

Electronic Supplementary Information:

**Selenium Substitution Effects on Excited-State
Properties and Photophysics of Uracil: A MS-
CASPT2 Study**

Qin Peng¹, Yun-Hua Zhu¹, Teng-Shuo Zhang¹, Xiang-Yang Liu^{2,*}, Wei-Hai
Fang¹, Ganglong Cui^{1,*}

¹Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, China and ²College of Chemistry and Materials Science, Sichuan Normal University, Chengdu 610068, China

Email: xiangyangliu@sicnu.edu.cn; ganglong.cui@bnu.edu.cn

I. Tables

Table S1. Energies of all MS-CASPT2 Optimized Excited-State Minimum-Energy Structures in S_1 , S_2 , T_1 , and T_2 States of 2SeU, 4SeU, and 24SeU Relative to their Corresponding S_0 Minima (in kcal/mol).

System	structure	S_0	$S_1(n\pi^*)$	$S_2(\pi\pi^*)$	$T_1(\pi\pi^*)$	$T_2(n\pi^*)$
2SeU	S1T-MIN	29.0	65.8	76.1	58.6	61.4
	S2P-MIN	12.2	74.4	78.1	65.4	74.8
	S2T-MIN	38.2	68.3	71.8	58.7	62.2
	T1P-MIN	4.6	72.9	82.8	60.2	72.5
	T1T-MIN	29.0	66.2	74.0	57.2	61.9
	T2P-MIN	4.2	70.6	84.3	63.2	70.4
	T2T-MIN	32.8	66.3	73.0	61.7	63.4
4SeU	S1-MIN	5.4	51.0	71.2	47.6	50.1
	S2-MIN	11.2	53.9	68.0	50.0	53.4
	T1-MIN	4.2	51.2	70.3	47.1	50.3
	T2-MIN	4.3	51.0	71.4	47.4	50.0
24SeU	S1-MIN	5.0	48.7	68.6	44.8	47.8
	S2-MIN	11.0	52.9	65.0	48.4	52.0
	T1-MIN	4.9	49.0	67.9	44.5	48.0
	T2-MIN	4.5	48.8	69.1	44.8	47.7

Table S2. MS-CASPT2 Energies of all Intersection Structures Relative to Their Corresponding S_0 Minima (in kcal/mol).

System	structure	S_0	$S_1(n\pi^*)$	$S_2(\pi\pi^*)$	$T_1(\pi\pi^*)$	$T_2(n\pi^*)$
2SeU	S2S1	45.8	72.4	74.2	62.1	64.4
	S2S1T2	13.3	75.2	78.9	67.6	74.9
	S1T2T1	27.0	74.5	95.5	73.8	75.0
	T2T1	26.6	71.5	90.1	66.6	70.0
	T2T1S0	64.0	79.4	80.8	63.3	64.0
4SeU	S2S1	46.5	80.6	83.8	75.7	77.3
	T1S0	57.9	66.6	96.8	61.0	74.2
24SeU	S2S1	27.7	73.2	74.5	68.3	70.7
	T1S0	53.4	63.0	86.1	57.6	66.8

Table S3. MS-CASPT2 Calculated Vertical Excitation Energies (eV) and Oscillator Strength at the MS-CASPT2 Optimized S_0 Minima of 2SeU, 4SeU and 24SeU.

System	States	VEE (eV)	Osc.	Configuration	Weight
2SeU	S_1 ($n\pi^*$)	3.33	0.59618359E-05	22222u200d0	0.779878
	S_2 ($\pi\pi^*$)	3.80	0.29236149	22222u00d0	0.764233
	S_3 ($\pi\pi^*$)	4.28	0.11169655	22222ud000	0.706180
4SeU	S_1 ($n\pi^*$)	2.38	0.61096490E-05	22222u2d000	0.879147
	S_2 ($\pi\pi^*$)	3.40	0.43728392	22222ud000	0.583175
				2222u22d000	0.156715
	S_3 ($\pi\pi^*$)	4.21	0.14768350E-01	2222u22d000	0.560885
24SeU	S_1 ($n\pi^*$)	2.38	0.92562809E-06	u22222d000	0.867133
	S_2 ($\pi\pi^*$)	3.15	0.18982392	2222u22d000	0.486569
				22222u200d0	0.115125
				22222u2d000	0.615997
	S_3 ($\pi\pi^*$)	3.37	0.60032308E-01	2222u22d000	0.105966
				22222u200d0	0.374354
				2222u2200d0	0.199343
	S_4 ($\pi\pi^*$)	3.69	0.19493457	2222u22d000	0.122111

II. Figures

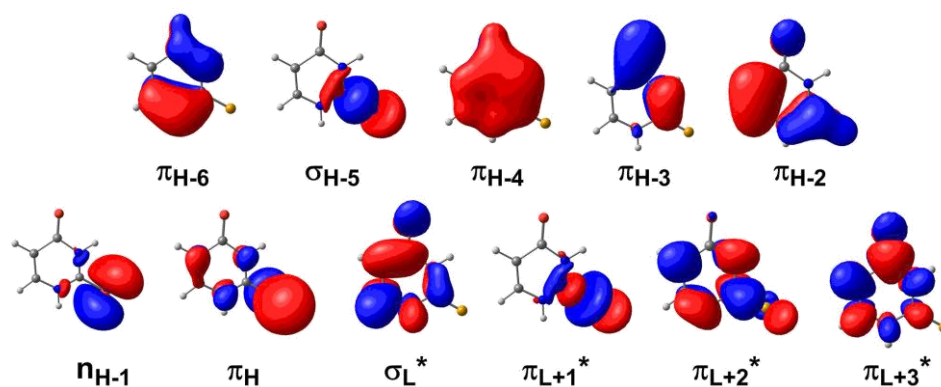


Figure S1. Molecular orbitals of 2SeU used as active space in all MS-CASPT2 calculations.

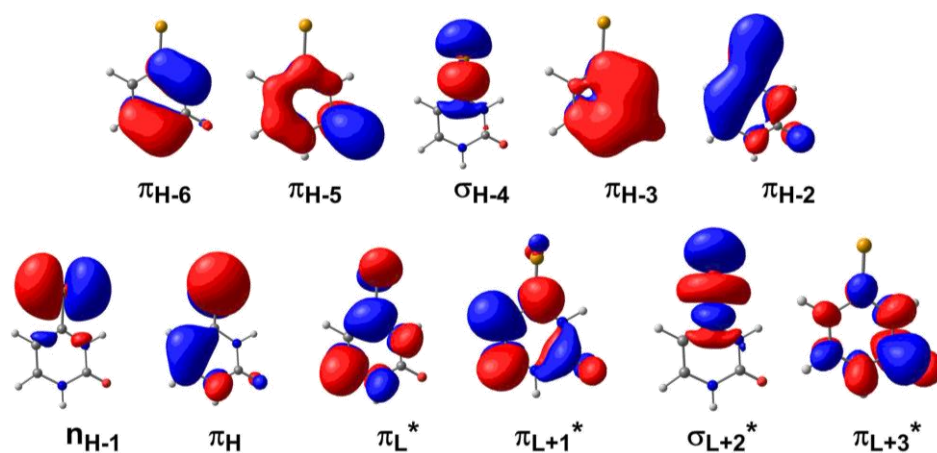


Figure S2. Molecular orbitals of 4SeU used as active space in all MS-CASPT2 calculations.

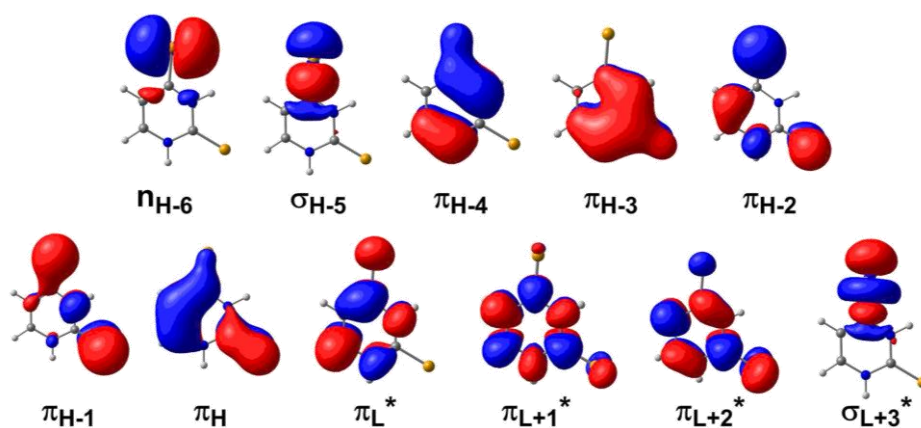


Figure S3. Molecular orbitals of 24SeU used as active space in all MS-CASPT2 calculations.

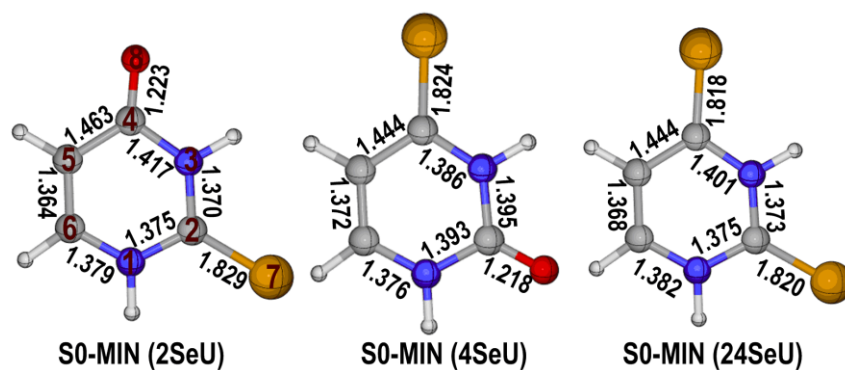


Figure S4. MS-CASPT2 optimized ground-state minimum-energy structures of 2SeU, 4SeU, and 24SeU. Also shown are selected bond lengths and atomic numbering.

