

Theoretical Characterization of Sulfur-to-Selenium Substitution in an Emissive RNA Alphabet: Impact on H-bonding Potential and Photophysical Properties

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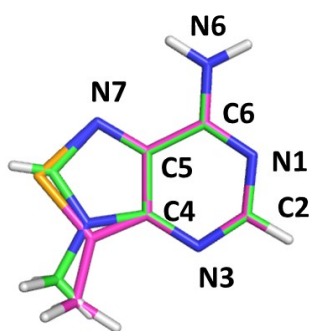


Figure S1: Superimposition of a modified ^{ts}A base (in magenta) and natural A base in cyan. Calculated RMSD between the heavy atoms is 0.19 Å. Identical heavy atoms skeleton for modified ^{ts}A and unmodified A base have also been marked.

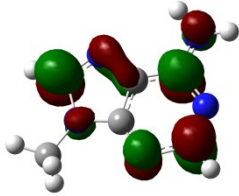
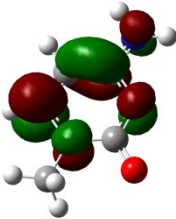
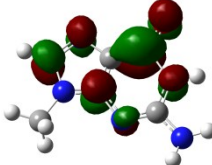
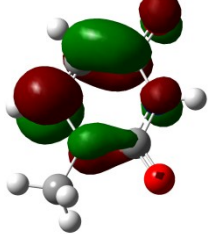
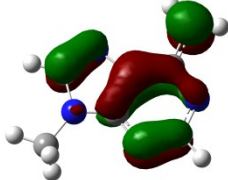
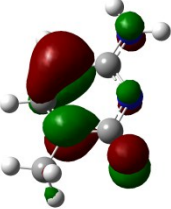
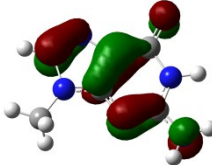
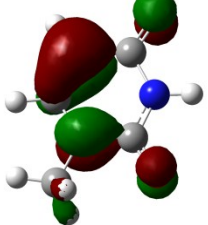
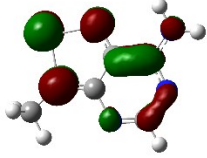
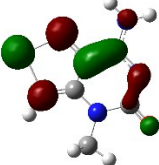
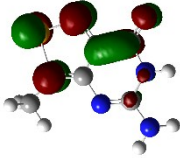
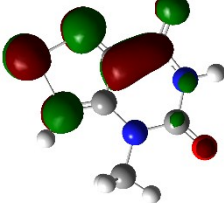
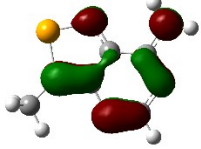
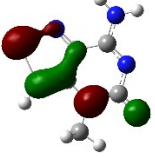
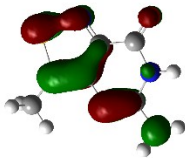
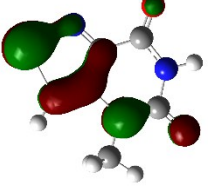
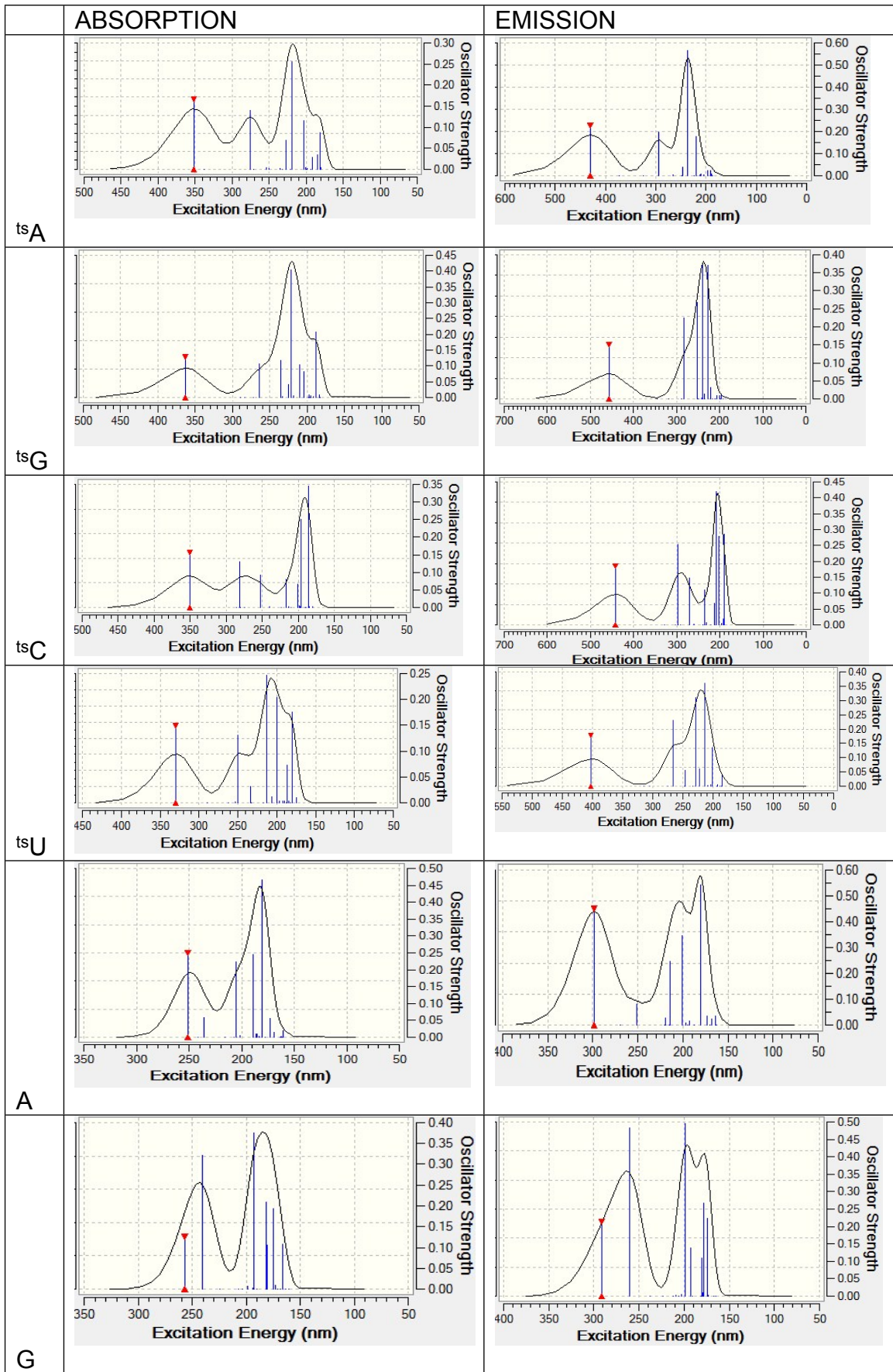
L				
H				
A	C	G	U	
L				
H				
tsA	tsC	tsG	tsU	

Figure S2. Shapes of Molecular orbitals representing HOMO (H) and LUMO (L) for the Natural and the non-natural ts-bases.



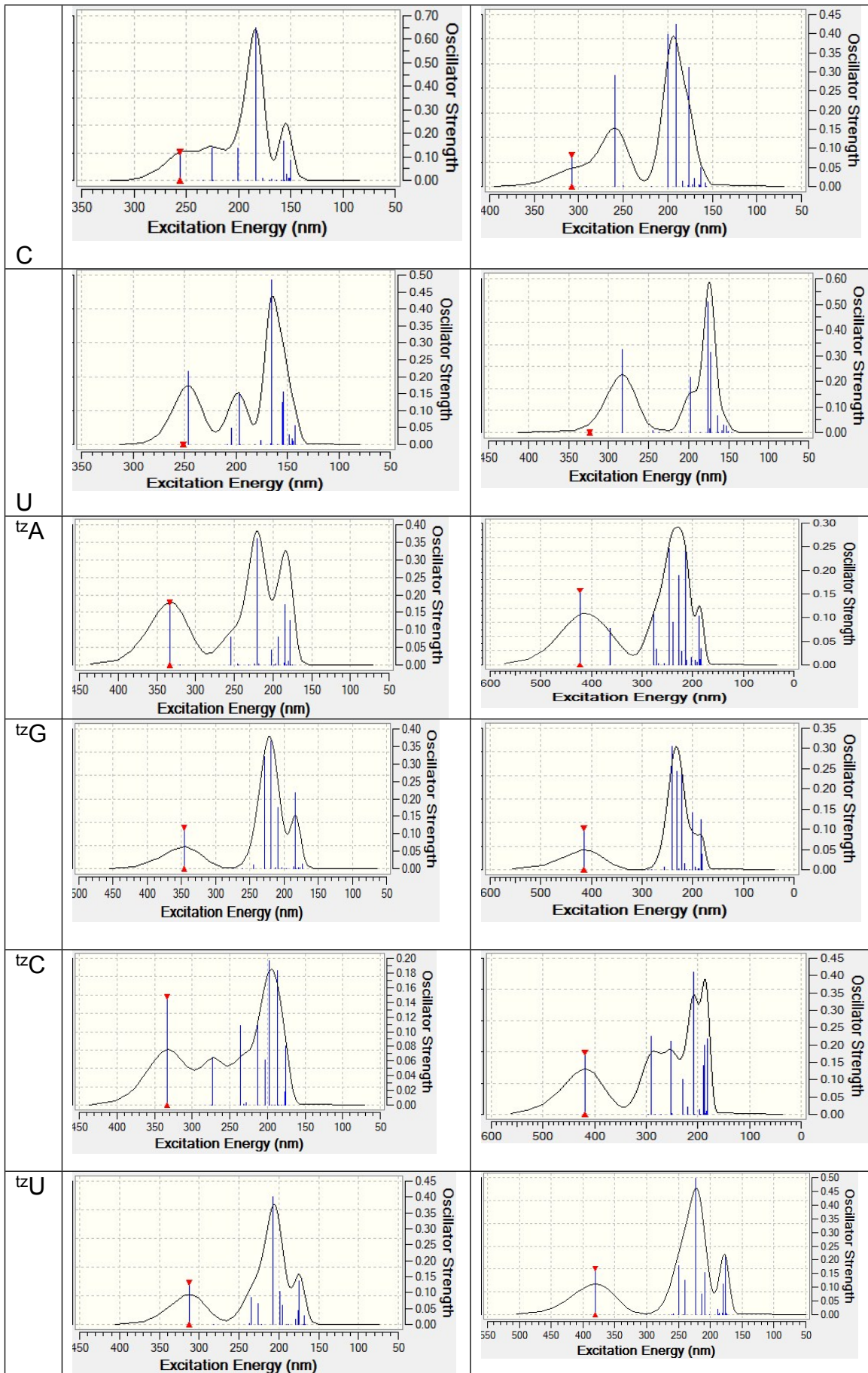


Figure S3. Calculated absorption and emission spectra (in nm).

