

Supporting Information:

MS-CASPT2 Studies on the Photophysics of Selenium-Substituted Guanine Nucleobase

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Table S1. MS-CASPT2 Computed Energies (in eV) of Five Lowest Electronic States i.e. $S_2(^1\pi\pi^*)$, $S_1(^1n\pi^*)$, $T_2(^3n\pi^*)$, $T_1(^3\pi\pi^*)$, and S_0 at Different Minima

	S_0	$S_1(^1n\pi^*)$	$S_2(^1\pi\pi^*)$	$T_1(^3\pi\pi^*)$	$T_2(^3n\pi^*)$
S0-MIN	0.00	0.61	1.22	0.81	0.80
S1-MIN	2.61	2.46	2.65	2.52	2.48
S2-MIN	2.39	3.30	3.04	3.13	3.19
T1-MIN	2.40	2.35	2.33	2.24	2.29
T2-MIN	2.56	2.39	2.50	2.42	2.36
T3-MIN	3.55	3.99	4.36	4.12	4.17

Table S2. Spin-Orbit Couplings (SOC in cm^{-1}) of 6-Selenoguanine (6SeGua) Computed at MS-CASPT2 Level.

Structure	States	SOC (cm^{-1})
S1-MIN	S1/T1	437
S1-MIN	S1/T2	14
S2S1T2	S2/T2	435
S2S1T2	S1/T2	39
S0T1	T1/S0	252
T2T1S0	T1/S0	508

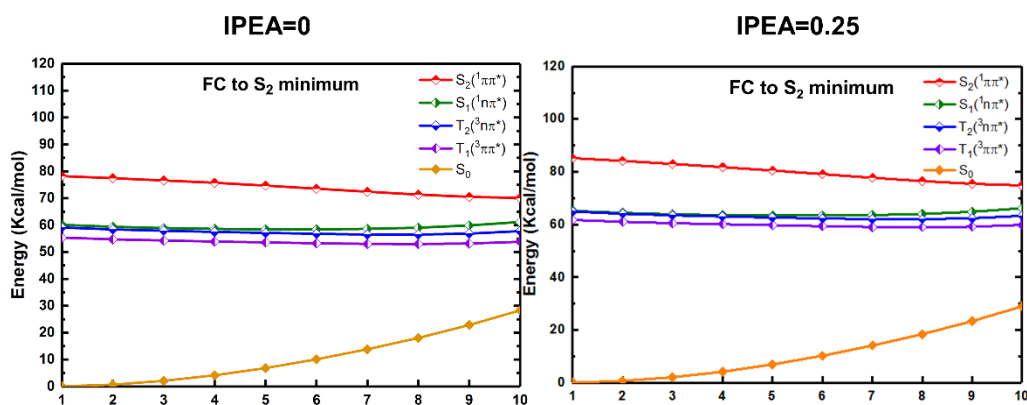


Figure S1. MS-CASPT2 calculated linearly interpolated internal coordinate (LIIC) paths connecting Franck-Condon point and S_2 minimum with different IPEA values.

Cartesian Coordinates

S0-MIN

C	0.44060186	-0.84507053	0.00941773
C	1.77902712	-0.40144277	-0.00578424
C	1.27371405	1.75753545	-0.01700194
C	-0.59900283	0.13376642	-0.00064814
C	1.63827505	-2.60492038	0.01238129
H	1.98364711	-3.63919152	0.01811614
N	-0.06300046	1.42833558	-0.02316954
H	-0.75515764	2.17530907	-0.10462044
N	2.25530236	0.87718838	-0.00416404
N	1.56077340	3.11273974	-0.10231715
H	0.97137032	3.69831195	0.48774337
H	2.54823975	3.27414051	0.08961270
N	2.53214811	-1.55082542	-0.00274545
H	3.54558410	-1.59832262	-0.01506383
N	0.37115754	-2.22960760	0.02031779
Se	-2.40439983	-0.10656631	-0.00261418

S1-MIN

C	0.43753321	-0.84279676	-0.07698105
C	1.77077050	-0.40269378	-0.00674995
C	1.26512865	1.76316288	0.00282361
C	-0.58874624	0.13908909	-0.16483743
C	1.63925635	-2.61004017	-0.01640878
H	1.97896042	-3.64461262	-0.00002207
N	-0.09051499	1.47268579	-0.04356049
H	-0.65625366	2.20759920	-0.46667281
N	2.24273422	0.89295237	0.06491055
N	1.54941070	3.12865668	-0.06624313
H	0.98029928	3.67619256	0.57987604
H	2.53996677	3.27577240	0.12555561
N	2.52111242	-1.55545427	0.02473679
H	3.53370103	-1.60454615	0.07866562
N	0.36325500	-2.22059471	-0.07764417
Se	-2.40833242	-0.19399228	0.40201170

S2-MIN

C	0.43734270	-0.84908936	-0.17129357
C	1.78294530	-0.40341131	0.00318393
C	1.26259215	1.75687836	-0.05118791
C	-0.57423601	0.12712670	-0.38100177
C	1.63562057	-2.60832223	-0.02890278
H	1.97825154	-3.64256403	0.01248422

N	-0.04180893	1.42571955	-0.26125392
H	-0.72309525	2.17725096	-0.36930973
N	2.24180564	0.86276419	0.07716941
N	1.57512933	3.10658118	-0.03603340
H	0.87628762	3.69315353	0.41742694
H	2.50202383	3.25563158	0.35805373
N	2.52371818	-1.55204957	0.08148857
H	3.52862060	-1.60027339	0.21662345
N	0.37569864	-2.23056389	-0.18270497
Se	-2.30261591	-0.03745328	0.67471783

T1-MIN

C	0.42315945	-0.84847708	0.13686556
C	1.76322945	-0.39805927	-0.00563927
C	1.24815516	1.75992091	0.00325648
C	-0.61292810	0.13307843	0.29989982
C	1.63936296	-2.60628281	0.03906793
H	1.98698020	-3.63823931	0.01507284
N	-0.06713274	1.44987637	0.13139633
H	-0.73840978	2.21047555	0.07049527
N	2.23881517	0.87452381	-0.05440728
N	1.55310297	3.10771503	-0.14461030
H	1.02756896	3.71981784	0.47749219
H	2.55567677	3.25147161	-0.03636022
N	2.51601483	-1.54085161	-0.05348515
H	3.52539657	-1.58033783	-0.16016352
N	0.36663852	-2.22359366	0.15718298
Se	-2.34734917	-0.18965774	-0.51660361

T2-MIN

C	0.44064062	-0.84776160	-0.11797008
C	1.76729940	-0.40313250	-0.00833153
C	1.26279429	1.75686537	-0.01427084
C	-0.60006637	0.13200205	-0.25408039
C	1.64040654	-2.61375256	-0.02254937
H	1.98289018	-3.64698952	0.00583850
N	-0.07249655	1.45139079	-0.14876991
H	-0.67234591	2.21054382	-0.46522658
N	2.24163431	0.88330357	0.08050814
N	1.55573110	3.11898027	-0.05416116
H	0.94053353	3.67581770	0.53820302
H	2.52958784	3.26462978	0.20849294
N	2.51845322	-1.55080278	0.04125052
H	3.52915851	-1.59438986	0.12907770

N	0.36671992	-2.22276903	-0.12025549
Se	-2.35265942	-0.13255526	0.56170452

S2T1T2

C	0.00000000	0.00000000	0.00000000
C	1.44229000	0.00000000	0.00000000
C	1.65783000	0.00000000	2.25373000
C	-0.59927000	0.22073000	1.22317000
C	0.54120000	-0.12626000	-2.04952000
H	0.52286000	-0.19687000	-3.13719000
N	0.23882000	0.31598000	2.28556000
H	-0.13551000	0.40241000	3.22303000
N	2.27540000	0.06164000	1.01497000
N	2.30796000	0.52996000	3.40328000
H	3.00356000	-0.14043000	3.72958000
H	2.82228000	1.38331000	3.15818000
N	1.73796000	-0.06645000	-1.35992000
H	2.66853000	-0.16695000	-1.74930000
N	-0.52989000	-0.07618000	-1.28076000
Se	-2.47290000	0.40825000	1.46861000

T2T1S0

C	0.52516396	-0.90114467	0.18157102
C	1.85157484	-0.45142869	-0.09141164
C	1.26514631	1.68456982	-0.16078999
C	-0.52510938	0.03267055	0.28523922
C	1.75634970	-2.64840156	0.10837270
H	2.12683012	-3.67381114	0.12814331
N	-0.03086527	1.30507438	0.08472531
H	-0.75209641	2.03608751	0.11554632
N	2.26914670	0.81659619	-0.25708657
N	1.50449023	3.02747481	-0.38957012
H	0.94358865	3.66512293	0.17119714
H	2.49781146	3.24280971	-0.33598929
N	2.61901338	-1.58215175	-0.13346502
H	3.61874526	-1.62288744	-0.30910646
N	0.50333713	-2.29033365	0.30146882
Se	-3.09480912	0.84103484	0.66067446

S0T1

C	0.37669696	-0.85003083	0.22811035
C	1.70482149	-0.39909719	-0.07468723
C	1.21729542	1.76184033	0.10829590
C	-0.67748731	0.14240235	0.41513149

C	1.59074295	-2.60586328	0.09052875
H	1.94585773	-3.63668668	0.08226068
N	-0.06155549	1.45754608	0.41671739
H	-0.67564311	2.22631769	0.67530528
N	2.17140629	0.86309318	-0.18181761
N	1.59672408	3.08213880	0.18000795
H	0.89807619	3.77798371	-0.06117336
H	2.51626349	3.25237161	-0.21392824
N	2.45029660	-1.54311377	-0.15586400
H	3.44897642	-1.58618374	-0.33791034
N	0.34240089	-2.22934048	0.32647233
Se	-1.76658647	-0.23199658	-1.13798925

