

Supporting Information

On the Reaction Mechanism of Tirapazamine Reduction Chemistry: Unimolecular N–OH Homolysis, Step-Wise Dehydration or Triazene Ring-Opening

Jian Yin, Rainer Glaser,^{*,§} and Kent S. Gates^{*,§,‡}

Contribution from the Departments of Chemistry and Biochemistry, University of Missouri, Columbia, Missouri 65211

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Table S1. Results for the TPZ-Derived Species Computed at the B3LYP/6-31G* and QCI/6-31G*//B3LYP/6-31G* Levels

#	$E_{\text{tot}}^{\text{a}}$	$VZPE^{\text{b}}$	TE^{b}	S^{c}	NI	ν_1	ν_2	$E(\text{QCI/DFT})$
7	-640.267262	90.91	97.90	106.57	0	24	94	-638.490493
TS3	-640.251891	87.78	94.45	103.87	1	-1555	50	-638.451958
9	-640.275913	89.89	97.41	111.48	0	26	46	-638.502338
11a	-563.855075	74.90	80.11	91.55	0	89	167	-562.281834
11b	-563.854232	74.87	80.10	91.69	0	84	166	-562.281278
8	-640.246045	90.35	97.37	106.56	0	21	100	-638.477432
TS4	-640.237025	87.54	94.31	104.77	1	-980	44	-638.437665
10	-640.275156	90.00	97.55	112.01	0	20	53	-640.275156
12a	-563.854434	74.97	80.25	92.10	0	77	137	-562.285410
12b	-563.853003	75.01	80.32	92.59	0	62	138	-562.283305
13	-640.262991	90.75	97.89	107.32	0	46	53	-638.494889
TS5	-640.240731	86.43	93.54	105.56	1	-1510	50	-638.4546959
15	-640.261481	91.32	98.51	106.51	0	46	94	-638.4870253
17	-563.831720	75.41	80.89	92.79	0	96	166	-562.2579309

(a) See text.

Table S2. Results for the TPZ-Derived Species Computed at the MP2(full)/6-31G* and QCI/6-31G*//MP2(full)/6-31G* Levels

#	$E_{\text{tot}}^{\text{a}}$	$VZPE^{\text{b}}$	TE^{b}	S^{c}	NI	ν_1	ν_2	$E(\text{QCI}/\text{MP2})$
7	-638.457274	91.21	98.38	106.48	0	47	91	-638.498055
TS3	-638.339050	90.67	97.06	101.73	1	-4325	46	-638.457544
9	-638.381118	92.12	99.46	110.43	0	27	38	-638.499262
11a	-562.168912	76.90	81.93	90.15	0	102	180	-562.278762
11b	-562.168338	76.91	81.94	90.18	0	99	181	-562.278212
8	-638.435695	90.71	97.84	105.73	0	49	116	-638.474738
TS4a	-638.319636	90.25	96.59	100.46	1	-3860	62	-638.431713
TS4b	-638.317479	92.39	98.54	99.23	1	-2064	41	-638.419380
10	-638.386696	93.64	101.02	111.02	0	21	61	-638.493338
12a	-562.174301	78.15	83.30	91.69	0	58	150	-562.273731
12b	-562.172040	78.60	83.78	92.91	0	31	152	-562.270186
13	-638.454456	91.11	98.39	108.07	0	42	58	-638.495070
TS5	-638.401675	91.35	98.17	103.51	1	-2042	65	-638.448593
15	-638.430272	94.90	102.03	106.22	0	47	95	-638.482515
17	-562.211486	79.09	84.40	91.72	0	99	174	-562.254313

(a) See text.