Table S1. Predicted photophysical properties of ts-bases based on isoselenazolo[4,3-*d*]pyrimidine nucleobase analogues. os. str. represents the oscillator strength. The $\Delta\lambda_{\text{abs}}(\text{calc-exp})$, and $\Delta\lambda_{\text{em}}(\text{calc-exp})$ values correspond to the difference between the computed and experimental values for tz-bases. MUE is the mean unsigned error.

	λ_{abs}	os. str.	$\Delta\lambda_{\text{abs}}$ (calc-exp)	λ_{em}	os. str.	$\Delta\lambda_{\text{em}}$ (calc-exp)
B3LYP						
tsA	351.2	0.165		429.4	0.226	
tsG	362.5	0.127		455.9	0.151	
tsC	350.6	0.157		441.1	0.186	
tsU	329.6	0.149		402.5	0.179	
A	250.8	0.249		298.8	0.449	
G	248.4	0.127		291.6	0.213	
C	255.7	0.119		308.0	0.082	
U	246.4	0.215		282.9	0.325	
tzA	332.6	0.176	-5.4	422.8	0.158	12.8
tzG	346.2	0.117	13.2	429.6		-29.4
tzC	332.7	0.147	7.7	417.8	0.179	6.8
tzU	312.5	0.131	0.5	380.3	0.167	-11.7
MUE			6.7			15.2
CAM-B3LYP						
tsA	329.2	0.212		408.4	0.285	
tsG	329.1	0.179		411.9	0.216	
tsC	321.1	0.209		394.0	0.254	
tsU	302.8	0.204		362.5	0.242	
A	235.0	0.343		285.5	0.532	
G	244.3	0.158		276.7	0.249	
C	244.1	0.167		276.8	0.254	
U	236.7	0.269		274.2	0.377	
tzA	310.6	0.227	-27.4	384.6	0.302	-25.4
tzG	313.2	0.165	-19.8	388.8	0.214	-70.2
tzC	303.4	0.200	-21.7	373.9	0.246	-37.1
tzU	285.0	0.185	-27.1	342.9	0.232	-49.2
MUE			24.0			45.5
M06						
tsA	347.7	0.187		421.7	0.261	
tsG	354.9	0.152		435.1	0.188	
tsC	345.5	0.185		424.5	0.228	
tsU	325.7	0.178		386.3	0.222	
A	249.2	0.273		298.7	0.469	
G	254.0	0.136		285.6	0.220	
C	253.4	0.142		288.3	0.197	
U	244.6	0.238		280.5	0.345	
tzA	327.2	0.194	-10.8	385.3	0.188	-24.7
tzG	335.5	0.133	2.5	404.5	0.178	-54.5

tzC	323.2	0.162	-1.8	400.9	0.201	-10.1
tzU	303.4	0.145	-8.6	363.0	0.189	-29.0
MUE			5.9			29.6

M11

tsA	316.1	0.244		396.9	0.327	
tsG	311.5	0.215		391.9	0.260	
tsC	307.6	0.240		378.8	0.289	
tsU	289.9	0.236		348.1	0.278	
A	229.7	0.403		281.5	0.570	
G	239.6	0.174		273.3	0.275	
C	240.6	0.199		273.7	0.304	
U	235.2	0.291		274.4	0.396	
tzA	299.4	0.262	-38.6	375.0	0.348	-35.0
tzG	298.3	0.200	-34.8	372.5	0.260	-86.5
tzC	293.4	0.236	-31.6	362.8	0.290	-48.2
tzU	275.7	0.223	-36.3	332.8	0.275	-59.2
MUE			35.3			57.2

RI-CC2

tsA	317.4					
tsG	326.9					
tsC	341.3					
tsU	317.5					
tzA	300.1		-37.9			
tzG	308.3		-24.7			
tzC	320.9		-4.1			
tzU	297.5		-14.5			
MUE			20.3			

Table S2. XYZ coordinates of the ts-modified bases in cWW and tHW geometries in gas phase and in water.

Gas phase optimized geometries:

A:tsU cWW

35

A:tsU SCF Done: -3455.06557809 A.U.

C	-7.244017	1.085797	0.000825
N	-2.204416	0.173710	-0.000456
C	-2.897969	1.324107	-0.000058
N	-4.214912	1.479570	0.000253
C	-4.850373	0.302032	0.000137
C	-4.265545	-0.961997	-0.000260
C	-2.857823	-1.005234	-0.000580
N	-2.161010	-2.148510	-0.001019
N	-5.225750	-1.951736	-0.000255
C	3.018334	3.191237	0.000051
N	2.455157	1.849387	-0.000056
C	1.074936	1.694908	-0.000290
O	0.307591	2.638659	-0.000405
N	0.602799	0.391030	-0.000386
C	1.312956	-0.784623	-0.000262
O	0.765385	-1.873518	-0.000321
C	2.782609	-0.585115	-0.000016
C	3.307051	0.754999	0.000081
H	-6.759817	2.058847	0.001054
H	-2.288477	2.219912	0.000030
H	-2.659937	-3.019338	-0.001024
H	3.634160	3.340813	-0.888415
H	-1.145153	-2.137044	-0.001200
H	-0.443614	0.309218	-0.000556
H	3.633850	3.340801	0.888735
H	2.201006	3.902941	-0.000087
H	-7.867821	0.996761	0.889785
H	-7.868052	0.997299	-0.888027
N	3.607859	-1.598067	0.000125
C	4.673286	0.785816	0.000317
Se	5.301099	-0.969043	0.000419
H	5.317199	1.647833	0.000433
N	-6.204868	0.072903	0.000390
C	-6.357011	-1.295858	0.000125
H	-7.337140	-1.746140	0.000243

tsA:U cWW

32

tsA:U SCF Done: -3307.39680776 A.U.

C	-4.482390	2.410521	0.000163
N	0.234010	0.211587	-0.000312

C	-0.233793	1.495274	-0.000274
N	-1.469083	1.902552	-0.000143
C	-2.408903	0.899022	-0.000028
C	-2.052110	-0.491930	-0.000048
C	-0.628515	-0.791179	-0.000203
N	-0.209875	-2.055511	-0.000239
N	-2.979323	-1.424101	0.000068
C	6.060711	1.839530	0.000205
N	5.191100	0.666424	0.000027
C	3.812452	0.907577	-0.000265
O	3.365303	2.038290	-0.000385
N	3.027783	-0.219554	-0.000314
C	3.455266	-1.537762	-0.000049
O	2.645736	-2.463225	-0.000109
C	4.892896	-1.700967	0.000295
C	5.682967	-0.609302	0.000328
H	5.301113	-2.697306	0.000515
H	-3.738710	3.206324	0.000294
H	0.548855	2.246037	-0.000367
H	-0.898506	-2.787385	-0.000170
H	5.867855	2.449403	-0.880253
H	6.761054	-0.687365	0.000587
H	0.788351	-2.271909	-0.000383
H	1.996000	-0.048546	-0.000516
H	7.096020	1.509576	-0.000360
H	5.868598	2.448691	0.881333
H	-5.116933	2.526387	0.880707
H	-5.116744	2.526528	-0.880502
C	-3.775954	1.098805	0.000121
Se	-4.586568	-0.579655	0.000235

tsA:tsU cWW

34

tsA:tsU SCF Done: -5801.29967978 A.U.

C	-6.354562	1.937608	0.000619
N	-1.355581	0.487204	-0.000477
C	-2.014768	1.685277	-0.000279
N	-3.297662	1.897888	-0.000013
C	-4.073274	0.762654	0.000089
C	-3.507485	-0.556910	-0.000088
C	-2.055377	-0.634789	-0.000392
N	-1.451387	-1.822478	-0.000592
N	-4.280627	-1.620433	0.000036
C	4.088278	3.132168	0.000378
N	3.424555	1.836753	0.000095
C	2.036895	1.788256	-0.000085
O	1.341929	2.785807	-0.000036
N	1.467009	0.522775	-0.000381
C	2.085647	-0.702473	-0.000467
O	1.456843	-1.747675	-0.000703
C	3.565377	-0.615682	-0.000250
C	4.190474	0.680421	0.000024
H	-5.742570	2.838603	0.000591

H	-1.355283	2.545889	-0.000349
H	-2.021242	-2.650177	-0.000398
H	4.713390	3.234758	-0.888172
H	-0.434922	-1.886397	-0.000652
H	0.418938	0.521064	-0.000462
H	4.713165	3.234483	0.889118
H	3.327548	3.904111	0.000401
H	-6.999227	1.954180	0.881278
H	-6.999499	1.954317	-0.879838
C	-5.454736	0.750208	0.000383
Se	-5.997944	-1.033071	0.000432
N	4.310338	-1.689116	-0.000308
C	5.555128	0.605992	0.000196
Se	6.046151	-1.192090	0.000000
H	6.264398	1.415054	0.000410

G:tsC cWW

37

G:tsC SCF Done: -3510.46545942 A.U.

C	-3.226194	3.141896	-0.000469
N	-2.628259	1.815023	-0.000409
C	-1.233385	1.667606	-0.000628
O	-0.522442	2.670889	-0.000754
N	-0.684829	0.413117	-0.000485
C	-1.407602	-0.688537	-0.000234
N	-0.832049	-1.877616	-0.000177
C	-2.871446	-0.601111	-0.000015
C	-3.451504	0.708644	-0.000105
C	7.261515	0.635007	0.001851
N	2.239393	0.199116	-0.000208
C	3.016566	1.328310	0.000158
N	2.367185	2.507615	0.000425
N	4.335865	1.297318	0.000389
C	4.824938	0.043876	0.000108
C	4.134349	-1.168151	-0.000304
C	2.710689	-1.124162	-0.000491
O	1.908293	-2.063116	-0.000808
N	5.015454	-2.230911	-0.000576
H	-3.846078	3.276126	0.888109
H	-1.422432	-2.692167	0.000001
H	7.234809	1.260833	0.893367
H	1.352063	2.576753	-0.000160
H	2.929887	3.337263	0.000367
H	8.191381	0.071054	-0.013087
H	7.218842	1.281475	-0.874004
H	-3.846394	3.275901	-0.888860
H	-2.428294	3.874552	-0.000705
H	0.201752	-1.968213	-0.000422
H	1.215877	0.305363	-0.000312
N	-3.645329	-1.655702	0.000277
C	-4.819575	0.674924	0.000145
Se	-5.368548	-1.107057	0.000490
H	-5.505062	1.504248	0.000148

N	6.149987	-0.292685	-0.000128
C	6.193210	-1.676959	-0.000319
H	7.136187	-2.200408	-0.000545

tsG:C cWW

34

tsG:C SCF Done: -3362.79447540 A.U.