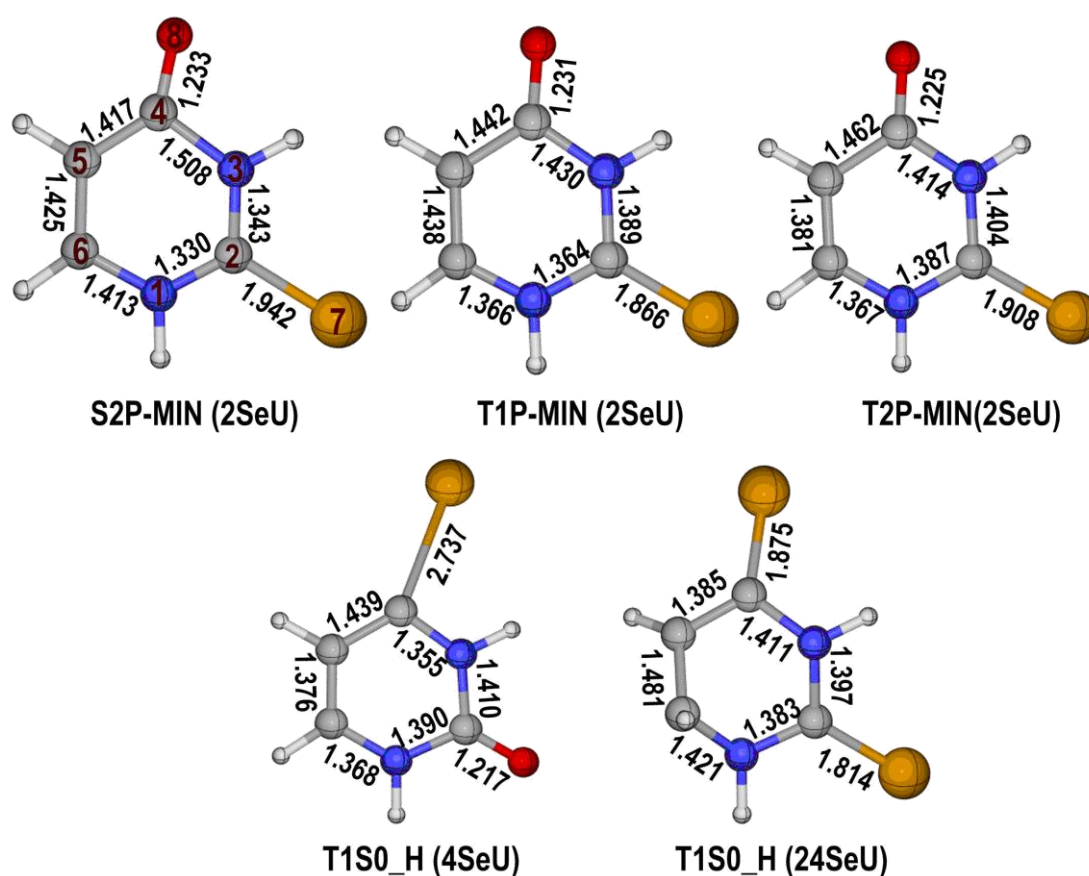


Figure S5. MS-CASPT2 optimized additional structures and intersections of 2SeU, 4SeU, and 24SeU. Also shown are selected bond lengths (in Å) and atomic numbering.

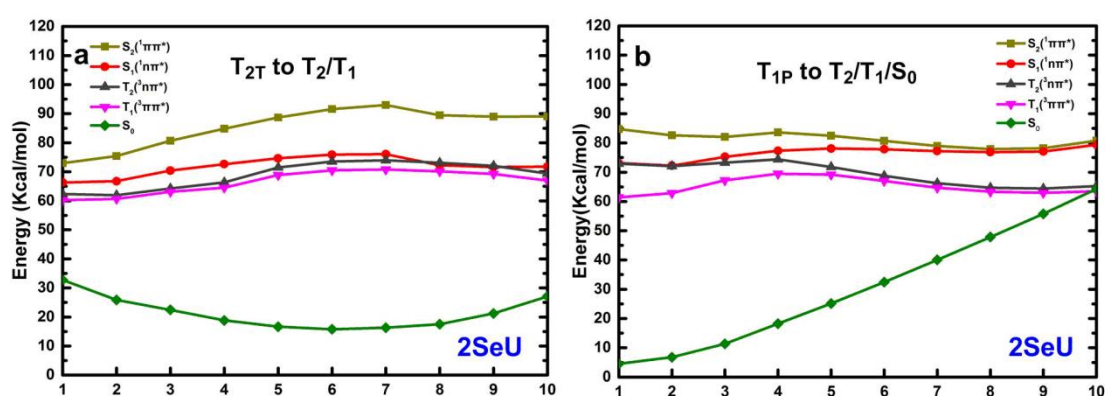


Figure S6. MS-CASPT2 calculated LIIC paths connecting T_{2T} and T_2/T_1 intersections (a), T_{1P} and $T_2/T_1/S_0$ intersections (b) of 2SeU.

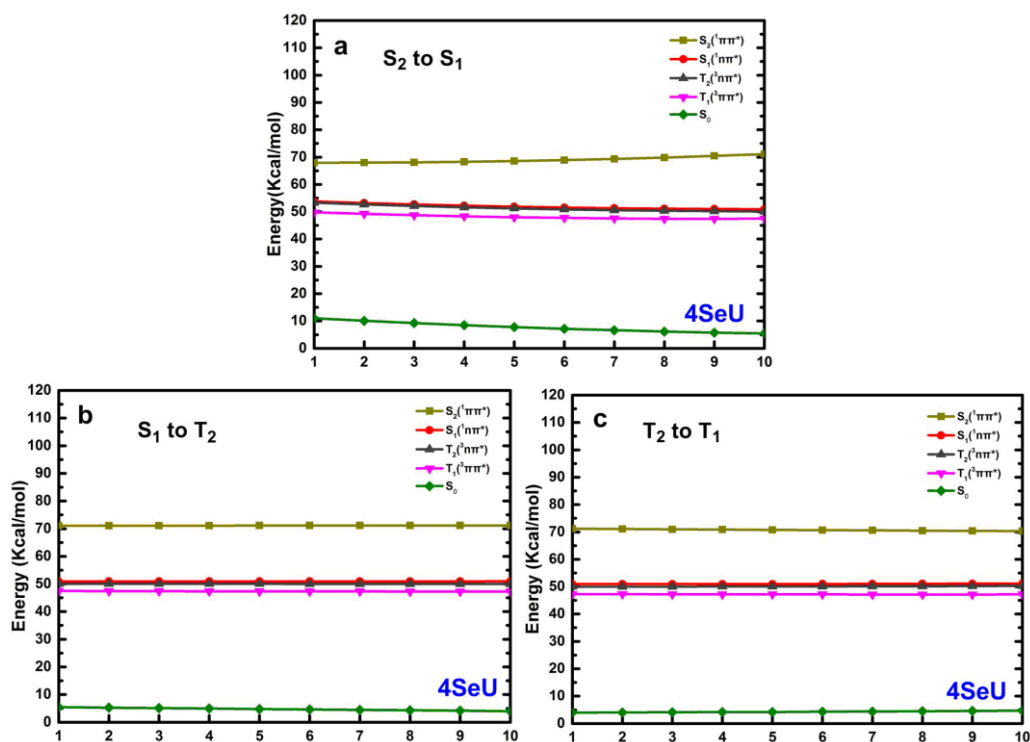


Figure S7. MS-CASPT2 calculated LIIC paths connecting S_2 and S_1 (a), S_1 and T_2 (b), T_2 and T_1 (c) and T_1 and T_1/S_0_H intersections (d) of 4SeU.

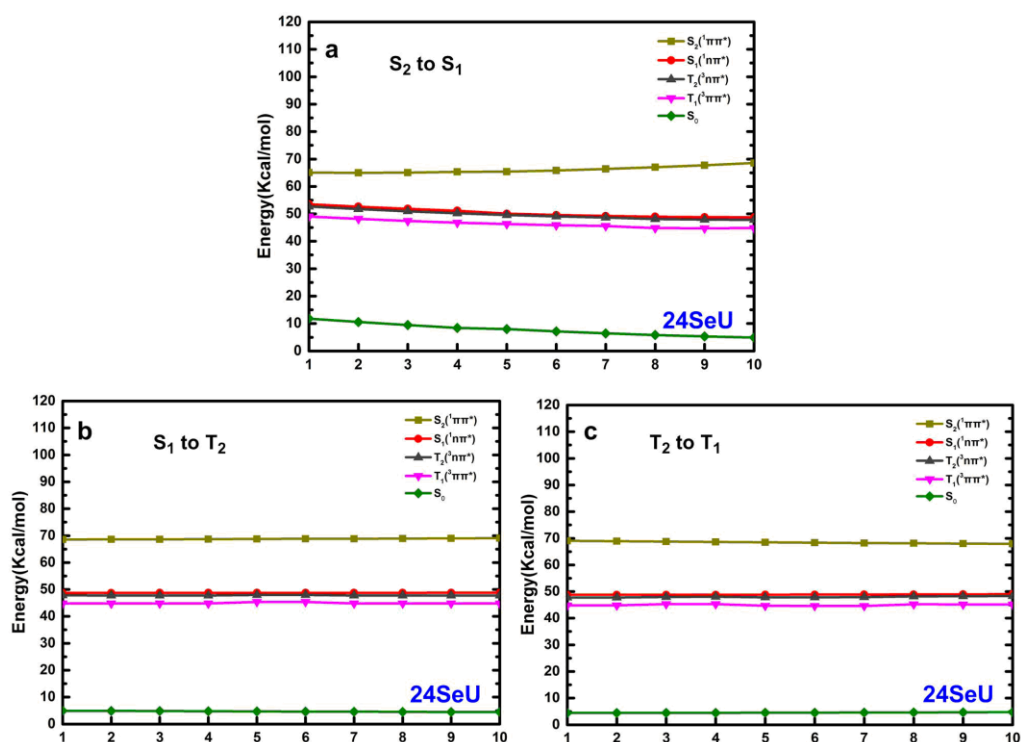


Figure S8. MS-CASPT2 calculated LIIC paths connecting S_2 and S_1 (a), S_1 and T_2 (b), T_2 and T_1 (c) and T_1 and T_1/S_0_H intersections (d) of 24SeU.