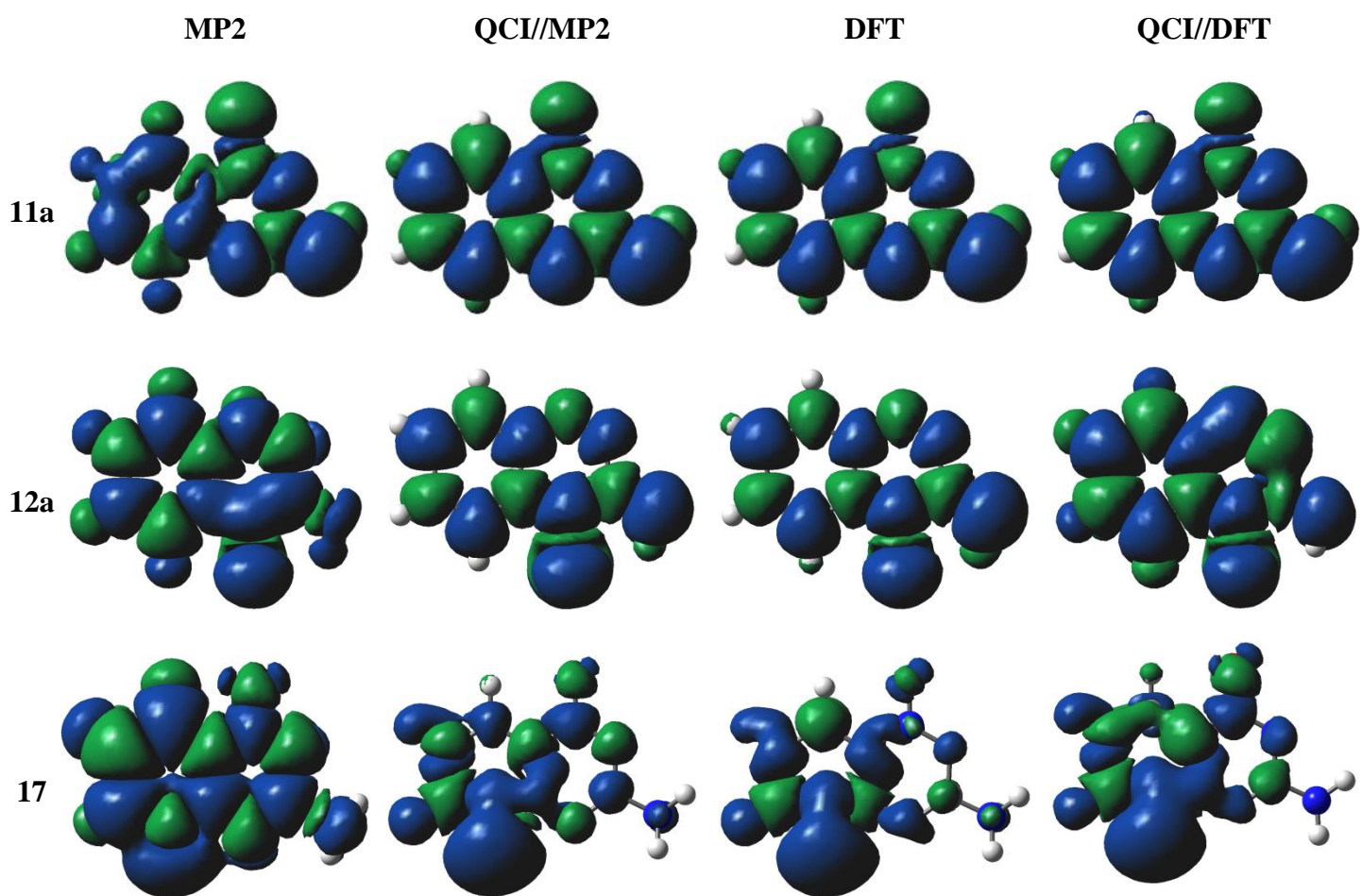


Figure S1. Spin Densities of **11a**, **12** and **17**. Isovalue for surfaces is 0.0004 au.

Cartesian Coordinates of Optimized Structures at DFT and MP2 levels

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B3LYP/6-31G* -640.267262

C	1.59741200	0.64137800	-0.00142000
C	-0.23298100	-0.71389700	-0.00071600
C	-1.06965300	0.42718200	0.00005000
H	-0.23623000	-2.86693300	-0.00149500
C	-0.86469100	-1.98212500	-0.00093800
C	-2.47125900	0.33702900	0.00044400
C	-3.05371200	-0.91423300	0.00007200
C	-2.24168500	-2.07234600	-0.00059400
H	-3.05245700	1.25080000	0.00106200
H	-4.13479900	-1.01013100	0.00031100
H	-2.71170900	-3.05193000	-0.00088800
N	-0.43769700	1.69315300	0.00064400
N	0.87423800	1.80563700	-0.00021900
N	1.12239400	-0.60427600	-0.00120200
N	2.93317800	0.82618500	-0.00382000
H	3.30103600	1.76414200	0.00210300
O	3.54116900	-2.05747400	0.00373100
H	2.56723500	-1.82152200	0.00118300
H	3.54139600	0.01167100	0.00136100
O	-1.12865000	2.72510900	0.00216500

MP2 (full) /6-31G* -638.4572735

C	1.58548600	0.66459900	-0.05878000
C	-0.22837900	-0.70572200	-0.03828800
C	-1.07789400	0.41484400	-0.00124900
H	-0.18380900	-2.85400800	-0.08510400
C	-0.83128800	-1.98182900	-0.05393700
C	-2.47368900	0.30893400	0.02979800
C	-3.02891300	-0.95698100	0.01176700
C	-2.20673900	-2.10145700	-0.02683300
H	-3.07403000	1.21105200	0.06174200
H	-4.10924100	-1.06870100	0.03250100
H	-2.66021000	-3.08912500	-0.03962500
N	-0.46577800	1.68888300	0.02909500
N	0.84875000	1.82199700	-0.00515400
N	1.13191600	-0.58197100	-0.06757800
N	2.92084900	0.88417600	-0.15115300
H	3.25332600	1.81234300	0.06954000
O	3.57211300	-2.06897000	0.17200500
H	2.61334700	-1.82990800	0.06328900
H	3.53510500	0.09047100	0.00310600
O	-1.17913100	2.71671400	0.08839600