C	-6.101165	1.636741	0.002356
N	-5.218112	0.474466	0.001304
C	-3.824929	0.715994	0.001157
O	-3.441049	1.885401	0.001933
N	-2.990502	-0.348998	0.000252
C	-3.454490	-1.597498	-0.000623
N	-2.569033	-2.595442	-0.001488
C	-4.862904	-1.863590	-0.000640
C	-5.691888	-0.795397	0.000367
C	4.621044	2.245722	0.000399
N	-0.129308	0.230922	-0.001904
C	0.346125	1.537114	-0.002171
N	-0.609194	2.489310	-0.003961
N	1.606441	1.848690	-0.001342
C	2.500002	0.802659	-0.000500
C	2.102972	-0.585188	-0.000346
C	0.661589	-0.891990	-0.000985
O	0.175635	-2.019605	-0.000753
N	3.002220	-1.539044	0.000405
H	-5.911631	2.247168	0.882898
H	-2.884650	-3.547519	-0.001818
H	-5.251852	-2.869238	-0.001379
H	-6.767326	-0.903216	0.000469
H	3.907346	3.068726	-0.001736
H	-1.604835	2.279742	-0.001101
H	-0.296417	3.441925	-0.001711
H	5.257949	2.343614	0.882082
H	5.261356	2.341876	-0.878991
H	-7.134172	1.297800	0.002077
H	-5.911650	2.248714	-0.877111
H	-1.558752	-2.400673	-0.001295
H	-1.147593	0.064464	-0.001816
Se	4.633154	-0.748174	0.001220
C	3.868764	0.958575	0.000262

tsG:tsC cWW

36

tsG:tsC SCF Done: -5856.70144956 A.U.

C	-4.252804	3.048012	-0.014044
N	-3.554782	1.770425	-0.006334
C	-2.153387	1.731265	-0.000787
O	-1.520568	2.784255	-0.002923
N	-1.509002	0.520596	0.006916
C	-2.147120	-0.630699	0.008152

N	-1.484234	-1.775448	0.014252
C	-3.612406	-0.656367	0.002738
C	-4.291156	0.604429	-0.004554
C	6.471035	1.636222	-0.009969
N	1.424261	0.558693	0.014112
C	2.138996	1.751567	0.012439
N	1.379573	2.866563	0.021886
N	3.434786	1.818713	0.005525
C	4.114425	0.622230	0.001301
C	3.461206	-0.664891	0.003762
C	1.988700	-0.693463	0.010383
O	1.298772	-1.709578	0.012241
N	4.163155	-1.772112	-0.000367
H	-4.884660	3.137221	0.871610
H	-2.009645	-2.633185	0.014448
H	5.927326	2.580158	-0.005501
H	0.363586	2.844394	0.009211
H	1.863977	3.744273	0.007511
H	7.121733	1.608598	0.866576
H	7.111092	1.610945	-0.894412
H	-4.877343	3.130576	-0.905518
H	-3.513923	3.840128	-0.013964
H	-0.452872	-1.786052	0.015334
H	0.394425	0.590129	0.015796
Se	5.913755	-1.305593	-0.008788
C	5.487831	0.515587	-0.005606
N	-4.302278	-1.768002	0.004258
C	-5.652676	0.465192	-0.009163
Se	-6.062141	-1.353639	-0.003871
H	-6.400424	1.238788	-0.014891

G:C cWW

35

GC SCF Done: -1016.55829586 A.U.

C	5.177651	-1.873432	0.000712
N	4.371713	-0.656981	0.000438
C	2.965665	-0.805937	0.000287
O	2.506393	-1.949056	0.000416
N	2.203781	0.310283	0.000012
C	2.746963	1.527564	-0.000112
N	1.928341	2.578868	-0.000357
C	4.170882	1.699818	0.000019
C	4.927771	0.579863	0.000292
C	-5.526976	-1.474330	0.000295
N	-0.693541	-0.045948	-0.000384
C	-1.229588	-1.307045	-0.000395
N	-0.359383	-2.334261	-0.000693
N	-2.529326	-1.539642	-0.000228
C	-3.257801	-0.408538	-0.000095
C	-2.823065	0.916782	-0.000099
C	-1.418403	1.157382	-0.000265
O	-0.817845	2.236069	-0.000269
N	-3.898748	1.782324	0.000065
C	-4.942408	1.004532	0.000127

N	-4.623773	-0.343078	0.000027
H	4.949565	-2.471523	0.880694
H	2.307984	3.507491	-0.000441
H	4.625059	2.677794	-0.000086
H	6.008013	0.616662	0.000412
H	-5.364223	-2.091764	-0.882489
H	0.650942	-2.204368	-0.000297
H	-0.748229	-3.258277	-0.000271
H	-5.970916	1.329246	0.000225
H	-5.366663	-2.089645	0.885025
H	-6.551153	-1.108151	-0.001547
H	6.230425	-1.601643	0.000891
H	4.949911	-2.471700	-0.879241
H	0.901544	2.452719	-0.000383
H	0.331759	0.056148	-0.000419

A:U cWW

33

AU SCF Done: -961.162576415 A.U.

C	-5.441806	-1.750925	0.015013
N	-0.614210	-0.050609	0.008849
C	-1.115993	-1.295685	0.004777
N	-2.391722	-1.659470	0.000266
C	-3.204962	-0.596617	-0.002289
C	-2.828861	0.744427	0.000368
C	-1.445308	1.011014	0.005753
N	-0.936066	2.248503	0.008038
N	-3.934576	1.568753	-0.008914
C	-4.946731	0.741058	-0.016071
N	-4.578431	-0.585918	-0.016641
C	5.076560	-2.047008	-0.007724
N	4.289461	-0.817442	-0.003978
C	2.897402	-0.962143	0.000800
O	2.374221	-2.060475	0.001642
N	2.192366	0.215500	0.004316
C	2.709973	1.501931	0.003138
O	1.966713	2.480154	0.006065
C	4.156190	1.564718	-0.001786
C	4.868764	0.421433	-0.005088
H	4.632486	2.530416	-0.002823
H	-4.884050	-2.600607	-0.370470
H	-0.372463	-2.084297	0.005635
H	-1.566621	3.029325	0.002563
H	-5.986346	1.028399	-0.027185
H	4.846354	-2.643097	0.873297
H	5.949670	0.424305	-0.008863
H	0.071716	2.397066	0.008273
H	1.149717	0.115978	0.007407
H	6.132011	-1.788343	-0.011079
H	4.840408	-2.641586	-0.888201
H	-6.317315	-1.578885	-0.608292
H	-5.762164	-1.974554	1.033196

tsA:A tHW

35

tsA:A SCF Done: -3359.90297437 A.U.

C	-7.001224	0.366428	0.451292
N	-1.913474	0.955210	0.194858
C	-2.882405	1.757603	0.658585
N	-4.190160	1.535499	0.700392
C	-4.497262	0.334138	0.198648
C	-3.606070	-0.606166	-0.312735
C	-2.243221	-0.253471	-0.300540
N	-1.276643	-1.056044	-0.769180
N	-4.269986	-1.739951	-0.732215
C	-5.526818	-1.481722	-0.480486
N	-5.737241	-0.245134	0.087983
C	5.500869	-1.465904	0.302632
N	2.857722	2.966061	-0.365117
C	4.169318	2.619244	-0.293149
N	4.698055	1.440197	-0.111572
C	3.788335	0.420616	-0.002152
C	2.368612	0.635933	-0.078861
C	1.943832	2.019728	-0.251284
N	0.647005	2.337032	-0.300572
N	1.544375	-0.387804	0.007736
H	-6.837141	1.033568	1.293964
H	-2.545494	2.711240	1.049103
H	-1.527091	-1.977638	-1.079167
H	-6.351595	-2.148566	-0.676633
H	6.215466	-0.649402	0.208874
H	4.858495	3.450602	-0.395449
H	-0.119000	1.688264	-0.104726
H	-7.711761	-0.407354	0.734339
H	-7.409211	0.944980	-0.378122
H	5.651474	-1.951373	1.268667
H	5.709561	-2.204206	-0.473635
H	-0.303001	-0.816660	-0.598441
H	0.428353	3.313484	-0.404669
Se	2.546752	-1.889674	0.239806
C	4.125003	-0.908672	0.177432

tsA:U tHW

32

tsA:U SCF Done: -3307.39339409 A.U.

C	-5.176550	1.793865	-0.002064
N	-4.313389	0.615047	-0.001726
C	-2.941176	0.836974	-0.000036
O	-2.480083	1.971484	0.001217
N	-2.165052	-0.285381	0.000088
C	-2.594067	-1.615304	-0.000666
O	-1.783999	-2.526448	0.000142
C	-4.038216	-1.758836	-0.002349
C	-4.817308	-0.661856	-0.002780

C	4.346181	-1.903523	-0.004764
N	2.616792	3.000313	-0.000701
C	3.837392	2.402304	-0.003536
N	4.125783	1.130252	-0.004191
C	3.035218	0.299745	-0.001437
C	1.686635	0.791146	0.001848
C	1.538517	2.239517	0.001910
N	0.328098	2.810738	0.004764
N	0.683398	-0.064483	0.004477
H	-4.984733	2.400474	0.880803
H	-4.457584	-2.750738	-0.003110
H	-5.895909	-0.727708	-0.003918
H	5.206106	-1.235354	-0.007998
H	4.674228	3.092377	-0.005579
H	-0.547911	2.302774	0.004512
H	-1.142671	-0.128181	0.001470
H	4.400734	-2.547129	-0.884665
H	4.406244	-2.545685	0.875831
H	-4.980502	2.402893	-0.882307
H	-6.213088	1.468597	-0.004986
H	0.295730	3.815463	0.003534
C	3.101591	-1.083113	-0.001549
Se	1.369214	-1.752911	0.002621

tsA:C tHW

33

tsA:C SCF Done: -3287.50151377 A.U.