Franck-Condon Point to the S2 Minimum

point1

C	0.44060186	-0.84507053	0.00941773
C	1.77902712	-0.40144277	-0.00578424
C	1.27371405	1.75753545	-0.01700194
C	-0.59900283	0.13376642	-0.00064814
C	1.63827505	-2.60492038	0.01238129
H	1.98364711	-3.63919152	0.01811614
N	-0.06300046	1.42833558	-0.02316954
H	-0.75515764	2.17530907	-0.10462044
N	2.25530236	0.87718838	-0.00416404
N	1.56077340	3.11273974	-0.10231715
H	0.97137032	3.69831195	0.48774337
H	2.54823975	3.27414051	0.08961270
N	2.53214811	-1.55082542	-0.00274545
H	3.54558410	-1.59832262	-0.01506383
N	0.37115754	-2.22960760	0.02031779
Se	-2.40439983	-0.10656631	-0.00261418

point2

C	0.43949540	-0.84214690	-0.00696570
C	1.78056300	-0.39987200	-0.00606940
C	1.27612390	1.75989710	-0.02130600
C	-0.59783640	0.13764370	-0.03664790
C	1.63598120	-2.60335780	0.00810570
H	1.98001980	-3.63803590	0.01711900
N	-0.05906740	1.43210560	-0.04581210
H	-0.74905320	2.18073270	-0.12840810
N	2.25707480	0.87678950	0.00158880
N	1.56852820	3.11422490	-0.09751790
H	0.96803290	3.70074920	0.48024870

H	2.55224790	3.27337610	0.11413560
N	2.53132480	-1.55008130	0.00354380
H	3.54482900	-1.59882290	0.00431820
N	0.36906270	-2.22626870	0.00204320
Se	-2.41904160	-0.13555230	0.07108430

point3

C	0.43843970	-0.83995350	-0.02378670
C	1.78182950	-0.39868260	-0.00624780
C	1.27770660	1.76172420	-0.02574680
C	-0.59651550	0.14050520	-0.07305780
C	1.63407930	-2.60220820	0.00372010
H	1.97702690	-3.63719980	0.01605910
N	-0.05561870	1.43498490	-0.06873460
H	-0.74369310	2.18500130	-0.15261830
N	2.25815020	0.87613060	0.00752620
N	1.57496160	3.11520400	-0.09277230
H	0.96341040	3.70263360	0.47230110
H	2.55445890	3.27231390	0.13871230
N	2.53048190	-1.54951270	0.01006230
H	3.54389210	-1.59923710	0.02421150
N	0.36742370	-2.22367960	-0.01670340
Se	-2.42774870	-0.15664310	0.14653530

point4

C	0.43745350	-0.83850090	-0.04109440
C	1.78282880	-0.39788380	-0.00635600
C	1.27846640	1.76301420	-0.03029820
C	-0.59501210	0.14234260	-0.11004060
C	1.63257570	-2.60148290	-0.00079270
H	1.97467200	-3.63669600	0.01493420
N	-0.05263430	1.43696610	-0.09203890
H	-0.73905470	2.18811060	-0.17736950
N	2.25852400	0.87520760	0.01366220
N	1.58005670	3.11568760	-0.08797190
H	0.95745710	3.70393120	0.46399940
H	2.55482980	3.27096670	0.16350840
N	2.52961660	-1.54913110	0.01679800
H	3.54276000	-1.59957770	0.04463370
N	0.36625810	-2.22185040	-0.03596600
Se	-2.43051260	-0.16972280	0.22385250

point5

C	0.43655550	-0.83782580	-0.05895530
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C	1.78355620	-0.39749910	-0.00642990
C	1.27837590	1.76374390	-0.03493240
C	-0.59329800	0.14311130	-0.14778280
C	1.63148960	-2.60120760	-0.00545840
H	1.97298000	-3.63654800	0.01373400
N	-0.05011360	1.43800940	-0.11584130
H	-0.73514150	2.19001530	-0.20280010
N	2.25816850	0.87400590	0.02002080
N	1.58374690	3.11566690	-0.08299910
H	0.95006730	3.70458140	0.45544280
H	2.55325760	3.26933410	0.18870830
N	2.52872830	-1.54895490	0.02374360
H	3.54141840	-1.59985540	0.06561870
N	0.36559610	-2.22081730	-0.05581020
Se	-2.42710230	-0.17437920	0.30320140

point6

C	0.43576420	-0.83799240	-0.07744320
C	1.78399970	-0.39756730	-0.00650440
C	1.27737490	1.76386850	-0.03961540
C	-0.59134450	0.14272920	-0.18647780
C	1.63085450	-2.60142430	-0.01031060
H	1.97199870	-3.63679250	0.01243790
N	-0.04807630	1.43804190	-0.14025780
H	-0.73198600	2.19062820	-0.22904920
N	2.25703240	0.87249960	0.02663360
N	1.58591230	3.11511360	-0.07772430
H	0.94107570	3.70449630	0.44673770
H	2.54957630	3.26740300	0.21451210
N	2.52781850	-1.54901080	0.03089160
H	3.53985230	-1.60008000	0.08720410
N	0.36548100	-2.22064430	-0.07631300
Se	-2.41704910	-0.16988790	0.38473890

point7

C	0.43509710	-0.83909270	-0.09662650
C	1.78413880	-0.39814300	-0.00661220
C	1.27536730	1.76332130	-0.04430190
C	-0.58912480	0.14107650	-0.22630410
C	1.63071720	-2.60219170	-0.01538980
H	1.97179920	-3.63747930	0.01101300
N	-0.04656460	1.43695690	-0.16538790
H	-0.72965270	2.18982000	-0.25623460
N	2.25503810	0.87065140	0.03353640

N	1.58637540	3.11397930	-0.07200330
H	0.93025840	3.70355880	0.43800630
H	2.54355510	3.26514530	0.24112860
N	2.52688970	-1.54933410	0.03822830
H	3.53804570	-1.60026090	0.10941690
N	0.36596870	-2.22142340	-0.09755160
Se	-2.39962380	-0.15520330	0.46854260

point8

C	0.43456710	-0.84124580	-0.11655250
C	1.78394220	-0.39929590	-0.00678250
C	1.27221920	1.76201310	-0.04892900
C	-0.58661730	0.13799790	-0.26739910
C	1.63113570	-2.60358390	-0.02074070
H	1.97247300	-3.63867060	0.00941190
N	-0.04564730	1.43461530	-0.19129360
H	-0.72824240	2.18742010	-0.28442470
N	2.25208130	0.86841190	0.04076650
N	1.58489940	3.11219430	-0.06567500
H	0.91733610	3.70162200	0.42939520
H	2.53489940	3.26251620	0.26876760
N	2.52594450	-1.54996870	0.04572770
H	3.53598050	-1.60040760	0.13225630
N	0.36712440	-2.22327380	-0.11958780
Se	-2.37381110	-0.12896350	0.55452000

point9

C	0.43417800	-0.84459330	-0.13722770
C	1.78336640	-0.40110930	-0.00703790
C	1.26775800	1.75983480	-0.05340890
C	-0.58381360	0.13330850	-0.30982420
C	1.63217500	-2.60568890	-0.02640950
H	1.97412830	-3.64043930	0.00757160
N	-0.04542290	1.43085050	-0.21797300
H	-0.72789620	2.18322250	-0.31360420
N	2.24803100	0.86572040	0.04835760
N	1.58118900	3.10966870	-0.05856060
H	0.90198250	3.69851080	0.42108560
H	2.52325920	3.25945260	0.29762780
N	2.52498330	-1.55096580	0.05334430
H	3.53363690	-1.60053050	0.15567410
N	0.36901630	-2.22633680	-0.14244890
Se	-2.33828630	-0.08952390	0.64229400

point10

C	0.43734270	-0.84908936	-0.17129357
C	1.78294530	-0.40341131	0.00318393
C	1.26259215	1.75687836	-0.05118791
C	-0.57423601	0.12712670	-0.38100177
C	1.63562057	-2.60832223	-0.02890278
H	1.97825154	-3.64256403	0.01248422
N	-0.04180893	1.42571955	-0.26125392
H	-0.72309525	2.17725096	-0.36930973
N	2.24180564	0.86276419	0.07716941
N	1.57512933	3.10658118	-0.03603340
H	0.87628762	3.69315353	0.41742694
H	2.50202383	3.25563158	0.35805373
N	2.52371818	-1.55204957	0.08148857
H	3.52862060	-1.60027339	0.21662345
N	0.37569864	-2.23056389	-0.18270497
Se	-2.30261591	-0.03745328	0.67471783

The S2 Minimum to the S1 Minimum

point1

C	0.43734270	-0.84908936	-0.17129357
C	1.78294530	-0.40341131	0.00318393
C	1.26259215	1.75687836	-0.05118791
C	-0.57423601	0.12712670	-0.38100177
C	1.63562057	-2.60832223	-0.02890278
H	1.97825154	-3.64256403	0.01248422
N	-0.04180893	1.42571955	-0.26125392
H	-0.72309525	2.17725096	-0.36930973
N	2.24180564	0.86276419	0.07716941
N	1.57512933	3.10658118	-0.03603340
H	0.87628762	3.69315353	0.41742694
H	2.50202383	3.25563158	0.35805373
N	2.52371818	-1.55204957	0.08148857
H	3.52862060	-1.60027339	0.21662345
N	0.37569864	-2.23056389	-0.18270497
Se	-2.30261591	-0.03745328	0.67471783

point2

C	0.43766610	-0.84925100	-0.16136210
C	1.78199280	-0.40382010	0.00294370
C	1.26288830	1.75754640	-0.04549950
C	-0.57545830	0.12793080	-0.35917150
C	1.63695470	-2.60903630	-0.02632900
H	1.97958520	-3.64321640	0.01284840

