

Supporting Information:

Rational Design of Photo-cleavable Alkoxyamines for Polymerization and Synthesis

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Supplementary Information

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Supplementary Figures

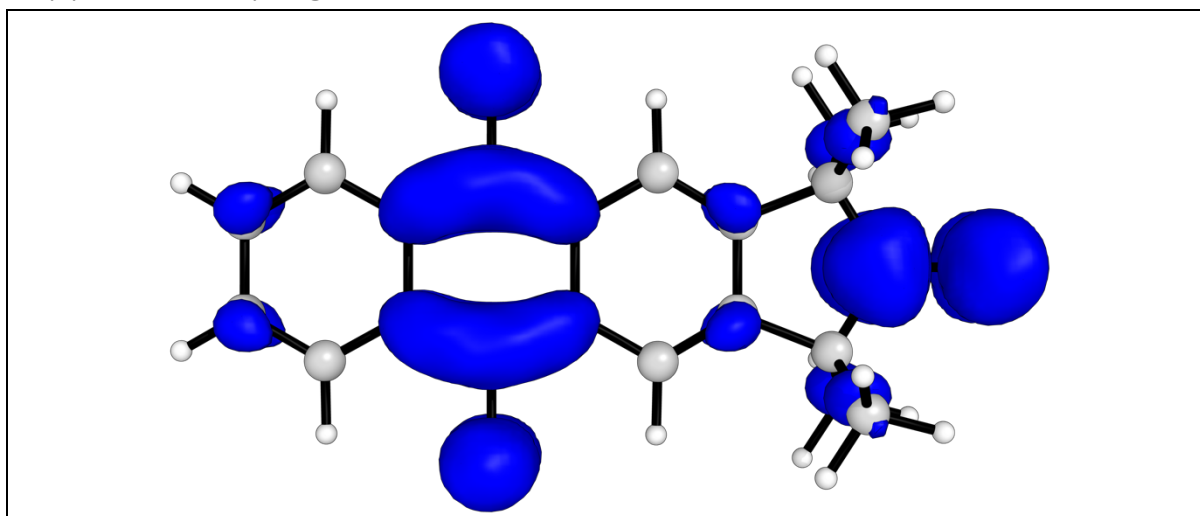


Figure S1. Spin density of anthraquinone-alkoxyamine triplet anion

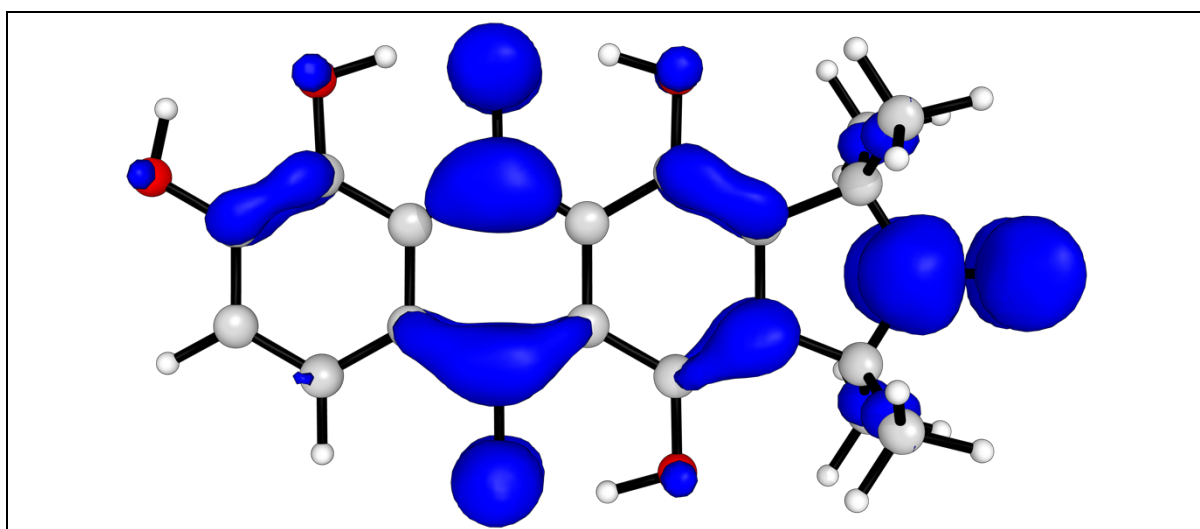


Figure S2. Spin density of 1,2,5,8-THAQ triplet anion

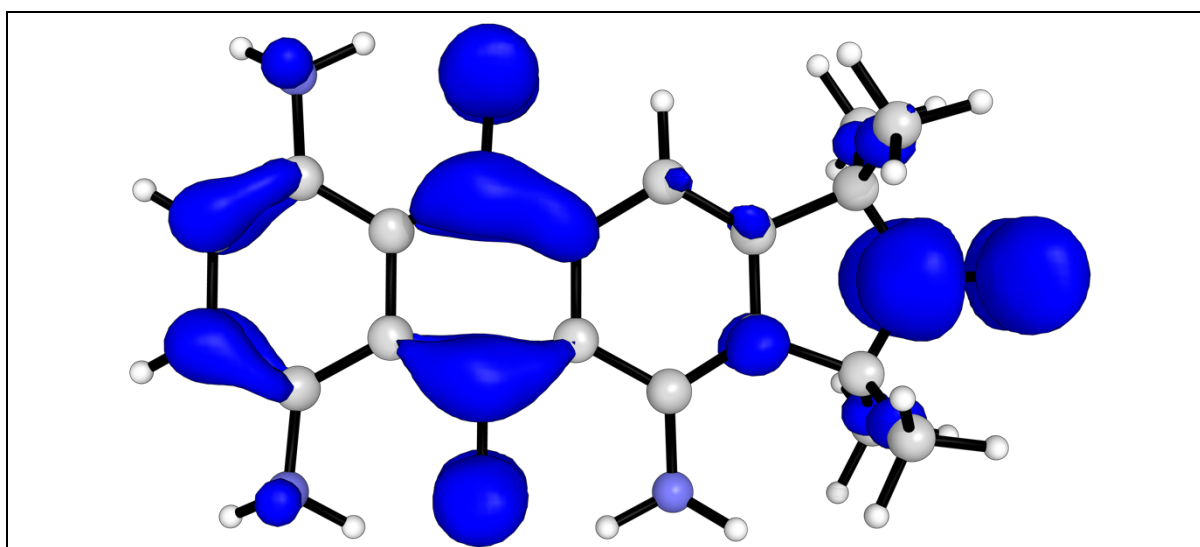


Figure S3. Spin density of 1,4,5-TAAQ triplet anion

Raw Energies

Table S1. Free energy components of all reported species

Structure	Gas			Solvent Electronic Energy (H)
	Zero-point Vibrational Energy (kJ mol ⁻¹)	Gibbs Free Energy (H)	Electronic Energy (H)	
Aq-STY	1284.7707	-1362.714547	-1363.147108	-1363.176845
Aq-STY radical cation	1283.1448	-1362.44675	-1362.877206	-1362.96369
Aq-EIB	1331.5978	-1438.130226	-1438.576377	-1438.605936
Aq-EIB radical cation	1330.2664	-1437.858393	-1438.30392	-1438.389465
Aq-EP	1256.9638	-1398.861173	-1399.278837	-1399.308678
Aq-EP radical cation	1256.9586	-1398.585688	-1399.003086	-1399.09057
Aq-Me	993.2202	-1092.551213	-1092.879409	-1092.902015
Aq-Me radical cation	994.2860	-1092.278009	-1092.605827	-1092.6926
1,2-DHAQ Aq-STY	1308.7470	-1513.126329	-1513.565931	-1513.596034
1,2-DHAQ Aq-EIB	1355.2516	-1588.542485	-1588.995826	-1589.026144
1,2-DHAQ Aq-EP	1281.1956	-1549.271507	-1549.697381	-1549.728315
1,2-DHAQ Aq-Me	1017.2067	-1242.962938	-1243.298124	-1243.321234
1,2,4-THAQ Aq-STY	1321.0531	-1588.334607	-1588.778172	-1588.808301
1,2,4-THAQ Aq-EIB	1367.3783	-1663.7508	-1664.208035	-1664.238335
1,2,4-THAQ Aq-EP	1293.3047	-1624.479857	-1624.909579	-1624.940506
1,2,4-THAQ Aq-Me	1029.2861	-1318.171263	-1318.51032	-1318.533403
1,2,5-THAQ Aq-STY	1322.1555	-1588.335024	-1588.779229	-1588.807749
1,2,5-THAQ Aq-EIB	1367.3144	-1663.75249	-1664.2089	-1664.237625
1,2,5-THAQ Aq-EP	1294.4951	-1624.480247	-1624.910728	-1624.940242
1,2,5-THAQ Aq-Me	1030.5087	-1318.171696	-1318.511383	-1318.533137
1,2,5,8-THAQ Aq-STY	1334.7939	-1663.540073	-1663.988305	-1664.015939
1,2,5,8-THAQ Aq-EIB	1382.1761	-1738.955443	-1739.418822	-1739.446483
1,2,5,8-THAQ Aq-EP	1309.6530	-1699.679723	-1700.116553	-1700.144401
1,2,5,8-THAQ Aq-Me	1043.1987	-1393.3772	-1393.720968	-1393.741813
1,5-DAAQ Aq-STY	1373.3381	-1473.376057	-1473.839381	-1473.8713
1,5-DAAQ Aq-EIB	1420.0344	-1548.792278	-1549.269672	-1549.301551
1,5-DAAQ Aq-EP	1347.1325	-1509.516822	-1509.967483	-1509.999591
1,5-DAAQ Aq-Me	1081.3977	-1203.214213	-1203.572913	-1203.597966
1,4-DAAQ Aq-STY	1370.1582	-1473.37495	-1473.838512	-1473.871804
1,4-DAAQ Aq-EIB	1418.1396	-1548.792402	-1549.268696	-1549.302015
1,4-DAAQ Aq-EP	1345.6826	-1509.516401	-1509.966516	-1510.000035
1,4-DAAQ Aq-Me	1078.2551	-1203.212036	-1203.570975	-1203.597153
1,4,5-TAAQ Aq-STY	1416.7762	-1528.70211	-1529.180522	-1529.214581
1,4,5-TAAQ Aq-EIB	1463.0219	-1604.117969	-1604.611276	-1604.64391
1,4,5-TAAQ Aq-EP	1390.9345	-1564.847844	-1565.314161	-1565.347666
1,4,5-TAAQ Aq-Me	1124.5789	-1258.54067	-1258.914224	-1258.941346
1,4,5,8-TAAQ Aq-STY	1462.0248	-1584.020974	-1584.51564	-1584.55009