C	-6.091759	0.976802	0.000064
N	-4.915908	0.113865	0.000039
C	-3.643424	0.755096	0.000324
O	-3.602996	1.975565	0.000218
N	-2.543520	-0.044166	0.000086
C	-2.639608	-1.363048	-0.000236
N	-1.492139	-2.059762	-0.000436
C	-3.908077	-2.026476	-0.000384
C	-5.007778	-1.235255	-0.000274
C	5.233554	-0.659804	-0.000326
N	1.587854	3.048134	-0.000197
C	2.942683	3.017346	-0.000469
N	3.744489	1.986062	-0.000449
C	3.106063	0.773285	-0.000183
C	1.671722	0.646321	0.000070
C	0.922523	1.903819	0.000065
N	-0.405745	1.901738	0.000304
N	1.121994	-0.551084	0.000336
H	-6.082098	1.618087	0.879280
H	-1.498347	-3.061846	-0.000525
H	-3.994669	-3.101221	-0.000636
H	-6.007876	-1.646216	-0.000436
H	5.724131	0.312615	-0.000444
H	3.412956	3.995188	-0.000589
H	-0.986635	1.061942	0.000273
H	-0.609740	-1.548696	-0.000200

H	-6.987385	0.359943	0.000084
H	-6.082164	1.618113	-0.879138
H	5.560103	-1.215652	-0.881255
H	5.560373	-1.215586	0.880543
H	-0.891115	2.783712	0.000230
C	3.759631	-0.444287	-0.000112
Se	2.469237	-1.782094	0.000355

tsG:G tHW

37

tsG:G SCF Done: -3510.45495019 A.U.

C	4.221057	-2.799449	0.009896
N	3.654833	2.326725	0.044208
C	4.770412	1.498349	0.073840
N	5.980750	2.156410	0.044355
N	4.713444	0.214257	0.075129
C	3.453033	-0.353849	0.020979
C	2.247639	0.421528	0.002561
C	2.336822	1.886671	0.013650
O	1.412775	2.681751	-0.010314
N	1.085928	-0.182375	-0.033145
C	-6.655482	1.338536	0.106902
N	-1.718116	0.378069	-0.097410
C	-2.369633	1.576386	-0.111268
N	-1.597801	2.685156	-0.215721
N	-3.680626	1.688164	-0.054069
C	-4.297088	0.489530	0.007816
C	-3.739565	-0.788313	0.022770
C	-2.313925	-0.901606	-0.031030
O	-1.600997	-1.899476	-0.024287
N	-4.727853	-1.748360	0.092710
C	-5.840489	-1.071952	0.119522
N	-5.650378	0.297570	0.067168
H	5.217283	-2.363331	0.066019
H	6.047265	3.020883	0.558392
H	-0.694091	0.353915	-0.114441
H	-6.427471	2.097152	-0.639387
H	-2.061577	3.565954	-0.092197
H	-6.832746	-1.491413	0.171072
H	4.085481	-3.465094	0.864100
H	4.162637	-3.410821	-0.892506
H	-7.628431	0.902056	-0.108357
H	-6.686151	1.816512	1.086864
H	-0.593540	2.642809	-0.104085
H	6.761064	1.537231	0.198138
H	3.771615	3.327158	-0.026319
C	3.202539	-1.709385	-0.002145
Se	1.349154	-1.971153	-0.045707

A:A tHW

36

AA SCF Done: -1013.67143104 A.U.

C	6.538731	0.591820	-0.181004
N	1.414091	0.787674	-0.097214
C	2.341696	1.735539	-0.292982
N	3.663015	1.612674	-0.309062
C	4.035459	0.345159	-0.096201
C	3.194988	-0.743390	0.117142
C	1.808884	-0.485060	0.109704
N	0.894386	-1.441741	0.304471
N	3.921986	-1.902858	0.290152
C	5.166496	-1.515211	0.185226
N	5.309300	-0.166561	-0.053612
C	-5.368156	-2.361611	-0.279960
N	-3.536449	2.393754	0.191681
C	-4.781039	1.918320	0.117134
N	-5.183287	0.653386	-0.004017
C	-4.141456	-0.179048	-0.038901
C	-2.791122	0.158767	0.033931
C	-2.498038	1.536278	0.149259
N	-1.255197	2.028917	0.225490
N	-2.010010	-0.981727	-0.023736
C	-2.868048	-1.965119	-0.132493
N	-4.173660	-1.551014	-0.145450
H	6.354531	1.447489	-0.825985
H	1.953285	2.734142	-0.460102
H	1.216925	-2.385128	0.424277
H	6.028732	-2.158396	0.264609
H	-5.786824	-2.269525	-1.282034
H	-5.566645	2.664186	0.158386
H	-0.411823	1.462254	0.115468
H	-2.611756	-3.010310	-0.201424
H	7.310394	-0.035448	-0.622574
H	6.879324	0.953172	0.789941
H	-5.118117	-3.402347	-0.086902
H	-6.113688	-2.027113	0.438123
H	-0.105187	-1.247631	0.208152
H	-1.168760	3.028456	0.284006

A:C tHW

34

AC SCF Done: -941.269596200 A.U.

C	-5.537308	1.148522	0.003169
N	-4.427325	0.203279	0.001569
C	-3.111384	0.750960	0.002509
O	-2.986252	1.965825	0.004625
N	-2.069487	-0.122965	0.000984
C	-2.259397	-1.432965	-0.001762
N	-1.173991	-2.220469	-0.003658
C	-3.575351	-2.001923	-0.002752
C	-4.615972	-1.135980	-0.000996
C	5.138651	-1.802018	0.020620
N	2.387020	2.512568	-0.001494
C	3.700761	2.288570	-0.005099

N	4.350510	1.123562	-0.005138
C	3.493541	0.100697	-0.003116
C	2.102096	0.165833	0.000011
C	1.535427	1.465034	0.000231
N	0.223263	1.695243	0.002029
N	1.566007	-1.111747	-0.002312
C	2.606530	-1.907983	-0.005982
N	3.802333	-1.241619	-0.010616
H	-5.481612	1.786736	0.883011
H	-1.277819	-3.217556	-0.005387
H	-3.738695	-3.067849	-0.004803
H	-5.642893	-1.474737	-0.001577
H	5.787277	-1.208986	-0.619988
H	4.323089	3.176579	-0.007789
H	-0.478397	0.954783	0.002422
H	-0.234679	-1.806438	-0.003337
H	2.566856	-2.985680	-0.011082
H	-6.475337	0.598116	0.002819
H	-5.482301	1.789002	-0.875082
H	5.108430	-2.827605	-0.341010
H	5.543938	-1.786783	1.032708
H	-0.101704	2.646366	0.001525

A:U tHW

33

AU SCF Done: -961.162938000 A.U.

C	4.659603	-1.923645	-0.000153
N	3.929290	-0.659225	-0.000052
C	2.538570	-0.730042	0.000028
O	1.962626	-1.811876	-0.000022
N	1.889983	0.468590	0.000191
C	2.461005	1.742802	0.000103
O	1.756352	2.739304	0.000224
C	3.913008	1.729813	-0.000129
C	4.568763	0.554831	-0.000197
C	-3.770288	2.742963	-0.000185
N	-3.224274	-2.357009	-0.000031
C	-4.307601	-1.574178	-0.000145
N	-4.375621	-0.242721	-0.000156
C	-3.157299	0.301057	-0.000028
C	-1.942847	-0.379086	0.000104
C	-2.005636	-1.787216	0.000100
N	-0.916514	-2.571591	0.000286
N	-0.897422	0.520388	0.000163
C	-1.461025	1.703289	0.000083
N	-2.828760	1.640004	-0.000020
H	4.401270	-2.508094	0.880880
H	4.438248	2.670074	-0.000278
H	5.648253	0.503328	-0.000377
H	-4.404141	2.695235	-0.884286
H	-5.256995	-2.097171	-0.000261
H	0.027378	-2.202649	0.000107
H	0.846206	0.426217	0.000230

H	-0.913985	2.633239	0.000107
H	-3.217490	3.679086	0.000297
H	-4.404935	2.694767	0.883314
H	4.401864	-2.507674	-0.881644
H	5.725452	-1.712515	0.000271
H	-1.057248	-3.565870	-0.000134

G:G tHW

38

GG SCF Done: -1164.21872153 A.U.

C	3.654108	3.264478	0.006334
N	4.136071	-1.773337	-0.064017
C	5.105963	-0.803346	-0.110243
N	6.406655	-1.233703	-0.125721
N	4.848899	0.478144	-0.093419
C	3.527136	0.751938	-0.007069
C	2.471805	-0.147308	0.041987
C	2.733710	-1.546352	0.008799
O	1.960124	-2.491386	0.036196
N	1.279078	0.523720	0.114144
C	1.589960	1.791915	0.106176
N	2.952141	1.993863	0.033843
C	-6.311390	-1.466708	-0.159205
N	-1.501093	-0.022732	0.144768
C	-2.030089	-1.277890	0.141961
N	-1.158248	-2.311812	0.263146
N	-3.322747	-1.520060	0.057720
C	-4.052237	-0.386934	-0.014957
C	-3.624466	0.939785	-0.018702
C	-2.216443	1.195990	0.063518
O	-1.604105	2.256274	0.068890
N	-4.702281	1.796552	-0.109831
C	-5.741653	1.012975	-0.159453
N	-5.416952	-0.330520	-0.102843
H	4.252707	3.343841	-0.899533
H	6.613335	-2.117885	-0.559429
H	-0.479712	0.091021	0.180699
H	0.866271	2.591955	0.143265
H	-6.246616	-1.968054	-1.125702
H	-1.539904	-3.228879	0.121200
H	-6.769557	1.331608	-0.231535
H	2.921854	4.067089	0.026635
H	4.311180	3.352241	0.870110
H	-6.047971	-2.182473	0.617445
H	-7.331844	-1.123747	-0.002123
H	-0.160241	-2.196046	0.147604
H	7.073889	-0.504334	-0.316962
H	4.399361	-2.747498	-0.031765

XYZ coordinates of In-Water optimized geometries:

A:tsU cWW

35

A:tsU solv SCF Done: -3455.08621610 A.U.