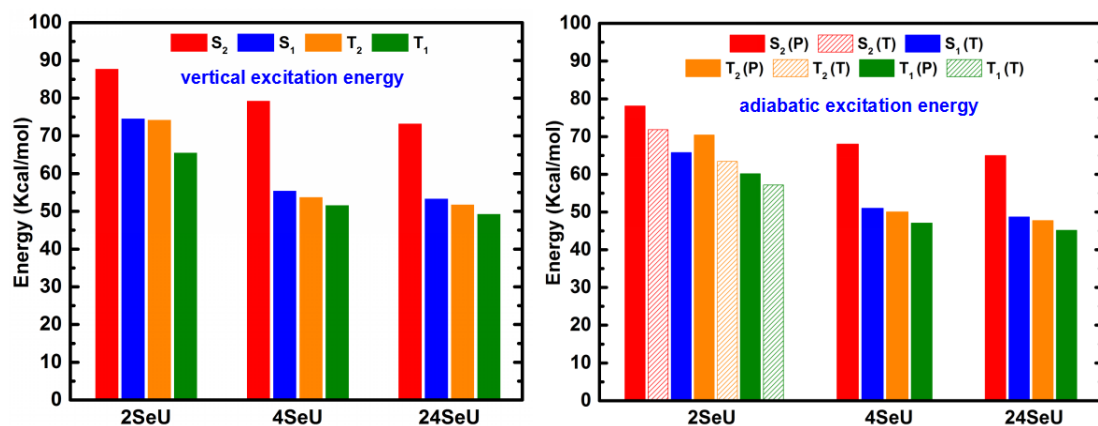


Figure S9. Comparison of vertical and adiabatic excitation energies to different excited states of 2SeU, 4SeU, and 24SeU based on the present MS-CASPT2 calculations.

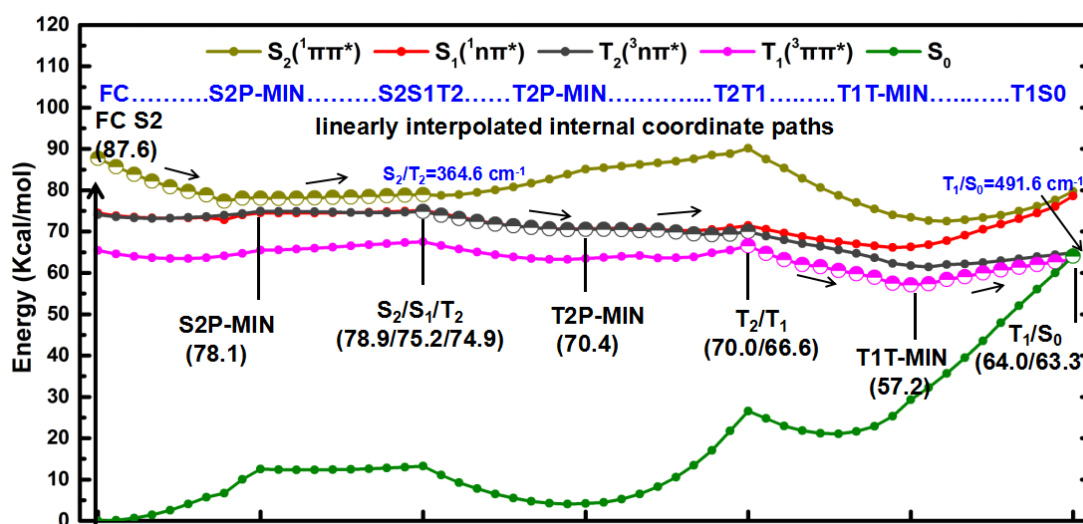


Figure S10. The other efficient excited-state relaxation pathways of 2SeU based on our MS-CASPT2 calculations. See main text for the main ones.

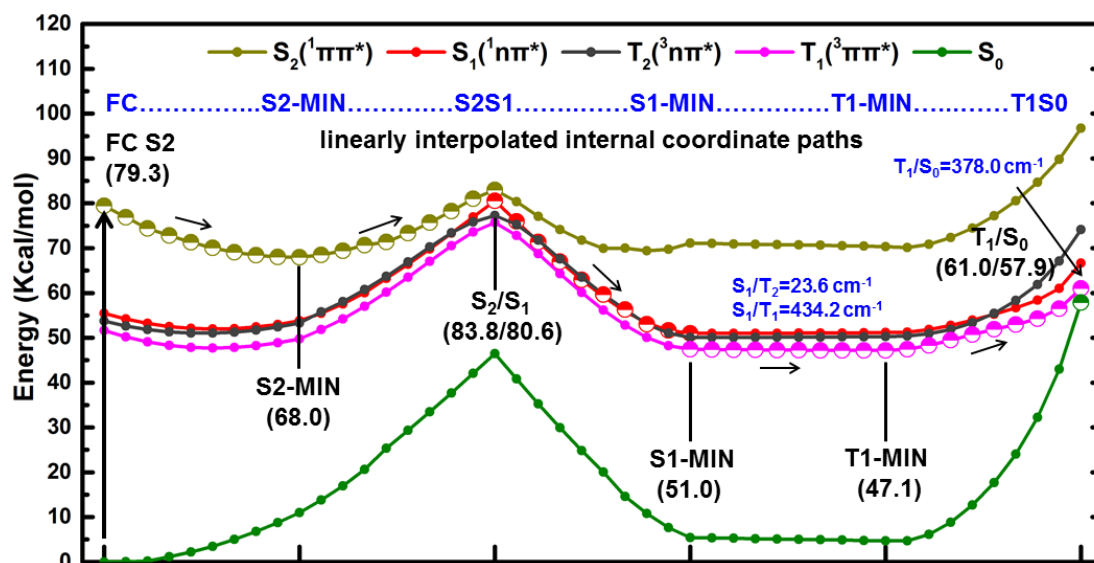


Figure S11. The efficient excited-state relaxation pathways of 4SeU proposed based on our MS-CASPT2 calculations.

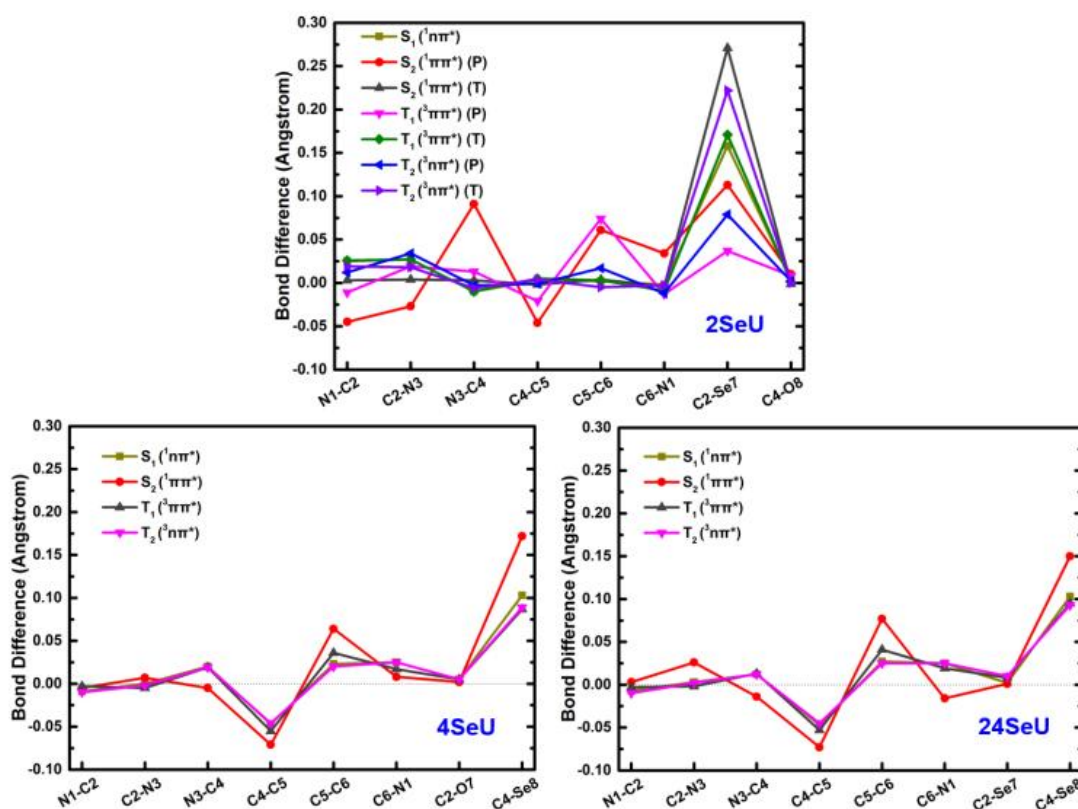


Figure S12. Bond-length changes (in angstrom) of excited-state minimum-energy structures of 2SeU, 4SeU, and 24SeU relative to corresponding ground-state structures.