1,4,5,8-TAAQ Aq-EIB	1510.4923	-1659.437017	-1659.947741	-1659.981403
1,4,5,8-TAAQ Aq-EP	1437.4259	-1620.161661	-1620.645389	-1620.67928
1,4,5,8-TAAQ Aq-Me	1170.3883	-1313.860758	-1314.250538	-1314.278712
AQ-NO radical	886.6340	-1052.69662	-1052.984009	-1053.00927
AQ-NO cation	889.4054	-1052.428996	-1052.719091	-1052.806342
AQ-NO anion	877.8209	-1052.723509	-1053.009311	-1053.087975
Pyridine	235.2370	-248.123997	-248.1861964	-248.1957941
Methyl-pyridine cation	332.9927	-287.746132	-287.8470342	-287.9292132
Methyl-pyridine cation	344.7885	-287.93308	-288.0288912	-288.039927
AQ-Me-Pyridine TS (ground state)	1225.5824	-1340.38196	-1340.789026	-1340.874367
AQ-Me-Pyridine TS (radical cation)	1230.2303	-1340.577063	-1340.982771	-1340.982784
AQ-BF ₃ -Me radical	1067.4275	-1455.652501	-1455.997519	-1456.020173
AQ-BF ₃ -Me-Pyridine TS (radical)	1309.5435	-1703.692401	-1704.123802	-1704.198845
AQ-BF ₃ -NO radical	964.8818	-1415.931595	-1416.242903	-1416.323595
AQ-BF ₃ -NO cation	968.6831	-1415.763854	-1416.07797	-1416.137472

Raw Vertical Excitation Energies and Oscillator Intensities

Table S2. Singlet vertical excitation energies and oscillator intensities for all reported functionalized species

Species		$n_N\pi^*$		$\pi\pi^*$	
		Energy (eV)	Oscillator Intensity	Energy (eV)	Oscillator Intensity
AQ-STY	14-DAAQ	4.1777	0.0042	2.6689	0.3589
	15-DAAQ	4.0611	0.0156	3.118	0.4818
	145-TAAQ	4.6377	0.0196	2.6317	0.4618
	1458-TAAQ	4.2553	0.0133	2.4451	0.5935
	12-DHAQ	3.5078	0.1929	3.808	0.0683
	125-THAQ	3.6511	0.0613	3.3336	0.4020
	124-THAQ	3.7212	0.0231	3.1384	0.3050
	1258-THAQ	3.6288	0.0633	2.9949	0.5039
AQ-EIB	14-DAAQ	4.1907	0.0048	2.6585	0.3597
	15-DAAQ	4.0847	0.0137	3.1157	0.4825
	145-TAAQ	4.7111	0.0217	2.627	0.4593
	1458-TAAQ	4.2867	0.0097	2.4416	0.5992
	12-DHAQ	3.8223	0.0762	3.5042	0.1957
	125-THAQ	3.7318	0.0211	3.3321	0.4018
	124-THAQ	3.7369	0.0240	3.1354	0.3048
	1258-THAQ	3.6729	0.0628	3.003	0.5054
AQ-EP	14-DAAQ	4.1947	0.0049	2.6585	0.3574
	15-DAAQ	4.0899	0.0135	3.118	0.4757
	145-TAAQ	4.6461	0.0199	2.6256	0.4587
	1458-TAAQ	4.2911	0.0095	2.4442	0.5937
	12-DHAQ	3.8272	0.0749	3.4988	0.1950

	125-THAQ	3.6693	0.0616	3.3322	0.3980
	124-THAQ	3.7425	0.0230	3.1306	0.3021
	1258-THAQ	3.4881	0.0143	3.0031	0.5010
AQ-ME	14-DAAQ	4.189	0.0049	2.6502	0.3509
	15-DAAQ	4.0801	0.0145	3.1034	0.4725
	145-TAAQ	4.6082	0.0160	2.6183	0.4501
	1458-TAAQ	4.2798	0.0097	2.4549	0.5745
	12-DHAQ	3.8161	0.0719	3.5001	0.1904
	125-THAQ	3.7316	0.0217	3.3344	0.3880
	124-THAQ	3.7316	0.0223	3.1307	0.2956
	1258-THAQ	3.6389	0.0591	3.0008	0.4846

Table S3. Vertical excitation energies of unfunctionalized species

Species	$n_N\pi^*$	$\pi\pi^*$	$n_O\pi^*$
AQ	N/A	4.3443	3.226
AQ-STY	3.963	4.3512	3.2686
AQ-EIB	3.9837	4.3585	3.2678
AQ-EP	3.9923	4.3654	3.264
AQ-ME	3.978	4.3661	3.2622

Open shell singlet vs triplet Mulliken Charges and Spin Densities

Table S4. Mulliken charge and spin densities of unfunctionalized anthraquinone-alkoxyamine

Atom	Open shell singlet biradical		Triplet biradical	
	Charge	Spin density	Charge	Spin density
C	-0.10846	-0.031765	-0.108436	0.031738
C	-0.10846	-0.031765	-0.108436	0.031738
C	0.112076	-0.005695	0.112151	0.00574
C	0.120078	-0.039274	0.120094	0.039206
C	0.120078	-0.039274	0.120094	0.039206
C	0.112076	-0.005695	0.112151	0.00574
C	-0.19528	-0.109268	-0.195363	0.111049
C	0.128339	-0.041434	0.12829	0.042139
C	0.128337	-0.041434	0.128288	0.042139
C	-0.19528	-0.109268	-0.195363	0.111049
C	0.164102	-0.005781	0.164232	0.006026
C	-0.714141	-0.05293	-0.714051	0.009406
C	-0.71413	-0.05293	-0.714049	0.009406
C	0.164102	-0.005781	0.164232	0.006026
O	-0.640164	-0.224921	-0.640125	0.224845
O	-0.640165	-0.224921	-0.640125	0.224845
C	0.401988	-0.002567	0.40223	0.04158
N	-0.41681	0.500614	-0.417318	0.493929
C	0.401987	-0.002568	0.402229	0.04158
O	0.0613	0.47028	0.061469	0.47018
C	0.2046	0.014093	0.204442	0.003107
C	0.204618	0.014096	0.20446	0.003111
C	0.204599	0.014092	0.204442	0.003107
C	0.204619	0.014096	0.204461	0.00311

Table S5. Mulliken charge and spin densities of 1,2,5,8-THAQ

Atom	Open shell singlet biradical		Triplet biradical	
	Charge	Spin density	Charge	Spin density
C	-0.175843	-0.071941	-0.176068	0.021774
C	-0.312048	-0.122344	-0.311778	0.070176
C	-0.042553	-0.017077	-0.042552	0.025053
C	-0.225538	-0.003295	-0.225717	0.012635
C	-0.311924	0.050501	-0.311813	-0.043246
C	-0.141847	-0.059469	-0.14175	0.065041
C	0.598017	-0.203833	0.598045	0.205617
C	0.367266	0.035231	0.367386	-0.035187
C	-0.206979	-0.021696	-0.206978	0.021625
C	0.139214	-0.114884	0.139191	0.116965
C	-0.348862	-0.050467	-0.348857	0.050311
C	0.195531	-0.044854	0.195505	0.04481
C	0.208096	-0.017196	0.20814	0.017041
C	-0.089107	-0.02531	-0.089052	0.025315
O	-0.793857	-0.156254	-0.793845	0.156139
O	-0.653962	-0.158507	-0.653987	0.158495
C	0.249899	0.004971	0.250301	0.025933
C	0.312623	0.001919	0.312927	0.033723
O	-0.128055	-0.006786	-0.128036	0.007028
O	-0.094833	-0.011844	-0.094728	0.011974
O	-0.166806	-0.007497	-0.166785	0.00749
O	-0.157636	-0.006407	-0.157619	0.006405
N	-0.393451	0.499972	-0.394056	0.492257
O	0.084843	0.471493	0.084978	0.470661
C	0.273622	0.008378	0.273385	0.008222
C	0.273602	0.008376	0.273366	0.008216
C	0.270263	0.009407	0.270167	0.007766
C	0.270327	0.009416	0.270231	0.00776

Table S6. Mulliken charge and spin densities of 1,4,5-TAAQ

Atom	Open shell singlet biradical		Triplet biradical	
	Charge	Spin density	Charge	Spin density
C	-0.779981	-0.037047	-0.780185	-0.008391
C	-0.432664	-0.07917	-0.432413	0.025587
C	0.49416	0.005561	0.4942	-0.009174
C	-0.353045	-0.005702	-0.353309	0.002228
C	-0.120744	-0.069384	-0.120495	0.071977
C	0.10312	-0.032459	0.103398	0.035732
C	-0.150756	-0.124366	-0.150857	0.12737
C	0.278006	0.022269	0.278132	-0.022206
C	0.42895	0.020539	0.428892	-0.020804
C	0.08615	-0.132708	0.086109	0.133476
C	-0.376592	-0.025833	-0.376571	0.025706
C	-0.322193	-0.016399	-0.322274	0.01645
C	0.177023	-0.07443	0.177023	0.074515
C	-0.025163	-0.084493	-0.025073	0.084333
O	-0.659081	-0.19665	-0.658968	0.196494
O	-0.70716	-0.165554	-0.707232	0.165631
C	0.260135	-0.006685	0.260211	0.057495

C	0.35315	-0.005622	0.353579	0.02496
N	0.091742	-0.002654	0.091674	0.003953
N	-0.0164	-0.015079	-0.016351	0.01507
N	-0.001887	-0.014135	-0.001885	0.01414
N	-0.432343	0.502511	-0.432763	0.495317
O	0.065143	0.470673	0.065248	0.470552
C	0.211326	0.02057	0.211128	0.004463
C	0.231488	0.01706	0.231458	-0.003378
C	0.294439	0.011759	0.294226	0.009538
C	0.303178	0.017431	0.3031	0.008968

Gas Phase Structure Cartesian Coordinates

AQ

C -5.5542621361 2.8671730276 -0.0005707914
 C -5.5553928268 1.4702787275 -0.0003878167
 C -4.3520608958 0.7711036819 -0.0001580017
 C -3.1406451909 1.4648425269 -0.0001114188
 C -3.1395090298 2.8687008519 -0.000294055
 C -4.3498002778 3.5643996518 -0.0005235729
 C -1.8609362499 3.6386818962 -0.0002545815
 C -0.5836115571 2.8666324118 0.0001367729
 C -0.5847476451 1.4627739964 0.000319575
 C -1.8633203812 0.6927930205 0.0001231641
 C 0.6278041074 3.5603712248 0.0003156014
 C 0.6255435961 0.767075508 0.0006813128
 C 1.8311359877 2.8611963207 0.000674359
 C 1.830005553 1.464301978 0.00085741
 O -1.8599489237 4.8583305143 -0.0002826175
 O -1.8643074414 -0.526855549 0.0004335117
 H -6.4933700431 3.4114803037 -0.0007498234
 H -6.4953804575 0.9274922326 -0.0004249258
 H -4.3359622897 -0.3139435 -0.0000159935
 H -4.3319453568 4.6494193146 -0.0006642678
 H 0.611705495 4.6454184319 0.0001691855
 H 0.6076888647 -0.3179442134 0.0008177362
 H 2.7711236541 3.4039828062 0.0008120227
 H 2.7691134445 0.919994835 0.0011372148

Aq-STY

C 0.7608793167 -1.5780146054 -6.6399304016
 C -0.5510961627 -1.6401042634 -6.1622310263
 C -0.8966922406 -0.9900335953 -4.9824137902
 C 0.0693910445 -0.2737871363 -4.2736895683
 C 1.385531441 -0.2116376599 -4.752905148
 C 1.7271523349 -0.8658869411 -5.937718598
 C 2.4416240203 0.5468117488 -4.016475131
 C 2.0475904993 1.2345062594 -2.7523087163
 C 0.727935208 1.1728706136 -2.2715653202
 C -0.3266470179 0.4167630976 -3.008834384
 C 0.3794787565 1.8220142723 -1.0852696761
 C 1.3550303525 2.52802586 -0.3939307328
 C 2.6611405179 2.5886124748 -0.8707404348