TS3

B3LYP/6-31G* -640.2518913

C	1.56928200	0.32632100	-0.28033400
C	-0.40638700	-0.77507500	-0.15946200
C	-1.07994200	0.46058600	0.01662300
H	-0.68569400	-2.90212100	-0.30888600
C	-1.19591200	-1.95435100	-0.17337700
C	-2.47093100	0.54370100	0.16974800
C	-3.20817500	-0.62542600	0.14650800
C	-2.56453900	-1.87401700	-0.02478800
H	-2.92641700	1.51718700	0.30271100
H	-4.28686900	-0.58569400	0.26098800
H	-3.16045600	-2.78211300	-0.03982600
N	-0.28669000	1.63241900	0.05317000
N	1.02373900	1.56902300	-0.07442600
N	0.93811000	-0.84448700	-0.31659100
N	2.91392900	0.33349800	-0.49949600
H	3.34650300	1.21510200	-0.22798800
O	3.95949200	-1.40692200	0.66238700
H	3.14804300	-1.91800300	0.85350500
H	3.52548700	-0.63324500	-0.22439700
O	-0.82756600	2.73758400	0.22208500

MP2 (full) /6-31G* -638.3390502

C	1.56035100	0.19405600	-0.36719400
C	-0.44237900	-0.76671100	-0.19735400
C	-1.02265300	0.46869400	0.01256400
H	-0.82804000	-2.86043900	-0.37499900
C	-1.28436100	-1.89076600	-0.20598700
C	-2.38754000	0.63771100	0.21491000
C	-3.16506600	-0.46391600	0.19829200
C	-2.60478100	-1.73590700	-0.01233200
H	-2.77548300	1.63542100	0.37616100
H	-4.23567300	-0.37306900	0.35108500
H	-3.25743100	-2.60369400	-0.02006700
N	-0.16554500	1.57664800	0.04161300
N	1.10072200	1.44495300	-0.11971500
N	0.89043100	-0.91417000	-0.41262400
N	2.91309600	0.14925600	-0.65364100
H	3.35466700	0.99615600	-0.28281100
O	3.70025800	-1.29299700	0.90866600
H	2.83241800	-1.73358300	1.01886400
H	3.48575000	-0.80309600	-0.13452900
O	-0.65882700	2.70381300	0.24376800

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B3LYP/6-31G* -640.246045

C	1.44512800	0.41184600	-0.01820300
C	-0.90294900	0.47640200	0.00066100
C	-0.84430800	-0.94676000	-0.00862100
H	-2.12753400	2.24459300	0.02041800
C	-2.13589700	1.16171000	0.01342700
C	-2.06792100	-1.67253100	-0.00564000
C	-3.26584500	-1.00117000	0.00607900
C	-3.29642300	0.42117800	0.01577100
H	-2.00834400	-2.75596800	-0.01265500
H	-4.20027500	-1.55405300	0.00827700
H	-4.25538000	0.93123200	0.02513100
N	0.32651100	-1.62777600	-0.01736800
N	1.44340800	-0.93941800	-0.02157400
N	0.28977100	1.16194400	-0.00276600
N	2.59739400	1.09729400	-0.03634700
H	3.47292700	0.58202400	0.00782400
O	0.36973700	2.44341400	0.00896000
H	2.52945400	2.10397700	0.01947900
O	4.26840400	-1.31418400	0.04648200
H	3.29372200	-1.53401100	0.01352500

MP2 (full) /6-31G* -638.4356948

C	1.44841200	0.42057700	-0.07099900
C	-0.91791200	0.46345800	0.01315700
C	-0.83792100	-0.94975200	-0.04121400
H	-2.14039500	2.23509600	0.09874200
C	-2.14410200	1.15072000	0.06423900
C	-2.05309300	-1.67854900	-0.02816800
C	-3.25492900	-1.00847700	0.02358400
C	-3.30376300	0.40721800	0.07261300
H	-1.99196800	-2.76241100	-0.06537200
H	-4.18355300	-1.57308300	0.03135000
H	-4.26567000	0.91123100	0.11209700
N	0.33424300	-1.64230200	-0.08245100
N	1.45385500	-0.91263800	-0.09733800
N	0.27523400	1.17324200	-0.01023600
N	2.59059400	1.14721200	-0.18057600
H	3.44840600	0.63677700	0.01565400
O	0.33894600	2.42762100	0.03744500
H	2.51194300	2.10792100	0.13377000
O	4.29657600	-1.32761500	0.21293700
H	3.33942400	-1.54534000	0.06564000