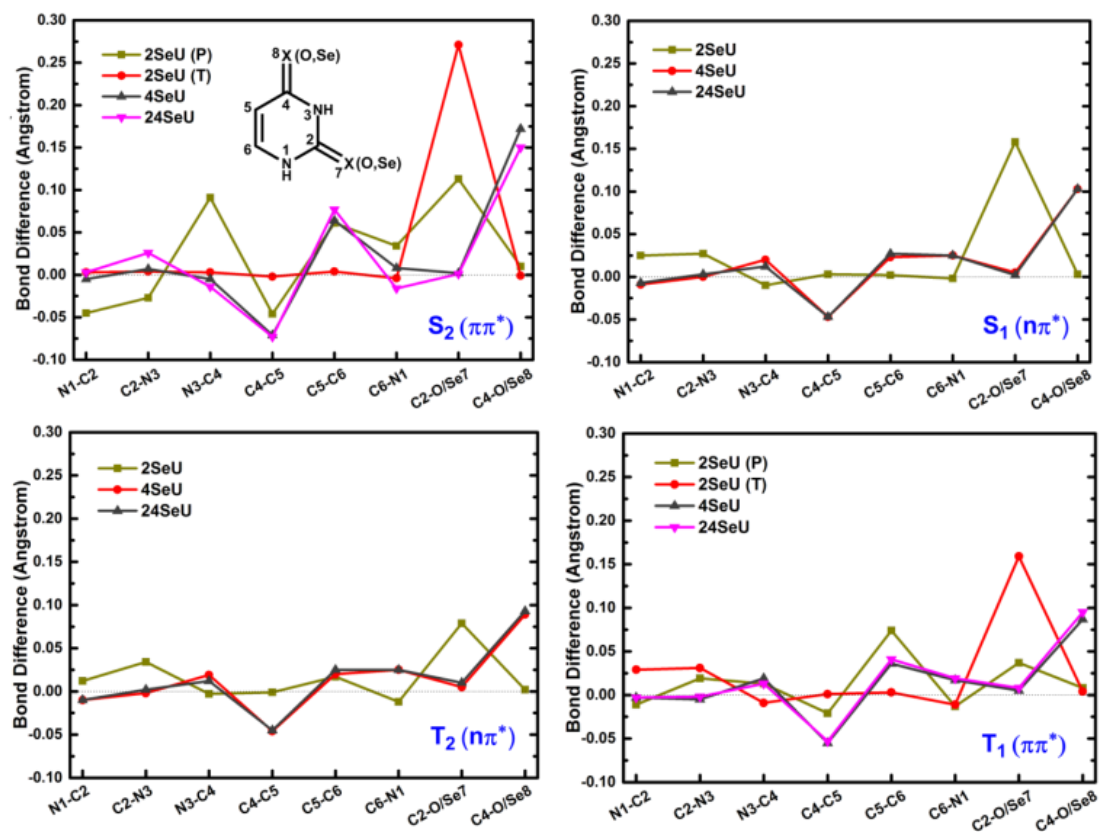


Figure S13. Comparison of selected bond lengths of 2SeU, 4SeU, and 24SeU related to same kinds of excited-state minima.

III. Cartesian Coordinates

S0-MIN (2SeU)

C	-0.14044724	-0.30709756	0.00020965
N	0.82878474	0.66080021	0.01037986
C	0.66212094	2.06796183	0.01504803
C	-0.74196134	2.47887751	0.00014152
C	-1.72385374	1.53249497	-0.00903999
N	-1.42335821	0.18632079	-0.00267915
H	-0.96974157	3.54506711	-0.00310666
H	-2.78965002	1.7730447	-0.02039461
Se	0.21506513	-2.10077111	-0.00823963

O	1.6382982	2.80410317	0.02867292
H	1.79414615	0.32754014	0.01464356
H	-2.16133828	-0.51253287	-0.01557747

S1-MIN (2SeU)

C	-0.13959437	-0.32682856	-0.27882533
N	0.8472649	0.66052117	-0.22123054
C	0.67265775	2.03403186	0.03051456
C	-0.73222134	2.42953669	0.16895013
C	-1.72081329	1.49951743	0.01207685
N	-1.44590693	0.1621199	-0.16359941
H	-0.95865727	3.48089489	0.34846587
H	-2.78397842	1.75556255	0.03159304
Se	0.18945841	-1.94665768	0.82420241
O	1.64181013	2.78310281	0.08187706
H	1.81569117	0.38030821	-0.37060876
H	-2.19764598	-0.45630039	-0.45335787

S2T-MIN (2SeU)

C	-0.1379933	-0.2832905	-0.43590512
N	0.83291622	0.66941372	-0.24186735
C	0.67068113	2.05210562	0.04012996
C	-0.73360076	2.44130439	0.15070239
C	-1.71995858	1.50508034	0.0029208
N	-1.42028866	0.18793458	-0.25489711
H	-0.96905597	3.48487623	0.36210612
H	-2.78361949	1.74271155	0.08060025

Se	0.16070855	-1.9716076	0.77726885
O	1.64764819	2.77633014	0.16200265
H	1.80248219	0.35625291	-0.3120562
H	-2.16185475	-0.50530244	-0.32094721

S2P-MIN (2SeU)

C	-0.16378606	-0.25393138	0.00426352
N	0.83698692	0.64227463	0.01161257
C	0.65238275	2.13866896	0.01297034
C	-0.71932947	2.49364489	0.00026691
C	-1.77896619	1.54101842	-0.01113035
N	-1.42356285	0.17302713	-0.00673383
H	-0.9551579	3.56028826	-0.00011369
H	-2.84504474	1.75596161	-0.01710931
Se	0.22884144	-2.15584788	-0.0117195
O	1.69926443	2.78937162	0.02329174
H	1.80170416	0.3143399	0.02140339
H	-2.14526774	-0.54300729	-0.01694376

T1T-MIN (2SeU)

C	-0.13125387	-0.31349857	-0.36378916
N	0.84719665	0.67324885	-0.21691297
C	0.67593769	2.04903413	0.02244565
C	-0.734844	2.4462708	0.10270978
C	-1.72185809	1.50604317	0.00259056
N	-1.4289868	0.18067392	-0.18038309
H	-0.96347914	3.49978191	0.26806121

H	-2.78612206	1.75035792	0.06084524
Se	0.14750191	-1.98787462	0.69465217
O	1.64150704	2.79121296	0.14689901
H	1.81834262	0.3652744	-0.26493157
H	-2.17587719	-0.504716	-0.26212882

T1P-MIN (2SeU)

C	-0.1568097	-0.28495995	0.00035181
N	0.85554219	0.66585829	-0.00403422
C	0.66870386	2.08394956	0.00839735
C	-0.71547251	2.48750513	0.00317928
C	-1.77136015	1.51072886	-0.00851372
N	-1.43702381	0.18597959	-0.00054659
H	-0.94028503	3.55452242	0.00570349
H	-2.83436357	1.7483767	-0.01630261
Se	0.20426683	-2.11610918	-0.00264575
O	1.66356489	2.8092538	0.02087591
H	1.81717441	0.33446451	0.0300733
H	-2.16587263	-0.52376082	-0.02648024

T2T-MIN (2SeU)

C	-0.03622457	-0.00032608	-0.02406491
N	1.21478886	0.05798954	-0.62362007
C	2.48247133	0.10941526	-0.00574362
C	2.41293356	0.05314545	1.45900789
C	1.20879282	-0.09025517	2.07201458
N	0.02999067	-0.11514353	1.36351298

H	3.3455553	0.08226516	2.02279092
H	1.10297515	-0.20582417	3.15434463
Se	-1.36145874	1.42058552	-0.68118149
O	3.49996485	0.15889599	-0.6833213
H	1.25244328	0.03576307	-1.64236252
H	-0.84333251	-0.26942108	1.85783593

T2P-MIN (2SeU)

C	-0.1568097	-0.28495995	0.00035181
N	0.85554219	0.66585829	-0.00403422
C	0.66870386	2.08394956	0.00839735
C	-0.71547251	2.48750513	0.00317928
C	-1.77136015	1.51072886	-0.00851372
N	-1.43702381	0.18597959	-0.00054659
H	-0.94028503	3.55452242	0.00570349
H	-2.83436357	1.7483767	-0.01630261
Se	0.20426683	-2.11610918	-0.00264575
O	1.66356489	2.8092538	0.02087591
H	1.81717441	0.33446451	0.0300733
H	-2.16587263	-0.52376082	-0.02648024

S2S1 (2SeU)

C	-0.14445319	-0.25900545	-0.40561198
N	0.83126495	0.67166234	-0.20959705
C	0.65944596	2.03703064	0.02262068
C	-0.74337197	2.44804214	0.13164539
C	-1.71484243	1.52233104	0.00119355

N	-1.41408582	0.19679032	-0.23507209
H	-0.96066171	3.48636079	0.32086578
H	-2.7659383	1.75813532	0.07089172
Se	0.20357581	-2.06622884	0.84368668
O	1.60759756	2.76729129	0.1118098
H	1.77906979	0.36294547	-0.30377804
H	-2.14953587	-0.46954618	-0.33859643

S2S1T2 (SeU)

C	-0.17219558	-0.25735525	-0.06658548
N	0.8238826	0.64659508	-0.01887582
C	0.64957647	2.11939933	0.01406802
C	-0.72625917	2.49501563	0.02136668
C	-1.77583198	1.55387003	-0.00540853
N	-1.43170685	0.1851277	-0.04586833
H	-0.94770995	3.56101972	0.0519736
H	-2.83867072	1.77268004	0.0015768
Se	0.29844225	-2.1959192	0.13900597
O	1.68355916	2.77699698	0.03144804
H	1.78435959	0.31589364	-0.02962136
H	-2.15938224	-0.5175112	-0.08302141

T2T1S0 (2SeU)

C	-0.08365563	-0.25158305	0.42634807
N	0.84230493	0.73176825	0.27604011
C	0.66389686	2.1160254	-0.00753494
C	-0.74401769	2.47455547	-0.15483411

C	-1.707284	1.51841315	-0.00515766
N	-1.36161639	0.21048494	0.27444493
H	-0.9979661	3.51345333	-0.36675904
H	-2.77621815	1.72748583	-0.09970475
Se	-0.00276368	-2.40670711	-0.94023982
O	1.62552565	2.86489532	-0.09400441
H	1.82069123	0.45292535	0.36310244
H	-2.09083226	-0.49590798	0.33835722

