.08541600	-0.36313400
H	-1.50990100	-1.29927500	-1.19354200
O	-3.02517500	-1.94873700	0.05026200
H	0.47986500	1.21903700	-1.49460500
H	-1.56837400	1.57712900	-0.68905500
N	-0.66569600	1.85904200	1.15094700
H	0.04824900	1.43051500	1.73474400
H	-0.30915900	2.75583900	0.83867600
N	-3.48576300	-0.21881700	-1.39855000
H	-3.79809700	-0.92764900	-2.06872500
H	-4.27316500	-0.11795700	-0.74951900

Coordinates for TS 16→18

FM

0 2

N	-2.15531800	1.59312800	-1.21573400
H	-2.45087000	2.20867100	-1.95628300
C	-0.87539900	1.11353700	-1.02699900
C	-0.95642300	0.30928700	0.10523000
N	0.00346900	-0.38089300	0.80244000
H	-0.06537000	1.35510600	-1.69019300
C	-2.94264600	1.05181800	-0.24218500
H	-4.00143200	1.25149500	-0.17671000
N	-2.26035800	0.28511500	0.56929100
C	1.40524900	-0.35652200	0.43799700
N	1.66816300	-0.57928300	-0.99069700
H	2.54029200	-0.19414700	-1.33070300
C	1.10046900	-1.55829500	-1.75612800
H	0.23989800	-2.03952500	-1.25856300
O	1.47253400	-1.86204200	-2.86982400
H	-0.32951400	-1.37417100	1.31375100
H	1.86661100	-1.14951900	1.03654900

N	2.09103300	0.88156900	0.78027300
H	1.57170300	1.67694100	0.41854000
H	2.11633900	0.97709400	1.79013800
N	-0.72001400	-2.66369700	1.52272200
H	-1.70260200	-2.69465000	1.23812300
H	-0.24852200	-3.36009000	0.94054900

Coordinates for TS **18**→**19**

FM

0 2

N	1.47541000	0.88794700	-0.20493800
H	2.30296600	1.45330200	-0.11493900
C	0.29973000	1.27678200	-0.89555600
C	-0.55907900	0.02321500	-0.75684000
N	-1.81048000	-0.06749600	-0.96133500
H	0.47894900	1.65493000	-1.89917000
C	1.34516400	-0.42987000	0.14138600
H	2.14704000	-0.94151300	0.65984300
N	0.22252700	-0.99387900	-0.17125100
C	-2.56676100	1.15380300	-1.28289800
N	-1.85146400	2.41988400	-1.08354200
H	-1.78388600	2.98022100	-1.92449000
C	-0.69298100	2.51590700	-0.25299500
H	-0.89754800	2.14509600	0.76828600
O	0.05137800	3.56796500	-0.34658800
H	-3.42813500	1.12162000	-0.60809700
N	-3.08121400	1.14542700	-2.64340800
H	-2.36256800	0.80098000	-3.27499000
H	-3.85939600	0.49802600	-2.70858400

Coordinates for TS **19**→**20**

FM

0 2

N	1.37978400	0.95737500	-0.00437200
H	2.22109600	1.50402400	0.08714800
C	0.28319500	1.34519700	-0.86791200
C	-0.52507500	0.04869800	-0.87695400
N	-1.76651300	-0.05418200	-1.12115600
H	0.64810900	1.56438400	-1.88186400
C	1.35155800	-0.41011900	0.04872100
H	2.16895500	-0.95010600	0.51298900
N	0.30248400	-0.99812800	-0.43572700
C	-2.54011500	1.15255900	-1.34909600
N	-1.81389000	2.41566700	-1.10542200
H	-2.39358100	3.24485200	-1.08521300
C	-0.58743600	2.54098900	-0.48230500
H	-0.90137000	1.99442300	1.04182600
O	-0.11697600	3.62097400	-0.10175800

H	-3.37410800	1.09900700	-0.63804600
N	-3.13329800	1.24406900	-2.67247800
H	-2.39995600	1.18599700	-3.37486600
H	-3.74518100	0.44514900	-2.81319100