TS4a

B3LYP/6-31G* -640.237025

C	1.43765100	0.10971200	-0.28135600
C	-0.88441500	0.47373900	-0.00998000

C	-1.00880600	-0.93693600	-0.08282600
H	-1.86393900	2.37551700	0.20671200
C	-2.00792800	1.30349500	0.15329500
C	-2.29966300	-1.50836300	0.00742900
C	-3.40294200	-0.69546100	0.16280700
C	-3.25310300	0.71109900	0.23656300
H	-2.37794900	-2.58911300	-0.04906500
H	-4.39468800	-1.13182200	0.23092500
H	-4.13327900	1.33525500	0.35976300
N	0.07427500	-1.76579700	-0.22037700
N	1.25571400	-1.24314200	-0.32133300
N	0.39320700	1.00212600	-0.09549800
N	2.66375500	0.61199600	-0.42750200
H	3.55372200	-0.01997500	-0.19322300
O	0.62248700	2.25743100	-0.02791500
H	2.70917500	1.60828000	-0.21986400
O	4.42337100	-0.64268400	0.67096900
H	3.94667500	-1.47611100	0.85769100

MP2 (full) /6-31G* -638.3196355

C	1.44867500	0.10102100	-0.29519900
C	-0.83004200	0.46431800	-0.01593300
C	-0.96460000	-0.91688700	-0.09626800
H	-1.77515600	2.37216000	0.21231900
C	-1.93597700	1.30258200	0.15457500
C	-2.25545300	-1.47443000	-0.00477700
C	-3.31932700	-0.67110200	0.15380800
C	-3.15236800	0.72972400	0.23430700
H	-2.33838100	-2.55452000	-0.06803800
H	-4.31825900	-1.08934500	0.22372500
H	-4.02990100	1.35617500	0.36306600
N	0.09790300	-1.74095900	-0.23372900
N	1.27080900	-1.22443100	-0.33748900
N	0.43194200	0.97724100	-0.10234500
N	2.67321200	0.61810400	-0.45518800
H	3.56759100	-0.07338000	-0.20377700
O	0.68526700	2.25348000	-0.01633500
H	2.71620100	1.58344800	-0.11559400
O	4.01154400	-0.72481700	0.76047000
H	3.34091000	-1.44488900	0.75338900

TS4b

MP2 (full) /6-31G* -638.3174791

C	-1.59040400	0.40808300	-0.15841200
C	0.80040300	0.51207200	-0.06831000
C	0.76095200	-0.88251800	-0.13061200
H	1.96420600	2.28624800	0.17551400
C	1.98809200	1.20390100	0.13191100
C	1.96382500	-1.57927600	-0.01702000

C	3.12603500	-0.90963900	0.19467700
C	3.13730000	0.48784900	0.26219400
H	1.92625000	-2.66135700	-0.09267100
H	4.05744900	-1.45740600	0.29742600
H	4.07592000	1.00786400	0.42662400
N	-0.38273300	-1.57190500	-0.47291600
N	-1.48340500	-0.90662100	-0.46139800
N	-0.39725900	1.18766100	-0.19483100
N	-2.73718500	0.90469100	0.16606500
H	-3.27878500	-0.27135000	0.51697800
O	-0.50565200	2.45417300	-0.13872400
H	-2.73344700	1.90828900	0.33188700
O	-3.07459600	-1.41621700	0.63118400
H	-3.48274600	-1.85554800	-0.14045200

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B3LYP/6-31G* -640.2759127

C	-1.51077700	0.82999500	-0.00002000
C	0.19505500	-0.69915600	-0.00010500
C	1.14105600	0.36037300	-0.00001100
H	-0.02947300	-2.84054200	-0.00016000
C	0.69233300	-2.03061900	-0.00009600
C	2.51558100	0.13117800	0.00007600
C	2.96719200	-1.18299800	0.00009300
C	2.05348700	-2.25998500	0.00001400
H	3.19144700	0.97738600	0.00012900
H	4.03433500	-1.38199200	0.00015800
H	2.42875100	-3.27886500	0.00004000
N	0.63407000	1.69447900	0.00000500
N	-0.65462000	1.92530800	0.00010100
N	-1.13517500	-0.47205000	-0.00020700
N	-2.81968000	1.07823700	-0.00003100
H	-2.94604400	2.09747000	0.00017700
O	-3.94236200	-1.81750100	0.00016700
H	-2.97236800	-1.77779100	0.00007100
H	-4.15388100	-0.87010200	-0.00022700
O	1.43630000	2.64248600	-0.00003800

MP2 (full) /6-31G* -638.3811178

C	1.46261000	-0.89524500	-0.00000600
C	-0.16402500	0.68049100	0.00000200
C	-1.13204600	-0.32224800	0.00000100
H	0.15535800	2.79479400	0.00000800
C	-0.60090300	2.01668300	0.00000500
C	-2.48382700	-0.05199600	-0.00000100
C	-2.87129800	1.25502600	0.00000000
C	-1.92494000	2.28857100	0.00000300
H	-3.18745700	-0.87475200	-0.00000200

H	-3.92838800	1.49993300	0.00000000
H	-2.26556900	3.31905700	0.00000500
N	-0.67938000	-1.66377400	0.00000000
N	0.56876000	-1.94384600	-0.00000500
N	1.15503900	0.40549500	0.00000400
N	2.75563800	-1.20632500	0.00001900
H	2.82871700	-2.23093000	0.00000300
O	3.88751700	1.82508600	-0.00002800
H	2.95284900	1.55746900	0.00003700
H	4.33131400	0.96350400	0.00008600
O	-1.53759800	-2.57478800	-0.00000800