S1T2T1 (2SeU)

C	-0.18989373	-0.2333557	0.15465192
N	0.84117148	0.64231789	-0.25373038
C	0.66971281	2.01745507	0.00867855
C	-0.73145387	2.40726519	0.18703818
C	-1.74084338	1.51308117	0.00876381
N	-1.50237552	0.16841613	-0.12264122
H	-0.92566944	3.45752948	0.350041
H	-2.79531867	1.81446259	-0.05162077
Se	0.34786281	-2.07820658	0.65164246
O	1.61267667	2.77512004	-0.03820909
H	1.81543696	0.38651761	-0.30319564
H	-2.21324136	-0.414794	-0.58136082

T2T1 (2SeU)

C	-0.15924101	-0.24677652	-0.35356898
N	0.85366153	0.6455785	0.04102621
C	0.66864729	2.03172532	-0.01228607

C	-0.72598657	2.44687482	-0.1667737
C	-1.73838112	1.52191275	-0.00866601
N	-1.44527426	0.16865581	0.08743318
H	-0.93721182	3.50957256	-0.23884828
H	-2.78604429	1.79500634	0.10331518
Se	0.2692993	-2.08338597	-0.2404061
O	1.60812095	2.79473829	0.16217545
H	1.76878868	0.35423369	0.35714814
H	-2.18831392	-0.4823267	0.27950897

S0-MIN (4SeU)

C	-3.35115637	-1.03221933	-0.08972848
N	-1.96634632	-0.87652924	-0.02766602
C	-1.24271184	0.30492859	0.00550401
C	-2.04238898	1.50728512	-0.00813004
C	-3.40975607	1.40885657	-0.07071763
N	-4.03179932	0.18246219	-0.10928913
H	-1.54554567	2.47549483	0.02584465
H	-4.06905391	2.27990775	-0.09283375
Se	0.58073574	0.30197632	0.05976409
O	-3.90844435	-2.11469578	-0.12416036
H	-5.04429335	0.10608374	-0.15345104
H	-1.44342261	-1.75334389	-0.01972904

S1-MIN (4SeU)

C	-3.34793679	-1.03059087	-0.07482367
N	-1.96338121	-0.89231903	0.02970701

C	-1.28373588	0.33745112	-0.00618086
C	-2.03355379	1.51539284	-0.03163195
C	-3.4262243	1.43632538	-0.06134112
N	-4.03155898	0.17248248	-0.05920378
H	-1.54069291	2.48914445	-0.02457455
H	-4.09184406	2.2984759	-0.09021341
Se	0.63858589	0.27019409	0.11431925
O	-3.8956946	-2.12054987	-0.15702963
H	-5.03836396	0.07946973	-0.14662163
H	-1.45978246	-1.76526934	-0.09699842

S2-MIN (4SeU)

C	-3.34646383	-1.02845857	-0.09306995
N	-1.95739013	-0.85601749	-0.00806956
C	-1.30772001	0.36204298	0.00879784
C	-2.03322803	1.52788635	-0.01642875
C	-3.46517342	1.44109574	-0.07161569
N	-4.03217647	0.17857683	-0.09205251
H	-1.53313431	2.49580564	-0.00120583
H	-4.14633039	2.29168843	-0.06736477
Se	0.67471396	0.13629188	0.05913403
O	-3.88643461	-2.12055518	-0.15145576
H	-5.04267396	0.07084966	-0.15872671
H	-1.39817185	-1.70899939	-0.01253508

T1-MIN (4SeU)

C	-3.34573572	-1.03423408	-0.08997732
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N	-1.96540552	-0.89076394	-0.01689222
C	-1.28401116	0.33720719	0.00459004
C	-2.02894411	1.50995009	-0.01341164
C	-3.43438585	1.43754681	-0.06334788
N	-4.02670328	0.1775229	-0.10105176
H	-1.52456867	2.47657458	0.01183489
H	-4.10108365	2.29836488	-0.08530925
Se	0.62556606	0.27993194	0.06752335
O	-3.9084814	-2.11937668	-0.13668927
H	-5.03638705	0.08082168	-0.15077038
H	-1.44404272	-1.76333848	-0.03109132

T2-MIN (4SeU)

C	-3.34434242	-1.03003036	-0.08878831
N	-1.96037202	-0.88908823	-0.01127294
C	-1.28254482	0.34200498	0.0080836
C	-2.03558112	1.52008142	-0.01334053
C	-3.42400066	1.43706932	-0.06081002
N	-4.0271254	0.17255155	-0.09185743
H	-1.54399332	2.4948202	0.00669816
H	-4.09283038	2.29679443	-0.08217167
Se	0.62831986	0.26700487	0.05813088
O	-3.89213337	-2.12269046	-0.14225122
H	-5.03457884	0.07758792	-0.16086926
H	-1.46500055	-1.77589877	-0.026144

S2S1 (4SeU)

C	-3.35299899	-0.98009955	-0.06664874
N	-1.99171918	-0.75535752	0.12954142
C	-1.35000164	0.39897063	0.24766431
C	-2.18501841	1.56825915	0.08646454
C	-3.51918976	1.4223278	-0.11420828
N	-4.0809566	0.17726829	-0.1816104
H	-1.74974956	2.55021006	0.1716095
H	-4.21013234	2.24883764	-0.20539688
Se	1.27123711	-0.25097037	-0.29933485
O	-3.82703791	-2.07437032	-0.13576704
H	-5.06100902	0.06356347	-0.33471805
H	-1.41760675	-1.57843238	0.09781171

T1S0_H (4SeU)

C	-3.35587382	-1.00148837	-0.09705277
N	-1.98674028	-0.7535969	0.12918412
C	-1.31906415	0.41945876	0.24636025
C	-2.16701595	1.57136037	0.0860478
C	-3.52278357	1.42832412	-0.09967797
N	-4.0799791	0.18192337	-0.180834
H	-1.73460718	2.57211892	0.13239677
H	-4.22458302	2.26480295	-0.1780374
Se	1.2778682	-0.23072141	-0.32091684
O	-3.84778898	-2.11086554	-0.19388059
H	-5.08033331	0.06258731	-0.3247446
H	-1.43328191	-1.61369669	0.19656248

T1S0_L (4SeU)

C	-3.27586115	-1.0137102	-0.13560803
N	-1.93154413	-0.84969748	0.24457746
C	-1.24794035	0.38572977	0.54130744
C	-2.06896938	1.55862787	0.25257207
C	-3.3624672	1.43551731	-0.14167149
N	-3.93984488	0.17848982	-0.34042542
H	-1.62553208	2.54919551	0.36968186
H	-4.02800923	2.28467734	-0.31413607
Se	0.20753268	0.00252812	-0.77553189
O	-3.7915849	-2.11265512	-0.25051024
H	-4.9017566	0.08437283	-0.64587281
H	-1.50820584	-1.71286884	0.59102437

S0-MIN (24SeU)

C	-4.43204937	-0.49269273	0.02576018
N	-3.06506004	-0.35307756	0.08547061
C	-2.42552362	0.87197595	0.08016801
C	-3.14060793	2.03622517	0.01452152
C	-4.58232964	1.99145474	-0.04690787
N	-5.11609458	0.69622021	-0.04439693
H	-1.33512719	0.83703748	0.13215728
H	-2.64001632	3.00398599	0.010381
Se	-5.25970737	-2.11374238	0.04084979
Se	-5.66496716	3.4501047	-0.11972664
H	-2.53429165	-1.21964215	0.13746236
H	-6.13398151	0.61270197	-0.08716817

S1-MIN (24SeU)

C	-4.43180202	-0.49059368	0.02719247
N	-3.07189152	-0.35581305	0.08384205
C	-2.39019254	0.87463318	0.07891205
C	-3.13860434	2.04995566	0.01408557
C	-4.53187415	1.97508063	-0.04611957
N	-5.12923783	0.69419183	-0.04030901
H	-1.30347464	0.82967296	0.12689961
H	-2.63417319	3.01802202	0.01242148
Se	-5.27390139	-2.1066434	0.03707861
Se	-5.72623915	3.47764157	-0.11682358
H	-2.55905823	-1.23147348	0.13667365
H	-6.13930734	0.58587715	-0.0852822

S2-MIN (24SeU)

C	-4.43267801	-0.49531652	0.02745334
N	-3.06455078	-0.34070582	0.08132934
C	-2.37206976	0.83649357	0.08026198
C	-3.13144562	2.06466242	0.01612205
C	-4.49832828	1.96796353	-0.0402388
N	-5.11416089	0.72525104	-0.03708755
H	-1.28528936	0.77467796	0.12878419
H	-2.63211915	3.03224605	0.01145506
Se	-5.27588356	-2.10961705	0.04136095
Se	-5.83271142	3.41132536	-0.12965424
H	-2.55754947	-1.22738068	0.12794611

H	-6.1329701	0.68095153	-0.07916131
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T1-MIN (24SeU)

C	-4.43454777	-0.49085368	0.02656528
N	-3.0702073	-0.35331765	0.08343339
C	-2.38273745	0.86756429	0.07879818
C	-3.14719675	2.04969012	0.01459503
C	-4.53487632	1.97598308	-0.04595834
N	-5.12566054	0.69183106	-0.04016269
H	-1.29620058	0.8215674	0.13012251
H	-2.65625349	3.02428807	0.01194301
Se	-5.26547696	-2.11911533	0.03806045
Se	-5.71638137	3.47856943	-0.12179575
H	-2.56129989	-1.23280856	0.13391683
H	-6.13891798	0.60715314	-0.08094673

T2-MIN (24SeU)