C 3.0206047466 1.9461524997 -2.0476226643
O 3.5838034875 0.6004133952 -4.4358640953
O -1.4711401892 0.3627431548 -2.5962655553
H 1.0268463045 -2.0866117235 -7.561093867
H -1.3025245801 -2.1969060675 -6.7129591521
H -1.9078949303 -1.0223344781 -4.590150798
H 2.7525831483 -0.801940217 -6.2867898229
H -0.6484188717 1.7558826347 -0.7395650791
C 1.2046352261 3.3222861476 0.8806608435
C 3.5246639052 3.4363185825 0.0297992603
H 4.031347034 1.9764051439 -2.4452059437
N 2.6453860996 3.5890150493 1.2454095402
C 4.8187108439 2.7008834165 0.386920378
C 3.8561087184 4.7657581759 -0.6642458311
C 0.5143772413 2.4817630326 1.9587019448
C 0.391686799 4.5963933611 0.6122521941
O 2.7848363692 4.8988257183 1.7580314241
C 3.2347448992 4.9524497047 3.1231898367
C 4.6128993851 4.343655079 3.3110754477
C 2.1816963599 4.4357180598 4.0840178042
C 2.2887787472 3.2056360551 4.7337659107
H 3.1646277439 2.5836420807 4.5794606006
C 1.266222084 2.7529329941 5.5678292703
H 1.3595630873 1.7901868575 6.0607541045
C 0.1247662214 3.5274884021 5.7614373207
H -0.67220351 3.1726821041 6.4073812872
C 0.0140559435 4.7660743284 5.127440827
H -0.8679979596 5.3800935608 5.2807944222
C 1.0400756598 5.2148468666 4.3008822072
H 0.9560353136 6.1788906597 3.8037640054
H 4.5940731777 1.7904294864 0.949058379
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H 5.3571679467 2.4263553389 -0.5258696473
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H 4.4180337107 4.5552315747 -1.579574148
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H 1.1345798339 1.6206033499 2.2206580422
H -0.4496671605 2.1214544481 1.5842363443
H 0.3245588713 3.0685944384 2.8592640891
H 0.2834952645 5.1782952512 1.5297073819
H -0.603324469 4.3105150683 0.257029875
H 0.8631880058 5.2254176983 -0.1462867282
H 3.3086585004 6.0366720647 3.2701371382
H 5.3281504915 4.842040484 2.651533372
H 4.6072520277 3.2767179925 3.0788362974
H 4.9425585177 4.4781525883 4.3453284084

Aq-STY radical cation

C 0.569465629 -1.2147661101 -6.8928359072
C -0.5435859756 -1.6676441625 -6.180190352
C -0.74914475 -1.2571080433 -4.866813685
C 0.160468623 -0.3896758217 -4.2604197377
C 1.28027153 0.0659460084 -4.9773508979
C 1.4803829451 -0.349910985 -6.2943612984

C 2.2687636341 0.9905466608 -4.3605821582
C 2.028104185 1.422400698 -2.9423542011
C 0.9120018684 0.9679466259 -2.2279328126
C -0.0822616692 0.0335935082 -2.8555733594
C 0.6989621606 1.3727615694 -0.9091083328
C 1.6138187223 2.2366920979 -0.3268228154
C 2.7213072079 2.6907595047 -1.0392705212
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H -1.6065901835 -1.5963826565 -4.2950175006
H 2.3514065367 0.0139815659 -6.829325942
H -0.1784963379 0.9968579472 -0.3889576419
C 1.5533147768 2.7782822018 1.087565875
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C 3.5310859115 5.0670325834 -0.7648148405
C 1.5433394539 1.633370633 2.1020612259
C 0.3683367494 3.7331318794 1.2854292013
O 3.1969670868 4.5219143684 1.9051971727
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C 4.1829559055 3.1412386157 3.7021315904
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C 1.5441989268 3.6211271995 5.0231356433
H 2.0848562208 2.6997711118 5.2205917661
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H -0.0467542184 3.123001822 6.3818720069
C -0.3550505766 5.0465158568 5.4659334643
H -1.2903982207 5.2311857141 5.9836858224
C 0.1626156953 6.0081070883 4.5951030429
H -0.3656611446 6.9425327958 4.4383103978
C 1.365619677 5.7722487503 3.9404238525
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Aq-EIB

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C 1.3771291447 3.6073931741 0.9232024323
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C 1.6640078743 3.738236651 5.696447256
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H 5.5079711492 5.1408262069 2.5002458865
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H 5.0684981109 4.9627148274 4.2113598501

Aq-EIB radical cation

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C 0.1998574573 -0.5739460028 -3.8801026674
C 1.33431056 -0.2386424045 -4.639200932
C 1.5524684693 -0.8516078192 -5.8737281998
C 2.3198714722 0.7637566912 -4.1539621151
C 2.058675276 1.4103989273 -2.8237014092
C 0.9284442308 1.0764442659 -2.0672854964
C -0.0614346354 0.0598430465 -2.560447283
C 0.6946140008 1.6826306724 -0.8308116743
C 1.6066424561 2.6201971134 -0.3735990783
C 2.7325029719 2.9520424782 -1.1274667476
C 2.9733498474 2.3556908755 -2.3544439102
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C 4.44455688 6.1229460353 3.3615690778

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O 1.3682323187 5.7238821856 3.5406803142
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Aq-EP

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C 0.1699716801 -0.472137239 -4.1488866296
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C 2.4593184557 0.5810200056 -4.0280989425
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C 0.4004383181 1.7782973604 -1.0597802838
C 1.3274911646 2.6042420003 -0.4409330382
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O -1.3553263659 0.0836942181 -2.429557275
H 1.1659588013 -2.3248110739 -7.4023337864
H -1.1056997298 -2.6201757504 -6.4485718581
H -1.7364482215 -1.4187190766 -4.348388538
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C 1.1629047166 3.4109499124 0.8263602945
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Aq-EP radical cation

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C 1.2564405473 -0.1153786417 -4.7664983015
C 1.4374652696 -0.6446589605 -6.0449676755
C 2.1969362126 0.9312552085 -4.2855336191
C 1.9770579913 1.4853170676 -2.9065026485
C 0.9253948493 1.027796316 -2.1034981481
C -0.0198829528 -0.0320122697 -2.5934897816
C 0.7294235012 1.5479107463 -0.8218710058
C 1.600889514 2.5235529268 -0.3666975157
C 2.6490272553 2.9801606423 -1.1680880859
C 2.850641688 2.470434621 -2.4400144716
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O -0.9239609176 -0.4149235721 -1.8770936347
H 0.7107751092 -2.0363471213 -7.5110265526
H -1.1528284952 -2.8453887486 -6.0890069728
H -1.4742360437 -1.8973701406 -3.8011617834
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H -0.1025475591 1.1702314861 -0.233194819
C 1.5272580726 3.2499571204 0.9611638484
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C 0.3774767799 4.2761033761 0.9585327039

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Aq-Me

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C 1.4685219714 -0.4055924676 -4.4640206263
C 1.8219452281 -1.1452621002 -5.5938014811
C 2.4731544023 0.5250043549 -3.8664548589
C 2.0680914088 1.301204515 -2.6575229102
C 0.785184148 1.1625754513 -2.1018860112
C -0.2186118526 0.234168179 -2.7006623879
C 0.4236954407 1.8947685648 -0.9669919013
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H -1.0877828648 -2.8376790395 -6.0635761267
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H 2.8188942973 -1.0199033627 -6.0034463209
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H 4.0265237051 5.9898344111 -0.3364532759
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H 3.4053113289 6.0771333863 3.3974792295

Aq-Me radical cation

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C 1.412479165 -0.3518681655 -4.497123692
C 1.7097070923 -1.0719824947 -5.6548423286
C 2.4388519872 0.5725040012 -3.947342629
C 2.0923247257 1.3364744553 -2.7003398755
C 0.8467538785 1.179133652 -2.080378114
C -0.1865195459 0.2426771923 -2.6406447561
C 0.5344320383 1.8913541526 -0.9206276314
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C 2.724538405 2.915458369 -1.0222726323
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H -1.2096429516 -2.7805613173 -5.9912999032
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C -5.5097294924 0.0638110075 -1.3827304494
C -9.5788118358 1.9659114487 -0.8336727007
C -8.620906576 2.8103484324 1.3371121451
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H -4.9956717344 4.6163013748 -1.5940169402
H -6.6929346966 4.1013789592 -1.4639707812
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H -6.6121921702 4.6086095396 0.9950982842
H -4.9097702832 5.0678951275 0.9167299569
H -5.261876835 0.1395590781 2.0822833967
H -4.7132930426 -1.1508622414 0.9843704001
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C -8.7257724903 -1.9415929528 0.3574799242
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H -9.4989971068 2.9769149372 -1.2415624916
H -10.5732922389 1.8384776552 -0.3969194417
H -8.6066616076 3.8090575188 0.8932065149
H -7.8042458924 2.7100390797 2.0531820012
H -9.5646043953 2.6723854626 1.8685145474
H -9.7911323355 -2.0730957588 0.5716796538
H -8.1783602274 -2.0917992343 1.2926549381
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H -7.1710810129 -2.7227423824 -0.9147891878

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C -2.5703931742 0.5930978207 -0.0041024465
C -1.4097812205 1.3696559017 0.0224512086
C -1.4952783709 2.7724968442 -0.0175230318
C -2.7392117934 3.4058696462 -0.091048349
C -0.2685499326 3.6046062889 0.0181821405
C 1.0309661101 2.9227628823 0.0944772384
C 1.1144570014 1.4989773845 0.1325686782
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C 3.4550693411 3.0473995771 0.2005436896
C 3.5460170071 1.6759796672 0.2371392159
C 2.3768706232 0.8887543835 0.2035762564
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C -1.5975614208 2.7420536096 0.0215451974
C -2.8240261909 3.4135275877 0.0003202389
C -0.346942691 3.5370196454 0.0687396108
C 0.933759611 2.816483517 0.0938785392
C 0.9768081274 1.3906318507 0.0735405193
C -0.2511755727 0.6097512364 0.0273734261
C 2.1098414568 3.5471637433 0.1381134861
C 3.3618219416 2.8682212605 0.1634863552
C 3.4137597317 1.4944016082 0.1443731684
C 2.2218995938 0.7426372562 0.0991548353
O -0.3857291255 4.7722537784 0.085871035
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H -2.8270261636 4.4997063336 0.0198859194
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C 1.9248615157 1.665402736 -0.0299322272
C 4.3351186243 1.1487095611 -0.3479174959
C 5.4013820122 0.1040486171 -0.3915294679
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C 3.7022281266 -1.6974405926 0.0905778802
C 6.7174325674 0.4939165362 -0.6452523736
C 7.726824327 -0.4616335797 -0.6905183039
C 7.426838815 -1.8106712753 -0.4826723315
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O 4.5956333784 2.3240195264 -0.5287966757
O 3.4401556192 -2.8723501327 0.2718080531
C -0.6093138402 2.1253766119 0.3143336776
C -1.1490153356 -0.301667483 0.6883486643
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AQ-NO cation

