

Supporting Information

Electron and Spin Density Analysis of Tirapazamine Reduction Chemistry

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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	$E(\text{QCI//DFT})$
1	-639.678114	85.99	92.03	95.41	0	93	148	-637.907715
2	-639.711867	83.99	90.22	98.15	0	79	142	-637.929009
1^a	-639.708876	85.60	91.77	96.44	0	88	145	-637.954372
2^a	-639.764211	83.85	90.14	98.72	0	73	140	-637.998826
3a	-640.255846	92.51	99.04	100.27	0	66	127	-638.481097
3a^a	-640.286462	92.38	98.90	100.28	0	65	127	-638.528656
3b	-640.254604	92.27	98.84	100.77	0	62	124	-638.478596
3c	-640.253006	92.05	98.69	101.20	0	60	123	-638.476334
TS1a	-640.245575	91.06	97.45	99.78	1	-599	63	-638.460305
TS1b	-640.241411	90.72	97.21	100.41	1	-620	65	-638.454990
5	-564.523585	83.65	89.11	91.33	0	97	169	-562.942367
4a	-640.257275	92.13	98.71	100.31	0	79	135	-638.477262
4b	-640.257851	92.15	98.77	100.65	0	75	135	-638.478871
4b^a	-640.288835	91.83	98.52	101.19	0	74	134	-638.525851
4c	-640.256642	91.99	98.62	100.66	0	78	134	-638.476356
4d	-640.257890	92.14	98.76	100.64	0	75	134	-638.478763
TS2	-640.234132	90.14	96.85	101.78	1	-277	76	-638.445798
6	-564.502755	83.15	88.62	90.98	0	111	149	-562.922577

a) Use 6-31+G*.

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 ^b	TE ^b	S ^c	NI	ν_1	ν_2	E(QCI//MP2)
1	-637.883804	85.95	92.25	96.90	0	91	143	-637.905899
2	-637.856961	87.68	93.66	96.83	0	70	157	-637.919811
1^a	-637.934724	86.13	92.27	96.15	0	82	138	-637.952790
2^a	-637.933091	87.60	93.56	96.54	0	81	161	-637.989793
3a	-638.402444	96.35	102.51	97.80	0	76	155	-638.477507
3a^a	-638.453952	96.15	102.27	97.55	0	80	156	-638.525108
3b	-638.399684	95.86	102.10	98.59	0	67	149	-638.475242
3c	-638.397440	95.49	101.84	99.22	0	65	148	-638.472663
TS1a	-638.344946	94.02	100.20	98.37	1	-900	65	-638.454947
TS1b	-638.341183	93.72	100.02	99.30	1	-944	62	-638.449703
5	-562.915413	83.76	89.40	92.33	0	94	164	-562.942361
4a	-638.396307	96.21	102.48	98.49	0	72	153	-638.474793
4b	-638.397171	96.25	102.56	98.85	0	69	151	-638.476264
4b^a	-638.447375	95.85	102.18	98.96	0	70	151	-638.523386
4c	-638.395578	95.88	102.30	99.53	0	70	152	-638.476264
4d	-638.396968	96.23	102.55	98.87	0	69	150	-638.475988
TS2	-638.333528	92.40	99.17	103.22	1	-417	57	-638.444155
6	-562.893672	83.16	88.81	92.11	0	106	141	-562.919976

a) Use 6-31+G*.

b) RMP2(full) energies are listed for closed-shell systems.

c) UQCISD//MP2(full) total energies in hartree: **1**: -637.894739 (6-31G*), -637.941059 (6-31+G*); **5**: -562.930537; **6**: -562.906432.

d) UQCISD//MP2(full) energy relative to RQCISD//MP2(full) energy in kcal/mol: **1**: 7.00 (6-31G*), 7.36 (6-31+G*); **5**: 7.42; **6**: 8.50.

Table S3. Mulliken Spin Populations Computed at QCI//MP2 Level

Atom/Group	SP-1	2	3a	4b	SP-5	SP-6
O(N1), HO(N1)	0.315	0.327	0.504	0.002	0.138	-
N1	0.230	0.428	0.368	0.047	0.087	-0.335
N2	-0.235	0.053	-0.040	0.157	-0.155	0.152
C3	0.185	-0.004	0.065	-0.091	0.040	-0.170
(C3)NH _n	0.044	0.005	0.014	-0.017	0.020	-0.045
N4	-0.281	0.077	0.021	0.350	-0.094	0.242
O(N4), HO(N4)	-0.246	0.021	0.001	0.488	-	0.214
Σ_1	0.012	0.908	0.933	0.936	0.035	0.058
C4a	0.158	-0.048	0.036	-0.069	0.023	-0.196
C5a	-0.161	-0.033	-0.062	0.046	-0.048	0.168
HC5	0.150	0.038	0.061	-0.011	0.081	-0.186
HC6	-0.145	0.056	-0.012	0.052	-0.074	0.162
HC7	0.131	-0.016	0.050	-0.007	0.051	-0.188
HC8, C8	-0.146	0.096	-0.008	0.052	-0.068	0.181
Σ_2	-0.012	0.092	0.067	0.064	-0.035	-0.058
Σ_α	1.214	1.102	1.121	1.193	0.440	1.119
Σ_β	-1.214	-0.102	-0.121	-0.193	-0.440	-1.119

(a) See Scheme 1 for atom numbering.

Table S4. Mulliken Atom and Fragment Charges Computed at QCI//MP2 level

Atom/Group	1	SP-1	2	3a	4b	5	SP-5	6	SP-6
O(N1), HO(N1)	-0.433	-0.426	-0.526	-0.393	-0.065	-0.412	-0.421	-	-
N1	0.053	0.030	0.006	-0.028	-0.221	0.081	0.101	-0.274	-0.290
N2	-0.295	-0.290	-0.400	-0.334	-0.323	-0.293	-0.307	-0.320	-0.315
C3	0.701	0.693	0.655	0.688	0.717	0.631	0.643	0.688	0.681
(C3)NH _n	-0.027	-0.028	-0.131	-0.060	-0.063	-0.058	-0.053	-0.035	-0.033
N4	-0.201	-0.186	-0.274	-0.369	-0.245	-0.543	-0.558	-0.174	-0.154
O(N4), HO(N4)	-0.538	-0.521	-0.676	-0.070	-0.417	-	-	-0.506	-0.504
Θ ₁	-0.740	-0.729	-1.346	-0.567	-0.617	-0.594	-0.595	-0.620	-0.615
C4a	0.306	0.289	0.316	0.259	0.277	0.235	0.242	0.309	0.294
C5a	0.246	0.258	0.211	0.267	0.269	0.246	0.238	0.166	0.175
HC5	0.075	0.065	-0.032	0.039	0.014	0.072	0.073	0.052	0.047
HC6	0.013	0.021	-0.069	0.006	0.014	-0.002	-0.002	0.008	0.014
HC7	0.042	0.033	-0.046	0.006	0.002	0.035	0.036	0.030	0.024
HC8, C8	0.058	0.064	-0.034	-0.011	0.043	0.009	0.008	0.054	0.061
Θ ₂ = -Θ ₁	0.740	0.729	0.346	0.567	0.617	0.594	0.595	0.620	0.615
Θ ₊	1.494	1.452	1.188	1.265	1.334	1.308	1.341	1.308	1.296
Θ ₋ = -Θ ₊ + n	-1.494	-1.452	-2.188	-1.265	-1.334	-1.308	-1.341	-1.308	-1.296

(a) See Scheme 1 for atom numbering.