Coordinates for TS **21**→**22**

FM

0 2

N	1.32121300	0.68706200	-0.78796700
H	2.11787400	1.13845000	-1.20751800
C	-0.03333300	1.04662000	-1.00063000
C	-0.74673500	0.07143400	-0.09707000
N	-1.99432800	0.14110600	0.18618500
H	-0.42362200	0.78342300	-2.10486500
C	1.32786500	-0.44001400	-0.02363200
H	2.25940700	-0.94143900	0.20711300
N	0.16651400	-0.85300600	0.39971900
C	-2.66539000	1.26906700	-0.45452500
N	-1.85218600	2.48304000	-0.57195600
H	-2.25264100	3.36862200	-0.29732800
C	-0.49314200	2.46675100	-0.76488000
O	0.22952500	3.43792000	-0.73892400
H	-3.53046500	1.54180400	0.15948800
N	-3.06127800	0.81744100	-1.78524700
H	-3.57106000	-0.05666900	-1.79137700
C	-1.25932300	0.44933600	-3.42567800
N	-1.39957000	0.20614100	-4.55531700
H	-3.46455900	1.52167100	-2.38862600

Coordinates for TS **21**→**22**

FM

0 2

N	1.42589800	0.95454700	-0.04032100
H	2.14711200	1.61419300	0.20953600
C	0.10775100	1.25454400	-0.25721500
C	-0.51154100	0.04034600	-0.56039400
N	-1.83644000	-0.09265300	-0.82289100
C	1.54457400	-0.39941800	-0.21927900
H	2.49233800	-0.90443900	-0.10682600
N	0.41107800	-0.98191700	-0.53240000
C	-2.50380400	1.05864600	-0.86135600
N	-1.95498400	2.27228900	-0.46300000
H	-2.53700900	3.09820800	-0.50478400
C	-0.59871700	2.50599500	-0.18866200
O	-0.15198400	3.60960100	0.07252400
H	-3.58339400	1.02308000	-0.81256600
N	-2.66159000	1.20606000	-2.91545200
H	-1.66997500	1.15051300	-3.17703800

H -3.00757600 0.26646200 -3.14321900

Coordinates for TS **21**→**24**

FM

0 2

N 1.39238200 0.92692600 0.28713100
H 2.00919500 1.57602500 0.75108000
C 0.20754600 1.24512400 -0.32787200
C -0.29513500 0.04158400 -0.82134200
N -1.45176400 -0.06754300 -1.52643500
C 1.54760300 -0.42352400 0.13863700
H 2.40768400 -0.94274700 0.53438000
N 0.56058100 -0.99052300 -0.51877000
C -2.15552400 1.05469100 -1.59895000
N -1.65204200 2.29737100 -1.21529200
H -2.26998400 3.09699400 -1.26691900
C -0.45980400 2.50344400 -0.49009900
O -0.11814200 3.60560300 -0.09834500
H -3.01093100 0.63063200 -0.14587900
N -3.28763600 1.14212900 -2.42298900
H -3.14761900 1.76927100 -3.20720000
H -3.55047000 0.21953900 -2.74674200

Coordinates for TS **15**→**24**

FM

0 2

N -2.23283200 -1.13224100 1.17841900
H -2.43910400 -1.75238500 1.94416500
C -1.23611100 -0.16764300 1.16565600
C -1.30362400 0.38166000 -0.09627400
N -0.58604200 1.43046600 -0.68960600
H -0.58260800 0.01191300 1.99721500
C -2.84135200 -1.11189300 -0.03365900
H -3.66115200 -1.76520400 -0.28918600
N -2.30524800 -0.20965400 -0.82849300
C 0.82399900 1.65787800 -0.46237800
H 1.06605000 2.56909600 -1.02489700
N 1.71167200 0.64090900 -1.02235600
N 1.03126000 1.84094700 0.98692400
H 1.95121300 2.24097500 1.14678700
H 2.68784900 0.91858600 -0.99407000
C 1.59983600 -0.74425300 -0.66197900
O 2.77649100 -1.43894400 -1.01184700
H 0.35013700 2.51280300 1.33239800
H -0.82858300 1.49334500 -1.66962700
H 0.68568500 -1.17890200 -1.06858500
N 1.79074000 -1.18428900 0.75520400
H 2.68077000 -1.86484600 0.14632600