N	-0.04809220	1.43092120	-0.23950130
H	-0.71407380	2.19014110	-0.38276430
N	2.24189850	0.86587020	0.07706700
N	1.57336880	3.10902010	-0.03965360
H	0.88528350	3.69125700	0.43569320
H	2.50884890	3.25797130	0.33407860
N	2.52419270	-1.55268850	0.07730970
H	3.53012020	-1.60068940	0.20477970
N	0.37499780	-2.23035090	-0.17167270
Se	-2.32188840	-0.06022560	0.64069380

point3

C	0.43795860	-0.84920570	-0.15149090
C	1.78095050	-0.40410420	0.00273970
C	1.26318230	1.75823150	-0.03969010
C	-0.57670100	0.12885720	-0.33735750
C	1.63809390	-2.60961580	-0.02381860
H	1.98064610	-3.64375550	0.01313510
N	-0.05413130	1.43611190	-0.21754360
H	-0.70525590	2.20059730	-0.39616460
N	2.24197180	0.86904600	0.07704770
N	1.57128600	3.11149020	-0.04307070
H	0.89463610	3.68935170	0.45389900
H	2.51490860	3.26035910	0.31010120
N	2.52448600	-1.55325100	0.07312510
H	3.53137450	-1.60109860	0.19293970
N	0.37418410	-2.22992350	-0.16069040
Se	-2.33930550	-0.08171050	0.60629900

point4

C	0.43822470	-0.84895760	-0.14168700
C	1.77982280	-0.40426230	0.00257060
C	1.26346640	1.75892940	-0.03375780
C	-0.57796590	0.12989490	-0.31556930
C	1.63904790	-2.61006140	-0.02137310
H	1.98144720	-3.64418110	0.01334440
N	-0.05993390	1.44128850	-0.19539280
H	-0.69667280	2.20865570	-0.40951650
N	2.24202380	0.87229480	0.07711230
N	1.56889550	3.11398140	-0.04628050
H	0.90436150	3.68744170	0.47202220
H	2.52021390	3.26277270	0.28613650
N	2.52460550	-1.55373420	0.06893500
H	3.53239130	-1.60149490	0.18110670

N	0.37326610	-2.22928610	-0.14976320
Se	-2.35490920	-0.10190160	0.57157290

point5

C	0.43846810	-0.84850820	-0.13195650
C	1.77861300	-0.40429150	0.00243630
C	1.26373240	1.75963640	-0.02769800
C	-0.57925550	0.13103510	-0.29381490
C	1.63982480	-2.61037150	-0.01899510
H	1.98199890	-3.64449050	0.01347420
N	-0.06550850	1.44644910	-0.17305630
H	-0.68834800	2.21433670	-0.42282940
N	2.24205180	0.87562040	0.07726380
N	1.56621180	3.11648350	-0.04927960
H	0.91447510	3.68553220	0.49003950
H	2.52477620	3.26518960	0.26219770
N	2.52455680	-1.55413370	0.06473940
H	3.53317660	-1.60187160	0.16928360
N	0.37225140	-2.22844030	-0.13889730
Se	-2.36874020	-0.12079570	0.53655260

point6

C	0.43869130	-0.84785740	-0.12230530
C	1.77732380	-0.40418790	0.00233800
C	1.26397220	1.76034990	-0.02150340
C	-0.58057300	0.13227170	-0.27210080
C	1.64043090	-2.61054320	-0.01668800
H	1.98231010	-3.64468020	0.01352070
N	-0.07086380	1.45159290	-0.15053760
H	-0.68029830	2.21764300	-0.43611370
N	2.24205310	0.87902760	0.07750740
N	1.56324990	3.11898780	-0.05206510
H	0.92499260	3.68363040	0.50792660
H	2.52860810	3.26758840	0.23829600
N	2.52434470	-1.55444450	0.06053870
H	3.53373540	-1.60222120	0.15747390
N	0.37114590	-2.22738590	-0.12809990
Se	-2.38083800	-0.13839130	0.50127280

point7

C	0.43889630	-0.84700320	-0.11273920
C	1.77595780	-0.40394630	0.00227730
C	1.26417840	1.76106870	-0.01516440
C	-0.58192200	0.13360030	-0.25043270

C	1.64087120	-2.61057240	-0.01445660
H	1.98238720	-3.64474520	0.01347810
N	-0.07600860	1.45672080	-0.12783700
H	-0.67253500	2.21855910	-0.44937890
N	2.24202480	0.88252210	0.07785010
N	1.56002510	3.12148660	-0.05463530
H	0.93592880	3.68174570	0.52565800
H	2.53172260	3.26994850	0.21444080
N	2.52397270	-1.55466050	0.05633320
H	3.53407180	-1.60253630	0.14568130
N	0.36995450	-2.22612060	-0.11737920
Se	-2.39124090	-0.15468750	0.46576490

point8

C	0.43908460	-0.84594140	-0.10326370
C	1.77451690	-0.40356010	0.00225680
C	1.26434400	1.76179300	-0.00866970
C	-0.58330660	0.13501940	-0.22881590
C	1.64114930	-2.61045340	-0.01230630
H	1.98223510	-3.64467940	0.01333900
N	-0.08095130	1.46183490	-0.10495160
H	-0.66506380	2.21704980	-0.46263010
N	2.24196460	0.88611090	0.07830070
N	1.55655270	3.12397330	-0.05698960
H	0.94729830	3.67988950	0.54320640
H	2.53413320	3.27225010	0.19063940
N	2.52344390	-1.55477460	0.05212340
H	3.53418880	-1.60280870	0.13390970
N	0.36868040	-2.22464020	-0.10674460
Se	-2.39998550	-0.16968310	0.43005630

point9

C	0.43925690	-0.84466610	-0.09388500
C	1.77300310	-0.40302150	0.00227990
C	1.26446290	1.76252400	-0.00200640
C	-0.58473140	0.13652940	-0.20725550
C	1.64126710	-2.61017950	-0.01024350
H	1.98185650	-3.64447570	0.01309490
N	-0.08570010	1.46693890	-0.08187660
H	-0.65788550	2.21305990	-0.47586630
N	2.24187020	0.88980160	0.07886970
N	1.55284850	3.12644280	-0.05912880
H	0.95911450	3.67807520	0.56054310

H	2.53585390	3.27447430	0.16689730
N	2.52276000	-1.55477910	0.04791020
H	3.53408900	-1.60302990	0.12216400
N	0.36732580	-2.22293870	-0.09620680
Se	-2.40710640	-0.18337550	0.39417000

point10

C	0.43753321	-0.84279676	-0.07698105
C	1.77077050	-0.40269378	-0.00674995
C	1.26512865	1.76316288	0.00282361
C	-0.58874624	0.13908909	-0.16483743
C	1.63925635	-2.61004017	-0.01640878
H	1.97896042	-3.64461262	-0.00002207
N	-0.09051499	1.47268579	-0.04356049
H	-0.65625366	2.20759920	-0.46667281
N	2.24273422	0.89295237	0.06491055
N	1.54941070	3.12865668	-0.06624313
H	0.98029928	3.67619256	0.57987604
H	2.53996677	3.27577240	0.12555561
N	2.52111242	-1.55545427	0.02473679
H	3.53370103	-1.60454615	0.07866562
N	0.36325500	-2.22059471	-0.07764417
Se	-2.40833242	-0.19399228	0.40201170

The S2 Minimum to S2S1T2 crossing point

point1

C	0.43734270	-0.84908936	-0.17129357
C	1.78294530	-0.40341131	0.00318393
C	1.26259215	1.75687836	-0.05118791
C	-0.57423601	0.12712670	-0.38100177
C	1.63562057	-2.60832223	-0.02890278
H	1.97825154	-3.64256403	0.01248422
N	-0.04180893	1.42571955	-0.26125392
H	-0.72309525	2.17725096	-0.36930973
N	2.24180564	0.86276419	0.07716941
N	1.57512933	3.10658118	-0.03603340
H	0.87628762	3.69315353	0.41742694
H	2.50202383	3.25563158	0.35805373
N	2.52371818	-1.55204957	0.08148857
H	3.52862060	-1.60027339	0.21662345
N	0.37569864	-2.23056389	-0.18270497
Se	-2.30261591	-0.03745328	0.67471783

point2

C	0.43655510	-0.85215450	-0.14922740
C	1.78381250	-0.40143360	0.01146190
C	1.25812510	1.76593120	-0.01741130
C	-0.56790580	0.12512040	-0.35269120
C	1.63697270	-2.60991340	-0.02303790
H	1.98125510	-3.64378990	0.01285760
N	-0.05180980	1.42438000	-0.24304700
H	-0.73182720	2.17757490	-0.33947580
N	2.24080820	0.86208090	0.08156460
N	1.55391530	3.12350600	-0.04485420
H	0.93203430	3.68991620	0.53021440
H	2.52906490	3.28312370	0.20424120
N	2.52545870	-1.55339950	0.07881210
H	3.53063010	-1.60213790	0.21059570
N	0.37546620	-2.23422380	-0.16361870
Se	-2.35427060	-0.07320050	0.56307620

point3

C	0.43533710	-0.85452510	-0.12675040
C	1.78390610	-0.39834040	0.02079800
C	1.25183010	1.77463380	0.01949960
C	-0.56337370	0.12281250	-0.32326230
C	1.63837270	-2.61041500	-0.01829300
H	1.98464510	-3.64380860	0.01113920
N	-0.06310160	1.42233760	-0.22245470
H	-0.74230750	2.17666530	-0.30673960
N	2.23826370	0.86255380	0.08812310
N	1.53166410	3.13845240	-0.04899100
H	1.01140230	3.68861010	0.63299230
H	2.53333110	3.30414850	0.04817500
N	2.52672850	-1.55338770	0.07609630
H	3.53216660	-1.60243880	0.20453250
N	0.37528660	-2.23718610	-0.14541500
Se	-2.39586620	-0.10873220	0.45001020

point4

C	0.43381640	-0.85612990	-0.10396050
C	1.78339170	-0.39421540	0.03132420
C	1.24419570	1.78294500	0.05997420
C	-0.56032890	0.12045410	-0.29267380
C	1.63972270	-2.60986850	-0.01497310
H	1.98819500	-3.64268840	0.00686340
N	-0.07521110	1.41981190	-0.19931340
H	-0.75392220	2.17483020	-0.27110390