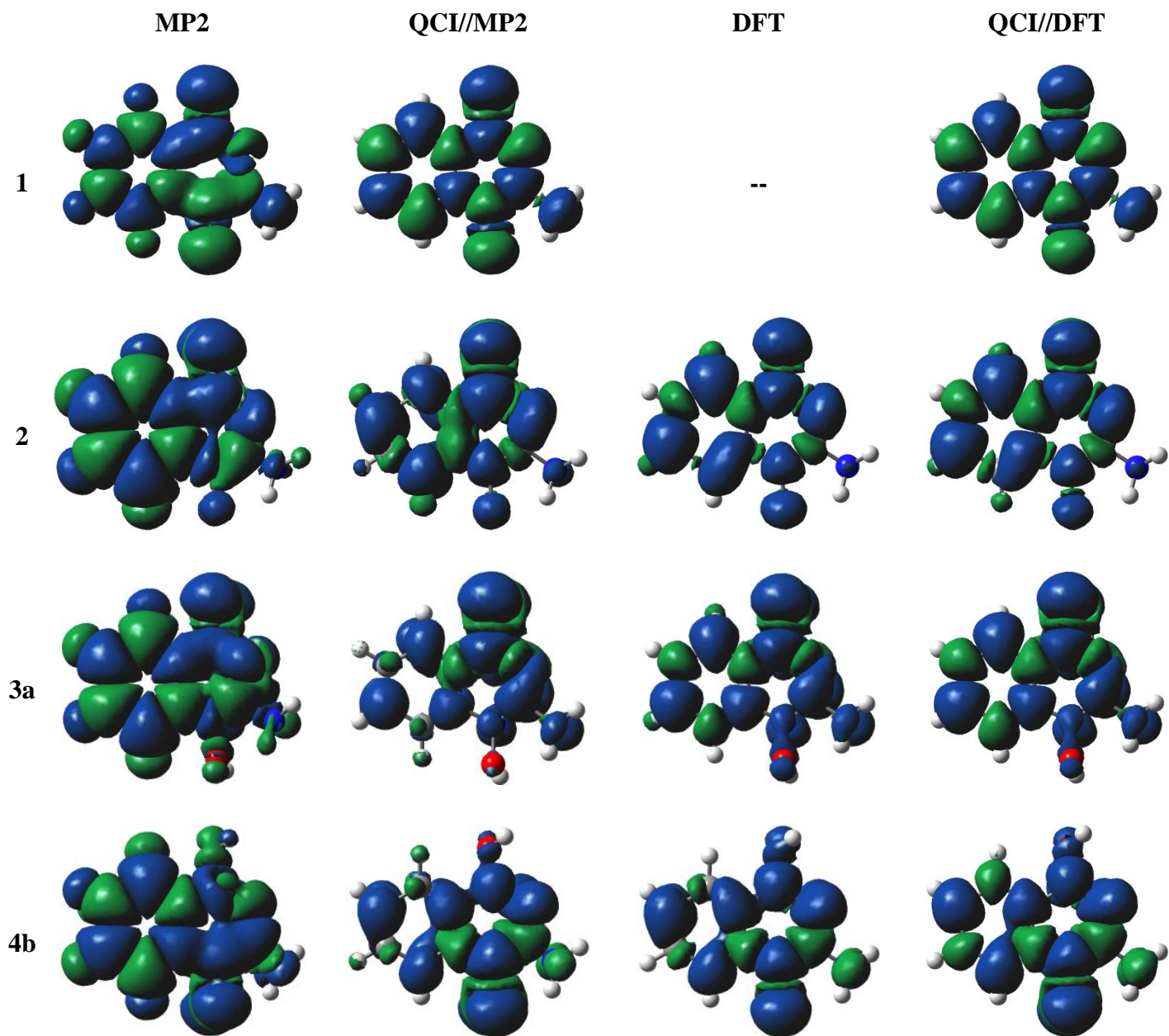
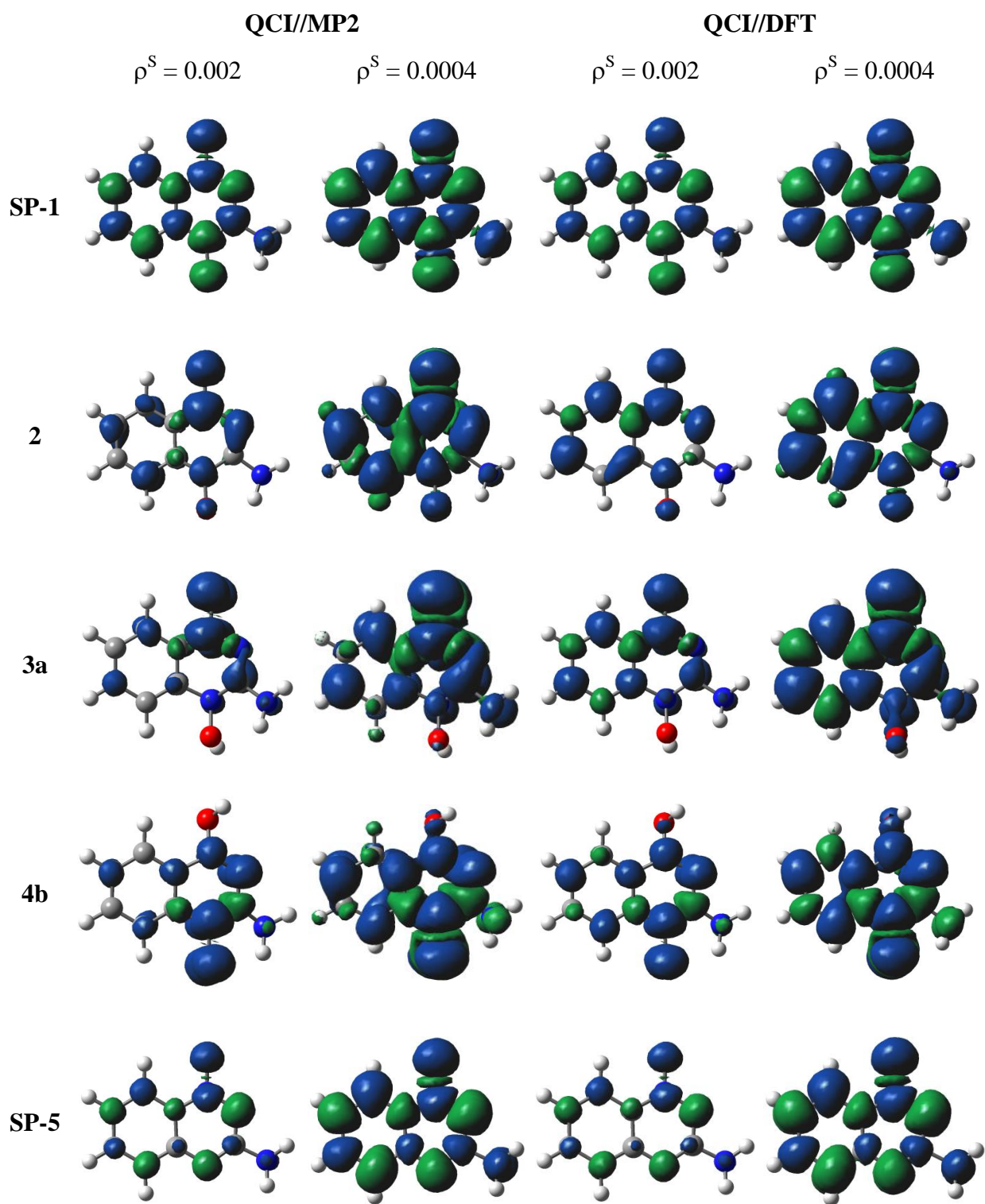


Figure S1. Spin Densities of **1**, **2**, **3a**, and **4b**. Isovalue for surfaces is 0.0004 au.



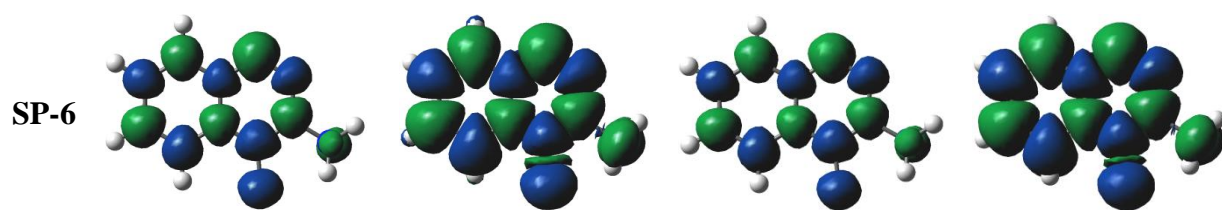


Figure 2 (expanded version). Spin density distributions computed at the UQCISD level based on the MP2 (left) and DFT structures, respectively, for radicals **2-4** and for spin-polarized singlet excited states of **1**, **5**, and **6**. See text for details.