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B3LYP/6-31G* -640.2751562

C	1.43975200	0.51318600	0.00007800
C	-0.99400900	0.47727200	-0.00003500
C	-0.86815200	-0.92816800	-0.00003200
H	-2.31047300	2.17692200	-0.00003600
C	-2.25100000	1.09546500	-0.00001100
C	-2.02719300	-1.71939800	0.00005200
C	-3.27604500	-1.11395800	0.00012800
C	-3.38195000	0.28968100	0.00008100
H	-1.90669500	-2.79774200	0.00005000
H	-4.17476900	-1.72251800	0.00020400
H	-4.36381600	0.75346100	0.00012900
N	0.36822300	-1.57311200	-0.00018300
N	1.44564000	-0.90048200	-0.00016400
N	0.18933400	1.21281600	-0.00009200
N	2.56377700	1.13197400	0.00039100
H	4.30705300	-0.24475400	-0.00004500
O	0.18498700	2.48324200	-0.00025100
H	2.39092000	2.14336200	0.00053100
O	4.62249800	-1.16400700	-0.00004000
H	3.78065800	-1.64546700	0.00026500

MP2 (full) /6-31G* -638.3866957

C	-1.43177400	0.55430100	-0.00002800
C	1.00991400	0.46554100	-0.00002200
C	0.87874300	-0.89855300	-0.00003800
H	2.33060200	2.14070100	0.00005400
C	2.25160900	1.06031000	0.00004100
C	1.98635900	-1.70214800	0.00000000
C	3.22504000	-1.13142000	0.00005500
C	3.34393500	0.24622100	0.00007600
H	1.84302700	-2.77842400	-0.00001900
H	4.11447200	-1.75239400	0.00007800
H	4.33322900	0.69398200	0.00011000
N	-0.40814500	-1.54261800	-0.00009000

N	-1.42969500	-0.91704200	-0.00013900
N	-0.17000100	1.20401000	-0.00003400
N	-2.52409200	1.13396600	-0.00002000
H	-4.24345400	-0.24772800	0.00014100
O	-0.14243700	2.49209100	-0.00000200
H	-2.38481300	2.15012200	-0.00007300
O	-4.61350800	-1.14689300	0.00015600
H	-3.80492300	-1.68158000	-0.00005000

11a

B3LYP/6-31G* -563.8550745

C	1.95754000	-0.67986400	-0.00003500
C	-0.31870600	-0.88814800	0.00000600
C	-0.45119000	0.52558400	0.00002900
H	-1.40853800	-2.74158400	-0.00004200
C	-1.51146300	-1.66165100	-0.00002200
C	-1.69363600	1.15897800	0.00003400
C	-2.83760800	0.37170600	0.00001000
C	-2.74255000	-1.03779800	-0.00002200
H	-1.73329700	2.24124100	0.00006400
H	-3.81427000	0.84581100	0.00001200
H	-3.65028500	-1.63401300	-0.00004600
N	0.74879400	1.29575700	0.00003100
N	1.92053100	0.71347300	-0.00004500
N	0.88332900	-1.50265700	0.00001600
N	3.16019100	-1.25524400	0.00003600
H	3.85783000	-0.50019200	0.00002700
O	0.66804000	2.53707400	-0.00003500

MP2 (full) /6-31G* -562.1689116

C	-1.93140400	-0.67154300	-0.00003500
C	0.31831100	-0.87763200	0.00000600
C	0.44978500	0.50903100	0.00003100
H	1.38923200	-2.72486500	-0.00002400
C	1.49656500	-1.64541500	-0.00001000
C	1.67533400	1.14328600	0.00002300
C	2.79454800	0.36681600	0.00000000
C	2.70078700	-1.03172000	-0.00001400
H	1.70854300	2.22537100	0.00004400
H	3.77291100	0.83624700	-0.00000100
H	3.61064900	-1.62366600	-0.00002900
N	-0.74105300	1.27210000	0.00007800
N	-1.88810700	0.70929600	0.00000100
N	-0.88055300	-1.49630400	-0.00001000
N	-3.14002200	-1.22794900	0.00001100
H	-3.82617600	-0.46310300	0.00003200
O	-0.64132100	2.52413500	-0.00007300

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B3LYP/6-31G* -563.8542322

C	-1.09424700	-1.76006000	0.00000000
C	0.80323100	-0.47240900	0.00000000
C	0.00000000	0.69671600	0.00000000
H	2.82773600	-1.20102600	0.00000000
C	2.21450900	-0.30608800	0.00000000
C	0.54999800	1.97818400	0.00000000
C	1.93281300	2.10516700	0.00000000
C	2.76149300	0.96097000	0.00000000
H	-0.11259700	2.83471900	0.00000000
H	2.38038800	3.09422300	0.00000000
H	3.84053200	1.08366500	0.00000000
N	-1.41674300	0.52004400	0.00000000
N	-1.95555500	-0.67213700	0.00000000
N	0.26088700	-1.70978200	0.00000000
N	-1.72031400	-2.94008000	0.00000000
H	-0.98193900	-3.65501400	0.00000000
O	-2.14235400	1.53028000	0.00000000