N	2.23451300	0.86404050	0.09734570
N	1.50908850	3.15148840	-0.04833910
H	1.11180110	3.68866720	0.72122930
H	2.51450530	3.31824720	-0.10624520
N	2.52755300	-1.55216020	0.07333400
H	3.53323460	-1.60145840	0.19854350
N	0.37511560	-2.23935360	-0.12844770
Se	-2.42738570	-0.14323030	0.33590270

point5

C	0.43210940	-0.85688470	-0.08093850
C	1.78242940	-0.38911790	0.04316540
C	1.23568700	1.79082370	0.10435610
C	-0.55848070	0.11827740	-0.26088830
C	1.64092590	-2.60827880	-0.01332130
H	1.99168490	-3.64045130	-0.00034370
N	-0.08768260	1.41701350	-0.17353590
H	-0.76608200	2.17236620	-0.23269620
N	2.22989390	0.86642260	0.10968710
N	1.48694610	3.16261030	-0.04303640
H	1.22986540	3.68918120	0.79090190
H	2.47305470	3.32504330	-0.25522240
N	2.52795910	-1.54982220	0.07054110
H	3.53384230	-1.59943110	0.19275740
N	0.37490290	-2.24060820	-0.11300910
Se	-2.44877110	-0.17576390	0.22104300

point6

C	0.43031540	-0.85668960	-0.05774790
C	1.78116320	-0.38307120	0.05643330
C	1.22671550	1.79823810	0.15288650
C	-0.55757530	0.11649050	-0.22787980
C	1.64189610	-2.60560260	-0.01350920
H	1.99492000	-3.63705820	-0.01074860
N	-0.10010360	1.41413890	-0.14512140
H	-0.77825270	2.16955490	-0.19177830
N	2.22472070	0.86961580	0.12553640
N	1.46601310	3.17173670	-0.03346960
H	1.36160800	3.68891740	0.83867200
H	2.41020890	3.32420500	-0.39521520
N	2.52797560	-1.54642200	0.06775630
H	3.53400240	-1.59651960	0.18731770
N	0.37459860	-2.24080840	-0.09932100
Se	-2.45992100	-0.20534580	0.10564900

point7

C	0.42850850	-0.85542480	-0.03443410
C	1.77970930	-0.37605020	0.07121810
C	1.21760750	1.80517610	0.20569140
C	-0.55741410	0.11527520	-0.19363860
C	1.64256670	-2.60173560	-0.01563120
H	1.99774910	-3.63239290	-0.02450040
N	-0.11212960	1.41136720	-0.11416100
H	-0.78998560	2.16665970	-0.14874690
N	2.21926160	0.87358290	0.14519560
N	1.44706000	3.17870140	-0.02027100
H	1.50260130	3.68628810	0.86203560
H	2.32791480	3.31542970	-0.52307170
N	2.52763140	-1.54193270	0.06503590
H	3.53373100	-1.59278860	0.18237220
N	0.37415900	-2.23978530	-0.08752540
Se	-2.46068610	-0.23099010	-0.01010840

point8

C	0.42672990	-0.85294760	-0.01102210
C	1.77814310	-0.36796880	0.08757920
C	1.20857220	1.81165600	0.26277170
C	-0.55787200	0.11478300	-0.15817300
C	1.64289870	-2.59650080	-0.01970000
H	2.00008200	-3.62624880	-0.04162270
N	-0.12350880	1.40885700	-0.08083880
H	-0.80094570	2.16392230	-0.10412780
N	2.21371280	0.87834730	0.16885460
N	1.43083140	3.18324320	-0.00430740
H	1.64817900	3.67930130	0.85944450
H	2.22877050	3.29845980	-0.63614940
N	2.52695350	-1.53623500	0.06244540
H	3.53304630	-1.58817880	0.17805470
N	0.37355330	-2.23734120	-0.07767380
Se	-2.45086160	-0.25176920	-0.12607500

point9

C	0.42497990	-0.84909020	0.01248690
C	1.77648640	-0.35866640	0.10553340
C	1.19967240	1.81773770	0.32399330
C	-0.55891580	0.11513190	-0.12150690
C	1.64288950	-2.58964030	-0.02564460
H	2.00190760	-3.61831850	-0.06200840

N	-0.13410650	1.40674260	-0.04542730
H	-0.81093720	2.16155780	-0.05856140
N	2.20817270	0.88400950	0.19656170
N	1.41802830	3.18498980	0.01334010
H	1.79364770	3.66549560	0.83040310
H	2.11593650	3.27313040	-0.73242150
N	2.52596400	-1.52909990	0.06004550
H	3.53196710	-1.58247960	0.17445920
N	0.37276930	-2.23325110	-0.06971570
Se	-2.43017710	-0.26686930	-0.24207720

point10

C	0.00000000	0.00000000	0.00000000
C	1.44229000	0.00000000	0.00000000
C	1.65783000	0.00000000	2.25373000
C	-0.59927000	0.22073000	1.22317000
C	0.54120000	-0.12626000	-2.04952000
H	0.52286000	-0.19687000	-3.13719000
N	0.23882000	0.31598000	2.28556000
H	-0.13551000	0.40241000	3.22303000
N	2.27540000	0.06164000	1.01497000
N	2.30796000	0.52996000	3.40328000
H	3.00356000	-0.14043000	3.72958000
H	2.82228000	1.38331000	3.15818000
N	1.73796000	-0.06645000	-1.35992000
H	2.66853000	-0.16695000	-1.74930000
N	-0.52989000	-0.07618000	-1.28076000
Se	-2.47290000	0.40825000	1.46861000

The S1 minimum to the T2 minimum

point1

C	0.43753321	-0.84279676	-0.07698105
C	1.77077050	-0.40269378	-0.00674995
C	1.26512865	1.76316288	0.00282361
C	-0.58874624	0.13908909	-0.16483743
C	1.63925635	-2.61004017	-0.01640878
H	1.97896042	-3.64461262	-0.00002207
N	-0.09051499	1.47268579	-0.04356049
H	-0.65625366	2.20759920	-0.46667281
N	2.24273422	0.89295237	0.06491055
N	1.54941070	3.12865668	-0.06624313
H	0.98029928	3.67619256	0.57987604
H	2.53996677	3.27577240	0.12555561
N	2.52111242	-1.55545427	0.02473679

H	3.53370103	-1.60454615	0.07866562
N	0.36325500	-2.22059471	-0.07764417
Se	-2.40833242	-0.19399228	0.40201170

point2

C	0.43780800	-0.84345460	-0.08152330
C	1.77039900	-0.40279800	-0.00711820
C	1.26508650	1.76265020	0.00091550
C	-0.59000760	0.13835710	-0.17446540
C	1.63942430	-2.61051880	-0.01737670
H	1.97948840	-3.64493570	0.00022700
N	-0.08858000	1.47039400	-0.05517860
H	-0.65839890	2.20872950	-0.46628730
N	2.24276190	0.89186670	0.06644300
N	1.55052750	3.12774360	-0.06479900
H	0.97615570	3.67625760	0.57566330
H	2.53951160	3.27461900	0.13483760
N	2.52087760	-1.55498470	0.02619420
H	3.53332550	-1.60344960	0.08371610
N	0.36360240	-2.22094160	-0.08243270
Se	-2.40369580	-0.18815360	0.42064470

point3

C	0.43809000	-0.84408140	-0.08606220
C	1.77001930	-0.40289090	-0.00748180
C	1.26499350	1.76209070	-0.00097040
C	-0.59127910	0.13762330	-0.18409520
C	1.63956970	-2.61098200	-0.01835050
H	1.97997850	-3.64524650	0.00046600
N	-0.08663160	1.46809260	-0.06674330
H	-0.66046250	2.20967180	-0.46584880
N	2.24275530	0.89077830	0.06798550
N	1.55154850	3.12678850	-0.06334600
H	0.97197980	3.67628680	0.57141600
H	2.53890070	3.27343250	0.14409850
N	2.52062110	-1.55450880	0.02764870
H	3.53291460	-1.60235540	0.08876170
N	0.36394420	-2.22125730	-0.08722190
Se	-2.39865600	-0.18206070	0.43920380

point4

C	0.43837930	-0.84467720	-0.09059750
C	1.76963210	-0.40297240	-0.00783990
C	1.26485040	1.76148480	-0.00283370

C	-0.59256120	0.13688740	-0.19372690
C	1.63969250	-2.61143060	-0.01933050
H	1.98043070	-3.64554630	0.00069420
N	-0.08466930	1.46578120	-0.07825400
H	-0.66244700	2.21042790	-0.46535620
N	2.24271560	0.88968740	0.06953880
N	1.55247440	3.12579240	-0.06188440
H	0.96777160	3.67628080	0.56713470
H	2.53813520	3.27221470	0.15333770
N	2.52034350	-1.55402730	0.02910080
H	3.53246920	-1.60126440	0.09380350
N	0.36428000	-2.22154180	-0.09201250
Se	-2.39321100	-0.17571540	0.45768600

point5

C	0.43867600	-0.84524150	-0.09512910
C	1.76923760	-0.40304230	-0.00819200
C	1.26465760	1.76083230	-0.00467450
C	-0.59385450	0.13614950	-0.20336040
C	1.63979220	-2.61186430	-0.02031700
H	1.98084410	-3.64583500	0.00091100
N	-0.08269280	1.46345920	-0.08971050
H	-0.66435480	2.21099940	-0.46480790
N	2.24264360	0.88859420	0.07110390
N	1.55330510	3.12475550	-0.06041440
H	0.96353110	3.67623920	0.56281960
H	2.53721540	3.27096630	0.16255480
N	2.52004480	-1.55354010	0.03055120
H	3.53198910	-1.60017720	0.09884240
N	0.36460950	-2.22179500	-0.09680520
Se	-2.38735810	-0.16911920	0.47608800

point6

C	0.43898010	-0.84577400	-0.09965660
C	1.76883600	-0.40310060	-0.00853740
C	1.26441550	1.76013300	-0.00649230
C	-0.59515940	0.13540950	-0.21299550
C	1.63986840	-2.61228300	-0.02131040
H	1.98121820	-3.64611250	0.00111560
N	-0.08070160	1.46112620	-0.10111240
H	-0.66618790	2.21138740	-0.46420240
N	2.24253990	0.88749870	0.07268160
N	1.55404060	3.12367790	-0.05893650
H	0.95925790	3.67616180	0.55847110