C	7.264508	1.086445	0.001487
N	2.219346	0.174951	-0.002414
C	2.912778	1.322786	-0.002613
N	4.230566	1.481716	-0.001506
C	4.869230	0.302457	-0.000067
C	4.282329	-0.961790	0.000337
C	2.873999	-1.005865	-0.000898
N	2.169617	-2.143426	-0.000665
N	5.246233	-1.949557	0.001936
C	-3.039162	3.189842	0.001437
N	-2.464923	1.848975	0.000460
C	-1.095535	1.694456	-0.000515
O	-0.315133	2.634761	-0.000517
N	-0.617577	0.390017	-0.001444
C	-1.327635	-0.780721	-0.001626
O	-0.775374	-1.874126	-0.002567
C	-2.791312	-0.584405	-0.000606
C	-3.316356	0.750590	0.000446
H	7.180360	1.713063	-0.884934
H	2.304100	2.219945	-0.003736
H	2.649900	-3.028680	0.000645
H	-3.655131	3.330495	0.890183
H	1.154651	-2.117335	-0.001372
H	0.424500	0.310493	-0.001974
H	-3.656254	3.331302	-0.886402
H	-2.230619	3.910474	0.001253
H	8.232362	0.591763	0.002454
H	7.179175	1.714106	0.887060
N	-3.618125	-1.600354	-0.000605
C	-4.682928	0.780481	0.001358
Se	-5.310582	-0.968764	0.000839
H	-5.337651	1.637096	0.002241
N	6.221349	0.075409	0.001337
C	6.378368	-1.289369	0.002482
H	7.363322	-1.733361	0.003711

tsA:U cWW

32

tsA:U solv SCF Done: -3307.41261443 A.U.

C	-4.513715	2.399604	-0.000234
N	0.225362	0.220017	0.000201
C	-0.246752	1.497811	0.000139
N	-1.484000	1.905464	0.000032
C	-2.424772	0.899367	-0.000020
C	-2.062129	-0.489624	0.000043
C	-0.638038	-0.786604	0.000159

N	-0.208443	-2.045074	0.000218
N	-2.990735	-1.421926	-0.000007
C	6.091684	1.833881	0.000169
N	5.210684	0.665565	-0.000045
C	3.840468	0.905293	-0.000002
O	3.383236	2.038152	0.000565
N	3.050666	-0.217681	0.000089
C	3.477639	-1.535007	-0.000073
O	2.656285	-2.457836	-0.000040
C	4.908326	-1.701322	-0.000280
C	5.702188	-0.610005	-0.000217
H	5.322537	-2.696830	-0.000414
H	-3.784608	3.208411	-0.000017
H	0.531764	2.254100	0.000186
H	-0.879817	-2.797340	0.000187
H	5.905546	2.441513	-0.883010
H	6.781463	-0.691396	-0.000287
H	0.792607	-2.245479	0.000295
H	2.023261	-0.045391	0.000357
H	7.122550	1.492470	-0.000283
H	5.906099	2.440833	0.883939
H	-5.150909	2.505263	0.879414
H	-5.150468	2.505357	-0.880193
C	-3.793407	1.095458	-0.000132
Se	-4.600290	-0.582698	-0.000150

tsA:tsU cWW

34

tsA:tsU solv SCF Done: -5801.31752120 A.U.

C	-6.380230	1.930493	0.000660
N	-1.366278	0.489835	-0.000422
C	-2.025530	1.683041	-0.000173
N	-3.309894	1.898953	0.000086
C	-4.088744	0.762862	0.000107
C	-3.520796	-0.555456	-0.000138
C	-2.068636	-0.634440	-0.000407
N	-1.457235	-1.815931	-0.000628
N	-4.297963	-1.617297	-0.000102
C	4.114910	3.128822	0.000262
N	3.437784	1.836673	0.000034
C	2.060686	1.788440	-0.000160
O	1.354289	2.785200	-0.000143
N	1.483800	0.523912	-0.000407
C	2.101773	-0.697406	-0.000472
O	1.467800	-1.746184	-0.000722
C	3.575679	-0.614505	-0.000200
C	4.201964	0.675987	0.000040
H	-5.781834	2.840237	0.000658
H	-1.368108	2.546250	-0.000192
H	-2.008413	-2.660206	-0.000568
H	4.740458	3.221667	-0.888015
H	-0.440671	-1.865848	-0.000725
H	0.439642	0.524219	-0.000489

H	4.740176	3.221505	0.888755
H	3.365081	3.910451	0.000215
H	-7.025789	1.938374	0.880541
H	-7.026100	1.938574	-0.878990
C	-5.471197	0.750056	0.000365
Se	-6.015374	-1.030994	0.000277
N	4.321371	-1.691356	-0.000173
C	5.566723	0.599980	0.000266
Se	6.057177	-1.192845	0.000182
H	6.286840	1.402383	0.000471

G:tsC cWW

37

G:tsC solv SCF Done: -3510.48987422 A.U.

C	-3.212079	3.137451	-0.000070
N	-2.616601	1.806230	-0.000251
C	-1.235081	1.645762	-0.000768
O	-0.503933	2.642956	-0.001115
N	-0.690053	0.387169	-0.000916
C	-1.427060	-0.707028	-0.000579
N	-0.858239	-1.901997	-0.000733
C	-2.886075	-0.607810	-0.000042
C	-3.452131	0.704571	0.000114
C	7.275673	0.666148	0.002421
N	2.240479	0.174249	-0.000721
C	3.003902	1.317463	-0.000113
N	2.341107	2.482654	0.000103
N	4.327902	1.300916	0.000330
C	4.836815	0.057315	0.000017
C	4.156905	-1.159341	-0.000616
C	2.735595	-1.132998	-0.001014
O	1.954293	-2.096767	-0.001508
N	5.049896	-2.215828	-0.000749
H	-3.831857	3.269183	0.887974
H	-1.444153	-2.723713	-0.000438
H	7.242965	1.290353	0.894268
H	1.321795	2.530320	-0.000354
H	2.884026	3.332945	0.000382
H	8.206415	0.104689	-0.009426
H	7.230822	1.307561	-0.876475
H	-3.832526	3.269129	-0.887654
H	-2.416171	3.871281	-0.000393
H	0.164772	-1.993039	-0.001053
H	1.211964	0.268222	-0.000889
N	-3.673894	-1.655274	0.000313
C	-4.820374	0.688372	0.000645
Se	-5.388901	-1.082497	0.000960
H	-5.504766	1.521477	0.000875
N	6.164946	-0.268288	0.000154
C	6.225770	-1.646985	-0.000163
H	7.176497	-2.159377	-0.000180

tsG:C cWW

34

tsG:C solv SCF Done: -3362.81631162 A.U.

C	-6.085123	1.668152	0.002536
N	-5.209643	0.497425	0.001234
C	-3.823162	0.714633	0.000916
O	-3.412975	1.883615	0.001821
N	-2.996581	-0.356108	-0.000337
C	-3.484204	-1.600872	-0.001138
N	-2.616789	-2.614948	-0.002178
C	-4.891645	-1.845876	-0.000895
C	-5.706034	-0.766599	0.000308
C	4.618988	2.253781	0.000187
N	-0.131477	0.199087	-0.001736
C	0.330054	1.512082	-0.002336
N	-0.631966	2.450754	-0.004274
N	1.591906	1.835763	-0.001648
C	2.497621	0.800072	-0.000519
C	2.111686	-0.587060	-0.000076
C	0.673849	-0.907893	-0.000742
O	0.209141	-2.047585	-0.000446
N	3.021000	-1.534409	0.000954
H	-5.893922	2.274797	0.885260
H	-2.950251	-3.566027	-0.002669
H	-5.291390	-2.848617	-0.001586
H	-6.784348	-0.858026	0.000607
H	3.908854	3.079546	-0.001941
H	-1.628090	2.224204	-0.001517
H	-0.339490	3.414156	-0.002359
H	5.256745	2.349457	0.881057
H	5.259914	2.347546	-0.878572
H	-7.118794	1.333569	0.002556
H	-5.894451	2.276345	-0.879236
H	-1.612449	-2.437290	-0.001820
H	-1.153527	0.023012	-0.001708
Se	4.647969	-0.731867	0.001639
C	3.867267	0.966186	0.000278

tsG:tsC cWW

36

tsG:tsC solv SCF Done: -5856.72130767 A.U.

C	4.237271	3.046028	0.010485
N	3.541473	1.764146	0.005396
C	2.152306	1.709533	0.002833
O	1.498771	2.758710	0.005126
N	1.512184	0.495142	-0.002265
C	2.165344	-0.650806	-0.004107
N	1.509585	-1.801146	-0.008205
C	3.627161	-0.662657	-0.001536
C	4.291177	0.602532	0.003287
C	-6.471519	1.655589	0.003138
N	-1.420660	0.525553	-0.009134
C	-2.119461	1.729935	-0.010069

N	-1.347236	2.830187	-0.017452
N	-3.418869	1.812453	-0.006451
C	-4.115413	0.625537	-0.002245
C	-3.476835	-0.664878	-0.001850
C	-2.005434	-0.711776	-0.005553
O	-1.337100	-1.745993	-0.005250
N	-4.192777	-1.765713	0.002292
H	4.867278	3.132183	-0.875878
H	2.030805	-2.665287	-0.009295
H	-5.929257	2.600128	0.000794
H	-0.328195	2.787417	-0.007312
H	-1.810118	3.724194	-0.008392
H	-7.119334	1.627586	-0.875142
H	-7.115253	1.629549	0.884465
H	4.863612	3.127195	0.899914
H	3.500278	3.839038	0.011193
H	0.486438	-1.815288	-0.008426
H	-0.385724	0.544930	-0.009296
Se	-5.940541	-1.282385	0.006324
C	-5.491797	0.532119	0.002086
N	4.332922	-1.767192	-0.003529
C	5.654229	0.482359	0.005308
Se	6.086045	-1.326703	0.001155
H	6.400418	1.260512	0.008868

G:C cWW

35

GC solv SCF Done: -1016.58401367 A.U.