Cartesian Coordinates of Optimized Structures at DFT and MP2 levels

TPZ, 1

B3LYP/6-31G* -639.6781137

C	1.88750500	0.04826400	-0.01143700
C	-0.32701100	-0.71042800	-0.00121300
C	-0.73670500	0.64097400	-0.00379900
H	-0.93997200	-2.76138100	0.00365100
C	-1.29163000	-1.73724100	0.00126200
C	-2.10469300	0.97201800	-0.00537300
C	-3.03945900	-0.04219900	-0.00463500
C	-2.62842700	-1.39721800	-0.00082100
H	-2.37686100	2.02007100	-0.00646500
H	-4.09750100	0.20010200	-0.00668600
H	-3.37853900	-2.18271900	-0.00015400
N	0.24029900	1.64791200	0.00342300
N	1.53057900	1.34028200	-0.00217300
N	1.01976700	-1.00797500	0.00073400
N	3.19478000	-0.28376200	-0.05753300
H	3.87767300	0.42534200	0.15950300
O	1.47776500	-2.22305000	0.01947900
H	3.38285700	-1.26551100	0.11144300
O	-0.09315500	2.85353500	0.01597700

B3LYP/6-31+G* -639.7088763

C	1.88893500	0.03990200	-0.00718000
C	-0.32943300	-0.71151800	-0.00082000
C	-0.73691200	0.64175300	-0.00303600
H	-0.95381100	-2.76394300	0.00270300
C	-1.29723100	-1.73637400	0.00078800
C	-2.10447700	0.97770100	-0.00426600
C	-3.04299400	-0.03555600	-0.00401100
C	-2.63510100	-1.39202000	-0.00117600
H	-2.37868200	2.02582200	-0.00516800
H	-4.10060500	0.21012100	-0.00570800
H	-3.38695900	-2.17626100	-0.00086400
N	0.24651000	1.64443700	0.00278100
N	1.53115900	1.33466600	-0.00110500
N	1.01777900	-1.00879400	0.00171500
N	3.19722100	-0.28014000	-0.04393700
H	3.88401500	0.44257500	0.10994200
O	1.47416300	-2.23082600	0.01557500
H	3.42255700	-1.26093000	0.07789900
O	-0.08565100	2.85433900	0.01232800

MP2 (full) /6-31G* -637.8838041

C	1.88988300	0.04579500	-0.00510700
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C	-0.33285400	-0.70436000	0.00891300
C	-0.73474900	0.64208000	-0.01091500
H	-0.93151100	-2.76139600	0.00794000
C	-1.28705500	-1.73673700	0.00243200
C	-2.09745700	0.97413800	-0.00760600
C	-3.02706800	-0.04891700	-0.01058600
C	-2.62529600	-1.40208800	-0.00035800
H	-2.37420500	2.02224600	-0.01333800
H	-4.08558300	0.19625600	-0.01292700
H	-3.37583300	-2.18777400	-0.00369300
N	0.23648400	1.64903100	0.00666200
N	1.53126200	1.33128700	-0.00254700
N	1.01908600	-1.01504100	0.00111700
N	3.20823700	-0.29492800	-0.09380400
H	3.85681000	0.41220500	0.22910200
O	1.45578300	-2.21229600	0.02336600
H	3.38367300	-1.25532400	0.18913000
O	-0.09969000	2.87003100	0.02202900

MP2 (full) /6-31+G* -637.934724

C	1.89167500	0.03746100	0.00582400
C	-0.33517800	-0.70518800	0.02932800
C	-0.73440500	0.64277800	-0.03605500
H	-0.94373200	-2.76387100	0.01736000
C	-1.29208900	-1.73569200	0.00203900
C	-2.09693000	0.97902300	-0.00592900
C	-3.03134800	-0.04313300	-0.01519900
C	-2.63244900	-1.39784100	0.00830800
H	-2.37631700	2.02740800	-0.02148500
H	-4.08963100	0.20575100	-0.00870000
H	-3.38413500	-2.18323700	-0.00113100
N	0.24217100	1.64630100	0.00892500
N	1.53309500	1.32652800	-0.00212300
N	1.01722600	-1.01597700	-0.00809600
N	3.21256000	-0.29068200	-0.09029700
H	3.85867300	0.42671700	0.22056800
O	1.45300800	-2.22070600	0.01516900
H	3.41662200	-1.24848600	0.18815100
O	-0.09457000	2.87171700	0.02439000

Radical-Anion, 2

B3LYP/6-31G* -639.7118666

C	1.89064900	0.07604300	-0.03402000
C	-0.32902000	-0.71113900	-0.01284000
C	-0.74046100	0.65144500	-0.00891300
H	-0.90787400	-2.75190200	-0.00181000
C	-1.27804400	-1.73394000	-0.00494000
C	-2.11474400	0.95517100	-0.00292700

C	-3.05567900	-0.07945800	0.00051200
C	-2.64530900	-1.41501300	0.00102200
H	-2.39460000	2.00117300	0.00305900
H	-4.11641600	0.16583100	0.00460300
H	-3.38299100	-2.21515200	0.00576700
N	0.21694400	1.65227500	0.00515000
N	1.57118900	1.35745500	-0.02347800
N	1.03033700	-0.98634600	-0.01356000
N	3.22008100	-0.30193000	-0.08672900
H	3.83456000	0.34220000	0.39342200
O	1.50047400	-2.23957200	0.04387400
H	3.27128800	-1.28525300	0.18772000
O	-0.11774600	2.89385500	0.03240000

B3LYP/6-31+G* -639.7642105

C	1.89236800	0.06279400	-0.02739400
C	-0.33243000	-0.71240400	-0.01200400
C	-0.73904800	0.65267500	-0.00835000
H	-0.92904900	-2.75531700	-0.00209100
C	-1.28697900	-1.73237800	-0.00432400
C	-2.11323800	0.96411400	-0.00203700
C	-3.05928500	-0.06733800	0.00072200
C	-2.65388200	-1.40668200	0.00079400
H	-2.39477800	2.01023300	0.00364600
H	-4.11881300	0.18254500	0.00468300
H	-3.39478000	-2.20370800	0.00513300
N	0.22558600	1.64612600	0.00350800
N	1.57032600	1.34654600	-0.01662700
N	1.02714500	-0.99013000	-0.01525600
N	3.22281900	-0.29623300	-0.08173000
H	3.84759500	0.37908800	0.33819100
O	1.49183000	-2.25045600	0.04061800
H	3.33764000	-1.27206300	0.18836000
O	-0.10607800	2.89425300	0.02792900

MP2 (full) /6-31G* -637.8569613

C	-1.86137800	0.10087100	0.10383200
C	0.31854100	-0.69181100	-0.08804400
C	0.75842100	0.62383900	-0.02015500
H	0.87488500	-2.72514400	-0.09888000
C	1.24945900	-1.71109500	-0.03370600
C	2.07412300	0.90511400	0.11935900
C	3.00098300	-0.10154700	0.18600100
C	2.56767400	-1.39496500	0.09530500
H	2.35151600	1.95457800	0.15622300
H	4.05791800	0.12929600	0.28707300
H	3.29274200	-2.20762700	0.13405000
N	-0.23404200	1.64206100	-0.22716200
N	-1.52966700	1.36543200	0.20463200
N	-1.00411600	-0.94676300	-0.18383400

N	-3.13937100	-0.33217000	0.39445800
H	-3.85580900	0.29388000	0.04933100
O	-1.48750800	-2.20656600	-0.28216400
H	-3.19112600	-1.30575800	0.07620000
O	0.13417100	2.87886800	-0.22986200