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C 2.6390988245 -0.652017611 0.133670952
C 2.9395193231 0.6987535373 -0.0745614345
C 1.9337310555 1.6670712271 -0.0315894963
C 4.3488470672 1.1467926348 -0.3499495198
C 5.4067167525 0.1047701117 -0.3920219456
C 5.1047742977 -1.2528510672 -0.1827297621
C 3.715290662 -1.7020974514 0.0896438421
C 6.7223842537 0.4946019109 -0.6454134259
C7.731005479 -0.4630037874 -0.6900375727
C 7.4310786208 -1.8115096014 -0.4822449506
C 6.121381671 -2.2075898179 -0.2290034219
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H 5.8671324222 -3.2495704467 -0.0648481034
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H 2.20529077 2.7064642933 -0.198238666
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AQ-NO anion

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C 1.3244717412 -1.069123645 0.2886691238
C 2.6480750544 -0.6715067966 0.0582958363
C 2.9509531291 0.690388684 -0.1511656654
C 1.9288702606 1.6484770596 -0.1293220299

C 4.3420643892 1.1389412533 -0.3962760029
C 5.4193399455 0.0938506878 -0.4220671317
C 5.1189038892 -1.2570180465 -0.2142912271
C 3.7093911975 -1.7057805115 0.04123437
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C 7.7524934813 -0.4661423086 -0.6841352705
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C 6.1393806803 -2.2094034757 -0.2422456751
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H 1.1147068483 -2.1232695451 0.4476815441
H 2.1854773217 2.6915064543 -0.2928792943
H 6.9407796538 1.5400799737 -0.8141079049
H 8.7782861269 -0.1602588155 -0.8669889719

Me-Pyridine cation

C 6.7098238181 -0.4817046836 0.0784553169
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C 4.0336848064 -1.0867177338 -0.1022183506
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H 7.7444691532 -0.1680256352 0.1634572599
H 7.1011904152 -2.5413589018 -0.3031066723
H 4.6614962615 -3.1143186065 -0.4718819128
H 2.9705225974 -1.2848429077 -0.1659746872
H 3.7822102645 1.0337095713 0.294323719
C 6.2339967396 1.8665751236 0.5127580674
H 5.3637588329 2.5113027026 0.6138273667
H 6.8506619482 2.2071418077 -0.3193090508
H 6.8074368301 1.8730084441 1.4399702013

Me-Pyridine radical

C 6.7876051964 -0.6738679376 -0.0787672576
C 6.3042832512 -1.94803959 -0.152019179
C 4.9115683757 -2.206469831 -0.1345566813
C 4.0519715615 -1.0827105883 -0.064629642
C 4.5510234046 0.185438673 0.0080035265
N 5.9272521151 0.4176719627 0.0577692304
H 7.8447584788 -0.4373142192 -0.0878515814
H 7.0188711603 -2.7611672754 -0.2254274104
H 4.522192354 -3.2135033999 -0.1975676453
H 2.9741582543 -1.207242343 -0.0684806013
H 3.9258195112 1.0683707678 0.0642135361
C 6.431939507 1.7543057788 -0.1696985204
H 6.482626694 1.9953829613 -1.2409954287
H 7.4325134271 1.8436825845 0.2593309541
H 5.7801567089 2.4786524561 0.3240067003

Pyridine

C 6.6750398156 -0.4735834979 0.079142692
C 6.3237493266 -1.7976694055 -0.1809671347
C 4.9727070511 -2.1181849295 -0.2750436774
C 4.0353973606 -1.1034893983 -0.1053619085
C 4.4945480047 0.187858353 0.1511808604
N 5.787080458 0.5099120037 0.244111609
H 7.721333803 -0.1885511145 0.1589907815
H 7.0930109649 -2.5521517824 -0.3053571732
H 4.6569042693 -3.1372341515 -0.4763475008
H 2.9709231146 -1.3017461392 -0.1691755282
H 3.7895158315 1.0041400621 0.2888869795

AQ-Me-Pyridine Transition state (neutral)

C 0.3191256666 0.9835642651 0.4673311532
C 0.2844490868 -0.3029101618 1.0230901161
C 1.3798326794 -1.1467650727 0.9226388879
C 2.5261959981 -0.6961052841 0.2584081968
C 2.5609866447 0.594535304 -0.2990874248
C 1.4495006235 1.4383349153 -0.1940756126
C 3.7686592821 1.0921812918 -1.0148340705
C 4.9480598163 0.1764788208 -1.1115112032
C 4.9133708537 -1.1094582595 -0.5561692533
C 3.6957661514 -1.6123462608 0.1533531707
C 6.0968426393 0.6206441158 -1.7686285819
C 7.2046964366 -0.2138348749 -1.8699726962
C 7.1700724261 -1.4965972904 -1.3160724998
C 6.027648994 -1.9438107195 -0.661216622
O 3.8047875675 2.2056218183 -1.5093603508
O 3.6716531411 -2.7359055445 0.6252016059
C -0.9818889779 1.6984196868 0.7356276281
C -1.0421517572 -0.537794502 1.7018076644
H 8.0366687031 -2.1452929358 -1.3965063791
H 5.9740851083 -2.9346723458 -0.2220663786
N -1.8556654264 0.5512434137 1.0988247948
O -2.9569193237 0.9016053856 1.8409656559
C -4.5137189899 0.3891182843 0.5566742395

C -1.5648554569 2.3766971475 -0.5051578492
C -0.8298684105 2.7405874241 1.8562780599
C -0.9155451857 -0.4422242728 3.2314982556
C -1.6795865359 -1.8784908873 1.3335562773
H -4.811129645 -0.2517045299 1.3786293283
H -3.6068668253 0.1284604996 0.0117669742
H -4.7642973031 1.4396787333 0.6474176595
H -1.6381161075 1.6590854464 -1.3280283581
H -0.9540603772 3.2276249647 -0.8256116818
H -2.5679152947 2.7443741757 -0.261503542
H -0.291699866 2.3382416373 2.7165421949
H -1.8295156116 3.0368747985 2.1837907091
H -0.2812625348 3.6142286164 1.4888188186
H -0.3433464492 0.4350472237 3.5389848044
H -0.4139891429 -1.3321410315 3.6261360447
H -1.9209787818 -0.3618042198 3.65217759
H -1.7366181979 -1.9830512958 0.2457839853
H -2.6932292807 -1.9072204868 1.748740688
H -1.1143666955 -2.721724005 1.7450552213
C -6.9691986512 0.0593670039 -0.3506152914
C -7.9290264691 -0.3145519215 -1.2791607837
C -7.5086570834 -0.8459095133 -2.4976883717
C -6.1463958732 -0.9850525123 -2.7458544348
C -5.2453220461 -0.5877414005 -1.765843124
N -5.6644298978 -0.0809309999 -0.6046794435
H -7.2182936289 0.4804086828 0.6195443372
H -8.9802935538 -0.1902406836 -1.0479516551
H -8.2360456044 -1.1474980291 -3.2440173496
H -5.7790464943 -1.3934514093 -3.6798683807
H -4.1673026431 -0.6648307725 -1.8848998824
H 1.3798455951 -2.149194321 1.341992043
H 1.5032469717 2.4295963006 -0.6359217724
H 6.0969993222 1.620922598 -2.1893128829
H 8.0981514151 0.1323969897 -2.3799952281

AQ-Me-Pyridine Transition state (radical)

C 0.6165326073 1.2511737919 0.1986082118
C 0.32054352 -0.101740876 0.3749506237
C 1.3184989191 -1.0621197195 0.3242196287
C 2.6319337808 -0.6484994587 0.0924978789
C 2.9290915424 0.7089882865 -0.0879837886
C 1.9170665256 1.669892464 -0.0357047576
C 4.3362619109 1.1657768085 -0.3399311407
C 5.4021534037 0.1276807342 -0.3847393756
C 5.1032547755 -1.2331909144 -0.2037118771
C 3.7088472594 -1.6917081654 0.0404136404
C 6.7199058139 0.5269917511 -0.6118683217
C 7.7334552024 -0.4249745671 -0.657706284
C 7.4362147924 -1.7782531138 -0.4777477554
C 6.1246124535 -2.1830739785 -0.2514536607
O 4.5752606238 2.3469326576 -0.4986691058
O 3.4296323 -2.8650993159 0.1949441444
C -0.6128197585 2.115748662 0.3108973689

C -1.153682711 -0.3422750568 0.6202450884
H 8.2304043875 -2.5165661066 -0.5141722129
H 5.8708831846 -3.2283513328 -0.1089516546
N -1.6561975197 1.0607115131 0.4872713349
O -2.8272128981 1.450059385 0.8346669924
C -4.3194514119 0.5663656539 0.352681582
C -0.9230207862 2.9040386511 -0.9635903909
C -0.5866571562 3.0248383503 1.5435358079
C -1.4254743425 -0.8495513038 2.0406107115
C -1.7517905414 -1.2668198685 -0.4472503623
H -4.20169799 -0.2650793498 1.030170899
H -4.0205105627 0.4708841375 -0.6820818429
H -4.9086153776 1.4185786469 0.656954991
H -0.9441181078 2.2453710545 -1.8358327435
H -0.1457705128 3.656549757 -1.1189833491
H -1.8846782508 3.4143523837 -0.8646309179
H -0.3971705456 2.4476982829 2.4521210119
H -1.5348288824 3.5574319713 1.643340225
H 0.218063976 3.7546130447 1.4247058481
H -0.9798132904 -0.1845001161 2.7838327979
H -0.9790525947 -1.8412502282 2.1511192807
H -2.4974865979 -0.9321671907 2.2365185231
H -1.6675960432 -0.819394422 -1.4414839399
H -2.794688121 -1.5171905542 -0.2410415333
H -1.1852071666 -2.201643758 -0.4498504039
C -7.0506053232 -0.5454287925 0.7170395523
C -8.2762780607 -1.128602433 0.4178045723
C -8.5311579827 -1.5005782899 -0.9001630017
C -7.5554993101 -1.2767228454 -1.8682331909
C -6.3576942723 -0.6872766142 -1.4792304919
N -6.1154224392 -0.3325485858 -0.2141987179
H -6.8054474703 -0.2357510303 1.7305115023
H -9.0088411119 -1.2836585876 1.2013072883
H -9.4776916361 -1.9575479821 -1.1691141389
H -7.7139747677 -1.5496800713 -2.905032481
H -5.5682035394 -0.4906227937 -2.2009432537
H 1.1267378644 -2.1236139194 0.4594250836
H 2.1822265149 2.7142052496 -0.1785113103
H 6.9277967734 1.5830919874 -0.7488240566
H 8.7580199516 -0.1144098833 -0.8337335277

AQ-BF₃-Me (radical)