C	5.159882	-1.901142	0.000751
N	4.361674	-0.676714	0.000418
C	2.963718	-0.802136	0.000408
O	2.478158	-1.942395	0.000682
N	2.210026	0.320280	0.000072
C	2.777426	1.531209	-0.000245
N	1.977169	2.598445	-0.000551
C	4.198312	1.682739	-0.000235
C	4.939689	0.552260	0.000096
C	-5.535768	-1.488053	0.000004
N	-0.692644	-0.021909	-0.000261
C	-1.218187	-1.291336	-0.000363
N	-0.342123	-2.306631	-0.000653
N	-2.520220	-1.534305	-0.000282
C	-3.262495	-0.414152	-0.000098
C	-2.833574	0.911721	0.000011
C	-1.433829	1.164238	-0.000105
O	-0.855021	2.260575	-0.000010
N	-3.915915	1.773316	0.000222
C	-4.957981	0.985570	0.000156
N	-4.628946	-0.354498	-0.000052
H	4.930568	-2.495138	0.883068
H	2.373538	3.525097	-0.000752
H	4.663504	2.656862	-0.000483
H	6.021676	0.572705	0.000128

H	-5.372957	-2.101661	-0.884799
H	0.669485	-2.161549	-0.000348
H	-0.713622	-3.242511	-0.000471
H	-5.990508	1.302310	0.000232
H	-5.374879	-2.100201	0.886184
H	-6.558335	-1.119266	-0.001408
H	6.212947	-1.633629	0.000785
H	4.930722	-2.495524	-0.881347
H	0.960175	2.486503	-0.000482
H	0.336274	0.089162	-0.000353

A:U cWW

33

AU solv SCF Done: -961.181251018 A.U.

C	-5.472560	-1.741974	-0.000424
N	-0.629782	-0.060356	0.000529
C	-1.137882	-1.300701	0.000489
N	-2.415248	-1.662493	0.000260
C	-3.228299	-0.595944	0.000054
C	-2.844223	0.743688	0.000051
C	-1.459210	1.005842	0.000301
N	-0.938052	2.237302	0.000377
N	-3.949655	1.570179	-0.000186
C	-4.965993	0.742726	-0.000392
N	-4.599338	-0.581187	-0.000299
C	5.117098	-2.034440	-0.000289
N	4.312813	-0.812119	-0.000214
C	2.929829	-0.961662	0.000123
O	2.400264	-2.062850	0.000361
N	2.214866	0.210255	0.000203
C	2.727349	1.497472	-0.000016
O	1.968261	2.471434	0.000102
C	4.165997	1.569400	-0.000358
C	4.886508	0.428620	-0.000445
H	4.644882	2.535466	-0.000542
H	-5.290433	-2.348780	-0.885896
H	-0.399428	-2.095069	0.000650
H	-1.550633	3.036725	-0.000018
H	-6.007767	1.029077	-0.000646
H	4.893309	-2.628681	0.883310
H	5.968780	0.439162	-0.000696
H	0.071817	2.368028	0.000276
H	1.177699	0.106240	0.000378
H	6.167683	-1.759545	-0.000668
H	4.892738	-2.628938	-0.883569
H	-6.505586	-1.403839	-0.001633
H	-5.292175	-2.347758	0.886113

tsA:A tHW

35

tsA:A solv SCF Done: -3359.92051681 A.U.

C	-6.993500	0.403064	0.460829
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N	-1.892040	0.902267	0.218342
C	-2.844848	1.721290	0.683637
N	-4.158164	1.523546	0.715626
C	-4.488428	0.333036	0.196411
C	-3.612178	-0.618764	-0.322466
C	-2.241556	-0.294657	-0.297915
N	-1.280758	-1.099006	-0.772608
N	-4.302590	-1.728407	-0.767522
C	-5.557585	-1.442845	-0.520319
N	-5.739474	-0.211991	0.062149
C	5.498925	-1.473155	0.260885
N	2.847411	2.974899	-0.379217
C	4.160104	2.628801	-0.332424
N	4.694342	1.449961	-0.157770
C	3.787928	0.425686	-0.021572
C	2.369165	0.643071	-0.067437
C	1.935251	2.023334	-0.241190
N	0.638970	2.332069	-0.264585
N	1.546108	-0.379683	0.048660
H	-6.990414	0.602760	1.531182
H	-2.488510	2.665413	1.082930
H	-1.518067	-2.028247	-1.081266
H	-6.400650	-2.083106	-0.736225
H	6.225109	-0.671076	0.139034
H	4.847536	3.461032	-0.453005
H	-0.113696	1.664677	-0.077989
H	-7.808347	-0.276054	0.223527
H	-7.138617	1.340936	-0.072887
H	5.664598	-1.947909	1.229611
H	5.678283	-2.226692	-0.507716
H	-0.309150	-0.862575	-0.592340
H	0.391254	3.305500	-0.369075
Se	2.548528	-1.881158	0.264941
C	4.125738	-0.904006	0.160675

tsA:U tHW

32

tsA:U solv SCF Done: -3307.41057415 A.U.

C	-5.171170	1.821666	-0.000003
N	-4.318865	0.631340	-0.000005
C	-2.949363	0.829705	0.000026
O	-2.457548	1.954559	0.000070
N	-2.188846	-0.305754	0.000002
C	-2.640318	-1.623079	-0.000061
O	-1.834480	-2.548950	0.000029
C	-4.078811	-1.745897	-0.000044
C	-4.843005	-0.635087	-0.000038
C	4.356784	-1.912763	-0.000061
N	2.622469	3.004855	-0.000007
C	3.843978	2.409997	-0.000131
N	4.137308	1.137713	-0.000109
C	3.048639	0.299357	-0.000050
C	1.699865	0.789569	0.000022

C	1.542839	2.237828	0.000052
N	0.331812	2.797307	0.000118
N	0.697401	-0.066220	0.000068
H	-4.971072	2.423643	0.883906
H	-4.521759	-2.729140	-0.000042
H	-5.923989	-0.686936	-0.000044
H	5.225437	-1.256441	-0.000736
H	4.680160	3.103024	-0.000051
H	-0.536191	2.272613	0.000117
H	-1.169253	-0.158141	0.000038
H	4.406222	-2.557362	-0.879317
H	4.406873	-2.556338	0.879915
H	-4.971179	2.423578	-0.883982
H	-6.209686	1.504636	0.000071
H	0.274908	3.805208	0.000112
C	3.118804	-1.083345	-0.000051
Se	1.385510	-1.751635	0.000023

tsA:C tHW

33

tsA:C solv SCF Done: -3287.52244490 A.U.

C	6.100950	0.980807	-0.000423
N	4.918540	0.123565	-0.000131
C	3.653168	0.750592	-0.000162
O	3.600409	1.981265	-0.000528
N	2.551399	-0.041280	0.000029
C	2.652226	-1.368150	0.000349
N	1.513618	-2.070861	0.000571
C	3.921811	-2.022954	0.000460
C	5.018320	-1.229411	0.000196
C	-5.238224	-0.679671	-0.000044
N	-1.592364	3.051915	0.000388
C	-2.949009	3.023718	0.000707
N	-3.751719	1.993113	0.000383
C	-3.116568	0.773904	0.000131
C	-1.684712	0.649944	0.000045
C	-0.931492	1.900662	0.000096
N	0.397265	1.894310	0.000018
N	-1.132852	-0.547133	-0.000137
H	6.098996	1.618757	-0.882128
H	1.525754	-3.078020	0.000759
H	4.008182	-3.098880	0.000714
H	6.021442	-1.635858	0.000230
H	-5.748546	0.282184	0.000078
H	-3.417781	4.003690	0.000374
H	0.979368	1.052030	-0.000057
H	0.627767	-1.572965	0.000406
H	6.990075	0.356001	-0.000423
H	6.099212	1.619067	0.881058
H	-5.555138	-1.242292	0.879755
H	-5.555187	-1.242099	-0.879949
H	0.884928	2.777883	0.000111
C	-3.766468	-0.447374	-0.000058

Se -2.472046 -1.779630 -0.000363

tsG:G tHW

37

tsG:G solv SCF Done: -3510.48999224 A.U.

C	4.328332	-2.749180	-0.045203
N	3.605159	2.364519	0.020829
C	4.750657	1.575188	0.004285
N	5.922601	2.258283	-0.053685
N	4.728506	0.280503	-0.002645
C	3.488621	-0.320918	-0.006274
C	2.258181	0.416266	0.014309
C	2.315662	1.884397	0.029726
O	1.354666	2.644704	0.045733
N	1.110625	-0.220931	0.017219
C	-6.668214	1.428497	-0.038073
N	-1.744775	0.280911	0.008330
C	-2.349010	1.510544	-0.021575
N	-1.538059	2.581631	-0.049338
N	-3.662175	1.670472	-0.029644
C	-4.330610	0.502191	-0.007621
C	-3.818308	-0.792839	0.021697
C	-2.401838	-0.960215	0.030604
O	-1.744918	-2.003702	0.053744
N	-4.843582	-1.720826	0.036648
C	-5.934455	-1.001547	0.016753
N	-5.690928	0.355720	-0.010660
H	5.313232	-2.284949	-0.043658
H	5.954619	3.218607	0.258382
H	-0.718104	0.223933	0.012467
H	-6.540939	2.032626	-0.935182
H	-1.963193	3.494282	-0.044127
H	-6.944660	-1.383334	0.020237
H	4.253356	-3.404471	0.824455
H	4.242899	-3.375947	-0.934724
H	-7.665111	0.995062	-0.035222
H	-6.551550	2.068515	0.835294
H	-0.527083	2.504098	-0.009256
H	6.757818	1.714124	0.106029
H	3.698020	3.379065	0.011291
C	3.283275	-1.685853	-0.022087
Se	1.443157	-2.002964	-0.008248

A:A tHW

36

AA solv SCF Done: -1013.69101355 A.U.

C	6.533336	-0.633287	0.117619
N	1.400935	-0.755902	0.098821
C	2.314922	-1.726727	0.230923
N	3.639369	-1.622488	0.227931
C	4.029573	-0.349846	0.066263

C	3.200656	0.759604	-0.081289
C	1.810135	0.522096	-0.059910
N	0.898370	1.489795	-0.193522
N	3.946889	1.912550	-0.223808
C	5.188872	1.498083	-0.163198
N	5.309150	0.140855	0.011464
C	-5.350419	2.387260	0.176295
N	-3.545805	-2.407060	-0.154831
C	-4.790878	-1.922456	-0.114529
N	-5.187938	-0.654002	-0.025398
C	-4.142423	0.179992	0.021084
C	-2.794518	-0.171716	-0.014205
C	-2.502802	-1.550625	-0.103567
N	-1.258314	-2.040444	-0.144242
N	-2.004411	0.960987	0.050390
C	-2.856996	1.955317	0.123738
N	-4.164521	1.550927	0.111186
H	6.576610	-1.139140	1.080916
H	1.911550	-2.726798	0.355882
H	1.204588	2.445101	-0.285337
H	6.064431	2.126513	-0.238681
H	-5.940766	2.133039	1.055073
H	-5.580378	-2.665859	-0.159577
H	-0.424373	-1.455681	-0.059914
H	-2.593460	3.001004	0.187056
H	7.382717	0.038730	0.025488
H	6.575906	-1.379004	-0.674602
H	-5.043418	3.428190	0.236498
H	-5.960717	2.241006	-0.713307
H	-0.100166	1.281640	-0.119882
H	-1.145339	-3.041440	-0.190909

A:C tHW

34

AC solv SCF Done: -941.292956955 A.U.