C	-4.43062594	-0.48811129	0.02919472
N	-3.07305457	-0.35433338	0.08933332
C	-2.39242854	0.87662372	0.08144236
C	-3.14061785	2.04971996	0.01024706
C	-4.535644	1.97535281	-0.05818738
N	-5.1295225	0.69315673	-0.04458249
H	-1.3054357	0.83245092	0.12296965
H	-2.63573378	3.0176125	0.00688839
Se	-5.27464082	-2.11174709	0.04172569
Se	-5.71315053	3.47979286	-0.09286082

H	-2.5606194	-1.22983099	0.14570014
H	-6.13828274	0.57986462	-0.10329947

S2S1T2T1 (24SeU)

C	-4.42461029	-0.49705063	-0.23891612
N	-3.04591162	-0.31320527	0.05055852
C	-2.42418164	0.81538626	0.07519885
C	-3.15207521	2.04166516	-0.09586622
C	-4.52563615	1.91711799	-0.06862704
N	-5.12020072	0.73773166	-0.06977621
H	-1.36393989	0.79850385	0.28024005
H	-2.65981566	2.99441357	-0.05027602
Se	-5.23204182	-2.14701003	0.15169109
Se	-5.71288734	3.47951068	0.02610657
H	-2.55134691	-1.17585797	0.20477426
H	-6.11710913	0.6693461	-0.03653656

T1S0_H (24SeU)

C	-4.32999136	-0.41840171	0.11740087
N	-3.01792017	-0.24199511	0.51711669
C	-2.35471066	0.84538203	-0.11235978
C	-3.11713061	2.06847574	0.22954099
C	-4.44440094	1.99818926	-0.15994544
N	-4.87998272	0.70270761	-0.50897041
H	-2.07011865	0.67478457	-1.16600011
H	-2.78853175	2.77413031	0.99622143
Se	-5.2445454	-1.97199308	0.3178362

Se	-5.6818788	3.39903494	-0.00870183
H	-2.53729502	-1.1053969	0.76938662
H	-5.8632503	0.59563374	-0.76295406

T1S0_L (24SeU)

C	-4.46948221	-0.42437006	0.06265968
N	-3.12905071	-0.28880925	0.27414488
C	-2.42717036	0.91050917	0.12696904
C	-3.07711704	2.04060307	-0.28004933
C	-4.49702099	2.02076779	-0.62311157
N	-5.09659362	0.73370022	-0.35861313
H	-1.36449534	0.86900535	0.38240609
H	-2.54228834	2.99374243	-0.32451506
Se	-5.35876265	-2.00811743	0.27192342
Se	-5.6320634	3.00328761	0.71695473
H	-2.65896077	-1.13190188	0.59782256
H	-6.07675099	0.60213433	-0.61802016

Franck-Condon Point to the S2T Minimum (2SeU)

Point1

C	-0.1471527	-0.3064334	-0.0358515
N	0.8242543	0.6595264	-0.0071162
C	0.6614139	2.0673407	0.0147302
C	-0.7418085	2.4807164	0.0096096
C	-1.7264321	1.5366085	-0.007978

N	-1.4291825	0.1902221	-0.0228979
H	-0.9680185	3.5472029	0.0218028
H	-2.7915256	1.7804802	-0.011669
Se	0.2472685	-2.1201455	0.0642495
O	1.6394655	2.8007318	0.0355319
H	1.7893938	0.3255899	-0.0083628
H	-2.1696126	-0.5060276	-0.0419904

Point2

C	-0.1471527	-0.3064334	-0.0358515
N	0.8242543	0.6595264	-0.0071162
C	0.6614139	2.0673407	0.0147302
C	-0.7418085	2.4807164	0.0096096
C	-1.7264321	1.5366085	-0.007978
N	-1.4291825	0.1902221	-0.0228979
H	-0.9680185	3.5472029	0.0218028
H	-2.7915256	1.7804802	-0.011669
Se	0.2472685	-2.1201455	0.0642495
O	1.6394655	2.8007318	0.0355319
H	1.7893938	0.3255899	-0.0083628
H	-2.1696126	-0.5060276	-0.0419904

Point3

C	-0.1527356	-0.3056055	-0.0718064
N	0.820454	0.6584017	-0.0239529
C	0.660959	2.0666033	0.0145313
C	-0.7415432	2.4817287	0.0188867

C	-1.7285168	1.5395739	-0.007077
N	-1.4340203	0.1934201	-0.0432082
H	-0.9665792	3.5482081	0.0462875
H	-2.7929738	1.7861984	-0.0032394
Se	0.2734884	-2.1340287	0.1369862
O	1.6406229	2.7975124	0.0424255
H	1.7855036	0.3242685	-0.0310202
H	-2.1765955	-0.5004684	-0.068755

Point4

C	-0.1571499	-0.3045783	-0.1084044
N	0.8174373	0.6574488	-0.0411073
C	0.6607631	2.0657516	0.0145312
C	-0.7411718	2.4818996	0.0283182
C	-1.7301059	1.5413822	-0.0064732
N	-1.437839	0.1959251	-0.0641065
H	-0.9654496	3.5480541	0.0712375
H	-2.7940013	1.790182	0.0048467
Se	0.293535	-2.1424612	0.2118177
O	1.6417584	2.7944629	0.0497869
H	1.7825295	0.3236154	-0.0543078
H	-2.1822423	-0.4958698	-0.096081

Point5

C	-0.160233	-0.3033187	-0.1465816
N	0.8153551	0.6567298	-0.059777
C	0.6608645	2.0647562	0.0148292

C	-0.7406834	2.4811032	0.0383379
C	-1.7311454	1.541904	-0.0063236
N	-1.4405005	0.1976707	-0.0862044
H	-0.9646775	3.5465521	0.0977594
H	-2.794571	1.792241	0.0125511
Se	0.3065331	-2.1447836	0.2910304
O	1.6428558	2.7915985	0.0581367
H	1.7806304	0.323737	-0.0794753
H	-2.1863647	-0.4923778	-0.1242247

Point6

C	-0.161673	-0.3017945	-0.1875061
N	0.8144803	0.6563615	-0.0814172
C	0.6613445	2.0635421	0.0155246
C	-0.7400414	2.4790638	0.0494898
C	-1.7315127	1.5408512	-0.0067703
N	-1.4417315	0.1984903	-0.110237
H	-0.9643351	3.5432974	0.1272231
H	-2.7945876	1.7919573	0.0199153
Se	0.310715	-2.1394062	0.377377
O	1.6438998	2.7889213	0.0680597
H	1.780096	0.3248333	-0.1080694
H	-2.1885911	-0.4903052	-0.1535314

Point7

C	-0.1609652	-0.2999733	-0.2325749
N	0.8152303	0.6565352	-0.1077065

C	0.6623444	2.0619658	0.016675
C	-0.7391685	2.4752971	0.0624303
C	-1.730988	1.537713	-0.0078673
N	-1.4410824	0.1980766	-0.1370233
H	-0.9645121	3.537585	0.1612507
H	-2.7938711	1.7885941	0.0271831
Se	0.3031222	-2.1234367	0.4739194
O	1.6448873	2.7863971	0.0801243
H	1.7813765	0.3272396	-0.1418721
H	-2.1883099	-0.4901812	-0.1844807

Point8

C	-0.1573695	-0.2978289	-0.2832846
N	0.8181729	0.6575341	-0.140361
C	0.6640847	2.0597892	0.0182292
C	-0.7379235	2.4690428	0.0778815
C	-1.7292188	1.5316752	-0.009456
N	-1.4378842	0.1959266	-0.167327
H	-0.9652978	3.5283161	0.2015721
H	-2.7921201	1.7809796	0.0349783
Se	0.2792859	-2.0922166	0.5834697
O	1.6458494	2.7839257	0.0947084
H	1.7850962	0.3314718	-0.1826653
H	-2.1846117	-0.4928032	-0.2176872

Point9

C	-0.1498983	-0.295361	-0.3409217
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N	0.8240018	0.6597341	-0.1807981
C	0.6668813	2.0566682	0.0199571
C	-0.7360725	2.4592162	0.0965356
C	-1.725686	1.521542	-0.0110123
N	-1.4312235	0.191282	-0.2015878
H	-0.9667398	3.5139384	0.2497334
H	-2.7888694	1.7673943	0.0444831
Se	0.233014	-2.0388993	0.7074967
O	1.6468776	2.7813277	0.1117614
H	1.7920379	0.3382482	-0.2318346
H	-2.1762597	-0.4992783	-0.2537546

Point10

C	-0.1373659	-0.2926468	-0.4061048
N	0.8334737	0.663566	-0.2297819
C	0.6711439	2.0521692	0.0214369
C	-0.733258	2.444414	0.1189562
C	-1.7196849	1.5056954	-0.0115315
N	-1.4199602	0.1830797	-0.2395644
H	-0.9687796	3.4924745	0.306766
H	-2.7834507	1.7455148	0.0575104
Se	0.1564462	-1.9542279	0.8445965
O	1.648139	2.778378	0.13062
H	1.8030767	0.3484471	-0.2899895
H	-2.1617167	-0.5110517	-0.2928557

The S2T to S2S1 crossing point

Point1

C	-0.1379933	-0.2832906	-0.4359052
N	0.8329165	0.6694139	-0.2418674
C	0.6706813	2.0521062	0.04013
C	-0.733601	2.4413051	0.1507024
C	-1.7199591	1.5050808	0.0029208
N	-1.4202891	0.1879346	-0.2548972
H	-0.9690562	3.4848772	0.3621062
H	-2.7836203	1.742712	0.0806003
Se	0.1607086	-1.9716082	0.7772691
O	1.6476487	2.7763309	0.1620027
H	1.8024827	0.356253	-0.3120563
H	-2.1618554	-0.5053026	-0.3209473

Point2

C	-0.1386768	-0.2799389	-0.4345536
N	0.8328327	0.6700304	-0.2389544
C	0.6694173	2.0504438	0.0396158
C	-0.7347157	2.441822	0.1507598
C	-1.7193843	1.5069459	0.0035448
N	-1.4196125	0.1892436	-0.2539338
H	-0.9681693	3.4845119	0.3613251
H	-2.7816539	1.7442241	0.0807701
Se	0.1654503	-1.9832526	0.7802183
O	1.6431281	2.7753313	0.1589553
H	1.7999874	0.3574276	-0.3124502
H	-2.16054	-0.5009767	-0.3252392