C -7.1352472878 0.7769159552 -0.5559329065
C -6.2921310143 1.6743407504 -1.2184319384
C -4.9168948927 1.4758213269 -1.2037940184
C -4.3844648055 0.3746706838 -0.5300440224
C -2.9155609081 0.165512538 -0.5146843407
C -2.3867703895 -1.059779755 0.1707620163
C -1.0054776312 -1.240902345 0.117998982
C -0.4455001732 -2.3549188518 0.7328718106
C -1.2297951134 -3.3015657187 1.3696445707
C -2.6566825204 -3.1866187771 1.3940430152
C -3.2249396024 -1.9896293144 0.8113749256
C -4.6869962048 -1.7087337401 0.8788645464

C -5.224165852 -0.5244245809 0.1329136333
C -6.6052712644 -0.3161026653 0.1206458037
C -0.3481399718 -4.4149739429 1.9199947903
N 0.9854095864 -3.742055886 1.8399649502
C 1.0133052942 -2.7350568593 0.7522156128
O -5.4658032699 -2.3931195522 1.5245392249
O -2.1584589301 0.953882865 -1.0517256034
O 2.0197709203 -4.6835186064 1.7046325057
C 2.9428174479 -4.5501173571 2.7750779611
H -8.2091424601 0.9340645608 -0.5682813695
H -6.7116316174 2.5266792163 -1.7431931831
H -4.2362620818 2.1564505212 -1.7045948142
H -0.4039428105 -0.49980078 -0.3991485377
C -3.4381166067 -4.2446896702 1.8961031326
H -7.2406922108 -1.0213946964 0.6451280671
C -0.4446082736 -5.6937565365 1.068691578
C -0.5642012161 -4.7495316603 3.4015518999
C 1.4458230607 -3.2759980812 -0.6202057553
C 1.9264996505 -1.5771440852 1.1588606312
H 3.4179247101 -3.5640414032 2.7676257071
H 3.695579438 -5.3247491049 2.613777401
H 2.4506734116 -4.7012010293 3.7408544629
B -3.3320643196 -4.6142463042 -1.1582027142
H -4.5142933739 -4.2029988484 1.9095345976
H -2.9548933372 -5.1357557447 2.266328873
H -0.3249306645 -5.4857575885 0.0041150931
H -1.4168893465 -6.1725834771 1.2078617757
H 0.3359888999 -6.3931618802 1.3752449775
H -0.5781029726 -3.8346304331 3.9985407082
H 0.2719655427 -5.3718976694 3.7350233368
H -1.4814678377 -5.3115553755 3.5852358042
H 0.7729526076 -4.0533532712 -0.985585916
H 2.4565070107 -3.6858775095 -0.5580977793
H 1.4396148138 -2.4571054614 -1.3461903762
H 1.6455449313 -1.2004960099 2.1452354914
H 1.8665255552 -0.7608862554 0.4320927159
H 2.9666654934 -1.9163526497 1.1902065479
F -2.2213322592 -4.027366345 -1.5586105847
F -4.4752902475 -3.9605453523 -1.1981507547
F -3.3079669071 -5.8814232426 -0.7938625353

AQ-BF₃-Me-Pyridine transition state (radical)

C -7.459087872 -0.1852848423 -0.8280663193
C -6.8567281627 0.6872993837 -1.7407715872
C -5.4758228362 0.8428969365 -1.7500470376
C -4.6940045186 0.1101160538 -0.8538678382
C -3.2143652052 0.2505145908 -0.8723536193
C -2.4152158224 -0.7533567321 -0.0952014288
C -1.0448422682 -0.7927714218 -0.3471654265
C -0.3060604276 -1.7805463114 0.2765523498
C -0.9022172293 -2.7324404429 1.1030864647
C -2.2846301752 -2.7328345035 1.3701414685
C -3.0214607775 -1.6710341416 0.779103201
C -4.4750319551 -1.4728488877 1.0867530599

C -5.2973167067 -0.7536210262 0.064181889
C -6.6845801292 -0.8939126548 0.083943639
C 0.1298968589 -3.7114861221 1.6513093646
N 1.3753952974 -3.126278646 1.054200892
C 1.1730789112 -2.0022057155 0.1075117499
O -4.9799596056 -1.7891959704 2.1453410214
O -2.66227156 1.1085154066 -1.5400470987
O 2.5293487905 -3.6887895149 1.0660837388
C 3.1977068235 -4.5436144145 2.5678731855
H -8.5375923707 -0.3088854989 -0.8307001178
H -7.4693547437 1.2424318109 -2.4441692
H -4.9819716558 1.5174376006 -2.4420041555
H -0.6101808244 -0.0684132451 -1.0293570394
C -2.9708771767 -3.8732733749 2.0208899227
H -7.1275556685 -1.5679012343 0.8094779609
C -0.0156478649 -5.1441069312 1.1231385991
C 0.2076395452 -3.631718391 3.187261573
C 1.5397471269 -2.4549732482 -1.3100742298
C 2.0271817734 -0.8146298053 0.5552194811
H 2.9785717799 -3.6925956837 3.1956449791
H 4.1433931768 -4.6043110558 2.0490567425
H 2.5007445413 -5.3629549886 2.4937428596
B -3.6571593429 -4.7947781678 0.800304459
H -3.7710143672 -3.5573792099 2.6858214503
H -2.2889276462 -4.5197984743 2.573760325
H -0.1518294082 -5.1413089431 0.0403993186
H -0.9040591478 -5.6142155214 1.5434393536
H 0.8663792114 -5.739992647 1.377950781
H 0.6504000749 -2.680198306 3.4979157725
H 0.7792291934 -4.4591314347 3.6172646015
H -0.8017856974 -3.6772127691 3.5968586617
H 0.9359082621 -3.3162619843 -1.6062704483
H 2.600265125 -2.7137791055 -1.3653065758
H 1.3340916996 -1.6363660859 -2.0044714091
H 1.7624022748 -0.5099787584 1.5714548463
H 1.8447516811 0.0300529394 -0.1140449565
H 3.0889267258 -1.0738597271 0.5127391154
F -2.6399816337 -5.1912758954 -0.1080458799
F -4.6057800371 -4.0143276403 0.1088298945
F -4.2503132926 -5.9286539408 1.3657550274
N 4.005779845 -5.4548282731 4.1588712398
C 5.1983905996 -5.0745884014 4.6242645466
H 5.7027138763 -4.2846980781 4.0728592786
C 5.7677423292 -5.653656196 5.752074928
H 6.7383932967 -5.3209713694 6.1008377304
C 5.0631794438 -6.6587288998 6.4110100019
H 5.4783398786 -7.1312837512 7.2950087487
C 3.8194742221 -7.0489819533 5.9218017237
H 3.2382469103 -7.8257602055 6.4046660499
C 3.3250699758 -6.416935974 4.7862549853
H 2.3590268788 -6.6841682046 4.3638373858

AQ-BF₃-NO radical anion

C -7.0479733083 0.4162185825 -1.0595347312

C -6.2231323601 1.3871272561 -1.6388365104
C -4.8571270376 1.3836288224 -1.3831278253
C -4.3117506757 0.396302826 -0.5587833664
C -2.84313737 0.3639084261 -0.3011507582
C -2.2849503874 -0.8691172054 0.3293526807
C -0.9009829853 -1.0269974103 0.2981992306
C -0.3707059652 -2.213796039 0.7744915895
C -1.1864349002 -3.2506192949 1.2360239857
C -2.5898358928 -3.1276073876 1.2782851996
C -3.1149620593 -1.8786516462 0.8568410185
C -4.5696755438 -1.5661025155 0.9887892973
C -5.1375437591 -0.5641414095 0.0281689737
C -6.5108060122 -0.5487742412 -0.2148435189
C -0.3427172652 -4.4421478816 1.6663091592
N 1.0262213676 -3.8953579403 1.450980796
C 1.0936137037 -2.5652313706 0.8219328809
O -5.2815673623 -2.0013532191 1.873112127
O -2.1263108405 1.2882882256 -0.6533477097
O 2.0700593312 -4.57793703 1.6738667834
H -8.1132455771 0.4167423125 -1.2708645224
H -6.6511301978 2.1420815734 -2.2916957614
H -4.1925022221 2.1264444892 -1.8128037328
H -0.2843677753 -0.2309421131 -0.1086312705
C -3.486965054 -4.2789161244 1.5607027613
H -7.1264756544 -1.3077378733 0.256459034
C -0.5024802707 -5.6854823569 0.7842275843
C -0.4631077735 -4.7871101581 3.1554137912
C 1.7187024609 -2.6837311435 -0.5725894222
C 1.9113397672 -1.6219582478 1.7073111665
B -4.1437506541 -4.8201609188 0.1281770689
H -4.3095768213 -4.0019667678 2.2181112335
H -2.9448927263 -5.1089275222 2.0139372015
H -0.4487095942 -5.4140918779 -0.2728201996
H -1.471308184 -6.16044801 0.9407448135
H 0.3036880962 -6.3845928522 1.027456313
H -0.3607814689 -3.8834691066 3.7639181373
H 0.3394722963 -5.4832455609 3.4165160206
H -1.4259935977 -5.2502510586 3.3751335351
H 1.1215869363 -3.3483703616 -1.2024611707
H 2.731068145 -3.0884017513 -0.4827058799
H 1.763690505 -1.6988156711 -1.0475892405
H 1.4515039436 -1.5339527442 2.6955446381
H 1.9593773575 -0.6277662805 1.2525839285
H 2.925389902 -2.0164658705 1.8193728352
F -3.1133565818 -5.2493385647 -0.7428029902
F -4.8569294162 -3.7669491053 -0.5029785752
F -5.0140965179 -5.8935858814 0.3919734009

AQ-BF₃-NO neutral

C -7.0705673232 0.5130600985 -0.9988480409
C -6.2345797553 1.4803781838 -1.5663507403
C -4.8652378677 1.4423879108 -1.3333448248
C -4.3293801465 0.4231635053 -0.5425749676
C -2.8659897578 0.3635499719 -0.3072656482

C -2.3151972817 -0.8819912468 0.3288490402
 C -0.9289184313 -1.0326876551 0.2952193146
 C -0.407151634 -2.2140496435 0.7833736867
 C -1.2228599008 -3.2396121732 1.2625334261
 C -2.6241479806 -3.1285420591 1.295888892
 C -3.1479474793 -1.8815833009 0.8534245132
 C -4.6166211037 -1.5848675854 0.9479757441
 C -5.1662783785 -0.5388833708 0.0313732821
 C -6.542180454 -0.4869643583 -0.1896226029
 C -0.4072866059 -4.4281752089 1.7342933839
 N 0.9920675521 -3.9038650775 1.4870593371
 C 1.0520831265 -2.5702279592 0.7922153569
 O -5.3387917071 -2.0986628668 1.7773212065
 O -2.1175844264 1.2570738315 -0.6627043226
 O 1.9646129004 -4.4940190045 1.8040953295
 H -8.1386634044 0.5438384799 -1.1893666158
 H -6.6564178012 2.2614501245 -2.1906905385
 H -4.1941759725 2.183642438 -1.7549078335
 H -0.3197759317 -0.2363333664 -0.1214733262
 C -3.4840184793 -4.3048846776 1.518647155
 H -7.1714392691 -1.2406396451 0.2716182245
 C -0.4918365348 -5.7225343679 0.9026392607
 C -0.4876661008 -4.6994932207 3.245125846
 C 1.6190786249 -2.8390526522 -0.6125030125
 C 1.9510155193 -1.64635493 1.6147242018
 B -3.8865531194 -4.8469108565 -0.0258729446
 H -4.407003343 -4.0726016161 2.0416273171
 H -2.9720064033 -5.1142301488 2.0407698176
 H -0.3978282146 -5.5133585472 -0.1640137433
 H -1.4825831106 -6.1551466215 1.0391421579
 H 0.2758948648 -6.4227399141 1.2434375136
 H -0.2895748049 -3.7881817123 3.8155132421
 H 0.2160561524 -5.4846594447 3.5313314705
 H -1.5028544356 -5.0268421152 3.470791975
 H 0.9802220061 -3.5300709726 -1.1672784521
 H 2.6396204271 -3.2258901033 -0.5501045391
 H 1.6263980074 -1.8838138487 -1.1425561022
 H 1.5608958964 -1.5212125084 2.6276783406
 H 1.9502473086 -0.6691375409 1.1267177848
 H 2.9749303248 -2.0256878793 1.6496123239
 F -2.6842598401 -5.0449236412 -0.7626288524
 F -4.64971643 -3.8534736837 -0.6626714932
 F -4.5795992816 -6.05000902 0.0781494566