C	-5.546199	1.146991	0.000103
N	-4.426375	0.210087	0.000298
C	-3.120046	0.747157	-0.001015
O	-2.984400	1.971881	-0.002070
N	-2.073464	-0.116425	-0.001043
C	-2.265339	-1.435289	0.000396
N	-1.185863	-2.223630	0.000332
C	-3.580044	-1.998466	0.001907
C	-4.619541	-1.132932	0.001752
C	5.124321	-1.836220	0.000099
N	2.405211	2.519539	0.001118
C	3.721314	2.288092	0.001871
N	4.362674	1.120309	0.001554
C	3.502337	0.094609	0.000299
C	2.111485	0.174279	-0.000565
C	1.550471	1.472043	-0.000125
N	0.235560	1.703685	-0.000962

N	1.561439	-1.094784	-0.001887
C	2.594677	-1.903084	-0.001780
N	3.796266	-1.247925	-0.000456
H	-5.500373	1.784412	0.881078
H	-1.290574	-3.225653	0.001583
H	-3.740605	-3.065925	0.003069
H	-5.648225	-1.469689	0.002775
H	5.674534	-1.520759	-0.884870
H	4.348411	3.174112	0.002856
H	-0.467676	0.961430	-0.001339
H	-0.248029	-1.814592	-0.000585
H	2.543962	-2.982141	-0.002622
H	-6.476655	0.585548	0.001008
H	-5.501228	1.782983	-0.881947
H	5.029067	-2.918964	-0.001051
H	5.673042	-1.522516	0.886623
H	-0.089202	2.657630	-0.000353

A:U tHW

33

AU solv SCF Done: -961.181544343 A.U.

C	-4.642012	-1.953854	0.000497
N	-3.929770	-0.675332	0.000138
C	-2.544802	-0.716999	-0.000030
O	-1.936914	-1.784655	0.000288
N	-1.915721	0.495112	-0.000220
C	-2.516127	1.751759	-0.000395
O	-1.824279	2.766067	-0.000368
C	-3.960317	1.712068	-0.000150
C	-4.594771	0.522792	0.000071
C	3.829115	2.730403	0.000412
N	3.207662	-2.369383	-0.000087
C	4.304015	-1.603245	0.000154
N	4.391926	-0.273711	0.000194
C	3.180332	0.293556	0.000076
C	1.955809	-0.368955	-0.000110
C	1.994205	-1.779346	-0.000227
N	0.894184	-2.542660	-0.000477
N	0.922488	0.546243	-0.000172
C	1.509765	1.719512	-0.000021
N	2.875011	1.634725	0.000148
H	-4.375723	-2.530553	-0.882910
H	-4.510992	2.639310	-0.000142
H	-5.674610	0.451667	0.000247
H	4.459344	2.677695	0.886585
H	5.246229	-2.141732	0.000139
H	-0.040817	-2.148908	-0.000469
H	-0.876201	0.468685	-0.000201
H	0.991026	2.666407	-0.000003
H	3.283877	3.670601	0.000067
H	4.460056	2.677457	-0.885235
H	-4.375929	-2.529980	0.884346
H	-5.709781	-1.756117	0.000310

H	1.001341	-3.546925	-0.000430
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G:G tHW

38

GG solv SCF Done: -1164.25837797 A.U.

C	-3.844693	3.236104	-0.048352
N	-4.034898	-1.820984	0.047187
C	-5.065684	-0.911436	0.047990
N	-6.319923	-1.408625	0.039171
N	-4.874134	0.392200	0.023140
C	-3.573543	0.734397	-0.011004
C	-2.465714	-0.104575	-0.016324
C	-2.664829	-1.510084	0.016799
O	-1.823359	-2.411133	0.021554
N	-1.305340	0.637156	-0.049785
C	-1.698990	1.884504	-0.064063
N	-3.068587	2.007112	-0.042211
C	6.287941	-1.548916	0.001139
N	1.496360	0.066329	-0.030037
C	1.981040	-1.213920	-0.063781
N	1.080411	-2.211065	-0.130094
N	3.274383	-1.499296	-0.048381
C	4.050447	-0.401086	-0.000910
C	3.664579	0.936503	0.034271
C	2.269237	1.239284	0.019757
O	1.716277	2.340783	0.044242
N	4.774614	1.760841	0.079368
C	5.791544	0.940020	0.071494
N	5.418866	-0.386874	0.023463
H	-4.454570	3.298835	0.851246
H	-6.492254	-2.375714	0.271068
H	0.472759	0.219036	-0.042891
H	-1.042306	2.740493	-0.087168
H	6.090331	-2.185328	0.862535
H	1.433775	-3.155533	-0.096573
H	6.833539	1.222554	0.098413
H	-3.161540	4.080622	-0.081223
H	-4.496040	3.263314	-0.920146
H	6.122788	-2.127250	-0.906811
H	7.321946	-1.214679	0.031125
H	0.075819	-2.074559	-0.060984
H	-7.074746	-0.755931	0.187725
H	-4.253130	-2.815383	0.062488

Size Expanded base pairs:

XYZ coordinates for In Gas Phase optimized geometries:

A:xtsU cWW

41

A:xtsU SCF Done: -3608.76362437 A.U.

C	8.398763	0.553677	-0.000192
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N	3.293363	0.158125	0.000268
C	4.099672	1.232211	0.000175
N	5.425724	1.253018	0.000057
C	5.937876	0.016937	0.000036
C	5.227817	-1.181302	0.000127
C	3.823018	-1.081080	0.000252
N	3.012396	-2.147005	0.000368
N	6.082665	-2.263397	0.000077
C	-1.590875	3.667786	0.000231
N	-1.192389	2.265817	0.000240
C	0.168309	1.988221	0.000396
O	1.021498	2.856361	0.000427
N	0.523550	0.652041	0.000322
C	-0.309820	-0.429105	0.000182
O	0.127961	-1.574158	0.000149
C	-1.752285	-0.111147	0.000072
C	-2.172502	1.269843	0.000094
H	8.015585	1.570764	-0.000343
H	3.584064	2.185202	0.000202
H	3.420106	-3.064071	0.000329
H	-2.181666	3.894613	0.888749
H	2.002702	-2.030923	0.000437
H	1.555865	0.468182	0.000409
H	-2.181452	3.894667	-0.888416
H	-0.692050	4.272033	0.000358
H	9.010335	0.401785	-0.889104
H	9.010310	0.402047	0.888783
N	7.262182	-0.348515	-0.000084
C	7.274688	-1.725626	-0.000056
H	8.204129	-2.272974	-0.000135
C	-3.510781	1.571669	-0.000027
C	-2.652797	-1.135655	-0.000069
C	-4.046206	-0.860707	-0.000193
C	-4.474524	0.525697	-0.000168
C	-5.848586	0.638783	-0.000294
Se	-6.585626	-1.053595	-0.000449
N	-4.960863	-1.824209	-0.000332
H	-6.432256	1.544960	-0.000307
H	-2.299279	-2.155960	-0.000087
H	-3.857813	2.591937	-0.000013

xtsA:U cWW

38

xtsA:U SCF Done: -3461.08148239 A.U.

N	-1.454713	0.312814	-0.000019
C	-1.064136	1.620581	-0.000023
N	0.143237	2.091058	-0.000032
C	1.163915	1.162687	-0.000024
C	0.890084	-0.259878	-0.000003
C	-0.524176	-0.624850	-0.000016
N	-0.916974	-1.904407	-0.000015
C	-7.354296	1.669491	0.000063
N	-6.428775	0.539938	0.000057

C	-5.063066	0.847924	-0.000035
O	-4.671946	1.999004	-0.000075
N	-4.224407	-0.239689	-0.000052
C	-4.588489	-1.576147	-0.000026
O	-3.734560	-2.461581	-0.000059
C	-6.015976	-1.809749	0.000040
C	-6.858240	-0.757783	0.000078
H	-6.375065	-2.824825	0.000064
H	-1.888171	2.326354	-0.000026
H	-0.249558	-2.650753	-0.000123
H	-7.191363	2.287762	0.880700
H	-7.931251	-0.888065	0.000132
H	-1.913556	-2.132815	-0.000103
H	-3.200188	-0.021548	-0.000106
H	-8.372349	1.289571	0.000372
H	-7.191787	2.287455	-0.880872
C	2.470873	1.603094	-0.000028
C	1.911227	-1.180945	0.000030
H	1.736574	-2.247524	0.000063
H	2.652873	2.668387	-0.000036
C	3.258889	-0.748245	0.000027
C	3.535638	0.678564	-0.000012
N	4.278400	-1.608564	0.000053
C	4.896584	0.962671	-0.000025
Se	5.799190	-0.651415	0.000022
C	5.533712	2.311854	-0.000002
H	5.224210	2.882176	-0.879032
H	5.225613	2.881524	0.879951
H	6.620979	2.257382	-0.000882

G:xtsC cWW

43

G:xtsC SCF Done: -3664.15307780 A.U.

C	1.767724	3.627670	0.000212
N	1.359666	2.228449	-0.000185
C	-0.006173	1.933086	-0.000961
O	-0.827750	2.850071	-0.001376
N	-0.412081	0.631040	-0.001140
C	0.439434	-0.372761	-0.000779
N	-0.055919	-1.604759	-0.000883
C	1.892784	-0.143441	-0.000336
C	2.330102	1.234534	0.000011
C	-8.354116	0.089709	0.000905
N	-3.313241	0.159875	-0.000875
C	-4.200259	1.205567	-0.000232
N	-3.672445	2.443232	-0.000094
N	-5.510177	1.041707	0.000260
C	-5.870745	-0.254172	0.000162
C	-5.061896	-1.390673	-0.000413
C	-3.650197	-1.203036	-0.000981
O	-2.757277	-2.057041	-0.001579
N	-5.831795	-2.536695	-0.000318
H	2.360279	3.852270	-0.888145

H	0.545919	-2.405618	-0.000473
H	-8.380202	0.729805	0.882141
H	-2.667912	2.609444	-0.000692
H	-4.314850	3.212801	0.000181
H	-8.385839	0.722664	-0.885349
H	-9.223140	-0.564258	0.006291
H	2.359798	3.851869	0.888987
H	0.872925	4.236721	0.000091
H	-1.083242	-1.756636	-0.001285
H	-2.304176	0.364480	-0.001235
C	3.672381	1.529607	0.000493
N	-7.155412	-0.722205	0.000772
C	-7.059242	-2.103811	0.000529
H	-7.944917	-2.719294	0.000929
C	2.802869	-1.164486	-0.000278
H	2.505520	-2.202554	-0.000619
H	4.019667	2.549443	0.000745
C	4.196255	-0.896447	0.000212
C	4.632548	0.484922	0.000623
N	5.103111	-1.868123	0.000308
C	6.008710	0.587865	0.001082
Se	6.732299	-1.109040	0.001006
H	6.599202	1.489547	0.001447

xtsG:C cWW

40

xtsG:C SCF Done: -3516.49066420 A.U.