MP2 (full) /6-31+G* -637.9330909

C	-1.85185500	0.08795800	0.12284800
C	0.31938300	-0.68853700	-0.11939000
C	0.75596400	0.62602000	-0.04088100
H	0.88976400	-2.72916700	-0.13204800
C	1.25270400	-1.71063000	-0.05190100
C	2.06298000	0.91398700	0.15410600
C	2.99226300	-0.09197600	0.23854900
C	2.56512900	-1.38980400	0.12284000
H	2.34230100	1.96317600	0.20795900
H	4.04463300	0.14034200	0.37978200
H	3.29227600	-2.19973900	0.17648600
N	-0.25111900	1.63414700	-0.26846800
N	-1.51047500	1.35364600	0.24226500
N	-1.00302300	-0.93810300	-0.24947400
N	-3.11203700	-0.33845800	0.47559300
H	-3.84656700	0.31646800	0.23453400
O	-1.48135900	-2.20414800	-0.33617300
H	-3.23660600	-1.30365100	0.15982100
O	0.11528200	2.87312800	-0.28669700

Radical 2+H⁺, 3a

B3LYP/6-31G* -640.2558457

C	-1.88860200	0.13879100	-0.03274200
C	0.35723200	-0.69028600	0.11693700
C	0.78112600	0.65032900	0.03841900
H	0.94236300	-2.75061100	0.08742900
C	1.28425200	-1.72343500	0.04409200
C	2.14108800	0.94777300	-0.09440600
C	3.06732600	-0.09092700	-0.15729500
C	2.64296400	-1.42021300	-0.09551600
H	2.43054100	1.99008400	-0.14683000
H	4.12362900	0.14000900	-0.25866400
H	3.36492100	-2.22929000	-0.15175200
N	-0.18381300	1.66912400	0.10849000
N	-1.52451100	1.37729500	-0.13290900
N	-1.02685500	-0.90483300	0.34703600
N	-3.20991400	-0.20619400	-0.18131700
H	-3.76510700	0.54757900	-0.56713600
O	-1.48786600	-2.19120500	-0.04155500
H	-1.71631700	-2.60966800	0.80726600
H	-3.36699900	-1.11133600	-0.60633400

O 0.14915300 2.89161700 0.15780400

B3LYP/6-31+G* -640.2864618

C	-1.88761400	0.13409600	-0.04863300
C	0.35763700	-0.68916700	0.11412100
C	0.78139600	0.65272300	0.03901700
H	0.94597700	-2.75277200	0.07650000
C	1.28435700	-1.72401500	0.03510000
C	2.14175400	0.95176800	-0.09908700
C	3.06856200	-0.08838300	-0.16812600
C	2.64398300	-1.41924800	-0.10814900
H	2.43618800	1.99345200	-0.14894200
H	4.12469300	0.14277400	-0.27343700
H	3.36627200	-2.22808400	-0.16946200
N	-0.18933800	1.66600100	0.12106500
N	-1.51971400	1.37338600	-0.14721800
N	-1.02631800	-0.89969200	0.35089400
N	-3.20675700	-0.20625500	-0.21724800
H	-3.76234000	0.54666900	-0.60603400
O	-1.48811900	-2.19441300	0.00579500
H	-1.69938700	-2.60216100	0.86438800
H	-3.37736100	-1.11752300	-0.62471700
O	0.14066800	2.89152800	0.18717800

MP2 (full) /6-31G* -638.4024439

C	-1.85192000	0.16032400	-0.10621400
C	0.35361700	-0.67621000	0.15621200
C	0.79358000	0.62106900	0.06800400
H	0.87806000	-2.72853200	0.08806500
C	1.23338800	-1.70659200	0.03176400
C	2.11115300	0.89745000	-0.13508600
C	2.99803300	-0.13533700	-0.24921600
C	2.55906400	-1.42584800	-0.17095400
H	2.41212100	1.93753600	-0.19167500
H	4.05140100	0.07592100	-0.40537300
H	3.26363900	-2.24667300	-0.26663500
N	-0.17483500	1.64822600	0.22435400
N	-1.47714100	1.39120500	-0.24319900
N	-1.02541700	-0.84055900	0.43465500
N	-3.13919400	-0.21091000	-0.37252200
H	-3.66089500	0.52402700	-0.83785100
O	-1.49302000	-2.15301400	0.15348500
H	-1.77590800	-2.46695700	1.03435900
H	-3.24628300	-1.13568200	-0.77149000
O	0.19458000	2.86745000	0.28157900

spins	(S**2,0)	(S**2,1)	PUHF	PMP2	PMP3	PMP4
annihilated						
s+1	0.66356	0.71548	-636.535265	-638.429159	-638.456554	-638.566386
s+1,s+2	0.75494	0.74980	-636.530225	-638.424399	-638.452258	-638.562090
s+1 to s+3	0.74988	0.75007	-636.530522	-638.424619	-638.452345	-638.562177

s+1 to s+4 0.75000 0.75000 -636.530515 -638.424607 -638.452328 -638.562160
s+1 to s+5 0.75000 0.75000 -636.530515
s+1 to s+6 0.75000 0.75000 -636.530515

MP2 (full) /6-31+G* -638.4539516

C	-1.84481000	0.15848300	-0.13084200
C	0.35201100	-0.67303700	0.16704700
C	0.79509800	0.62247000	0.07502000
H	0.86895000	-2.73165400	0.08593300
C	1.22502600	-1.70928400	0.02697700
C	2.10860200	0.89738600	-0.14910400
C	2.99250600	-0.13979600	-0.27671000
C	2.55029400	-1.42999500	-0.19112900
H	2.41620100	1.93652500	-0.20975300
H	4.04468800	0.06824500	-0.44804600
H	3.25181100	-2.25280700	-0.29836500
N	-0.18284800	1.64511200	0.25113300
N	-1.46236000	1.39066500	-0.27132000
N	-1.02646100	-0.82544000	0.44909200
N	-3.12044300	-0.21746000	-0.43934300
H	-3.63324400	0.50612800	-0.93490900
O	-1.49673900	-2.14604300	0.22626700
H	-1.77768600	-2.43125900	1.11951400
H	-3.22686600	-1.15526600	-0.81167800
O	0.18781100	2.86511600	0.32908500

3b

B3LYP/6-31G* -640.2546043

C	-1.89667100	0.11663000	-0.01861500
C	0.36475800	-0.68936300	-0.13397400
C	0.77036000	0.65635400	-0.02695900
H	0.97463100	-2.74032100	-0.20089100
C	1.30573600	-1.71283100	-0.10466900
C	2.12856700	0.96507900	0.10576000
C	3.06766500	-0.06390300	0.13462000
C	2.66211700	-1.39651700	0.03356600
H	2.40688700	2.00860600	0.18469700
H	4.12138200	0.17850400	0.23614300
H	3.39588800	-2.19649100	0.05303100
N	-0.20130500	1.66763000	-0.06562700
N	-1.55550500	1.36552700	0.03453900
N	-1.01822700	-0.93218000	-0.31411200
N	-3.19664700	-0.25049800	0.22543900
H	-3.83962400	0.53121200	0.20274900
O	-1.46931400	-2.21943500	0.02417500
H	-1.39080400	-2.28866200	1.00055700
H	-3.51339500	-1.08785500	-0.24683400
O	0.12326700	2.89305600	-0.06536200

MP2 (full) /6-31G* -638.3996841

C	-1.86570100	0.14074100	0.03665200
C	0.35906200	-0.67295500	-0.17902200
C	0.78072400	0.63096800	-0.05368200
H	0.91704500	-2.71796100	-0.21433000
C	1.25569800	-1.69505900	-0.09567300
C	2.09879100	0.91430600	0.15033000
C	3.00013000	-0.11083800	0.23132700
C	2.58091000	-1.40508400	0.10986900
H	2.38851900	1.95518400	0.23863000
H	4.05086300	0.11141000	0.38977900
H	3.29761100	-2.21858800	0.16896300
N	-0.18587000	1.65578900	-0.18175000
N	-1.52210000	1.38366800	0.13783400
N	-1.01916700	-0.87615000	-0.42633400
N	-3.11677400	-0.26269500	0.41646800
H	-3.76086300	0.51543200	0.51098700
O	-1.47460000	-2.18119900	-0.15098600
H	-1.36866500	-2.29602100	0.82212200
H	-3.48155800	-1.06388200	-0.08514300
O	0.17544300	2.88090700	-0.18068100