Solvent Phase Structure Cartesian Coordinates and Free Energies

AQ-NO singlet anion

G = -1052.802338 H

C 0.6098448143 1.2475474061 0.1061418982
 C 0.3080444666 -0.1054217491 0.3152183202
 C 1.3104260152 -1.0646231621 0.2942455422
 C 2.6327687223 -0.6660034777 0.061817631
 C 2.9352071109 0.6919769928 -0.1521474694

C 1.9159048114 1.6521288862 -0.1302279888
C 4.3324687475 1.1370772493 -0.4036595073
C 5.4059201764 0.0964093998 -0.425008071
C 5.1051978599 -1.2560839403 -0.2077403454
C 3.7009846695 -1.7015395649 0.048481034
C 6.7254048811 0.4853099949 -0.664111993
C 7.7397533991 -0.4670651645 -0.6863170547
C 7.4403472149 -1.8143357834 -0.468685625
C 6.1269325574 -2.2073793145 -0.2302070886
O 4.6048362979 2.3133844787 -0.5874221961
O 3.4494327535 -2.8811615746 0.2404278998
C -0.6455096581 2.0744526501 0.2219489213
C -1.1687783622 -0.2659323344 0.5752475286
H 8.2325901725 -2.5564281382 -0.4857720083
H 5.8767742593 -3.2494386602 -0.0595261973
N -1.6947249934 1.0279202763 0.0544973331
O -2.9220241864 1.3830789552 0.595341511
C -0.7948294995 3.0984280112 -0.9035704918
C -0.6918086494 2.8127934394 1.57260953
C -1.4385865578 -0.5086563204 2.0712853684
C -1.7977707746 -1.4051000991 -0.2286145728
H -0.7190098652 2.6078695458 -1.8790332638
H -0.0349101861 3.886108968 -0.8400153342
H -1.784039965 3.561556501 -0.8269361803
H -0.4030320941 2.1706077061 2.4083822034
H -1.7216609089 3.1439883942 1.7330719602
H -0.0178658333 3.6770050892 1.5606192769
H -0.9056463216 0.200012232 2.7097377661
H -1.1302849976 -1.5214645571 2.3551821071
H -2.5109924325 -0.3846007656 2.2435603546
H -1.5634772404 -1.2969997392 -1.292064392
H -2.8850036985 -1.3553919697 -0.107710591
H -1.4512522743 -2.3866784405 0.1156716833
H 1.0971839517 -2.1182819681 0.4535819511
H 2.1699909626 2.69521462 -0.2984478396
H 6.9401601785 1.5359720002 -0.8304473097
H 8.7647154764 -0.1616180729 -0.8726343006

AQ-NO triplet anion

G = -1052.839037 H

C -6.1107577405 1.9926353538 -0.0359244503
C -6.1057568344 0.5784904141 -0.014791921
C -4.9081604896 -0.1050430092 0.0114734982
C -3.6729639909 0.5840049515 0.0177936988
C -3.6779901832 2.0052992042 -0.0034469776
C -4.9180273593 2.6850994285 -0.0302218686
C -2.4401970145 2.780418654 0.0016129758
C -1.1950916845 2.0157003776 0.0297181383
C -1.1900576192 0.5921559677 0.0509929058
C -2.4297215708 -0.181845284 0.0458905536
C 0.0350601033 2.7154846406 0.0357660137
C 1.2208557798 2.01985638 0.0620106457
C 1.2258554682 0.6060493161 0.0831394071
C 0.0450108517 -0.0984194813 0.0778180206

O -2.4431886708 4.0374612019 -0.0171608547
O -2.4238218648 -1.4388779786 0.064641305
C 2.6240120341 2.5781572101 0.0723615089
N 3.41291867 1.3211274377 0.1014985918
C 2.6329233041 0.0582422318 0.1100226503
O 4.6809348438 1.32585482 0.1177924539
H -7.0543738764 2.5307165766 -0.0566115829
H -7.0455424144 0.0333724429 -0.019291727
H -4.8815513207 -1.19052959 0.0279958982
H -4.8990959935 3.7707559888 -0.0461467528
H 0.0060117768 3.8020608521 0.0191358017
H 0.0236479802 -1.1851855862 0.0936695817
C 2.9292832715 3.4033955071 1.3244096886
C 2.9628812008 3.3660584073 -1.1949751748
C 2.9438873166 -0.727031382 1.3861424128
C 2.9774920228 -0.7647649554 -1.1332363702
H 2.6924453914 2.8360276135 2.2293614672
H 2.3294836956 4.3185962922 1.3191943242
H 3.9888052878 3.6761528481 1.3416034785
H 2.7502773977 2.77189303 -2.0886819269
H 4.0225429827 3.6387808965 -1.1918572824
H 2.3633400251 4.2806438442 -1.2330465736
H 2.7029424575 -0.1345624296 2.2737585524
H 4.0053099226 -0.9916528145 1.4113734866
H 2.3505758401 -1.6461983716 1.4083399519
H 2.7607821398 -0.199094706 -2.0442789781
H 2.3844419226 -1.6842992859 -1.1438922263
H 4.0390569409 -1.0297670146 -1.1220823442

AQ-NO open-shell singlet anion

G = -1052.837980 H

C -6.1107577405 1.9926353538 -0.0359244503
C -6.1057568344 0.5784904141 -0.014791921
C -4.9081604896 -0.1050430092 0.0114734982
C -3.6729639909 0.5840049515 0.0177936988
C -3.6779901832 2.0052992042 -0.0034469776
C -4.9180273593 2.6850994285 -0.0302218686
C -2.4401970145 2.780418654 0.0016129758
C -1.1950916845 2.0157003776 0.0297181383
C -1.1900576192 0.5921559677 0.0509929058
C -2.4297215708 -0.181845284 0.0458905536
C 0.0350601033 2.7154846406 0.0357660137
C 1.2208557798 2.01985638 0.0620106457
C 1.2258554682 0.6060493161 0.0831394071
C 0.0450108517 -0.0984194813 0.0778180206
O -2.4431886708 4.0374612019 -0.0171608547
O -2.4238218648 -1.4388779786 0.064641305
C 2.6240120341 2.5781572101 0.0723615089
N 3.41291867 1.3211274377 0.1014985918
C 2.6329233041 0.0582422318 0.1100226503
O 4.6809348438 1.32585482 0.1177924539
H -7.0543738764 2.5307165766 -0.0566115829
H -7.0455424144 0.0333724429 -0.019291727
H -4.8815513207 -1.19052959 0.0279958982

H -4.8990959935 3.7707559888 -0.0461467528
H 0.0060117768 3.8020608521 0.0191358017
H 0.0236479802 -1.1851855862 0.0936695817
C 2.9292832715 3.4033955071 1.3244096886
C 2.9628812008 3.3660584073 -1.1949751748
C 2.9438873166 -0.727031382 1.3861424128
C 2.9774920228 -0.7647649554 -1.1332363702
H 2.6924453914 2.8360276135 2.2293614672
H 2.3294836956 4.3185962922 1.3191943242
H 3.9888052878 3.6761528481 1.3416034785
H 2.7502773977 2.77189303 -2.0886819269
H 4.0225429827 3.6387808965 -1.1918572824
H 2.3633400251 4.2806438442 -1.2330465736
H 2.7029424575 -0.1345624296 2.2737585524
H 4.0053099226 -0.9916528145 1.4113734866
H 2.3505758401 -1.6461983716 1.4083399519
H 2.7607821398 -0.199094706 -2.0442789781
H 2.3844419226 -1.6842992859 -1.1438922263
H 4.0390569409 -1.0297670146 -1.1220823442

AQ-NO radical

G = -1052.723378 H
C -6.130916885 1.9839633626 -0.036369304
C -6.1259767569 0.5870009713 -0.0154892281
C -4.919994146 -0.1066477876 0.0113391898
C -3.7117442562 0.5928713247 0.0174102303
C -3.7167066898 1.996150113 -0.0035650709
C -4.9298720535 2.6866142559 -0.0304112368
C -2.4418119856 2.7713602216 0.0023035891
C -1.1601682738 2.0069056981 0.0307863183
C -1.1551973462 0.6012246827 0.0517977045
C -2.4314006496 -0.1727828868 0.0463144632
C 0.0434211016 2.7166951351 0.0362246232
C 1.2381636852 2.0122709164 0.0625645724
C 1.2431092709 0.6137701921 0.0834683406
C 0.0533802727 -0.0995568756 0.078319484
O -2.4455919573 3.990945004 -0.0156212495
O -2.4265549503 -1.3923549971 0.0648345439
C 2.6367500354 2.5771038141 0.0726155875
N 3.425935413 1.3211859413 0.1022921931
C 2.6456534904 0.0593933792 0.1102501604
O 4.6922937087 1.3259114038 0.1188358893
H -7.0724538213 2.5236182971 -0.0572829029
H -7.0636720413 0.040317955 -0.020165272
H -4.8993502868 -1.1914600378 0.0278071696
H -4.9169011331 3.7715529077 -0.0463750204
H 0.0207436781 3.8027311904 0.01975258
H 0.0383844246 -1.185733245 0.0943165958
C 2.9306361587 3.4043735359 1.3255955907
C 2.9641668262 3.365827497 -1.196819365
C 2.9452489648 -0.7279564917 1.3873665881
C 2.9787751863 -0.7645853968 -1.1350773745
H 2.6945633169 2.8375065538 2.2308769129
H 2.3310246136 4.3194556141 1.3159022615

H 3.9893768116 3.6779094743 1.3430191766
H 2.7519348912 2.7715193544 -2.0903272615
H 4.0231212025 3.6390853367 -1.1944799991
H 2.3649202178 4.2805668342 -1.2309778689
H 2.7050808745 -0.1359663799 2.2753248398
H 4.0058948325 -0.9933591828 1.4128451702
H 2.3521215678 -1.6471347352 1.4050939114
H 2.7624473346 -0.1987629614 -2.0459276668
H 2.3860114799 -1.6841488316 -1.1418199473
H 4.0396338733 -1.0301611574 -1.1246789182