H	2.53614180	3.26968830	0.17174940
N	2.51972470	-1.55304740	0.03200050
H	3.53147410	-1.59909430	0.10387940
N	0.36493230	-2.22201610	-0.10160060
Se	-2.38109450	-0.16227370	0.49440660

point7

C	0.43929150	-0.84627420	-0.10417970
C	1.76842750	-0.40314690	-0.00887550
C	1.26412430	1.75938660	-0.00828710
C	-0.59647650	0.13466740	-0.22263220
C	1.63992060	-2.61268650	-0.02231080
H	1.98155220	-3.64637880	0.00130720
N	-0.07869540	1.45878130	-0.11245920
H	-0.66794840	2.21159290	-0.46353820
N	2.24240510	0.88640100	0.07427290
N	1.55468100	3.12255970	-0.05745080
H	0.95495180	3.67604820	0.55408910
H	2.53491460	3.26838130	0.18092070
N	2.51938290	-1.55254940	0.03344940
H	3.53092400	-1.59801610	0.10891550
N	0.36524790	-2.22220500	-0.10639940
Se	-2.37441710	-0.15518050	0.51263830

point8

C	0.43961030	-0.84674170	-0.10869820
C	1.76801220	-0.40318100	-0.00920550
C	1.26378450	1.75859290	-0.01005860
C	-0.59780630	0.13392320	-0.23227040
C	1.63994830	-2.61307470	-0.02331880
H	1.98184530	-3.64663380	0.00148520
N	-0.07667380	1.45642410	-0.12375040
H	-0.66963820	2.21161710	-0.46281340
N	2.24223970	0.88530120	0.07587860
N	1.55522620	3.12140110	-0.05595780
H	0.95061250	3.67589800	0.54967400
H	2.53353430	3.26704610	0.19006840
N	2.51901940	-1.55204600	0.03489840
H	3.53033850	-1.59694320	0.11395170
N	0.36555580	-2.22236090	-0.11120220
Se	-2.36732270	-0.14784120	0.53077920

point9

C	0.43993640	-0.84717600	-0.11321160
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C	1.76759020	-0.40320280	-0.00952680
C	1.26339620	1.75775160	-0.01180640
C	-0.59914920	0.13317690	-0.24190990
C	1.63995080	-2.61344740	-0.02433460
H	1.98209680	-3.64687740	0.00164880
N	-0.07463630	1.45405400	-0.13498560
H	-0.67125920	2.21146050	-0.46202630
N	2.24204440	0.88419950	0.07749970
N	1.55567620	3.12020200	-0.05445790
H	0.94623980	3.67571080	0.54522570
H	2.53200110	3.26568350	0.19919160
N	2.51863390	-1.55153740	0.03634820
H	3.52971740	-1.59587600	0.11898910
N	0.36585570	-2.22248340	-0.11600980
Se	-2.35980810	-0.14025740	0.54882580

point10

C	0.44064062	-0.84776160	-0.11797008
C	1.76729940	-0.40313250	-0.00833153
C	1.26279429	1.75686537	-0.01427084
C	-0.60006637	0.13200205	-0.25408039
C	1.64040654	-2.61375256	-0.02254937
H	1.98289018	-3.64698952	0.00583850
N	-0.07249655	1.45139079	-0.14876991
H	-0.67234591	2.21054382	-0.46522658
N	2.24163431	0.88330357	0.08050814
N	1.55573110	3.11898027	-0.05416116
H	0.94053353	3.67581770	0.53820302
H	2.52958784	3.26462978	0.20849294
N	2.51845322	-1.55080278	0.04125052
H	3.52915851	-1.59438986	0.12907770
N	0.36671992	-2.22276903	-0.12025549
Se	-2.35265942	-0.13255526	0.56170452

The S1 minimum to the T1 minimum

point1

C	0.43753321	-0.84279676	-0.07698105
C	1.77077050	-0.40269378	-0.00674995
C	1.26512865	1.76316288	0.00282361
C	-0.58874624	0.13908909	-0.16483743
C	1.63925635	-2.61004017	-0.01640878
H	1.97896042	-3.64461262	-0.00002207
N	-0.09051499	1.47268579	-0.04356049
H	-0.65625366	2.20759920	-0.46667281

N	2.24273422	0.89295237	0.06491055
N	1.54941070	3.12865668	-0.06624313
H	0.98029928	3.67619256	0.57987604
H	2.53996677	3.27577240	0.12555561
N	2.52111242	-1.55545427	0.02473679
H	3.53370103	-1.60454615	0.07866562
N	0.36325500	-2.22059471	-0.07764417
Se	-2.40833242	-0.19399228	0.40201170

point2

C	0.43695080	-0.84768760	-0.05405660
C	1.77233490	-0.40446910	-0.00666260
C	1.26654590	1.76601350	0.00234350
C	-0.58599920	0.14003890	-0.11582840
C	1.64317680	-2.61224740	-0.00999300
H	1.98518450	-3.64613520	0.00237280
N	-0.08562060	1.47409640	-0.02478970
H	-0.67373440	2.21244290	-0.40921080
N	2.24509680	0.89086210	0.05168990
N	1.55458600	3.12946810	-0.07434070
H	0.99054710	3.68441850	0.56961480
H	2.54682620	3.27549120	0.10878700
N	2.52440840	-1.55545150	0.01675410
H	3.53792830	-1.60245130	0.05348580
N	0.36577630	-2.22520460	-0.05238970
Se	-2.44572160	-0.19780350	0.30168390

point3

C	0.43612850	-0.85161110	-0.03134890
C	1.77328860	-0.40570500	-0.00644580
C	1.26708280	1.76810860	0.00197630
C	-0.58459770	0.14052300	-0.06715290
C	1.64618370	-2.61382970	-0.00360900
H	1.99018360	-3.64711490	0.00473140
N	-0.08139560	1.47456510	-0.00637460
H	-0.68917740	2.21602660	-0.35159510
N	2.24667900	0.88878700	0.03879610
N	1.55867610	3.12951460	-0.08234250
H	0.99946650	3.69179660	0.55917660
H	2.55246470	3.27452150	0.09236780
N	2.52677930	-1.55504020	0.00900920
H	3.54091890	-1.60016370	0.02880290
N	0.36778570	-2.22883170	-0.02737390
Se	-2.47218060	-0.20016560	0.20084240

point4

C	0.43506990	-0.85455590	-0.00875020
C	1.77366490	-0.40640160	-0.00611530
C	1.26679010	1.76945780	0.00173740
C	-0.58452740	0.14058820	-0.01854940
C	1.64829170	-2.61479120	0.00274780
H	1.99396770	-3.64756000	0.00703480
N	-0.07779900	1.47412140	0.01181000
H	-0.70257750	2.21844710	-0.29380830
N	2.24754430	0.88672700	0.02616620
N	1.56170900	3.12881320	-0.09030540
H	1.00712940	3.69835890	0.54853510
H	2.55692960	3.27290270	0.07615210
N	2.52825600	-1.55422960	0.00141600
H	3.54271880	-1.59770030	0.00443150
N	0.36929090	-2.23146970	-0.00248640
Se	-2.48817230	-0.20132690	0.09944420

point5

C	0.43376800	-0.85649510	0.01387430
C	1.77347920	-0.40655180	-0.00568360
C	1.26570260	1.77005330	0.00165100
C	-0.58579460	0.14026790	0.03029200
C	1.64949100	-2.61512600	0.00908720
H	1.99651580	-3.64746960	0.00926270
N	-0.07479460	1.47276660	0.02992050
H	-0.71392800	2.21977540	-0.23578210
N	2.24774020	0.88468030	0.01373100
N	1.56367800	3.12736530	-0.09828900
H	1.01357740	3.70411820	0.53766570
H	2.56023160	3.27066810	0.05997190
N	2.52884330	-1.55302400	-0.00612040
H	3.54333980	-1.59507710	-0.01984000
N	0.37028440	-2.23309640	0.02240950
Se	-2.49384790	-0.20147380	-0.00269040

point6

C	0.43220400	-0.85738210	0.03668090
C	1.77272850	-0.40613880	-0.00516160
C	1.26383780	1.76986810	0.00174820
C	-0.58842960	0.13958190	0.07972260
C	1.64974300	-2.61481750	0.01542110
H	1.99776920	-3.64683430	0.01139120