3c

B3LYP/6-31G* -640.2530062

C	1.90498600	0.10214600	-0.05009000
C	-0.36451300	-0.68686400	-0.14484100
C	-0.76153400	0.66061600	-0.02591400
H	-0.99489000	-2.73171300	-0.24734200
C	-1.31719200	-1.70242000	-0.13752800
C	-2.11950800	0.97814700	0.09927200
C	-3.06652100	-0.04262900	0.10850200
C	-2.67129200	-1.37810200	-0.00568900
H	-2.38973300	2.02273300	0.19078300
H	-4.11897200	0.20720800	0.20520300
H	-3.41165500	-2.17215100	-0.00176200
N	0.21559600	1.66429800	-0.03798100
N	1.56568900	1.35177800	0.03639000
N	1.01477000	-0.95378100	-0.31216600
N	3.22165500	-0.24891600	-0.00208300
H	3.85299000	0.45684700	0.34733100
O	1.44129700	-2.21544800	0.17071100
H	1.15497100	-2.25019900	1.11015300
H	3.43797100	-1.21822700	0.17496900
O	-0.10144700	2.89125800	0.00044900

MP2 (full) /6-31G* -638.3974397

C	1.87903200	0.12069800	0.01901600
C	-0.36161100	-0.67007600	-0.18190200
C	-0.77065300	0.63872300	-0.05120100
H	-0.95115700	-2.70796000	-0.25014000
C	-1.27462200	-1.68147400	-0.11702300
C	-2.08946300	0.93401100	0.13787700
C	-3.00372000	-0.08076600	0.20122900

C	-2.59937000	-1.37959700	0.07453800
H	-2.36790600	1.97734600	0.23240400
H	-4.05345200	0.15366300	0.34869600
H	-3.32590700	-2.18523700	0.11759300
N	0.20352600	1.65476800	-0.15415600
N	1.53681600	1.36540100	0.14645400
N	1.01367100	-0.90268000	-0.41345200
N	3.17182700	-0.24866800	0.18848200
H	3.77623900	0.44965200	0.59945800
O	1.43666500	-2.19840200	-0.02284100
H	1.08700900	-2.31253000	0.89270300
H	3.37264100	-1.22459700	0.34715800
O	-0.14865300	2.88325200	-0.12145500

3e, TS (3a, 3b)

B3LYP/6-31G* -640.2440772

C	1.87554600	0.11817900	0.00381200
C	-0.37507500	-0.70129000	-0.09461900
C	-0.78648300	0.64629400	-0.02190100
H	-0.97548000	-2.75583300	-0.11272300
C	-1.31220800	-1.72768500	-0.06421600
C	-2.14286300	0.95592100	0.07172000
C	-3.08351400	-0.07642100	0.09407600
C	-2.67256400	-1.40739800	0.03012500
H	-2.42477400	2.00004700	0.12610000
H	-4.13968700	0.16615200	0.16317400
H	-3.40552300	-2.20821300	0.05078700
N	0.18882800	1.66880100	-0.05143000
N	1.54012500	1.36514000	0.05103800
N	1.00261900	-0.92547900	-0.22280600
N	3.23588400	-0.30281800	0.10108400
O	1.43252000	-2.23339900	0.07262700
O	-0.14098500	2.89326900	-0.05491900
H	3.78502600	0.13651500	-0.63676100
H	3.62903500	0.01395400	0.98620100
H	2.40990000	-2.11668500	0.02236200

MP2 (full) /6-31G* -638.3875354

C	1.84749900	0.13305200	0.05756200
C	-0.37684800	-0.68671500	-0.11501600
C	-0.79676100	0.62391800	-0.03103400
H	-0.93142400	-2.73129200	-0.10815900
C	-1.27524500	-1.70598100	-0.04606500
C	-2.11572100	0.91357300	0.11696700
C	-3.02625600	-0.10827700	0.18162100
C	-2.60669100	-1.40148500	0.09612600
H	-2.40459100	1.95713200	0.17080200
H	-4.08159200	0.12025900	0.29188300
H	-3.32809900	-2.21176500	0.14446800
N	0.17768200	1.65091000	-0.18044000

N	1.52722800	1.37733600	0.14764600
N	0.99349600	-0.87780900	-0.25334000
N	3.18237500	-0.31397000	0.28349500
O	1.42961600	-2.21210000	-0.17401600
O	-0.17812900	2.87706000	-0.18330600
H	3.79489700	0.12455100	-0.40485800
H	3.48332500	0.03213600	1.19511000
H	2.39025700	-2.07449100	0.02683700

3f, SOSP

B3LYP/6-31G* -640.2437634

C	1.59881800	-0.99729300	0.00000000
C	0.00000000	0.80156500	0.00000000
C	-1.00120300	-0.19637000	0.00000000
H	0.44558400	2.89519000	0.00000000
C	-0.33889800	2.14859500	0.00000000
C	-2.34481100	0.17458500	0.00000000
C	-2.68573200	1.53121000	0.00000000
C	-1.69445400	2.50957000	0.00000000
H	-3.08972900	-0.61111800	0.00000000
H	-3.73359300	1.81611600	0.00000000
H	-1.96244000	3.56172500	0.00000000
N	-0.62631500	-1.55829400	0.00000000
N	0.71297300	-1.94053100	0.00000000
N	1.31454900	0.33993800	0.00000000
N	3.00036000	-1.27056000	0.00000000
O	2.33858400	1.28797600	0.00000000
O	-1.49887500	-2.47854300	0.00000000
H	3.23921300	-1.83047800	0.81742900
H	3.23921300	-1.83047800	-0.81742900
H	3.13078700	0.69853600	0.00000000

MP2 (full) /6-31G* -638.3866782

C	1.57303900	-1.00911500	0.00000000
C	0.00000000	0.79464100	0.00000000
C	-0.99916000	-0.16561300	0.00000000
H	0.48416000	2.85438700	0.00000000
C	-0.31041300	2.11796600	0.00000000
C	-2.30596000	0.21632500	0.00000000
C	-2.62370600	1.55236800	0.00000000
C	-1.63692300	2.49101800	0.00000000
H	-3.06138800	-0.56080000	0.00000000
H	-3.66695300	1.85215300	0.00000000
H	-1.88691900	3.54757700	0.00000000
N	-0.64509700	-1.53593200	0.00000000
N	0.69270300	-1.95882300	0.00000000
N	1.29944600	0.31665600	0.00000000
N	2.97126900	-1.28550400	0.00000000
O	2.32492600	1.27061600	0.00000000

O	-1.54717600	-2.44549000	0.00000000
H	3.19108900	-1.85536900	0.81725100
H	3.19108900	-1.85536900	-0.81725100
H	3.11740700	0.67610000	0.00000000

TS1a

B3LYP/6-31G* -640.2455746

C	1.85923800	0.11864000	-0.19142300
C	-0.33050500	-0.68227200	-0.20115700
C	-0.77130500	0.64040300	0.01731600
H	-0.94799400	-2.72529000	-0.43663400
C	-1.28982700	-1.70786000	-0.28280400
C	-2.13741500	0.93770000	0.16033000
C	-3.05924500	-0.08992900	0.09111900
C	-2.63371600	-1.41584700	-0.13084400
H	-2.42410500	1.96909000	0.32409600
H	-4.11692500	0.12705600	0.20587300
H	-3.36626000	-2.21578200	-0.18362900
N	0.18354600	1.66600800	0.03246800
N	1.49893900	1.38253500	-0.03690800
N	1.02032400	-0.96079600	-0.36736400
N	3.19776500	-0.15971800	-0.24231700
H	3.78737600	0.59097400	0.09402000
O	1.52443300	-2.13468400	0.77391500
H	1.63165500	-2.86398200	0.13732700
H	3.41425400	-1.07799400	0.12832000
O	-0.16260400	2.87152300	0.13286600