1,2,5,8-THAQ-NO singlet anion

G = -1353.6269 H

C -3.9193737818 2.7450037137 -0.0302420633
C -3.9051664937 1.3695737405 0.0126539548
C -2.6840687691 0.6516215042 0.0408281439
C -1.4776772014 1.3621857519 0.0041989739
C -1.4917668093 2.7951932771 -0.0371795815
C -2.7147472264 3.4859673485 -0.0437869709
C -0.2460548736 3.5371707889 -0.0623624403
C 1.0261351567 2.8022586899 -0.0655211825
C 1.0508719613 1.3895484178 -0.0285941886
C -0.2151784669 0.6265865597 0.0191320945
C 2.2333808313 3.5066079745 -0.1063031768
C 3.4574975196 2.8052785397 -0.1133654975
C 3.4676688633 1.4196569808 -0.0779223038
C 2.26363933 0.7134474691 -0.0346479818
O -0.2315952547 4.7953168953 -0.084161813
O -0.1891629097 -0.615426067 0.0697925644
C -5.3384540698 3.2586623462 0.0008708429
C -5.3131438539 0.8310382636 0.0834245694
O -2.7301262569 -0.6842154932 0.1076432429
O -2.7962988354 4.8225452863 -0.0546019874
O 2.3321656945 4.8481508398 -0.1413874225
O 4.615781856 3.4961875893 -0.1544736618
H 4.4215844227 0.9022373134 -0.0843647644
H 1.4129405084 5.2069084574 -0.1291187475
H 4.4181132336 4.4461476317 -0.1752712684
H 2.2637216066 -0.3704988156 -0.0058164776
H -1.7905876515 -0.9986296391 0.1119794455
H -1.8785912701 5.1759797433 -0.0659341801
N -6.0919920333 2.0232001486 -0.3601666615
O -7.4015226344 2.0265338619 0.0972687244
C -5.6442994467 4.316313287 -1.0637877618
C -5.6776538838 3.8306695478 1.3881870929
C -5.6338601582 0.3501127713 1.5100679146
C -5.601668492 -0.3047525739 -0.9020569957
H -5.2754210184 3.9926534072 -2.0426159925
H -5.2067117985 5.2880836128 -0.819613691
H -6.7333989642 4.4142101277 -1.1239967075
H -5.3940508184 3.151163632 2.195904111
H -6.7606297713 3.9734633679 1.4310255164
H -5.1650116101 4.7859186421 1.5426414797
H -5.3400328374 1.0797921493 2.2688624086

H -5.1173816876 -0.5924534057 1.7196663143
H -6.7162245659 0.208825705 1.5746891762
H -5.2472852323 -0.0422749899 -1.9041810954
H -6.6885436883 -0.4320961257 -0.9450060684
H -5.1386486191 -1.2462582731 -0.5948158867

1,2,5,8-THAQ-NO triplet anion

G = -1353.67933 H

C -3.9058481954 2.7635972747 0.0879188656
C -3.8950410671 1.3612764979 0.1325061313
C -2.7032690785 0.6499417208 0.1226091725
C -1.4771116861 1.3671710978 0.0660132708
C -1.4888218984 2.7980793045 0.0205480065
C -2.7299059877 3.4944222923 0.0323276068
C -0.2569396034 3.5317741949 -0.0367830765
C 0.9829272799 2.7979516063 -0.0473608115
C 1.0081473721 1.3767951906 -0.002572525
C -0.2337894816 0.6270164625 0.0555283545
C 2.2082508695 3.502466374 -0.1035707245
C 3.4158564395 2.8124211133 -0.1146716092
C 3.433110233 1.4116455789 -0.0703096912
C 2.2441025334 0.7051640735 -0.0150292594
O -0.2462231528 4.8307356055 -0.0786285456
O -0.2287189771 -0.6468154321 0.0961541776
C -5.3117743558 3.3111111428 0.1088241258
C -5.2901601953 0.7913078115 0.1889690706
O -2.7133181047 -0.6961207677 0.16600871
O -2.7783501644 4.8453643684 -0.009528036
O 2.2645319444 4.8528491821 -0.1483194561
O 4.5868562984 3.503018445 -0.1689493691
H 4.3922344307 0.9026907567 -0.080364422
H 1.3033287166 5.1513567407 -0.1314264854
H 4.3745272669 4.4490714802 -0.1934161429
H 2.2448430143 -0.3788502723 0.0196479706
H -1.7319147466 -0.9548016208 0.1473420385
H -1.8280395725 5.1465320393 -0.0453231673
N -6.0850644242 2.0449892345 0.1704833108
O -7.3523519574 2.035938924 0.2052334443
C -5.6792621383 4.0721573081 -1.1674564721
C -5.6105557017 4.1528724876 1.3518880144
C -5.5745098101 0.0241295811 1.4829006505
C -5.643473255 -0.0567776727 -1.0356094079
H -5.4718421282 3.4635014276 -2.0528450519
H -5.0936544106 4.9930731418 -1.2267825182
H -6.7440555875 4.3236370605 -1.1514281584
H -5.3539651955 3.6018739853 2.2618113611
H -6.6751353664 4.4044383714 1.3778807882
H -5.0244040965 5.0748060112 1.3200978891
H -5.3314926982 0.6368409346 2.3563180938
H -4.9684401502 -0.8850566534 1.5099775355
H -6.6335578619 -0.2481193478 1.5242235256
H -5.449436499 0.4981527226 -1.9585008423
H -6.7027700296 -0.3290326125 -1.0015303736
H -5.0383488209 -0.9669871653 -1.0372659686

1,2,5,8-THAQ-NO open-shell singlet anion

G = -1353.678270 H

C -3.9058481954 2.7635972747 0.0879188656
C -3.8950410671 1.3612764979 0.1325061313
C -2.7032690785 0.6499417208 0.1226091725
C -1.4771116861 1.3671710978 0.0660132708
C -1.4888218984 2.7980793045 0.0205480065
C -2.7299059877 3.4944222923 0.0323276068
C -0.2569396034 3.5317741949 -0.0367830765
C 0.9829272799 2.7979516063 -0.0473608115
C 1.0081473721 1.3767951906 -0.002572525
C -0.2337894816 0.6270164625 0.0555283545
C 2.2082508695 3.502466374 -0.1035707245
C 3.4158564395 2.8124211133 -0.1146716092
C 3.433110233 1.4116455789 -0.0703096912
C 2.2441025334 0.7051640735 -0.0150292594
O -0.2462231528 4.8307356055 -0.0786285456
O -0.2287189771 -0.6468154321 0.0961541776
C -5.3117743558 3.3111111428 0.1088241258
C -5.2901601953 0.7913078115 0.1889690706
O -2.7133181047 -0.6961207677 0.16600871
O -2.7783501644 4.8453643684 -0.009528036
O 2.2645319444 4.8528491821 -0.1483194561
O 4.5868562984 3.503018445 -0.1689493691
H 4.3922344307 0.9026907567 -0.080364422
H 1.3033287166 5.1513567407 -0.1314264854
H 4.3745272669 4.4490714802 -0.1934161429
H 2.2448430143 -0.3788502723 0.0196479706
H -1.7319147466 -0.9548016208 0.1473420385
H -1.8280395725 5.1465320393 -0.0453231673
N -6.0850644242 2.0449892345 0.1704833108
O -7.3523519574 2.035938924 0.2052334443
C -5.6792621383 4.0721573081 -1.1674564721
C -5.6105557017 4.1528724876 1.3518880144
C -5.5745098101 0.0241295811 1.4829006505
C -5.643473255 -0.0567776727 -1.0356094079
H -5.4718421282 3.4635014276 -2.0528450519
H -5.0936544106 4.9930731418 -1.2267825182
H -6.7440555875 4.3236370605 -1.1514281584
H -5.3539651955 3.6018739853 2.2618113611
H -6.6751353664 4.4044383714 1.3778807882
H -5.0244040965 5.0748060112 1.3200978891
H -5.3314926982 0.6368409346 2.3563180938
H -4.9684401502 -0.8850566534 1.5099775355
H -6.6335578619 -0.2481193478 1.5242235256
H -5.449436499 0.4981527226 -1.9585008423
H -6.7027700296 -0.3290326125 -1.0015303736
H -5.0383488209 -0.9669871653 -1.0372659686

1,2,5,8-THAQ-NO radical

G = -1353.547363 H

C -3.923652785 2.7499316139 0.0887912468
C -3.9091362856 1.3750207317 0.1324579249

C -2.6944890126 0.6539155381 0.1222445918
C -1.4935715665 1.3685374397 0.0663992618
C -1.5076039495 2.7962040785 0.0210196134
C -2.7243081167 3.4919640785 0.032110455
C -0.2530089066 3.5403115371 -0.0372722784
C 1.015248518 2.8046341483 -0.0485196033
C 1.038587369 1.3903624457 -0.0037900299
C -0.22416 0.6292199425 0.0552790629
C 2.2229972706 3.506381561 -0.1041986632
C 3.4473686931 2.8013972109 -0.1151784846
C 3.4545945797 1.4163797634 -0.0709291097
C 2.2495017346 0.7124101859 -0.0152748475
O -0.2502874571 4.793024336 -0.0774888818
O -0.2102632281 -0.6101227092 0.0946354956
C -5.3255361848 3.3078455406 0.1093436793
C -5.2978573405 0.7898967395 0.1892795956
O -2.7519345042 -0.6822721955 0.1666340798
O -2.8188252226 4.8273070071 -0.0080572294
O 2.3298718797 4.8452518283 -0.1501518445
O 4.6050767383 3.4872079452 -0.1689721345
H 4.4070873016 0.8966494523 -0.0803922508
H 1.4211419131 5.220866346 -0.137316354
H 4.4155296712 4.4388836303 -0.1942865089
H 2.2493874562 -0.3713941459 0.0195010458
H -1.8156301891 -1.0063751331 0.1513045866
H -1.9056289364 5.1905103487 -0.0447118828
N -6.095603908 2.0407422696 0.1711455927
O -7.3607536913 2.0280093533 0.2060339018
C -5.6884697355 4.0671969111 -1.1692199568
C -5.6192657612 4.1482014416 1.3545750059
C -5.571731584 0.0233885955 1.4857616272
C -5.6409716397 -0.0574270818 -1.0386061982
H -5.4677536028 3.464600278 -2.0552339837
H -5.1240073458 5.001041829 -1.2227528608
H -6.7575734907 4.2972361833 -1.155447495
H -5.3493393221 3.6031978353 2.2639564799
H -6.687921445 4.3787760383 1.3846390241
H -5.0543449935 5.0825534065 1.3172177051
H -5.3160563861 0.631675023 2.3584213163
H -4.9834492124 -0.8969257743 1.5071807151
H -6.6343852266 -0.2311806863 1.531177871
H -5.4344066883 0.4933067044 -1.9610690821
H -6.70409166 -0.3124266121 -1.009462152
H -5.0532037471 -0.9783049801 -1.0332380466