MP2 (full) /6-31G* -562.1683384

C	-1.05765700	-1.75087300	0.00000000
C	0.80175000	-0.45366100	0.00000000
C	0.00000000	0.68366300	0.00000000
H	2.81654400	-1.16563400	0.00000000
C	2.19620800	-0.27563200	0.00000000
C	0.52167700	1.96135500	0.00000000
C	1.87691600	2.09679200	0.00000000
C	2.71403600	0.97236000	0.00000000
H	-0.15554200	2.80589500	0.00000000
H	2.31637700	3.08901100	0.00000000
H	3.79038400	1.11288300	0.00000000
N	-1.40213300	0.48952200	0.00000000
N	-1.92030500	-0.67860000	0.00000000
N	0.27968000	-1.69809700	0.00000000
N	-1.68337100	-2.92758400	0.00000000
H	-0.94619400	-3.64273600	0.00000000
O	-2.13203100	1.51248400	0.00000000

12a

B3LYP/6-31G* -563.854434

C	-0.03284800	0.00017000	0.00314000
C	-0.01594400	0.00065700	2.43991600
C	1.38979200	0.00048800	2.32448200
H	-1.72470500	0.00130900	3.74408600
C	-0.64276900	0.00121200	3.69341000

C	2.17133200	0.00085600	3.48950000
C	1.55788000	0.00143000	4.73477800
C	0.15375700	0.00159900	4.83062200
H	2.16031700	0.00174400	5.63778300
H	-0.31745900	0.00204300	5.80907900
N	2.04516100	-0.00012200	1.09058600
N	1.38225000	-0.00024400	0.00712800
N	-0.74246400	0.00027900	1.25230500
N	-0.64350300	0.00039700	-1.12424700
O	-2.01404400	0.00020600	1.25092200
H	-1.65500100	0.00065200	-0.94450300
H	3.25050300	0.00068600	3.37573500

MP2 (full) /6-31G* -562.174301

C	-0.05226200	-0.00001000	0.01468900
C	-0.01042600	0.00078600	2.46016100
C	1.35587200	0.00060900	2.35294000
H	-1.70993200	0.00137800	3.74945800
C	-0.62814400	0.00125400	3.69242000
C	2.13773700	0.00087000	3.47689400
C	1.54465900	0.00133100	4.70534700
C	0.16413800	0.00152300	4.80017900
H	2.14951700	0.00154800	5.60599400
H	-0.30145500	0.00188700	5.78126900
N	2.02634200	0.00008100	1.07672400
N	1.41704800	-0.00005400	0.04304400
N	-0.72738600	0.00043200	1.26778000
N	-0.61287600	0.00005200	-1.08734300
O	-2.01701500	0.00061000	1.27411300
H	-1.63000900	0.00036600	-0.95181400
H	3.21644500	0.00070100	3.35286800

12b

B3LYP/6-31G* -563.8530033

C	2.00248300	-0.20383700	-0.00009200
C	-0.32496700	0.46883100	-0.00003500
C	-0.62901500	-0.90865400	-0.00001900
H	-1.07198600	2.48174900	-0.00001600
C	-1.34115700	1.43283300	-0.00000400
C	-1.97293400	-1.31551700	0.00002000
C	-2.98318400	-0.36531500	0.00004100
C	-2.66183100	1.00501000	0.00003100
H	-4.02306600	-0.67671800	0.00007100
H	-3.45842400	1.74321500	0.00005200
N	0.35760700	-1.89280300	-0.00003100
N	1.58398100	-1.55894100	-0.00002000
N	1.02476900	0.83376700	-0.00007900
N	3.24586800	0.11661400	0.00012600
O	1.36643400	2.05243600	-0.00000200

H	3.78093300	-0.75771500	0.00025500
H	-2.18088400	-2.38058400	0.00003200

MP2 (full) /6-31G* -562.1720401

C	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.43381542
C	1.36716844	0.00000000	2.37172474
H	-1.72876691	0.00004474	3.67984113
C	-0.64627441	0.00003973	3.65033335
C	2.11944258	0.00005607	3.51476583
C	1.49710900	0.00012053	4.72528383
C	0.11580706	0.00010151	4.77689999
H	2.07612061	0.00017301	5.64257167
H	-0.37908570	0.00014478	5.74377373
N	2.06827193	-0.00005269	1.11354955
N	1.48100415	-0.00028661	0.07265640
N	-0.70011609	0.00000123	1.22879097
N	-0.59799845	-0.00052137	-1.08085685
O	-1.98223039	-0.00016735	1.23836145
H	0.09643255	-0.00087873	-1.83321786
H	3.20110577	0.00005382	3.41834019