N	-0.07235060	1.47047140	0.04813810
H	-0.72321120	2.22005710	-0.17740940
N	2.24729810	0.88264380	0.00141570
N	1.56453730	3.12515590	-0.10635730
H	1.01881310	3.70906610	0.52654210
H	2.56233940	3.26784740	0.04363900
N	2.52851650	-1.55142290	-0.01370440
H	3.54275590	-1.59231160	-0.04424650
N	0.37074100	-2.23367000	0.04747010
Se	-2.48900640	-0.20073330	-0.10582960

point7

C	0.43034760	-0.85714530	0.05984130
C	1.77139030	-0.40513530	-0.00455980
C	1.26119620	1.76885310	0.00206650
C	-0.59248990	0.13853670	0.13013100
C	1.64897360	-2.61383610	0.02175950
H	1.99762230	-3.64563500	0.01338940
N	-0.07043790	1.46717130	0.06666360
H	-0.73039050	2.21931050	-0.11855630
N	2.24623310	0.88061270	-0.01085930
N	1.56419530	3.12215250	-0.11458090
H	1.02278870	3.71317060	0.51513270
H	2.56317120	3.26446940	0.02694410
N	2.52721680	-1.54942150	-0.02145070
H	3.54089660	-1.58942600	-0.06904550
N	0.37061410	-2.23312390	0.07286410
Se	-2.47304140	-0.19917250	-0.21027950

point8

C	0.42815590	-0.85568300	0.08353620
C	1.76942160	-0.40350080	-0.00389070
C	1.25776050	1.76693320	0.00264760
C	-0.59806440	0.13712460	0.18193680
C	1.64706520	-2.61213810	0.02810690
H	1.99591010	-3.64384250	0.01521560
N	-0.06902770	1.46276020	0.08571130
H	-0.73540250	2.21752340	-0.05907500
N	2.24454490	0.87858020	-0.02317940
N	1.56250500	3.11830280	-0.12303860
H	1.02539080	3.71637130	0.50339590
H	2.56258350	3.26056670	0.00965560
N	2.52484540	-1.54701150	-0.02948550
H	3.53764070	-1.58645100	-0.09451530

N	0.36982960	-2.23136090	0.09876440
Se	-2.44487270	-0.19679360	-0.31632570

point9

C	0.42557190	-0.85285540	0.10794580
C	1.76675870	-0.40117950	-0.00317160
C	1.25349720	1.76400210	0.00353550
C	-0.60527710	0.13532230	0.23558200
C	1.64384570	-2.60966300	0.03445540
H	1.99239260	-3.64141600	0.01681150
N	-0.06808710	1.45708150	0.10550230
H	-0.73814840	2.21464750	0.00117870
N	2.24221870	0.87653690	-0.03563510
N	1.55925110	3.11353350	-0.13182130
H	1.02641920	3.71857330	0.49127560
H	2.56035530	3.25618340	-0.00848150
N	2.52125680	-1.54418290	-0.03794800
H	3.53280740	-1.58343320	-0.12095280
N	0.36827840	-2.22824600	0.12533650
Se	-2.40285410	-0.19352330	-0.42415290

point10

C	0.42315945	-0.84847708	0.13686556
C	1.76322945	-0.39805927	-0.00563927
C	1.24815516	1.75992091	0.00325648
C	-0.61292810	0.13307843	0.29989982
C	1.63936296	-2.60628281	0.03906793
H	1.98698020	-3.63823931	0.01507284
N	-0.06713274	1.44987637	0.13139633
H	-0.73840978	2.21047555	0.07049527
N	2.23881517	0.87452381	-0.05440728
N	1.55310297	3.10771503	-0.14461030
H	1.02756896	3.71981784	0.47749219
H	2.55567677	3.25147161	-0.03636022
N	2.51601483	-1.54085161	-0.05348515
H	3.52539657	-1.58033783	-0.16016352
N	0.36663852	-2.22359366	0.15718298
Se	-2.34734917	-0.18965774	-0.51660361

The T2 minimum to the T1 minimum

point1

C	0.44064062	-0.84776160	-0.11797008
C	1.76729940	-0.40313250	-0.00833153
C	1.26279429	1.75686537	-0.01427084

C	-0.60006637	0.13200205	-0.25408039
C	1.64040654	-2.61375256	-0.02254937
H	1.98289018	-3.64698952	0.00583850
N	-0.07249655	1.45139079	-0.14876991
H	-0.67234591	2.21054382	-0.46522658
N	2.24163431	0.88330357	0.08050814
N	1.55573110	3.11898027	-0.05416116
H	0.94053353	3.67581770	0.53820302
H	2.52958784	3.26462978	0.20849294
N	2.51845322	-1.55080278	0.04125052
H	3.52915851	-1.59438986	0.12907770
N	0.36671992	-2.22276903	-0.12025549
Se	-2.35265942	-0.13255526	0.56170452

point2

C	0.43994630	-0.85251760	-0.09109370
C	1.77011230	-0.40510310	-0.00838350
C	1.26540870	1.76122710	-0.01328500
C	-0.59474460	0.13528450	-0.19664980
C	1.64528190	-2.61577500	-0.01510090
H	1.99007220	-3.64840440	0.00836440
N	-0.07014980	1.45685740	-0.11899250
H	-0.68538760	2.21492680	-0.40734490
N	2.24524990	0.88240160	0.06495130
N	1.56185500	3.12175090	-0.06365600
H	0.95674850	3.68484890	0.53302210
H	2.54005090	3.26638910	0.18270410
N	2.52328090	-1.55140210	0.03160730
H	3.53568300	-1.59327010	0.09869620
N	0.36937260	-2.22759710	-0.09050210
Se	-2.41449430	-0.14823570	0.44512300

point3

C	0.43895930	-0.85623240	-0.06441430
C	1.77209030	-0.40648750	-0.00810710
C	1.26686140	1.76458480	-0.01200860
C	-0.59114620	0.13765480	-0.13951590
C	1.64899600	-2.61712400	-0.00774410
H	1.99572240	-3.64924250	0.01071440
N	-0.06833420	1.46088440	-0.08952700
H	-0.69704990	2.21806870	-0.34965030
N	2.24775340	0.88147020	0.05010230
N	1.56637940	3.12351310	-0.07286600
H	0.97103760	3.69275500	0.52764720

H	2.54852180	3.26727670	0.15754960
N	2.52688030	-1.55157230	0.02239270
H	3.54052020	-1.59198890	0.06913390
N	0.37139640	-2.23135250	-0.06111690
Se	-2.46030230	-0.16082630	0.32687010

point4

C	0.43769700	-0.85890200	-0.03785340
C	1.77329640	-0.40728590	-0.00754630
C	1.26723510	1.76696850	-0.01045660
C	-0.58923270	0.13918100	-0.08243620
C	1.65158920	-2.61780860	-0.00048350
H	1.99987800	-3.64951570	0.01287040
N	-0.06700710	1.46353650	-0.06029360
H	-0.70731520	2.22007580	-0.29216070
N	2.24925250	0.88051820	0.03586380
N	1.56939530	3.12429950	-0.08188770
H	0.98353170	3.69960210	0.52201730
H	2.55513020	3.26733500	0.13285070
N	2.52931750	-1.55132340	0.01349590
H	3.54376570	-1.59055970	0.04017790
N	0.37281570	-2.23403870	-0.03200340
Se	-2.49106330	-0.17070160	0.20730560

point5

C	0.43615440	-0.86049920	-0.01126580
C	1.77376390	-0.40748830	-0.00673650
C	1.26659020	1.76839220	-0.00862340
C	-0.58899290	0.13991810	-0.02505480
C	1.65306440	-2.61782420	0.00669240
H	2.00253070	-3.64922350	0.01481640
N	-0.06613610	1.46484850	-0.03113770
H	-0.71617880	2.22102500	-0.23480140
N	2.24982880	0.87955260	0.02212570
N	1.57095030	3.12412600	-0.09082040
H	0.99433830	3.70543870	0.51608220
H	2.55996310	3.26659870	0.10838440
N	2.53061920	-1.55065830	0.00478630
H	3.54546580	-1.58899430	0.01155470
N	0.37362820	-2.23563600	-0.00299780
Se	-2.50730340	-0.17819500	0.08645600

point6

C	0.43430380	-0.86096590	0.01554920
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C	1.77349250	-0.40707100	-0.00570740
C	1.26496060	1.76884950	-0.00648540
C	-0.59044890	0.13990660	0.03308270
C	1.65337600	-2.61714910	0.01380400
H	2.00361110	-3.64835190	0.01653260
N	-0.06569900	1.46482020	-0.00184390
H	-0.72363710	2.22096260	-0.17742690
N	2.24953390	0.87857880	0.00876710
N	1.57104040	3.12298930	-0.09976810
H	1.00352750	3.71029230	0.50979490
H	2.56305190	3.26509380	0.08388700
N	2.53076250	-1.54957250	-0.00388750
H	3.54560430	-1.58730690	-0.01706560
N	0.37380020	-2.23609350	0.02611790
Se	-2.50899380	-0.18360100	-0.03589050

point7

C	0.43209260	-0.86020290	0.04283760
C	1.77244320	-0.40599210	-0.00448650
C	1.26235060	1.76830990	-0.00400380
C	-0.59366360	0.13917290	0.09251970
C	1.65241710	-2.61574020	0.02087360
H	2.00296930	-3.64687090	0.01798770
N	-0.06568310	1.46341000	0.02785250
H	-0.72967920	2.21990210	-0.11984220
N	2.24838480	0.87760120	-0.00434280
N	1.56960060	3.12086340	-0.10884170
H	1.01111720	3.71416560	0.50310440
H	2.56435950	3.26283760	0.05905710
N	2.52966350	-1.54805410	-0.01270070
H	3.54408800	-1.58551790	-0.04606870
N	0.37325830	-2.23531900	0.05560310
Se	-2.49543260	-0.18718440	-0.16008930

point8

C	0.42943900	-0.85805650	0.07087910
C	1.77053180	-0.40418600	-0.00310440
C	1.25873130	1.76671450	-0.00112690
C	-0.59874870	0.13772960	0.15387910
C	1.65000010	-2.61352820	0.02791540
H	2.00034920	-3.64473050	0.01912960
N	-0.06608450	1.46052790	0.05825340
H	-0.73427970	2.21782020	-0.06182750
N	2.24635960	0.87662400	-0.01734540