Point3

C	-0.1393651	-0.2765931	-0.433187
N	0.8327237	0.6706437	-0.2360263
C	0.6681507	2.0487752	0.0391039
C	-0.7358312	2.4423418	0.1508066
C	-1.7188143	1.5088131	0.0041642
N	-1.4189299	0.1905548	-0.252962
H	-0.9672835	3.4841491	0.3605186
H	-2.779692	1.7457416	0.0809293
Se	0.1702296	-1.9949196	0.7831007
O	1.6386146	2.7742992	0.1558961
H	1.7974659	0.3586262	-0.3127962
H	-2.1592051	-0.4966197	-0.3294899

Point4

C	-0.1400585	-0.2732531	-0.4318055
N	0.8325896	0.6712538	-0.2330831
C	0.6668814	2.0471004	0.0385945
C	-0.7369474	2.4428645	0.1508427
C	-1.7182492	1.5106826	0.0047787
N	-1.4182413	0.1918682	-0.2519817
H	-0.9663989	3.4837888	0.3596863
H	-2.7777345	1.7472648	0.0810777
Se	0.1750467	-2.0066087	0.7859168
O	1.6341081	2.7732343	0.1528254
H	1.7949182	0.3598487	-0.3130945

H	-2.1578508	-0.4922319	-0.333699
Point5			
C	-0.1407569	-0.2699191	-0.4304089
N	0.8324303	0.6718608	-0.230125
C	0.6656094	2.0454192	0.0380876
C	-0.7380643	2.4433902	0.1508679
C	-1.7176891	1.5125544	0.0053882
N	-1.417547	0.1931837	-0.2509929
H	-0.9655154	3.483431	0.3588281
H	-2.7757814	1.7487935	0.0812151
Se	0.1799017	-2.0183191	0.7886666
O	1.6296089	2.7721365	0.1497434
H	1.7923445	0.3610948	-0.3133455
H	-2.1564772	-0.4878135	-0.3378666
Point6			
C	-0.1414605	-0.2665909	-0.4289973
N	0.8322457	0.6724646	-0.2271518
C	0.6643347	2.0437316	0.0375834
C	-0.7391818	2.4439187	0.150882
C	-1.7171338	1.5144286	0.0059926
N	-1.4168469	0.1945013	-0.2499956
H	-0.9646331	3.4830756	0.357944
H	-2.7738328	1.750328	0.0813414
Se	0.1847946	-2.0300501	0.7913504
O	1.6251168	2.7710056	0.1466506

H	1.7897449	0.3623643	-0.3135493
H	-2.1550845	-0.4833648	-0.3419924
Point7			
C	-0.1421693	-0.2632686	-0.4275706
N	0.8320358	0.6730653	-0.2241636
C	0.6630574	2.0420375	0.0370818
C	-0.7403	2.4444502	0.1508849
C	-1.7165835	1.516305	0.0065918
N	-1.4161413	0.1958212	-0.2489896
H	-0.9637517	3.4827226	0.3570336
H	-2.7718887	1.7518683	0.0814564
Se	0.1897257	-2.0418011	0.7939686
O	1.6206322	2.7698413	0.1435473
H	1.7871196	0.3636569	-0.3137064
H	-2.1536729	-0.4788861	-0.3460763

Point8			
C	-0.1428834	-0.2599523	-0.4261288
N	0.8318007	0.6736628	-0.2211604
C	0.6617774	2.0403368	0.0365831
C	-0.7414187	2.4449846	0.1508765
C	-1.7160381	1.5181839	0.0071856
N	-1.41543	0.1971431	-0.2479748
H	-0.9628714	3.4823721	0.3560968
H	-2.769949	1.7534145	0.0815599
Se	0.1946949	-2.0535713	0.7965213

O	1.616155	2.7686436	0.1404338
H	1.7844687	0.3649723	-0.313817
H	-2.1522426	-0.4743776	-0.3501181

Point9

C	-0.1436029	-0.2566419	-0.4246718
N	0.8315403	0.6742571	-0.2181423
C	0.6604948	2.0386295	0.0360873
C	-0.7425381	2.445522	0.1508566
C	-1.7154977	1.5200653	0.0077738
N	-1.4147134	0.1984672	-0.2469513
H	-0.961992	3.4820239	0.3551335
H	-2.7680138	1.7549666	0.0816518
Se	0.1997024	-2.0653602	0.7990089
O	1.6116854	2.7674121	0.1373105
H	1.7817923	0.3663104	-0.3138813
H	-2.1507938	-0.4698395	-0.3541176

Point10

C	-0.1443278	-0.2533375	-0.4231998
N	0.8312545	0.6748483	-0.2151092
C	0.6592094	2.0369154	0.0355945
C	-0.743658	2.4460623	0.150825
C	-1.7149623	1.5219492	0.0083564
N	-1.4139914	0.1997934	-0.2459188
H	-0.9611136	3.4816781	0.3541435
H	-2.7660832	1.7565248	0.0817318

Se	0.2047484	-2.077167	0.8014316
O	1.6072234	2.7661467	0.1341777
H	1.7790905	0.3676709	-0.3138998
H	-2.1493265	-0.4652722	-0.3580748

The S1 Minimum to S1T2T1 crossing point

Point1

C	-0.1395944	-0.3268287	-0.2788254
N	0.8472651	0.6605214	-0.2212306
C	0.6726579	2.0340324	0.0305146
C	-0.7322215	2.4295374	0.1689502
C	-1.7208138	1.4995178	0.0120769
N	-1.4459073	0.1621199	-0.1635995
H	-0.9586575	3.4808959	0.348466
H	-2.7839792	1.755563	0.031593
Se	0.1894585	-1.9466582	0.8242026
O	1.6418106	2.7831036	0.0818771
H	1.8156917	0.3803083	-0.3706089
H	-2.1976466	-0.4563005	-0.453358

Point2

C	-0.1447153	-0.3185832	-0.2312508
N	0.8510957	0.6620628	-0.2228022
C	0.6737646	2.0356463	0.0279853
C	-0.7321304	2.4285228	0.1696839
C	-1.7243653	1.5025482	0.0117302
N	-1.4555201	0.1635472	-0.1573924

H	-0.9567778	3.4796974	0.3458082
H	-2.786722	1.7646005	0.0222995
Se	0.2119832	-1.9789793	0.8014703
O	1.638878	2.7878348	0.0676552
H	1.8190145	0.3786755	-0.3608497
H	-2.2064417	-0.4497608	-0.4642795

Point3

C	-0.1498384	-0.3101201	-0.1840821
N	0.8538573	0.662787	-0.2251461
C	0.6745364	2.0364015	0.0254634
C	-0.731986	2.4270676	0.1708259
C	-1.727475	1.5050975	0.0114907
N	-1.4643127	0.1646921	-0.1516508
H	-0.9544228	3.4780465	0.3440959
H	-2.7889958	1.7728278	0.0133169
Se	0.2329633	-2.0061828	0.7795646
O	1.6358874	2.7911308	0.0537714
H	1.8215953	0.3777869	-0.3517658
H	-2.2137457	-0.4437223	-0.475826

Point4

C	-0.1550059	-0.3013244	-0.1371561
N	0.8555536	0.6626904	-0.228206
C	0.6749722	2.0363139	0.0229436
C	-0.7317997	2.4252059	0.172372
C	-1.7301881	1.5072182	0.0113575

N	-1.4723235	0.1655995	-0.1463531
H	-0.9515978	3.475985	0.3432955
H	-2.7908445	1.7803422	0.0046117
Se	0.2525787	-2.0286984	0.7584962
O	1.6328286	2.7930451	0.040164
H	1.8234206	0.3775876	-0.3433936
H	-2.2195308	-0.4381528	-0.4880736

Point5

C	-0.1602629	-0.2920725	-0.0902832
N	0.8561669	0.6617554	-0.2319192
C	0.6750664	2.0353876	0.0204227
C	-0.7315868	2.4229672	0.1743216
C	-1.7325516	1.5089569	0.0113317
N	-1.4795678	0.1663155	-0.1414698
H	-0.9483052	3.4735503	0.3433736
H	-2.7923122	1.787232	-0.0038526
Se	0.2709972	-2.0468748	0.7382244
O	1.6296936	2.7936055	0.0267653
H	1.8244539	0.3780149	-0.335764
H	-2.2237282	-0.4330256	-0.5010925

Point6

C	-0.1656569	-0.2822295	-0.0432485
N	0.8556561	0.6599488	-0.2362164
C	0.6748079	2.0336136	0.0178991
C	-0.7313657	2.4203772	0.1766778

C	-1.7346136	1.5103542	0.0114165
N	-1.4860345	0.1668864	-0.1369629
H	-0.9445446	3.4707765	0.3442979
H	-2.7934422	1.7935757	-0.0121168
Se	0.2883693	-2.0609818	0.7186616
O	1.6264753	2.7928129	0.0135013
H	1.8246348	0.378999	-0.3289058
H	-2.2262225	-0.4283208	-0.5149459

Point7

C	-0.1712366	-0.2716458	0.0041884
N	0.8539534	0.6572211	-0.2410206
C	0.6741789	2.0309701	0.0153739
C	-0.7311596	2.4174584	0.1794484
C	-1.7364225	1.5114445	0.0116161
N	-1.4916824	0.1673599	-0.1327847
H	-0.9403126	3.4676946	0.3460373
H	-2.7942773	1.7994412	-0.0202278
Se	0.3048214	-2.0712123	0.6996734
O	1.6231673	2.7906405	0.0002913
H	1.8238777	0.3804659	-0.3228486
H	-2.2268442	-0.4240257	-0.5296889