H 2.23293700 -0.40233100 1.24847500

Coordinates for TS **24**→**25**

FM

0 2

N	-2.57156800	-0.90831600	0.76840200
H	-3.09250200	-1.28712500	1.54184700
C	-1.58847400	0.07080500	0.85206800
C	-1.16676300	0.24722200	-0.44708400
N	-0.24072000	1.13315500	-1.01338700
H	-1.29840500	0.53478500	1.77558800
C	-2.69672900	-1.25090700	-0.53794000
H	-3.39992500	-1.99284800	-0.88363600
N	-1.86611900	-0.57240800	-1.29871800
C	0.94045800	1.62639500	-0.34028900
H	1.37420600	2.35857500	-1.03640800
N	2.06110100	0.70004700	-0.08361600
N	0.54414900	2.19283600	0.93765900
H	1.34167300	2.62853700	1.38614400
H	2.71955800	0.63301500	-0.84914400
C	1.93847200	-0.45135000	0.65211300
O	1.29937800	-1.77949900	-0.68815200
H	-0.18195000	2.88681200	0.79493600
H	-0.06857900	0.87166300	-1.97504200
H	1.08010300	-0.46058200	1.31327700
N	2.91175300	-1.31607900	0.89236100
H	1.18568500	-2.58449800	-0.16153800
H	3.68929800	-1.14849300	0.24780100

Coordinates for TS **25**→**26**

FM

0 2

N	2.49212600	0.54098000	0.86866000
H	2.98992700	1.00682500	1.60968400
C	1.34489700	-0.22094300	1.01726200
C	1.01284200	-0.59939500	-0.26257300
N	-0.03970400	-1.40700400	-0.72398900
H	0.88748600	-0.41638000	1.96939400
C	2.79580400	0.57313900	-0.45428400
H	3.65326800	1.09885000	-0.84468600
N	1.92014000	-0.10295000	-1.16696600
C	-1.41378000	-1.15583400	-0.30742100
H	-2.02139900	-1.77740600	-0.98024300
N	-1.93241800	0.20577100	-0.48408100
N	-1.53941300	-1.51013600	1.09513600
H	-2.51113500	-1.48282200	1.38542600
H	-2.13788400	0.45092200	-1.44363900
C	-1.68763900	1.26486900	0.36481700

H	-1.17623700	-2.44629500	1.23293100
H	0.03754000	-1.50251700	-1.72864000
H	-1.37186800	0.96229600	1.35681700
N	-1.87992100	2.51623800	0.12898800
H	-2.19329200	2.69186000	-0.82754400
H	-3.21333300	3.31570300	0.93681500

Coordinates for TS **26**→**27**

FM

0 2

N	1.66563500	1.26268300	0.70538600
H	1.92432300	1.89452500	1.44356700
C	0.78281000	0.18788300	0.83131500
C	0.85571600	-0.41816200	-0.44674300
N	0.05323600	-1.48901500	-0.84584100
H	0.64596000	-0.30928400	1.77846700
C	2.09836700	1.31723100	-0.60204000
H	2.75789400	2.08493200	-0.97233300
N	1.59442800	0.31470600	-1.31124900
C	-1.27317100	-1.54782300	-0.20448300
H	-1.90402500	-2.13279800	-0.88859200
N	-1.95865400	-0.28021500	-0.01143100
N	-1.09535200	-2.16084900	1.10433000
H	-1.99787200	-2.29874600	1.54589000
H	-2.38806300	0.05577800	-0.86684100
C	-1.30330700	0.78634400	0.68979100
H	-0.62476000	-3.05340300	1.00498700
H	0.00038600	-1.53309500	-1.85626600
H	-1.59882100	0.89544200	1.73529300
N	-1.37999400	2.01183900	-0.02699100
H	-1.12643300	2.80417600	0.55050300
H	-0.77355300	2.00171200	-0.84439300