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B3LYP/6-31G* -640.262991

C	-1.66188400	-0.82098800	-0.01262600
C	0.10159500	0.61495600	-0.00767600
C	0.98922900	-0.48566600	-0.00226300
H	-0.02013100	2.76083400	-0.01144200
C	0.66155900	1.91594400	-0.00910000
C	2.38506800	-0.32550600	0.00005100
C	2.90092100	0.95463300	-0.00348000
C	2.03252700	2.07209200	-0.00745800
H	3.01305700	-1.20775100	0.00478800
H	3.97589500	1.10493900	-0.00256700
H	2.45429500	3.07330900	-0.00943400
N	0.41669700	-1.77833500	0.00782900
N	-0.89150800	-1.95058800	0.00266700
N	-1.24946600	0.43882400	-0.01043700
O	-2.60977200	2.96897200	0.03307400
H	-2.23328400	2.04627800	0.00075700
O	1.15187800	-2.77837100	0.02460900
N	-2.99521200	-1.07212000	-0.05734600
H	-3.31230500	-2.01431600	0.11322600
H	-3.63204600	-0.30535700	0.09953300

MP2 (full) /6-31G* -638.454456

C	-1.63217900	-0.87395100	-0.01343700
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C	0.08719000	0.61057700	-0.00625700
C	1.00684800	-0.45362900	-0.00645900
H	-0.11248200	2.74998000	-0.01028000
C	0.59694300	1.92707500	-0.00964000
C	2.39294400	-0.25500200	-0.00311700
C	2.85929200	1.04668700	-0.00950900
C	1.96220800	2.13457800	-0.01004900
H	3.05402900	-1.11418500	-0.00018300
H	3.92997100	1.23077000	-0.00975700
H	2.34932200	3.15008200	-0.01373700
N	0.47921600	-1.76419300	0.01245300
N	-0.82658800	-1.98140400	0.00399300
N	-1.26397600	0.39510400	-0.00990800
O	-2.72020200	2.92223300	0.04472300
H	-2.32374600	2.01521300	0.00457100
O	1.25643800	-2.74571700	0.03833200
N	-2.96005300	-1.17886000	-0.09366600
H	-3.22223400	-2.11835900	0.17443500
H	-3.60441500	-0.43816400	0.15121900

TS5

B3LYP/6-31G* -640.240731

C	-1.79518900	0.84784200	-0.00030800
C	0.41669600	0.38025900	0.01309200
C	0.12793400	-1.00701300	-0.00152800
H	2.01527500	2.03249800	0.06391000
C	1.78511000	0.72013400	0.02376500
C	1.13271400	-1.99048900	-0.00991900
C	2.45451600	-1.59352100	-0.00525800
C	2.78686600	-0.21247800	0.01008500
H	0.84083000	-3.03318600	-0.02117700
H	3.24698100	-2.33563100	-0.01298200
H	3.82980000	0.09257300	0.01184500
N	-1.23808100	-1.37403900	-0.00305600
N	-2.19078000	-0.46299800	-0.00169000
N	-0.55916500	1.32636400	0.01489800
O	1.79842700	3.16415900	-0.02542700
H	0.81915800	3.12266100	-0.05123100
O	-1.55353000	-2.57509400	-0.00224100
N	-2.83480000	1.72205900	-0.04354200
H	-3.76209900	1.36744100	0.13604400
H	-2.64121200	2.69301200	0.14907900

MP2 (full) /6-31G* -638.4016749

C	1.71525600	1.00852300	-0.02595300
C	-0.43703700	0.35426700	-0.08124100
C	-0.00574700	-1.00788900	-0.01174900
H	-2.20383600	1.82016600	-0.25258700

C	-1.81869900	0.55086300	-0.15083500
C	-0.92220100	-2.05680100	0.04198400
C	-2.22308400	-1.79031700	0.01874600
C	-2.68154700	-0.43201000	-0.05724200
H	-0.52816900	-3.06602600	0.09822000
H	-2.95834300	-2.58795500	0.06052900
H	-3.75133800	-0.23501700	-0.06040500
N	1.35267200	-1.25234000	0.02332900
N	2.21042800	-0.24478500	0.00975300
N	0.42241900	1.37336400	-0.08509600
O	-2.24086900	2.86736400	0.17079600
H	-1.28022600	3.02386900	0.29074500
O	1.81005100	-2.42904900	0.06309500
N	2.64955800	2.00031900	0.05348500
H	3.60397500	1.73049300	-0.14792800
H	2.35729200	2.91222800	-0.27226800