N	1.56649250	3.11769690	-0.11816110
H	1.01705430	3.71703180	0.49594860
H	2.56376430	3.25984010	0.03355690
N	2.52716180	-1.54608250	-0.02185800
H	3.54072690	-1.58365870	-0.07589750
N	0.37187790	-2.23316600	0.08574450
Se	-2.46508970	-0.18919550	-0.28652580

point9

C	0.42622580	-0.85430290	0.09996980
C	1.76762080	-0.40155730	-0.00160210
C	1.25403690	1.76397190	0.00220540
C	-0.60587430	0.13557690	0.21784740
C	1.64583150	-2.61041020	0.03492120
H	1.99535320	-3.64185690	0.01987100
N	-0.06690760	1.45602590	0.08968140
H	-0.73739450	2.21465010	-0.00317020
N	2.24339390	0.87565210	-0.03039310
N	1.56148940	3.11340990	-0.12785850
H	1.02119020	3.71882950	0.48824660
H	2.56104060	3.25610860	0.00701590
N	2.52300020	-1.54362870	-0.03159950
H	3.53521070	-1.58178040	-0.10705350
N	0.36946500	-2.22941750	0.11683380
Se	-2.41539580	-0.18988980	-0.41545540

point10

C	0.42315945	-0.84847708	0.13686556
C	1.76322945	-0.39805927	-0.00563927
C	1.24815516	1.75992091	0.00325648
C	-0.61292810	0.13307843	0.29989982
C	1.63936296	-2.60628281	0.03906793
H	1.98698020	-3.63823931	0.01507284
N	-0.06713274	1.44987637	0.13139633
H	-0.73840978	2.21047555	0.07049527
N	2.23881517	0.87452381	-0.05440728
N	1.55310297	3.10771503	-0.14461030
H	1.02756896	3.71981784	0.47749219
H	2.55567677	3.25147161	-0.03636022
N	2.51601483	-1.54085161	-0.05348515
H	3.52539657	-1.58033783	-0.16016352
N	0.36663852	-2.22359366	0.15718298
Se	-2.34734917	-0.18965774	-0.51660361

The T1 minimum to the T2T1S0 crossing point

point1

C	0.42315945	-0.84847708	0.13686556
C	1.76322945	-0.39805927	-0.00563927
C	1.24815516	1.75992091	0.00325648
C	-0.61292810	0.13307843	0.29989982
C	1.63936296	-2.60628281	0.03906793
H	1.98698020	-3.63823931	0.01507284
N	-0.06713274	1.44987637	0.13139633
H	-0.73840978	2.21047555	0.07049527
N	2.23881517	0.87452381	-0.05440728
N	1.55310297	3.10771503	-0.14461030
H	1.02756896	3.71981784	0.47749219
H	2.55567677	3.25147161	-0.03636022
N	2.51601483	-1.54085161	-0.05348515
H	3.52539657	-1.58033783	-0.16016352
N	0.36663852	-2.22359366	0.15718298
Se	-2.34734917	-0.18965774	-0.51660361

point2

C	0.40747510	-0.88460250	0.13175140
C	1.75448460	-0.39824130	-0.00531930
C	1.25595620	1.74487400	-0.00234590
C	-0.61065410	0.10986330	0.26826690
C	1.67074490	-2.60976540	0.04360530
H	2.04310560	-3.63329720	0.02397260
N	-0.05638280	1.42783390	0.11765110
H	-0.71846630	2.19949590	0.06360520
N	2.23832490	0.86449020	-0.05617400
N	1.55565050	3.09390330	-0.14265580
H	1.01755900	3.70361710	0.47080130
H	2.55594500	3.24501360	-0.02460340
N	2.52890750	-1.52669320	-0.04646370
H	3.53959200	-1.54849840	-0.14572720
N	0.38840790	-2.26227940	0.15284020
Se	-2.49236400	-0.04433280	-0.48974450

point3

C	0.39522120	-0.91818550	0.12407840
C	1.74755430	-0.39976720	-0.00546100
C	1.26195370	1.73007830	-0.00780340
C	-0.60822150	0.08557850	0.23390920
C	1.69999200	-2.61326710	0.04729790
H	2.09443030	-3.62872850	0.03250330

N	-0.04762590	1.40531890	0.10143610
H	-0.70088950	2.18755570	0.05330310
N	2.23766360	0.85459410	-0.05680390
N	1.55591340	3.08042940	-0.14008160
H	1.00413910	3.68742760	0.46363760
H	2.55349360	3.23928860	-0.01055110
N	2.54144430	-1.51463020	-0.03946490
H	3.55314710	-1.52031480	-0.13033320
N	0.40994270	-2.29754000	0.14626010
Se	-2.61987240	0.10354330	-0.45246650

point4

C	0.38781260	-0.94715400	0.11369730
C	1.74388750	-0.40257990	-0.00590670
C	1.26614280	1.71633050	-0.01284480
C	-0.60530970	0.06158610	0.19777790
C	1.72628870	-2.61692030	0.04995160
H	2.13896310	-3.62532360	0.04036300
N	-0.04101530	1.38306460	0.08335120
H	-0.68722840	2.17410560	0.04007720
N	2.23746960	0.84552490	-0.05591730
N	1.55398530	3.06801480	-0.13704250
H	0.98759100	3.67217930	0.45567700
H	2.54838290	3.23493860	0.00547570
N	2.55402200	-1.50556480	-0.03236730
H	3.56652870	-1.49771840	-0.11373570
N	0.43063180	-2.32765730	0.13720260
Se	-2.72986640	0.24855490	-0.40629900

point5

C	0.38689300	-0.96909590	0.10064600
C	1.74520240	-0.40660020	-0.00640200
C	1.26862960	1.70451620	-0.01718940
C	-0.60143190	0.03962870	0.16088860
C	1.74878160	-2.62090850	0.05133410
H	2.17452390	-3.62405450	0.04710870
N	-0.03672810	1.36197180	0.06402070
H	-0.67948350	2.15848730	0.02434930
N	2.23855470	0.83803010	-0.05306810
N	1.55022870	3.05744630	-0.13370600
H	0.96852950	3.65893670	0.44657350
H	2.54096160	3.23257710	0.02313850
N	2.56718490	-1.50054000	-0.02505880
H	3.58038030	-1.48293110	-0.09575190

N	0.44980760	-2.35069860	0.12550770
Se	-2.82374840	0.38461580	-0.35293080

point6

C	0.39408760	-0.98165490	0.08519470
C	1.75320810	-0.41169950	-0.00661160
C	1.26966980	1.69546580	-0.02061310
C	-0.59596940	0.02149980	0.12421250
C	1.76667810	-2.62539130	0.05123490
H	2.19904740	-3.62586070	0.05224080
N	-0.03481920	1.34289820	0.04402700
H	-0.67962810	2.13993290	0.00645610
N	2.24179800	0.83279710	-0.04785650
N	1.54519020	3.04946730	-0.13025210
H	0.94778070	3.64870960	0.43601210
H	2.53177740	3.23276550	0.04205860
N	2.58150320	-1.50055080	-0.01742870
H	3.59537070	-1.47811800	-0.07626910
N	0.46683670	-2.36479740	0.11115370
Se	-2.90424530	0.50591770	-0.29409920

point7

C	0.41070850	-0.98303180	0.06781490
C	1.76923590	-0.41767110	-0.00617870
C	1.26966310	1.68977110	-0.02302350
C	-0.58823580	0.00859670	0.08853190
C	1.77933010	-2.63037720	0.04954020
H	2.21090330	-3.63132740	0.05534510
N	-0.03510020	1.32640430	0.02385830
H	-0.68897320	2.11757220	-0.01330510
N	2.24797160	0.83031610	-0.04010090
N	1.53941810	3.04463410	-0.12685860
H	0.92615210	3.64219230	0.42380360
H	2.52138580	3.23598180	0.06179500
N	2.59737960	-1.50629300	-0.00936740
H	3.61194930	-1.48494080	-0.05525190
N	0.48123290	-2.36846430	0.09428890
Se	-2.97473520	0.60801820	-0.23143160

point8

C	0.43761720	-0.97224270	0.04908580
C	1.79401350	-0.42423100	-0.00478200
C	1.26911110	1.68769680	-0.02448170
C	-0.57750720	0.00165190	0.05436440

C	1.78621580	-2.63560020	0.04625660
H	2.20896290	-3.64043050	0.05617710
N	-0.03710960	1.31262330	0.00389120
H	-0.70779150	2.09040560	-0.03461920
N	2.25762380	0.83080750	-0.02991950
N	1.53331030	3.04324230	-0.12368870
H	0.90423580	3.63962230	0.40993230
H	2.51018900	3.24261090	0.08184900
N	2.61488040	-1.51801980	-0.00076820
H	3.63012630	-1.50431320	-0.03272290
N	0.49271700	-2.36067400	0.07518330
Se	-3.03830890	0.68823200	-0.16629730

point9

C	0.47535590	-0.94892390	0.02960540
C	1.82773110	-0.43106520	-0.00213440
C	1.26858580	1.68926650	-0.02515350
C	-0.56295360	0.00086260	0.02200870
C	1.78678150	-2.64044990	0.04145360
H	2.19227970	-3.65247910	0.05460670
N	-0.04017100	1.30135310	-0.01560940
H	-0.73546990	2.05719410	-0.05716090
N	2.27111400	0.83425460	-0.01762040
N	1.52712210	3.04539210	-0.12090310
H	0.88239290	3.64088810	0.39447960
H	2.49844040	3.25298080	0.10170500
N	2.63366780	-1.53561190	0.00848460
H	3.64937310	-1.53655440	-0.00870310
N	0.50117990	-2.34059420	0.05410620
Se	-3.09714360	0.74486790	-0.09970490

point10

C	0.52516396	-0.90114467	0.18157102
C	1.85157484	-0.45142869	-0.09141164
C	1.26514631	1.68456982	-0.16078999
C	-0.52510938	0.03267055	0.28523922
C	1.75634970	-2.64840156	0.10837270
H	2.12683012	-3.67381114	0.12814331
N	-0.03086527	1.30507438	0.08472531
H	-0.75209641	2.03608751	0.11554632
N	2.26914670	0.81659619	-0.25708657
N	1.50449023	3.02747481	-0.38957012
H	0.94358865	3.66512293	0.17119714
H	2.49781146	3.24280971	-0.33598929