Coordinates for TS **27**→**28**

FM

0 2

N	1.77851200	-0.38702900	0.29905500
H	2.23480000	-0.18939200	1.17640900
C	0.32678200	-0.42238200	0.16147800
C	0.19173100	-1.34992800	-1.03737000
N	-0.90056800	-1.49223600	-1.68533800
H	-0.17318200	-0.84241700	1.03739700
C	2.27993900	-1.31502500	-0.57652100
H	3.34194000	-1.53403500	-0.58292300
N	1.43983600	-1.87013500	-1.39328200
C	-2.02002100	-0.76412900	-1.06443800
H	-2.80410800	-0.69324800	-1.82697700
N	-1.71469000	0.61295100	-0.66339700

N	-2.44184900	-1.50636100	0.12687700
H	-3.25916800	-1.05298100	0.52376100
H	-1.95988900	1.26333700	-1.39957800
C	-0.35224900	0.92648100	-0.22557400
H	-2.69073700	-2.45556300	-0.13844300
H	-1.58181500	-3.23026700	-2.12257200
H	-0.38571600	1.56920700	0.66140500
N	0.33049600	1.68718000	-1.26641200
H	1.23201700	2.01983900	-0.93851500
H	0.49519900	1.10571200	-2.08503500

Coordinates for TS **28**→**29**

FM

0 2

N	1.99134800	0.15177900	0.79915800
H	2.48496300	0.50337600	1.60577900
C	0.56516000	0.08257900	0.70409300
C	0.39268900	-0.90184400	-0.41282100
N	-0.72476500	-1.13562100	-0.99435700
H	0.07884300	-0.41351300	1.68562200
C	2.49410300	-0.82406300	-0.02314000
H	3.55691400	-1.03383600	-0.03466500
N	1.63307500	-1.44191400	-0.77173400
C	-1.84399400	-0.42537400	-0.35954100
H	-2.65778000	-0.38166800	-1.09261700
N	-1.59841100	0.95312300	0.05961400
N	-2.23191300	-1.20496200	0.81458300
H	-2.92244200	-0.74255000	1.39132100
H	-1.96433100	1.61527400	-0.61190100
C	-0.24057000	1.37044500	0.42341500
H	-2.46750000	-2.16879100	0.61349500
H	-0.27867800	1.98259100	1.33118500
N	0.30611200	2.21935100	-0.63027200
H	1.15612100	2.68368800	-0.32727200
H	0.52276000	1.67739900	-1.46326300
C	-0.72669900	-1.03970500	2.86406400
N	-0.96882600	-1.33762900	3.96229000

Coordinates for TS **29**→**30**

FM

0 2

N	1.86042600	0.57610800	0.97007500
H	2.23167600	1.19488900	1.67122300
C	0.53098900	0.42168200	0.60069000
C	0.53443000	-0.66268500	-0.36680800
N	-0.51481600	-1.12715400	-0.96270100
C	2.57227100	-0.33833600	0.22536700

H	3.64440100	-0.42445500	0.34408100
N	1.86360100	-1.06066600	-0.58806100
C	-1.75358600	-0.69175500	-0.33045300
H	-2.53621800	-0.69104500	-1.09906900
N	-1.75633700	0.67770100	0.23751800
N	-2.02015100	-1.62102500	0.76808100
H	-2.99177100	-1.55311200	1.05840500
H	-2.36434400	1.35040500	-0.20911000
C	-0.58591100	1.21681300	0.71774400
H	-1.84617500	-2.56741200	0.44172100
H	-0.64813300	2.11149900	1.31947300
N	-0.12089100	2.67789100	-0.95894000
H	0.84838600	2.97486200	-0.78864600
H	-0.00990100	1.95342700	-1.67902200