MP2 (full) /6-31G* -636.4963943

C	1.82182000	0.13424100	-0.21751100
C	-0.31079200	-0.66163600	-0.20841100
C	-0.76906100	0.61925000	0.02387400
H	-0.89060100	-2.70342000	-0.48033100
C	-1.25482900	-1.69714600	-0.30642700
C	-2.13405300	0.89839600	0.16621500
C	-3.00708800	-0.11550600	0.08190800
C	-2.55918000	-1.43027800	-0.15898200
H	-2.43243100	1.92383200	0.34505100
H	-4.07006600	0.07223500	0.19560200
H	-3.28668100	-2.23347800	-0.22606300
N	0.16057400	1.63185800	0.04790300
N	1.45247200	1.38232700	-0.04592600
N	1.01441700	-0.94029100	-0.37123100
N	3.14533600	-0.10982100	-0.29512800
H	3.74001300	0.65120900	0.00755000
O	1.56255000	-2.09215100	0.86269700
H	1.62037900	-2.85259700	0.25486300
H	3.40008800	-1.04095100	0.01002300

O	-0.21394900	2.83599200	0.16980200
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TS1b

B3LYP/6-31G* -640.2414114

C	1.86192800	0.07881700	-0.22550500
C	-0.33865100	-0.68347700	-0.22056400
C	-0.75804700	0.64489400	0.01256900
H	-0.97259900	-2.71393900	-0.47992700
C	-1.31178000	-1.69728900	-0.31599600
C	-2.12010600	0.96244400	0.15489200
C	-3.05568800	-0.05138100	0.06897300
C	-2.65038100	-1.38305800	-0.16566300
H	-2.39341500	1.99573400	0.32945600
H	-4.11058400	0.18026500	0.18099400
H	-3.39724400	-2.16877200	-0.23107800
N	0.21756800	1.65190800	0.04895000
N	1.52683600	1.35154500	-0.04886600
N	1.00385000	-0.98500900	-0.37539700
N	3.18737300	-0.22213600	-0.32276500
H	3.82363100	0.49285100	0.00267300
O	1.50146300	-2.18775100	0.77448800
H	1.18258200	-1.76915700	1.59937500
H	3.40425400	-1.17871400	-0.06847900
O	-0.10767200	2.85798500	0.18817500

MP2 (full) /6-31G* -638.3411833

C	1.82677000	0.08669600	-0.24817000
C	-0.31984300	-0.66202000	-0.22995600
C	-0.75193600	0.62534500	0.01942900
H	-0.91996200	-2.69093100	-0.51540900
C	-1.28076900	-1.68396600	-0.33647900
C	-2.11340100	0.92978500	0.15918200
C	-3.00196900	-0.06767800	0.06047900
C	-2.57857300	-1.39102500	-0.19091600
H	-2.39514100	1.95816200	0.34797700
H	-4.06211900	0.13800600	0.17049000
H	-3.32299500	-2.17792700	-0.26656100
N	0.20122000	1.61513900	0.05973000
N	1.48634900	1.34473100	-0.05193300
N	0.99745200	-0.97255300	-0.38021700
N	3.13408100	-0.18480100	-0.36242000
H	3.77937400	0.54677600	-0.09707500
O	1.52077500	-2.14221200	0.86467000
H	1.13936000	-1.70142600	1.65178600
H	3.38673700	-1.14864000	-0.18230800
O	-0.14835500	2.82165400	0.21452500

Radical 2+H+, 4a

B3LYP/6-31G* -640.2572751

C	-1.91446100	0.01559100	0.03276800
C	0.36364600	-0.73737100	-0.05877900
C	0.74498100	0.62090500	-0.09177400
H	0.98237800	-2.77607500	0.05701200
C	1.32279500	-1.74799800	0.03431200
C	2.10115600	0.95720300	-0.01656300
C	3.05277800	-0.05540300	0.08391800
C	2.66880600	-1.40256500	0.10297100
H	2.38502000	2.00194200	-0.04641500
H	4.10428700	0.20996200	0.14284000
H	3.42057700	-2.18255500	0.17498600
N	-0.26799800	1.56010400	-0.29710900
N	-1.57962300	1.27780300	-0.00379900
N	-1.00733300	-1.04081400	-0.10186900
N	-3.20030700	-0.37678600	0.25982200
H	-3.91775300	0.28723500	0.00828100
O	-1.43908600	-2.25851500	-0.12005900
H	-3.36052400	-1.35481000	0.04645000
O	0.05175900	2.88172100	0.01185200
H	-0.16675100	2.98432100	0.96206800

MP2 (full) /6-31G* -562.9154125

C	1.91375100	-0.56759700	-0.00347200
C	-0.32217700	-0.87523600	0.00649000
C	-0.51916100	0.51928900	-0.00778200
H	-1.32446700	-2.77209600	0.02091400
C	-1.47188200	-1.69586800	0.01158100
C	-1.79046900	1.10721900	-0.01275100
C	-2.89115900	0.27105200	-0.01057400
C	-2.73120300	-1.13026900	0.00365700
H	-1.87588100	2.18792800	-0.02127100
H	-3.88929100	0.70008600	-0.01696600
H	-3.60920100	-1.77109600	0.00597300
N	0.63424600	1.33324200	0.00352800
N	1.84684800	0.80196200	-0.00128400
N	0.92106400	-1.43843000	0.01202600
N	3.19872000	-1.03558600	-0.08207500
H	3.92090200	-0.39351800	0.21806700
H	3.31559500	-2.00226600	0.19338400
O	0.51624900	2.58138800	0.01895500

Radical 2+H+, 4b

B3LYP/6-31G* -640.2578511

C	1.91774400	0.01842100	-0.03864700
C	-0.36041000	-0.73745000	0.05344000
C	-0.74530400	0.61956100	0.08385600

H	-0.97190700	-2.77886300	-0.04678000
C	-1.31680300	-1.75224000	-0.02756700
C	-2.10351100	0.94880200	0.01165400
C	-3.05226300	-0.06709000	-0.07614900
C	-2.66415300	-1.41310800	-0.08930500
H	-2.39182700	1.99231600	0.01883800
H	-4.10464200	0.19498300	-0.13494500
H	-3.41337300	-2.19628100	-0.15354400
N	0.26461100	1.56474800	0.28344300
N	1.58058800	1.27736400	-0.01352200
N	1.01033100	-1.04001800	0.09568100
N	3.20543900	-0.37715400	-0.25002700
H	3.92253500	0.29492000	-0.02178700
O	1.44346100	-2.25673500	0.12527600
H	3.36926600	-1.35117600	-0.02384200
O	-0.08256000	2.84864200	-0.18534800
H	0.22417100	3.43289600	0.52992700

B3LYP/6-31+G* -640.2888353

C	1.91688800	0.00901300	-0.03909500
C	-0.36060600	-0.73825200	0.05084800
C	-0.74612000	0.62029900	0.08026000
H	-0.98309300	-2.78150300	-0.04109600
C	-1.32104100	-1.75198600	-0.02509000
C	-2.10476900	0.95487100	0.00702400
C	-3.05595600	-0.06054900	-0.07720200
C	-2.66890200	-1.40894800	-0.08636900
H	-2.39284300	1.99889300	0.01290200
H	-4.10829800	0.20270400	-0.13633500
H	-3.41975100	-2.19121300	-0.14795400
N	0.26778300	1.56026800	0.27318600
N	1.57866200	1.27316200	-0.02177300
N	1.00910900	-1.04047400	0.09890300
N	3.20782500	-0.37495200	-0.24316600
H	3.92375300	0.30702400	-0.03843000
O	1.44065000	-2.26289600	0.12510700
H	3.39710600	-1.34937400	-0.03750000
O	-0.08032200	2.85099100	-0.16712700
H	0.29988500	3.43599600	0.51225500

MP2 (full) /6-31G* -562.8936717

C	-1.88447600	-0.29924000	-0.00141600
C	0.35450200	0.44540400	0.00597500
C	0.69213800	-0.93024100	-0.00003600
H	1.00234100	2.49893900	0.00123700
C	1.32476000	1.46309200	0.00041400
C	2.06779000	-1.26919500	-0.00291700
C	3.02109300	-0.27525300	-0.00802600
C	2.65209800	1.09290700	-0.00462100
H	2.32663200	-2.32416300	-0.00430700