N	2.61901338	-1.58215175	-0.13346502
H	3.61874526	-1.62288744	-0.30910646
N	0.50333713	-2.29033365	0.30146882
Se	-3.09480912	0.84103484	0.66067446

The T1 minimum to S0T1 crossing point

point1

C	0.42315945	-0.84847708	0.13686556
C	1.76322945	-0.39805927	-0.00563927
C	1.24815516	1.75992091	0.00325648
C	-0.61292810	0.13307843	0.29989982
C	1.63936296	-2.60628281	0.03906793
H	1.98698020	-3.63823931	0.01507284
N	-0.06713274	1.44987637	0.13139633
H	-0.73840978	2.21047555	0.07049527
N	2.23881517	0.87452381	-0.05440728
N	1.55310297	3.10771503	-0.14461030
H	1.02756896	3.71981784	0.47749219
H	2.55567677	3.25147161	-0.03636022
N	2.51601483	-1.54085161	-0.05348515
H	3.52539657	-1.58033783	-0.16016352
N	0.36663852	-2.22359366	0.15718298
Se	-2.34734917	-0.18965774	-0.51660361

point2

C	0.41909590	-0.85306400	0.14403070
C	1.75818430	-0.40085690	-0.01498460
C	1.25168570	1.75960620	0.00973750
C	-0.61379350	0.13382420	0.31229060
C	1.63261920	-2.61111940	0.04600530
H	1.98135090	-3.64291020	0.02571370
N	-0.05906970	1.45113880	0.15995400
H	-0.72826200	2.21583080	0.13537320
N	2.23755270	0.86920830	-0.07216020
N	1.56115950	3.10708080	-0.11507510
H	0.98943110	3.74798090	0.43211700
H	2.56287000	3.27785220	-0.05118700
N	2.50791600	-1.54855980	-0.06450590
H	3.51633490	-1.59191190	-0.17881340
N	0.36207450	-2.23178370	0.17451670
Se	-2.30086340	-0.20093510	-0.58355250

point3

C	0.41474970	-0.85669910	0.15212120
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C	1.75278000	-0.40312730	-0.02386940
C	1.25364660	1.75935150	0.01719310
C	-0.61599800	0.13462280	0.32494360
C	1.62620800	-2.61488590	0.05270360
H	1.97600720	-3.64650300	0.03557360
N	-0.05264430	1.45229270	0.18897160
H	-0.71859140	2.22032320	0.20043810
N	2.23482660	0.86470120	-0.08914990
N	1.56851060	3.10590010	-0.08452130
H	0.95656810	3.77147910	0.38319070
H	2.56765580	3.29864950	-0.06568040
N	2.50000730	-1.55457330	-0.07551440
H	3.50740210	-1.60095570	-0.19766890
N	0.35795940	-2.23826110	0.19229560
Se	-2.25080160	-0.21093340	-0.65156650

point4

C	0.41010380	-0.85935460	0.16105880
C	1.74699360	-0.40486060	-0.03235160
C	1.25392810	1.75915430	0.02564900
C	-0.61966750	0.13545200	0.33776490
C	1.62013670	-2.61755270	0.05917940
H	1.97095730	-3.64899440	0.04472450
N	-0.04799610	1.45332950	0.21850670
H	-0.70957450	2.22394730	0.26574740
N	2.23056430	0.86104260	-0.10541410
N	1.57507060	3.10415530	-0.05284940
H	0.92918760	3.79036560	0.33101550
H	2.57020810	3.31363240	-0.08022520
N	2.49229110	-1.55885670	-0.08656360
H	3.49860390	-1.60741030	-0.21678400
N	0.35429930	-2.24300150	0.21052490
Se	-2.19682040	-0.21966690	-0.72052300

point5

C	0.40515040	-0.86099350	0.17075630
C	1.74081220	-0.40603080	-0.04046810
C	1.25244000	1.75902020	0.03518640
C	-0.62491730	0.13629560	0.35065810
C	1.61440680	-2.61908140	0.06542240
H	1.96619720	-3.65035210	0.05319530
N	-0.04523880	1.45423630	0.24864660
H	-0.70136410	2.22668350	0.33139900
N	2.22471010	0.85828570	-0.12093570

N	1.58078030	3.10182790	-0.01987520
H	0.90747390	3.80456850	0.27575040
H	2.57055800	3.32253020	-0.09530690
N	2.48476770	-1.56136700	-0.09769650
H	3.48994360	-1.61121610	-0.23618750
N	0.35109850	-2.24596110	0.22917930
Se	-2.13853250	-0.22706470	-0.79026380

point6

C	0.39989120	-0.86156040	0.18111280
C	1.73423650	-0.40658300	-0.04822820
C	1.24911340	1.75897180	0.04596050
C	-0.63185330	0.13715080	0.36352180
C	1.60901430	-2.61941630	0.07138860
H	1.96171160	-3.65052770	0.06096180
N	-0.04446350	1.45500210	0.27951870
H	-0.69409470	2.22850090	0.39754460
N	2.21722960	0.85650910	-0.13562660
N	1.58560610	3.09890550	0.01469880
H	0.89164030	3.81381440	0.21737060
H	2.56853330	3.32497580	-0.11154200
N	2.47743890	-1.56204170	-0.10894290
H	3.48142650	-1.61230000	-0.25587570
N	0.34835870	-2.24706990	0.24819210
Se	-2.07550280	-0.23295000	-0.86059470

point7

C	0.39433970	-0.86096810	0.19200880
C	1.72728640	-0.40641580	-0.05560380
C	1.24390390	1.75906150	0.05822920
C	-0.64057110	0.13803910	0.37624550
C	1.60395100	-2.61847080	0.07698980
H	1.95747340	-3.64944310	0.06792960
N	-0.04574010	1.45562580	0.31130680
H	-0.68788730	2.22935910	0.46441120
N	2.20811630	0.85583600	-0.14930090
N	1.58953970	3.09539050	0.05132920
H	0.88200050	3.81750710	0.15560910
H	2.56365460	3.32042180	-0.12973160
N	2.47031300	-1.56078100	-0.12031470
H	3.47306720	-1.61055630	-0.27579960
N	0.34607860	-2.24621780	0.26743880
Se	-2.00723990	-0.23700680	-0.93128720

point8

C	0.38852470	-0.85907280	0.20329820
C	1.72001160	-0.40535150	-0.06251070
C	1.23679950	1.75939360	0.07240440
C	-0.65115400	0.13902860	0.38870380
C	1.59920540	-2.61610270	0.08207440
H	1.95344190	-3.64696800	0.07390260
N	-0.04911680	1.45613280	0.34428040
H	-0.68285390	2.22921540	0.53233750
N	2.19740580	0.85646560	-0.16162830
N	1.59260300	3.09131740	0.09071240
H	0.87908440	3.81451060	0.08985890
H	2.55494320	3.30799970	-0.15095610
N	2.46341340	-1.55741890	-0.13179630
H	3.46490150	-1.60581640	-0.29584280
N	0.34425220	-2.24323270	0.28670730
Se	-1.93317590	-0.23871940	-1.00208560

point9

C	0.38249830	-0.85562640	0.21479500
C	1.71251130	-0.40307970	-0.06877360
C	1.22783900	1.76016820	0.08914960
C	-0.66366650	0.14027820	0.40074870
C	1.59476470	-2.61206790	0.08638810
H	1.94955970	-3.64287420	0.07851940
N	-0.05461400	1.45660910	0.37885020
H	-0.67909920	2.22804290	0.60184390
N	2.18520320	0.85873100	-0.17204370
N	1.59486240	3.08678440	0.13393870
H	0.88385860	3.80271580	0.01898780
H	2.54052030	3.28625120	-0.17675370
N	2.45679570	-1.55166850	-0.14332680
H	3.45700950	-1.59779210	-0.31577940
N	0.34286530	-2.23783640	0.30564160
Se	-1.85262220	-0.23725440	-1.07272570

point10

C	0.37669696	-0.85003083	0.22811035
C	1.70482149	-0.39909719	-0.07468723
C	1.21729542	1.76184033	0.10829590
C	-0.67748731	0.14240235	0.41513149
C	1.59074295	-2.60586328	0.09052875
H	1.94585773	-3.63668668	0.08226068
N	-0.06155549	1.45754608	0.41671739

H	-0.67564311	2.22631769	0.67530528
N	2.17140629	0.86309318	-0.18181761
N	1.59672408	3.08213880	0.18000795
H	0.89807619	3.77798371	-0.06117336
H	2.51626349	3.25237161	-0.21392824
N	2.45029660	-1.54311377	-0.15586400
H	3.44897642	-1.58618374	-0.33791034
N	0.34240089	-2.22934048	0.32647233
Se	-1.76658647	-0.23199658	-1.13798925