1,4,5-TAAQ-NO singlet anion

G = -1218.792343 H

C -5.3002078319 2.7445603644 -0.0399255825
C -5.2748728799 1.3612305393 -0.072359345
C -4.0479964504 0.6572036468 -0.0939385654
C -2.8369252373 1.4152924992 -0.0491137479
C -2.9080808394 2.8302937511 0.0026085515
C -4.1244018096 3.497533217 0.0030134327
C -1.6735076428 3.6617984847 0.055284845

C -0.366470323 2.9988393386 0.0597915719
C -0.2926074641 1.5638138213 -0.0080049254
C -1.5266338973 0.7544255725 -0.0768805208
C 0.8044393285 3.7754802578 0.1466794106
C 0.9593707623 0.9230544687 0.0110650219
C 2.0540580904 3.0950125469 0.1834434322
C 2.1247567216 1.7357310739 0.1177747667
O -1.7809282906 4.8937333881 0.1006712151
O -1.4462652665 -0.4880974063 -0.153583559
C -6.7225977506 3.242617915 -0.0914593724
C -6.6900074347 0.8187748793 -0.1352884497
N -4.0639346648 -0.7060445599 -0.1308215954
H -4.1380999449 4.581908154 0.0373113357
N 0.8286134165 5.1403754065 0.1671881637
H 2.964164594 3.6848296323 0.2580841869
H 3.0939673158 1.2434688031 0.139594698
H -0.04506112 5.63398199 0.2825675871
H 1.691295635 5.5965346208 0.4243216453
N 1.1588044265 -0.4286037431 -0.103255502
H -4.9300383297 -1.1704492521 -0.3523381469
H -3.1916814675 -1.190520233 -0.2831864372
H 0.3544560387 -1.0310896142 -0.0053145757
H 2.0621622995 -0.785784847 0.1722646764
N -7.470753122 2.0205719325 0.2946707052
O -8.7872357884 2.0087358911 -0.1437559906
C -7.0559355703 3.7824265668 -1.4940874139
C -7.0101563142 4.3373626719 0.9380559591
C -7.0211625742 -0.2798044026 0.8854269111
C -7.0446186402 0.318834024 -1.5486710463
H -6.7754803326 3.0799963914 -2.283001542
H -6.5291338681 4.7265650802 -1.6746220836
H -8.1356855199 3.944064857 -1.5502057764
H -6.7121654767 4.0070298395 1.9382713398
H -8.087165463 4.5361269625 0.9460084108
H -6.4847402429 5.2696429735 0.6995640867
H -6.5740932852 -0.0538767198 1.8585552589
H -6.7085905426 -1.2838030896 0.5765879012
H -8.1107672593 -0.2842362104 0.9966452023
H -6.6871349048 0.995487923 -2.3289690594
H -8.136028753 0.2678375919 -1.6086546673
H -6.6185523265 -0.6726869985 -1.7427824112

1,4,5-TAAQ-NO triplet anion

G = -1218.820115 H

C -5.285844656 2.7599451957 -0.1417364474
C -5.266219901 1.3560915972 -0.1702866884
C -4.0566752433 0.656732372 -0.1311304136
C -2.8242107245 1.4071438858 -0.0774372033
C -2.8883109654 2.8274009767 -0.0365843313
C -4.1287146665 3.4987959471 -0.0674568748
C -1.6861113519 3.6532207069 0.0457372442
C -0.3937070575 2.9904596952 0.031693722
C -0.3167505717 1.5512777076 -0.0404992914
C -1.528711052 0.7392158306 -0.0841013956

C 0.8059018421 3.7635490499 0.1188384674
C 0.9683229663 0.920529884 -0.0298630987
C 2.0304080337 3.1022346021 0.1713361875
C 2.1079830303 1.7138407675 0.0968615912
O -1.8154465436 4.9119864274 0.1349865872
O -1.4576775095 -0.5349775181 -0.1229923717
C -6.694284167 3.3000169997 -0.189412951
C -6.6706119428 0.7834595114 -0.2167480362
N -4.0505370842 -0.7203818083 -0.0940885237
H -4.1326660983 4.5829415928 -0.032572182
N 0.7993791046 5.156410302 0.0997411658
H 2.9415958398 3.6912752409 0.2483974781
H 3.0805428789 1.227077682 0.1161318065
H -0.1108043566 5.5600198131 0.3010770348
H 1.5907365984 5.5873430348 0.5590278998
N 1.146843815 -0.4525152176 -0.1930258943
H -4.8453208611 -1.2021023413 -0.4849721636
H -3.1314498839 -1.1323355169 -0.2366261055
H 0.307833491 -0.9963770806 -0.0240712005
H 1.9983058351 -0.8128773701 0.2172589906
N -7.466670513 2.0385463794 -0.1586128746
O -8.7337794462 2.0270096553 -0.2035718389
C -6.9931147172 4.0546153592 -1.4883490518
C -7.0539722901 4.1511478857 1.0288150055
C -7.0421200623 -0.0739774968 0.9981055588
C -7.0214019593 0.0625963478 -1.5256656936
H -6.7336255101 3.4448809378 -2.359060474
H -6.4067914449 4.9777180997 -1.5229545836
H -8.0565912298 4.3083900901 -1.5347707198
H -6.8471309937 3.606519147 1.954875641
H -8.1156578023 4.4143465815 0.99878581
H -6.4629385163 5.0718109295 1.0253265633
H -6.7980674539 0.4527707454 1.9254032899
H -6.5040447108 -1.0249055987 0.9890548426
H -8.1167400195 -0.2799832869 0.9794289727
H -6.7336991923 0.6690401361 -2.3893428525
H -8.1009736207 -0.1132421437 -1.5589363936
H -6.5201093161 -0.9065057378 -1.6007842036

1,4,5-THAQ-NO open-shell singlet anion

G = -1218.819063 H

C -5.285844656 2.7599451957 -0.1417364474
C -5.266219901 1.3560915972 -0.1702866884
C -4.0566752433 0.656732372 -0.1311304136
C -2.8242107245 1.4071438858 -0.0774372033
C -2.8883109654 2.8274009767 -0.0365843313
C -4.1287146665 3.4987959471 -0.0674568748
C -1.6861113519 3.6532207069 0.0457372442
C -0.3937070575 2.9904596952 0.031693722
C -0.3167505717 1.5512777076 -0.0404992914
C -1.528711052 0.7392158306 -0.0841013956
C 0.8059018421 3.7635490499 0.1188384674
C 0.9683229663 0.920529884 -0.0298630987
C 2.0304080337 3.1022346021 0.1713361875

C 2.1079830303 1.7138407675 0.0968615912
O -1.8154465436 4.9119864274 0.1349865872
O -1.4576775095 -0.5349775181 -0.1229923717
C -6.694284167 3.3000169997 -0.189412951
C -6.6706119428 0.7834595114 -0.2167480362
N -4.0505370842 -0.7203818083 -0.0940885237
H -4.1326660983 4.5829415928 -0.032572182
N 0.7993791046 5.156410302 0.0997411658
H 2.9415958398 3.6912752409 0.2483974781
H 3.0805428789 1.227077682 0.1161318065
H -0.1108043566 5.5600198131 0.3010770348
H 1.5907365984 5.5873430348 0.5590278998
N 1.146843815 -0.4525152176 -0.1930258943
H -4.8453208611 -1.2021023413 -0.4849721636
H -3.1314498839 -1.1323355169 -0.2366261055
H 0.307833491 -0.9963770806 -0.0240712005
H 1.9983058351 -0.8128773701 0.2172589906
N -7.466670513 2.0385463794 -0.1586128746
O -8.7337794462 2.0270096553 -0.2035718389
C -6.9931147172 4.0546153592 -1.4883490518
C -7.0539722901 4.1511478857 1.0288150055
C -7.0421200623 -0.0739774968 0.9981055588
C -7.0214019593 0.0625963478 -1.5256656936
H -6.7336255101 3.4448809378 -2.359060474
H -6.4067914449 4.9777180997 -1.5229545836
H -8.0565912298 4.3083900901 -1.5347707198
H -6.8471309937 3.606519147 1.954875641
H -8.1156578023 4.4143465815 0.99878581
H -6.4629385163 5.0718109295 1.0253265633
H -6.7980674539 0.4527707454 1.9254032899
H -6.5040447108 -1.0249055987 0.9890548426
H -8.1167400195 -0.2799832869 0.9794289727
H -6.7336991923 0.6690401361 -2.3893428525
H -8.1009736207 -0.1132421437 -1.5589363936
H -6.5201093161 -0.9065057378 -1.6007842036

1,4,5-TAAQ-NO radical

G = -1218.716835 H
C -5.2998378855 2.7404221131 -0.1575389447
C -5.2803581076 1.3556403032 -0.1949129183
C -4.0560269226 0.6459905774 -0.1563205025
C -2.8475308434 1.4083759005 -0.084590252
C -2.9177350649 2.8193881476 -0.0458676242
C -4.1306631951 3.4923479144 -0.0808922307
C -1.6826787169 3.6563000536 0.0380034918
C -0.3842506897 2.9966002226 0.0648415723
C -0.3071396967 1.5579907955 0.0029735767
C -1.5294492632 0.7466001076 -0.0673692706
C 0.7851920007 3.7763225018 0.1493151823
C 0.9474038372 0.9213644797 0.0216423206
C 2.0413902369 3.0975146912 0.1713291813
C 2.1152279529 1.7416254648 0.1084022787
O -1.804316857 4.887734757 0.0829071662
O -1.4520549203 -0.4980260017 -0.1145501184

C -6.7020152437 3.2922658711 -0.1977635857
C -6.6830996606 0.7783681279 -0.2578555388
N -4.0592982146 -0.7144474191 -0.1555086045
H -4.1453766627 4.5761249014 -0.0477183676
N 0.8023642339 5.1311349038 0.2161609368
H 2.949898308 3.6905146527 0.2380756285
H 3.0857839006 1.2520852558 0.1218001747
H -0.0663574579 5.6444875048 0.1863587304
H 1.6860908871 5.6155410929 0.2559454926
N 1.1488008948 -0.4231736749 -0.0630572804
H -4.9004145331 -1.2169570551 -0.3856519708
H -3.1704031271 -1.1883082247 -0.2383139305
H 0.3537911334 -1.0420890408 -0.0112058414
H 2.0760584733 -0.783251916 0.1060382699
N -7.474841553 2.0362124939 -0.2887377924
O -8.7409652437 2.0261534763 -0.3180449162
C -6.9652021041 4.1533499713 -1.4344963056
C -7.0751248052 4.0419923277 1.0833868807
C -7.0827957581 -0.0128920827 0.9933704918
C -6.9987692888 -0.0062389973 -1.5371303703
H -6.6937525381 3.6148376668 -2.3472607738
H -6.3765408393 5.0738731823 -1.3803331739
H -8.0259087244 4.4168353696 -1.4786034657
H -6.8852008513 3.4231505578 1.9652818415
H -8.1356748466 4.3080682288 1.0566750121
H -6.4838754514 4.9589706467 1.1633356672
H -6.8749253231 0.5670180952 1.897171416
H -6.5403720416 -0.9597761875 1.0561016031
H -8.154012196 -0.2298575303 0.9499492343
H -6.6391118122 0.5297214731 -2.4201295674
H -8.0837096454 -0.1244524309 -1.6120244481
H -6.555841774 -1.0052732688 -1.5279583548