C	-7.376131	1.325027	0.001172
N	-6.401084	0.238733	0.000669
C	-5.032074	0.592478	0.000436
O	-4.743111	1.788578	0.000669
N	-4.114907	-0.402286	-0.000029
C	-4.475587	-1.684004	-0.000231
N	-3.510839	-2.606106	-0.000656
C	-5.857551	-2.063315	-0.000014
C	-6.770144	-1.065364	0.000435
N	-1.318884	0.402107	-0.000529
C	-0.937801	1.737383	-0.000518
N	-1.957912	2.618550	-0.000815
N	0.295687	2.137426	-0.000350
C	1.290182	1.183804	-0.000246
C	0.984545	-0.233563	-0.000302
C	-0.429039	-0.634303	-0.000432
O	-0.817407	-1.805648	-0.000463
H	-7.237052	1.949465	0.881307
H	-3.747588	-3.580783	-0.000764
H	-6.164234	-3.097041	-0.000192
H	-7.833309	-1.259884	0.000630
H	-2.935448	2.336928	-0.000155
H	-1.713268	3.591105	-0.000270
H	-8.377906	0.902536	0.001320
H	-7.237493	1.949888	-0.878733
H	-2.520150	-2.328513	-0.000686

H	-2.319849	0.152826	-0.000513
C	1.958104	-1.194653	-0.000222
C	2.610811	1.573585	-0.000100
H	1.689677	-2.240764	-0.000270
H	2.839656	2.629811	-0.000063
C	3.324068	-0.810598	-0.000073
C	3.645698	0.606719	-0.000012
N	4.310808	-1.705492	-0.000002
C	5.012021	0.843390	0.000129
Se	5.866807	-0.803330	0.000189
C	5.695291	2.170292	0.000231
H	5.407455	2.751885	-0.879206
H	5.407390	2.751784	0.879715
H	6.780368	2.078741	0.000267

XYZ coordinates for In Water optimized structures:

A:xtsU cWW

41

A:xtsU SCF Done: -3608.78300243 A.U.

C	8.431906	0.544906	-0.000054
N	3.310878	0.162881	0.000206
C	4.118684	1.233004	0.000205
N	5.445500	1.255361	0.000131
C	5.961443	0.017921	0.000048
C	5.247011	-1.178975	0.000038
C	3.841458	-1.078677	0.000122
N	3.023956	-2.137781	0.000121
N	6.103927	-2.260574	-0.000065
C	-1.619877	3.669351	0.000087
N	-1.206012	2.268949	0.000039
C	0.144642	1.995932	0.000069
O	1.007297	2.863122	0.000321
N	0.508101	0.660578	0.000173
C	-0.320286	-0.422905	0.000105
O	0.130340	-1.566901	0.000247
C	-1.760578	-0.112817	0.000010
C	-2.183932	1.265261	-0.000015
H	8.063946	1.566992	-0.000211
H	3.606218	2.188485	0.000277
H	3.411534	-3.067371	0.000039
H	-2.212938	3.887264	0.888412
H	2.016478	-2.007112	0.000156
H	1.536268	0.481247	0.000316
H	-2.212896	3.887328	-0.888250
H	-0.730536	4.286306	0.000130
H	9.039408	0.381932	-0.888870
H	9.039260	0.382156	0.888905
N	7.283754	-0.347943	-0.000048
C	7.298803	-1.721593	-0.000103
H	8.231171	-2.267483	-0.000183
C	-3.522353	1.564006	-0.000076
C	-2.659818	-1.141564	-0.000024
C	-4.051951	-0.869958	-0.000101

C	-4.480687	0.514205	-0.000128
C	-5.856036	0.630021	-0.000197
Se	-6.596507	-1.055140	-0.000228
N	-4.971784	-1.832861	-0.000142
H	-6.441483	1.537422	-0.000228
H	-2.305358	-2.162677	0.000004
H	-3.879725	2.581513	-0.000092

xtsA:U cWW

38

xtsA:U SCF Done: -3461.10248748 A.U.

N	-1.448481	0.320658	0.000136
C	-1.054502	1.622180	0.000115
N	0.154588	2.095666	0.000067
C	1.177979	1.164807	0.000035
C	0.899772	-0.255777	0.000059
C	-0.515037	-0.621453	0.000108
N	-0.912082	-1.895124	0.000135
C	-7.389174	1.660311	0.000004
N	-6.450588	0.537668	0.000015
C	-5.093544	0.844793	0.000105
O	-4.693126	1.999002	0.000166
N	-4.249259	-0.237573	0.000092
C	-4.611568	-1.573935	-0.000002
O	-3.745159	-2.454860	-0.000002
C	-6.031829	-1.811248	-0.000095
C	-6.878410	-0.760388	-0.000085
H	-6.396437	-2.825958	-0.000173
H	-1.875652	2.332792	0.000145
H	-0.253274	-2.655998	0.000084
H	-7.234145	2.276215	0.883466
H	-7.952307	-0.895007	-0.000155
H	-1.910121	-2.111810	0.000153
H	-3.229629	-0.018227	0.000159
H	-8.401574	1.267462	0.000052
H	-7.234209	2.276160	-0.883509
C	2.485976	1.602833	-0.000019
C	1.919224	-1.180210	0.000036
H	1.732456	-2.246454	0.000057
H	2.678312	2.667518	-0.000034
C	3.267176	-0.749629	-0.000017
C	3.547779	0.674696	-0.000051
N	4.289677	-1.609869	-0.000043
C	4.910612	0.958256	-0.000113
Se	5.813471	-0.652253	-0.000117
C	5.551358	2.305054	-0.000104
H	5.241816	2.874752	-0.879416
H	5.243080	2.874160	0.880042
H	6.638079	2.246153	-0.000893

G:xtsC cWW

43

G:xtsC SCF Done: -3664.18027735 A.U.

C	1.761081	3.610628	-0.000430
N	1.352519	2.209025	-0.000435
C	-0.000562	1.905018	-0.000863
O	-0.837851	2.817288	-0.001320
N	-0.405926	0.601338	-0.000756
C	0.456208	-0.397439	-0.000356
N	-0.031393	-1.633167	-0.000202
C	1.904728	-0.160493	-0.000080
C	2.332024	1.217913	-0.000142
C	-8.375594	0.136174	0.000769
N	-3.314440	0.136283	-0.000442
C	-4.185699	1.199675	0.000403
N	-3.639024	2.423458	0.000952
N	-5.501981	1.055079	0.000700
C	-5.888413	-0.231920	0.000143
C	-5.093433	-1.376719	-0.000719
C	-3.681419	-1.212718	-0.001051
O	-2.810125	-2.095742	-0.001758
N	-5.879403	-2.515063	-0.001001
H	2.354193	3.832372	-0.888331
H	0.569537	-2.440851	0.000201
H	-8.396798	0.772011	0.884635
H	-2.627708	2.566782	0.000356
H	-4.261705	3.214748	0.001424
H	-8.400930	0.767404	-0.886322
H	-9.246937	-0.513731	0.004486
H	2.354051	3.832371	0.887563
H	0.869610	4.223438	-0.000508
H	-1.047386	-1.782190	-0.000482
H	-2.298418	0.325482	-0.000522
C	3.670941	1.523483	0.000074
N	-7.178720	-0.685206	0.000364
C	-7.104958	-2.063278	-0.000511
H	-8.001432	-2.665635	-0.000534
C	2.819824	-1.180265	0.000183
H	2.521052	-2.220094	0.000203
H	4.019853	2.543662	0.000013
C	4.209810	-0.901009	0.000414
C	4.634701	0.482691	0.000362
N	5.131661	-1.862834	0.000665
C	6.010688	0.601963	0.000603
Se	6.753831	-1.081279	0.000886
H	6.593951	1.510741	0.000629

xtsG:C cWW

40

xtsG:C SCF Done: -3516.51298103 A.U.

C	-7.361410	1.370780	0.001055
N	-6.396378	0.272691	0.000625
C	-5.030892	0.596903	0.000421
O	-4.711896	1.794047	0.000612

N	-4.124401	-0.406897	0.000021
C	-4.512891	-1.686053	-0.000164
N	-3.568290	-2.628709	-0.000560
C	-5.897039	-2.039195	0.000032
C	-6.792475	-1.026209	0.000428
N	-1.319127	0.367566	-0.000374
C	-0.949976	1.706062	-0.000329
N	-1.972905	2.576830	-0.000484
N	0.286218	2.114527	-0.000229
C	1.288435	1.167258	-0.000202
C	0.991563	-0.249876	-0.000265
C	-0.420921	-0.659770	-0.000354
O	-0.797646	-1.835295	-0.000389
H	-7.218914	1.991218	0.883415
H	-3.825891	-3.603065	-0.000680
H	-6.218288	-3.069802	-0.000124
H	-7.860387	-1.201234	0.000603
H	-2.950311	2.280296	-0.000093
H	-1.748037	3.558340	-0.000115
H	-8.365436	0.955554	0.001188
H	-7.219297	1.991575	-0.881116
H	-2.580947	-2.371716	-0.000645
H	-2.323667	0.111619	-0.000381
C	1.973077	-1.204391	-0.000232
C	2.608150	1.565040	-0.000085
H	1.711568	-2.253486	-0.000279
H	2.837024	2.622366	-0.000021
C	3.336161	-0.813058	-0.000127
C	3.648757	0.604105	-0.000045
N	4.333369	-1.700252	-0.000070
C	5.015182	0.851649	0.000084
Se	5.884713	-0.784083	0.000017
C	5.690670	2.181850	0.000220
H	5.397577	2.760373	-0.879235
H	5.397580	2.760202	0.879790
H	6.775765	2.095703	0.000210