H	4.07466600	-0.54208200	-0.01208800
H	3.42377100	1.85807100	-0.00926700
N	-0.22688000	-1.93788600	0.01620800
N	-1.51220500	-1.57755100	0.01347100
N	-0.99541000	0.76942000	0.00136600
N	-3.20053200	0.05787300	-0.09892700
H	-3.84450700	-0.66649600	0.19486300
H	-3.39391200	0.99897800	0.22900600
O	-1.42640500	1.95361500	0.01743600

spins	(S**2,0)	(S**2,1)	PUHF	PMP2	PMP3	PMP4
annihilated						
s+1	0.61841	0.69677	-636.539101	-638.429171	-638.457312	-638.566838
s+1,s+2	0.76094	0.75048	-636.531727	-638.422200	-638.451024	-638.560550
s+1 to s+3	0.74960	0.75018	-636.532298	-638.422619	-638.451178	-638.560704
s+1 to s+4	0.75001	0.74999	-636.532276	-638.422597	-638.451155	-638.560682
s+1 to s+5	0.75000	0.74999	-636.532277			
s+1 to s+6	0.75000	0.74999	-636.532277			

MP2 (full) /6-31+G* -638.4473753

C	1.89680800	0.06416800	-0.10879400
C	-0.36102100	-0.72705200	0.11140400
C	-0.74813900	0.59113000	0.13434600
H	-0.90377000	-2.76438100	-0.05559100
C	-1.26433900	-1.74064100	-0.04921800
C	-2.07491900	0.89543200	-0.03305800
C	-2.97743300	-0.11618100	-0.19316600
C	-2.58199400	-1.43236900	-0.19775300
H	-2.38419600	1.93375400	-0.03380900
H	-4.02756800	0.13151500	-0.32353600
H	-3.31333900	-2.22486700	-0.32515800
N	0.24526600	1.54098100	0.40677400
N	1.53233000	1.28406200	-0.10985600
N	1.02231900	-0.99109300	0.26968600
N	3.11977200	-0.35614700	-0.50199300
H	3.85182900	0.34277000	-0.51037100
O	1.47698200	-2.20009900	0.36810000
H	3.36063200	-1.30591500	-0.23772400
O	-0.16894100	2.81520300	-0.06467800
H	0.18049200	3.41475700	0.62397200

4c

B3LYP/6-31G* -640.2566421

C	-1.91683600	0.01458400	-0.00121500
C	0.36310500	-0.73649100	0.06275400
C	0.74522500	0.62153200	0.09611300
H	0.98191100	-2.77473600	-0.05561300
C	1.32297900	-1.74698900	-0.02942300
C	2.10228000	0.95699400	0.02714100
C	3.05410800	-0.05541900	-0.06960300

C	2.66922400	-1.40237300	-0.09258100
H	2.38603700	2.00179700	0.05659800
H	4.10599500	0.20954000	-0.12321400
H	3.42077300	-2.18280300	-0.16247400
N	-0.26663200	1.56474900	0.28507900
N	-1.58031200	1.27765200	0.00584900
N	-1.00730700	-1.04344800	0.09959600
N	-3.21625700	-0.37661300	-0.09058600
H	-3.88172200	0.31708800	-0.39626400
O	-1.43621900	-2.26129700	0.04776400
H	-3.34698000	-1.34460500	-0.35694100
O	0.05282000	2.87963700	-0.04956600
H	-0.14577400	2.95959400	-1.00635500

MP2 (full) /6-31G* -638.3955781

C	-1.90499200	0.05916200	0.04710700
C	0.36865900	-0.72369600	-0.10631400
C	0.74601900	0.59750000	-0.14061300
H	0.92628700	-2.75034000	0.07636900
C	1.28358000	-1.72684600	0.05168400
C	2.07529500	0.90860100	-0.01464700
C	2.98606200	-0.09269900	0.14143900
C	2.59973800	-1.40950500	0.16877200
H	2.37499900	1.94910100	-0.04666800
H	4.03729400	0.16283000	0.23977000
H	3.33821000	-2.19542200	0.29046500
N	-0.24230100	1.55211500	-0.40249300
N	-1.54307100	1.28573900	0.05456500
N	-1.01296400	-1.01236300	-0.21451800
N	-3.16809600	-0.34529200	0.26689300
H	-3.83599800	0.34595900	0.57449700
O	-1.45044200	-2.22886100	-0.18796300
H	-3.30595300	-1.32836000	0.45959600
O	0.11895500	2.84553300	0.01373500
H	-0.04408200	2.84635800	0.98409400

4d

B3LYP/6-31G* -640.257890

C	1.91937400	0.01425000	-0.00528300
C	-0.36138200	-0.73635200	0.05860800
C	-0.74558200	0.62097200	0.08735000
H	-0.97578600	-2.77650100	-0.04269800
C	-1.31970900	-1.74964300	-0.02109200
C	-2.10381100	0.95156100	0.02030900
C	-3.05416300	-0.06309500	-0.06304100
C	-2.66694600	-1.40936000	-0.07830300
H	-2.39070500	1.99552600	0.02543700
H	-4.10649900	0.20000000	-0.11752400
H	-3.41690800	-2.19205900	-0.13973600

N	0.26493100	1.56817600	0.27029800
N	1.58208000	1.27404600	-0.01029300
N	1.00880600	-1.04384400	0.09431600
N	3.22331200	-0.37806100	-0.07650700
H	3.87396000	0.30918400	-0.42783200
O	1.43679200	-2.26205000	0.05024900
H	3.34566100	-1.34515000	-0.35230300
O	-0.07747700	2.84416100	-0.22074200
H	0.23515900	3.43989700	0.48260700

MP2 (full) /6-31G* -638.3969683

C	1.90780900	0.05793000	-0.05527900
C	-0.36804900	-0.72349300	0.10785200
C	-0.74731600	0.59655400	0.12535000
H	-0.92271300	-2.75361300	-0.04572500
C	-1.28179500	-1.73062100	-0.03415900
C	-2.07614000	0.90321900	-0.00611500
C	-2.98641500	-0.10085800	-0.14518200
C	-2.59842400	-1.41739200	-0.15209800
H	-2.37682300	1.94323800	-0.00817400
H	-4.03750800	0.15237800	-0.25009100
H	-3.33586600	-2.20614400	-0.26167300
N	0.24369600	1.55367800	0.37848300
N	1.54725200	1.27802100	-0.07960100
N	1.01403500	-1.01181700	0.21663700
N	3.18028700	-0.35036100	-0.25260300
H	3.81357300	0.33538400	-0.63934200
O	1.44928700	-2.22957600	0.19476200
H	3.29700300	-1.32685200	-0.49116600
O	-0.14939700	2.80856500	-0.15897500
H	0.16830300	3.42501500	0.52725500

4e

B3LYP/6-31G* -640.2553899

C	-1.90985900	-0.00780900	-0.03490100
C	0.37373500	-0.73453400	0.05619800
C	0.74661900	0.62698600	0.08311100
H	1.01049300	-2.76724700	-0.04510700
C	1.34236100	-1.73635300	-0.02627900
C	2.09941000	0.97842900	0.00624600
C	3.05837500	-0.02748100	-0.08356900
C	2.68548800	-1.37842800	-0.09213000
H	2.37513900	2.02565700	0.01725400
H	4.10771000	0.24558200	-0.14559700
H	3.44457000	-2.15202400	-0.15609900
N	-0.27416500	1.54672500	0.28706700
N	-1.58034300	1.26064700	-0.00341400
N	-0.99473400	-1.04946700	0.09310200
N	-3.19473000	-0.40789500	-0.24610300

H	-3.91858100	0.24320900	0.01953000
O	-1.41734900	-2.27379700	0.11179500
H	-3.33569000	-1.39135200	-0.04080200
O	0.05046400	2.87391900	-0.06986700
H	-0.81753300	3.22027200	-0.35123200