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B3LYP/6-31G* -640.261481

C	1.52661500	0.67703800	0.02443300
C	-0.24499400	-0.74190100	0.01679100
C	-1.13636700	0.36604100	0.00148300
H	3.88437500	-2.15897300	0.73975000
C	-0.89181400	-1.98731100	0.01880500
C	-2.53556300	0.22392600	-0.01036700
C	-3.08557800	-1.04229700	-0.00696500
C	-2.23802400	-2.18579600	0.00743200
H	-3.14586300	1.11817400	-0.02246400
H	-4.16369900	-1.17155400	-0.01588000
H	-2.66689200	-3.18477200	0.00913900
N	-0.54878300	1.65530200	-0.00684500
N	0.75705200	1.81388100	0.00474900
N	1.10243500	-0.58795500	0.02839900
O	3.68027100	-1.81497600	-0.14345000
H	2.69857000	-1.75211600	-0.15013300
O	-1.27813000	2.66082800	-0.02648700
N	2.85354600	0.91211000	0.05817700
H	3.17814300	1.85892500	-0.06251800
H	3.48283700	0.11194300	-0.03943500

MP2 (full) /6-31G* -638.4302717

C	1.49450900	0.72014800	0.04607800
C	-0.23621200	-0.73638300	0.03317300
C	-1.14581400	0.33987800	0.00184400
H	3.99802300	-2.16106300	0.64046300
C	-0.84652800	-1.99252800	0.04005000
C	-2.53024900	0.14709800	-0.02216500
C	-3.02305600	-1.08339700	-0.01254900

C	-2.13709100	-2.20716300	0.01909800
H	-3.16282300	1.02773500	-0.04760500
H	-4.09432600	-1.25824500	-0.02984600
H	-2.54694200	-3.21420100	0.02560600
N	-0.61227300	1.62863300	-0.01838400
N	0.70388800	1.82505500	0.00421200
N	1.09698600	-0.56492700	0.05774600
O	3.73333800	-1.75342900	-0.19894500
H	2.75322400	-1.75130600	-0.16806000
O	-1.36060900	2.64080200	-0.05995500
N	2.81710100	0.97218200	0.11419100
H	3.12345200	1.91899400	-0.06000900
H	3.45428600	0.18658500	-0.02687700

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B3LYP/6-31G* -640.2525697

C	-1.87857400	-0.35420800	-0.01464800
C	0.20006900	0.54444100	-0.01033800
C	0.76576900	-0.75841700	-0.00093300
H	-0.70046900	3.76718300	0.86154600
C	1.13863300	1.58721300	-0.01632400
C	2.15408100	-0.98610700	-0.00290500
C	3.01095400	0.09623500	-0.01550000
C	2.49011900	1.42103800	-0.02429400
H	2.51281700	-2.00763900	0.00405900
H	4.08584400	-0.05871000	-0.01999700
H	3.16635300	2.27215300	-0.03884900
N	-0.13981700	-1.84610600	0.01621200
N	-1.44368000	-1.65220900	0.00732700
N	-1.14444600	0.74984000	-0.01103100
O	-1.03518100	3.67291700	-0.04249600
H	-1.29017400	2.72968200	-0.08680500
O	0.29430900	-3.00895900	0.04208700
N	-3.22917200	-0.24052800	-0.06229800
H	-3.79197400	-1.06409300	0.08449700
H	-3.64192200	0.67161400	0.05700800

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B3LYP/6-31G* -563.8317196

C	1.92112500	-0.55582700	-0.00565800
C	-0.29942700	-0.93524700	0.00338700
C	-0.54273400	0.46786100	-0.00384100
C	-1.47067500	-1.71028000	0.00832700
C	-1.83580900	1.02284800	-0.00802400
C	-2.92976700	0.18176600	-0.00546600
C	-2.74353600	-1.23013700	0.00329000
H	-1.93627000	2.10088600	-0.01301600

H	-3.93556500	0.59141600	-0.00968200
H	-3.60391000	-1.89468100	0.00550000
N	0.59391500	1.30972300	0.00189200
N	1.81302800	0.81032500	-0.00032400
N	0.95174400	-1.45805800	0.00670800
N	3.21007900	-0.99102800	-0.05393500
H	3.94226100	-0.32831200	0.15259600
H	3.37249000	-1.96728000	0.14238600
O	0.44807100	2.54441700	0.01121800

MP2 (full) /6-31G* -562.2114859

C	1.91498200	-0.53446000	-0.00268000
C	-0.29890200	-0.93271600	0.00535600
C	-0.54234500	0.47037700	-0.00781800
C	-1.46032900	-1.71129000	0.01308300
C	-1.83797500	0.99703700	-0.01344900
C	-2.87784500	0.17729300	-0.00926500
C	-2.67954100	-1.24815300	0.00508800
H	-1.94144300	2.07652500	-0.02192800
H	-3.89317400	0.56222000	-0.01522000
H	-3.54292100	-1.90887300	0.00929100
N	0.55863300	1.31122300	0.00322300
N	1.79022300	0.80699400	0.00401400
N	0.93333800	-1.45257700	0.00889500
N	3.20047100	-0.99397300	-0.07848500
H	3.92417500	-0.33784800	0.18545400
H	3.33482600	-1.95541500	0.20620200
O	0.42895200	2.56914800	0.01634700