Coordinates for TS **30**→**31**

FM

0 2

N	2.00431700	-0.30103700	0.90618700
H	2.55912300	0.33428300	1.45480700
C	0.69485900	-0.12713800	0.48044000
C	0.36853800	-1.35032200	-0.23531100
N	-0.76554100	-1.59090500	-0.80339600
C	2.40267500	-1.52880200	0.42500100
H	3.39738400	-1.90061300	0.63284900
N	1.50863800	-2.17014000	-0.26398000
C	-1.80420800	-0.64939900	-0.41582200
H	-2.50547000	-0.56599000	-1.25369300
N	-1.37461400	0.73979700	-0.12132700
N	-2.42384000	-1.16550300	0.80975400
H	-3.31883100	-0.70885900	0.96395700
H	-1.82754300	1.54844700	-0.73447300
C	-0.14850400	0.94497600	0.39185200
H	-2.58931400	-2.16027400	0.68450100
H	0.12240200	1.96287800	0.65611000
N	-2.13570100	2.41407000	-1.90178100
H	-1.29787500	2.86717100	-2.27876500
H	-2.49116500	1.86196300	-2.68813200

Coordinates for TS **31**→**32**

FM

0 2

N	1.87567200	0.62917400	0.59490600
H	2.26615800	1.37794300	1.14446900
C	0.54535700	0.32342800	0.42731300
C	0.53480600	-0.82409700	-0.40710600
N	-0.58294800	-1.40991400	-0.80383700
C	2.58214500	-0.31356500	-0.12364600

H	3.66255600	-0.29830000	-0.14750400
N	1.83295100	-1.18518600	-0.73847000
C	-1.70466900	-0.87470300	-0.24224900
H	-2.63232500	-1.18176600	-0.71626200
N	-1.79649000	0.32978400	0.42576700
N	-1.97229300	-2.13520700	1.28779200
H	-2.98344600	-2.01033900	1.42008600
C	-0.67315500	0.90996600	0.78691000
H	-1.90018700	-3.00860500	0.75166700
H	-0.73603200	1.84654500	1.33677900

Coordinates for TS **29**→**33**

FM

0 2

N	1.97114300	0.57982000	0.53706700
H	2.42538500	1.42098000	0.85559600
C	0.66095400	0.44518700	0.14430900
C	0.52625400	-0.87689800	-0.24213300
N	-0.64029100	-1.44751000	-0.68171800
C	2.56407200	-0.64897700	0.35179300
H	3.60877200	-0.81286800	0.56937100
N	1.72898300	-1.54412000	-0.10819800
C	-1.66008600	-0.59798000	-0.69185200
H	-2.55744800	-0.89337500	-1.22049400
N	-1.54778800	0.76674200	-0.52725000
N	-2.54406200	-1.35834200	1.07966200
H	-2.69947100	-2.33452300	0.80160900
H	-2.41380800	1.28413400	-0.52706900
C	-0.45392800	1.44049800	0.17074200
H	-1.71080800	-1.43849800	1.67409100
H	-0.73536800	1.68950400	1.20909300
N	-0.23035100	2.72988400	-0.48485400
H	0.31140000	3.35759600	0.09919400
H	0.24826700	2.60218400	-1.37165100

Coordinates for TS **33**→**34**

FM

0 1

N	-1.31464500	-1.32190100	0.10750600
H	-1.26887600	-2.31893100	0.25410600
C	-0.23902700	-0.46402600	0.04957600
C	-0.79793900	0.82616000	-0.02394700
N	-0.05485700	1.95876100	-0.07753000
C	-2.42925800	-0.53367000	0.07836600
H	-3.42216300	-0.95599800	0.12574000
N	-2.16392000	0.75243500	-0.01351400
C	1.23419100	1.73304700	-0.05367400
H	1.91786600	2.57409900	-0.03005400

N	1.83010300	0.51531900	-0.03011800
H	2.80457900	0.41744700	0.26193000
C	1.14363300	-0.69610200	0.07485300
H	2.84520400	-0.97569400	1.56731600
N	1.62289500	-1.94689700	-0.23298100
H	2.56399900	-2.11557900	0.10454800
H	1.31212600	-2.32896300	-1.12608300