MP2 (full) /6-31G* -638.3935646

C	1.89631800	0.04123400	-0.08145100
C	-0.38028900	-0.72387400	0.11039100
C	-0.74585700	0.59881700	0.14345200
H	-0.95268100	-2.74734000	-0.08714400
C	-1.29985200	-1.72024700	-0.06375300
C	-2.06723400	0.92671800	-0.00155000
C	-2.98415400	-0.06668700	-0.17298500
C	-2.61077400	-1.38801700	-0.19485300
H	-2.35663500	1.97039200	0.01605300
H	-4.03121700	0.19823900	-0.28882200
H	-3.35623300	-2.16534600	-0.32857100
N	0.25277600	1.53253500	0.44590000
N	1.54197200	1.26738900	-0.05576200
N	1.00013000	-1.01456200	0.22288800
N	3.12248700	-0.38477300	-0.45201600
H	3.87103800	0.29087400	-0.39127600
O	1.44116100	-2.22641500	0.30106700
H	3.31601900	-1.35245600	-0.21977100
O	-0.12714700	2.83227900	-0.03443400
H	0.72709000	3.14694000	-0.39611700

4f

B3LYP/6-31G* -640.2533814

C	1.71302400	-0.85743000	0.00000000
C	0.00000000	0.82449700	0.00000000
C	-0.95824300	-0.22190800	0.00000000
H	0.35611600	2.92167300	0.00000000
C	-0.41019900	2.15624500	0.00000000
C	-2.32872900	0.08573000	0.00000000
C	-2.71999800	1.42186800	0.00000000
C	-1.77207900	2.45367800	0.00000000
H	-3.05376300	-0.71863500	0.00000000
H	-3.77979200	1.65980100	0.00000000
H	-2.09540000	3.48997400	0.00000000
N	-0.45749000	-1.48942000	0.00000000
N	0.84544000	-1.85259300	0.00000000
N	1.36085900	0.48338100	0.00000000
N	3.04335800	-1.07972500	0.00000000
H	3.40977600	-2.01581200	0.00000000
O	2.29735500	1.38647700	0.00000000
H	3.62463900	-0.25181500	0.00000000
O	-1.34833800	-2.55777800	0.00000000

H	-0.74153900	-3.32235200	0.00000000
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TS2

B3LYP/6-31G* -640.2341324

C	-1.90144600	0.03105700	-0.09301000
C	0.31281200	-0.77754700	-0.00992700
C	0.71625800	0.56331800	-0.22127900
H	0.90140800	-2.82113700	0.29155000
C	1.25787100	-1.81020900	0.13736400
C	2.09702700	0.86444700	-0.25651300
C	3.01969800	-0.14731600	-0.10337200
C	2.59807900	-1.48674500	0.08832500
H	2.38114900	1.90295700	-0.37593500
H	4.08097600	0.08118300	-0.12450000
H	3.34177700	-2.26968200	0.20505100
N	-0.21241300	1.55110600	-0.43742700
N	-1.49308200	1.27470200	-0.35566000
N	-1.04602000	-1.04100500	0.04487200
N	-3.21585200	-0.25481000	0.03791000
H	-3.87688000	0.44554600	-0.26095000
O	-1.52518800	-2.22115900	0.22188800
H	-3.45676300	-1.23701200	0.00258600
O	0.26088300	2.98457200	0.75808500
H	-0.08745100	3.65884600	0.14502200

MP2 (full) /6-31G* -638.3335284

C	-1.88147800	0.01535100	-0.15793500
C	0.35437600	-0.72645700	-0.00973400
C	0.70237400	0.58818900	-0.27372200
H	0.98807300	-2.73413700	0.37483600
C	1.31504400	-1.72078400	0.17500600
C	2.06200500	0.91765300	-0.33666800
C	2.99580000	-0.03857100	-0.15638900
C	2.61698300	-1.36884700	0.09875600
H	2.31672100	1.95553500	-0.51803200
H	4.05032400	0.21397200	-0.20398100
H	3.38553000	-2.12271500	0.23958400
N	-0.23075100	1.56501500	-0.50045100
N	-1.52255700	1.23133100	-0.45120400
N	-0.98642000	-1.02050900	0.06354900
N	-3.16061800	-0.34226300	-0.08233600
H	-3.86779000	0.36493600	-0.21361900
O	-1.44071900	-2.21007300	0.31431100
H	-3.37784300	-1.30791300	0.12288100
O	0.08271900	2.72526900	0.99113100
H	-0.31920600	3.47454800	0.51201700

5

B3LYP/6-31G* -564.5235851

C	1.91580100	-0.56527100	-0.00622600
C	-0.31968600	-0.88158500	0.00279700
C	-0.51593500	0.52153100	-0.00414300
H	-1.33981000	-2.77377600	0.01262700
C	-1.47980300	-1.69787000	0.00744300
C	-1.79339700	1.10725600	-0.00784400
C	-2.89858500	0.28136600	-0.00540200
C	-2.73405000	-1.12472800	0.00280500
H	-1.87232900	2.18739100	-0.01234000
H	-3.89607800	0.70958600	-0.00939100
H	-3.61379800	-1.76263800	0.00494500
N	0.63966200	1.33328000	0.00169100
N	1.84638000	0.80259300	-0.00062500
N	0.91978100	-1.43684100	0.00620900
N	3.19355500	-1.03757700	-0.05689700
H	3.94025500	-0.39523600	0.16259000
H	3.32544100	-2.01543800	0.15429100
O	0.52682700	2.57196600	0.01225600

MP2 (full) /6-31G* -562.9154125

C	1.91375100	-0.56759700	-0.00347200
C	-0.32217700	-0.87523600	0.00649000
C	-0.51916100	0.51928900	-0.00778200
H	-1.32446700	-2.77209600	0.02091400
C	-1.47188200	-1.69586800	0.01158100
C	-1.79046900	1.10721900	-0.01275100
C	-2.89115900	0.27105200	-0.01057400
C	-2.73120300	-1.13026900	0.00365700
H	-1.87588100	2.18792800	-0.02127100
H	-3.88929100	0.70008600	-0.01696600
H	-3.60920100	-1.77109600	0.00597300
N	0.63424600	1.33324200	0.00352800
N	1.84684800	0.80196200	-0.00128400
N	0.92106400	-1.43843000	0.01202600
N	3.19872000	-1.03558600	-0.08207500
H	3.92090200	-0.39351800	0.21806700
H	3.31559500	-2.00226600	0.19338400
O	0.51624900	2.58138800	0.01895500

6

B3LYP/6-31G* -564.5027545

C	-1.87739100	-0.29611300	-0.01036600
C	0.34285000	0.45164500	-0.00130700
C	0.69620500	-0.92603500	0.00057000

H	1.00071700	2.49882700	-0.00173000
C	1.32308300	1.46491000	-0.00133500
C	2.07599800	-1.26636900	-0.00062500
C	3.02997400	-0.27687500	-0.00312300
C	2.64923800	1.09259200	-0.00309600
H	2.33215800	-2.32086600	0.00121100
H	4.08429500	-0.53678100	-0.00454300
H	3.41953900	1.85846800	-0.00490600
N	-0.23151000	-1.91945900	0.01261500
N	-1.49966100	-1.58845200	0.00720000
N	-1.00037700	0.75946200	-0.00000800
N	-3.18847600	0.03483700	-0.06489900
H	-3.85370100	-0.68689700	0.16816500
H	-3.39630600	1.00493100	0.13694900
O	-1.44828600	1.96438400	0.01702200

MP2 (full) /6-31G*

C	-1.88447600	-0.29924000	-0.00141600
C	0.35450200	0.44540400	0.00597500
C	0.69213800	-0.93024100	-0.00003600
H	1.00234100	2.49893900	0.00123700
C	1.32476000	1.46309200	0.00041400
C	2.06779000	-1.26919500	-0.00291700
C	3.02109300	-0.27525300	-0.00802600
C	2.65209800	1.09290700	-0.00462100
H	2.32663200	-2.32416300	-0.00430700
H	4.07466600	-0.54208200	-0.01208800
H	3.42377100	1.85807100	-0.00926700
N	-0.22688000	-1.93788600	0.01620800
N	-1.51220500	-1.57755100	0.01347100
N	-0.99541000	0.76942000	0.00136600
N	-3.20053200	0.05787300	-0.09892700
H	-3.84450700	-0.66649600	0.19486300
H	-3.39391200	0.99897800	0.22900600
O	-1.42640500	1.95361500	0.01743600