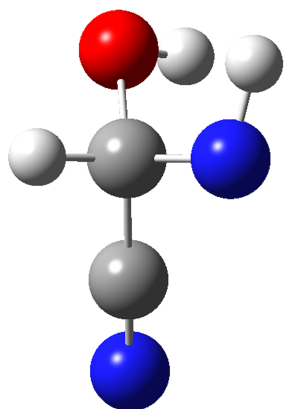
Coordinates for TS **34**→**35**

FM

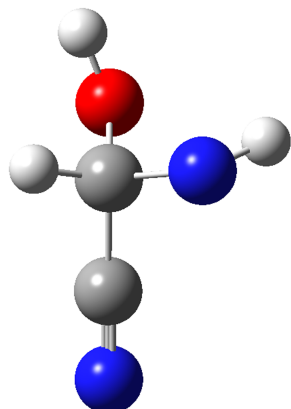
0 2

N	1.34733600	1.32140200	-0.01527700
H	1.36975600	2.32258900	-0.11908700
C	0.23938200	0.49206700	-0.01712300
C	0.76041300	-0.81556400	0.03252000
N	-0.01721900	-1.91428500	0.02094500
C	2.44261200	0.48884700	0.03028300
H	3.44690400	0.88707100	0.03257000
N	2.13786000	-0.78141900	0.06777200
C	-1.30561700	-1.65677100	-0.03641600
H	-1.98981800	-2.49881500	-0.03203900
N	-1.90914700	-0.43641400	-0.07636500
H	-3.09111400	-0.28208500	0.95588300
C	-1.14409400	0.67126300	-0.08026800
N	-1.78739100	1.88451700	-0.16902700
H	-2.78267800	1.81662400	0.00598400
H	-1.35127300	2.66438700	0.30099700

Structure of two conformers of 3.



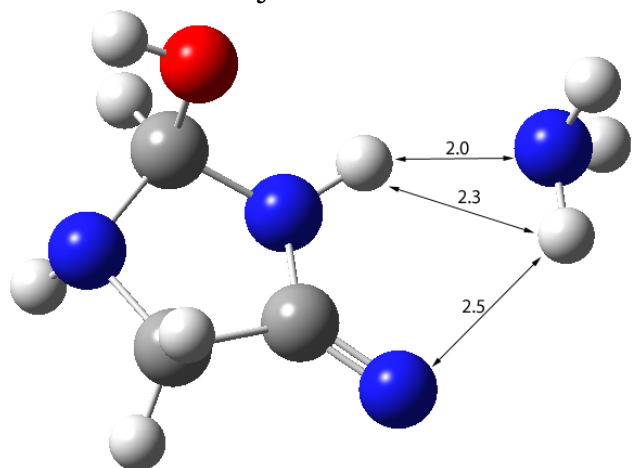
Structure of Isomer 1 of 3
B3LYP/6-311G(d,p) Energy
-262.6625629



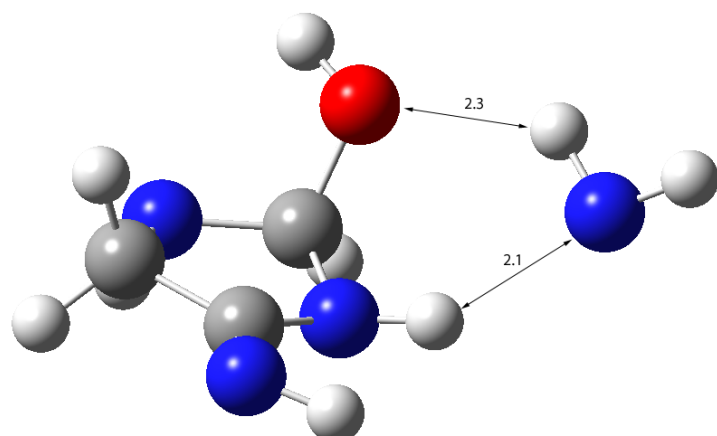
Structure of Isomer 2 of 3
B3LYP/6-311G(d,p) Energy
-262.6600117

List of Radical-Neutral Molecule Structures.

Structure of 8-NH₃



Structure of 9



Structure of 10-NH3