Point8

C	-0.1770513	-0.2601534	0.0522961
N	0.8509606	0.6535051	-0.2462447
C	0.673154	2.0274214	0.0128511

C	-0.7309963	2.4142311	0.1826455
C	-1.7380263	1.512256	0.0119355
N	-1.4964348	0.1677844	-0.1288756
H	-0.9356025	3.4643342	0.3485606
H	-2.7948585	1.8048843	-0.0282414
Se	0.3204469	-2.0776834	0.6810756
O	1.6197636	2.7870317	-0.0129532
H	1.8220679	0.3823388	-0.3176264
H	-2.2253598	-0.4201379	-0.545365

Point9

C	-0.1831479	-0.2475608	0.101376
N	0.8465436	0.6487149	-0.2517874
C	0.6716989	2.0229187	0.0103403
C	-0.730909	2.4107148	0.1862868
C	-1.7394714	1.512809	0.0123792
N	-1.5001706	0.1682099	-0.12516
H	-0.9304046	3.4607246	0.3518358
H	-2.7952245	1.8099459	-0.0362273
Se	0.3352923	-2.0804369	0.6626252
O	1.6162583	2.7818982	-0.0263296
H	1.8190568	0.3845415	-0.3132814
H	-2.2214584	-0.4166675	-0.5619995

Point10

C	-0.1895677	-0.233647	0.1517693
N	0.8405241	0.6427461	-0.2575264

C	0.6697695	2.0174001	0.0078583
C	-0.7309376	2.4069297	0.1903954
C	-1.7408007	1.5131152	0.0129493
N	-1.5027129	0.1686875	-0.1215407
H	-0.9247074	3.4568969	0.3558271
H	-2.7954095	1.814647	-0.0442757
Se	0.3493364	-2.0794382	0.6440052
O	1.6126464	2.7751165	-0.0399464
H	1.8146544	0.3870023	-0.3098683
H	-2.2147316	-0.4136437	-0.5795891

The T1T Minimum to T2T1S0 crossing point (2SeU)

Point1

C	-0.1312539	-0.3134987	-0.3637893
N	0.8471969	0.673249	-0.216913
C	0.6759379	2.0490347	0.0224457
C	-0.7348442	2.4462715	0.1027098
C	-1.7218586	1.5060436	0.0025906
N	-1.4289872	0.180674	-0.1803831
H	-0.9634794	3.4997829	0.2680613
H	-2.7861228	1.7503584	0.0608453
Se	0.147502	-1.9878752	0.6946524
O	1.6415075	2.7912137	0.1468991
H	1.8183431	0.3652745	-0.2649316
H	-2.1758778	-0.5047161	-0.2621289

Point2

C	-0.1351022	-0.2924942	-0.2789385
N	0.8657597	0.6851355	-0.1673778
C	0.6727851	2.0682216	0.017981
C	-0.7341597	2.463798	0.0756524
C	-1.7200043	1.5254135	0.002846
N	-1.4523148	0.1871112	-0.1322443
H	-0.96661	3.5218507	0.2017678
H	-2.7840378	1.7738021	0.0455692
Se	0.1698651	-2.1496138	0.5369
O	1.6267672	2.8281045	0.1205147
H	1.8310776	0.3577755	-0.2059131
H	-2.1859626	-0.5132925	-0.2066996

Point3

C	-0.1381054	-0.2760132	-0.1979758
N	0.8735932	0.6944081	-0.118043
C	0.6710002	2.0837667	0.014063
C	-0.7338863	2.4781588	0.0500857
C	-1.7193953	1.54012	0.0037256
N	-1.4657114	0.1932741	-0.0851636
H	-0.9693628	3.5393541	0.1380692
H	-2.7833294	1.7909026	0.0318229
Se	0.1880669	-2.2779317	0.3721085
O	1.6198675	2.8523456	0.0936151
H	1.8353805	0.3553182	-0.1439957
H	-2.1900543	-0.5178909	-0.1482539

Point4

C	-0.1414124	-0.2634173	-0.1214599
N	0.8691217	0.7013308	-0.0693775
C	0.6711519	2.0963714	0.0103538
C	-0.7339346	2.4902064	0.0254223
C	-1.7209168	1.5510959	0.0050938
N	-1.4702567	0.1992956	-0.0391638
H	-0.9717156	3.553271	0.0763319
H	-2.7847585	1.803311	0.0197026
Se	0.2073422	-2.378366	0.2034372
O	1.6226773	2.8632848	0.0669987
H	1.8298196	0.3581222	-0.0802605
H	-2.1890546	-0.5186935	-0.0870206

Point5

C	-0.1494837	-0.2541452	-0.0498016
N	0.8461727	0.7057678	-0.0220329
C	0.6744997	2.1059128	0.0064302
C	-0.7328482	2.5009225	0.0011995
C	-1.7250324	1.5600263	0.0070566
N	-1.471657	0.2047609	0.0061336
H	-0.9714618	3.5648742	0.0160552
H	-2.7884626	1.8142753	0.0095939
Se	0.2457115	-2.4522687	0.0327696
O	1.640243	2.8557552	0.0413046
H	1.8084078	0.3666408	-0.0160447
H	-2.1880256	-0.5167096	-0.022606

Point6

C	-0.070672	-0.2369871	-0.0044653
N	0.9184677	0.7167706	0.0208371
C	0.6668805	2.1220687	0.0042096
C	-0.7691209	2.4943565	-0.019869
C	-1.7468556	1.5304103	0.006936
N	-1.3222285	0.2347503	0.0311098
H	-1.0295947	3.5531636	-0.0318496
H	-2.815083	1.7635532	0.0030548
Se	-0.0582153	-2.5556321	-0.1072115
O	1.5894666	2.9244233	0.0282169
H	1.8805433	0.3790486	0.0538083
H	-2.0555246	-0.4701135	0.0252809

Point7

C	-0.1113488	-0.2362508	0.075162
N	0.8446643	0.7162247	0.0671875
C	0.6776876	2.1248009	-0.0019735
C	-0.7528512	2.5077525	-0.0450845
C	-1.7458339	1.5498541	0.0124514
N	-1.3708848	0.2298832	0.0869866
H	-1.0050155	3.5673614	-0.0962409
H	-2.8116493	1.7931897	-0.0034686
Se	0.1042276	-2.5833781	-0.2994354
O	1.6461632	2.8710877	-0.0024695
H	1.812097	0.3952439	0.1113766

H	-2.0991927	-0.4799568	0.1055662
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Point8

C	-0.1119981	-0.234225	0.1551311
N	0.8207293	0.719076	0.1174286
C	0.6811106	2.1269866	-0.0063111
C	-0.7516647	2.5082529	-0.071002
C	-1.7469066	1.5484244	0.0158172
N	-1.3598764	0.2326772	0.1383145
H	-1.0046951	3.5649926	-0.1613559
H	-2.8129607	1.7893709	-0.0133273
Se	0.1089561	-2.592336	-0.4919904
O	1.6636849	2.8538614	-0.0278659
H	1.7921913	0.4126058	0.1759861
H	-2.0905073	-0.4738744	0.179233

Point9

C	-0.1004941	-0.24033	0.2669084
N	0.8264613	0.7229524	0.1814135
C	0.676785	2.1242478	-0.0091853
C	-0.7484539	2.498748	-0.102037
C	-1.7333156	1.540252	0.0165102
N	-1.3562154	0.2270271	0.2025278
H	-1.0024116	3.549784	-0.2421366
H	-2.8007224	1.7712891	-0.0343653
Se	0.0584556	-2.5433633	-0.7171788
O	1.65416	2.8561684	-0.0608496

H	1.8009424	0.4272232	0.2492434
H	-2.0871279	-0.4781864	0.2592071

Point10

C	-0.0828775	-0.2556675	0.4131649
N	0.844505	0.7257034	0.2587337
C	0.667344	2.1125578	-0.0126741
C	-0.741034	2.4767646	-0.1403069
C	-1.7056353	1.5227288	0.0141412
N	-1.3610188	0.2116808	0.2800994
H	-0.9940261	3.5179992	-0.3416449
H	-2.7749249	1.7359881	-0.0659313
Se	-0.0257872	-2.4010854	-0.9698001
O	1.6303742	2.858875	-0.1053954
H	1.8229282	0.4430275	0.331917
H	-2.0917842	-0.49276	0.3477545

Franck-Condon Point to the S2 Minimum (4SeU)

Point1

C	-3.3518954	-1.0312853	-0.0906169
N	-1.9670165	-0.8760287	-0.0274168
C	-1.2412503	0.3055593	0.0062361
C	-2.0428533	1.5059303	-0.0093505
C	-3.4084251	1.4083578	-0.0689474
N	-4.0312053	0.1820941	-0.1093368
H	-1.5455476	2.4748206	0.0206575
H	-4.0690449	2.2789776	-0.0885552

Se	0.5809473	0.3040197	0.0614008
O	-3.9086706	-2.1150706	-0.1260851
H	-5.0440189	0.1065269	-0.1544282
H	-1.4452112	-1.7536941	-0.0181504

Point2

C	-3.3514573	-1.0309703	-0.0909006
N	-1.9663983	-0.8741933	-0.0249877
C	-1.2481853	0.3116323	0.006836
C	-2.0411113	1.5081057	-0.0101999
C	-3.4148019	1.4122164	-0.0695219
N	-4.0315911	0.1816581	-0.1075387
H	-1.5434277	2.476899	0.0179621
H	-4.0775393	2.2807935	-0.0864332
Se	0.5918674	0.2864883	0.0616134
O	-3.9067092	-2.1156709	-0.128939
H	-5.0442201	0.1025003	-0.1552584
H	-1.4406177	-1.7492515	-0.0172252

Point3

C	-3.3509454	-1.0306076	-0.0911766
N	-1.9657176	-0.8722647	-0.0225479
C	-1.2551021	0.3177626	0.0074093
C	-2.0394065	1.5102804	-0.0110559
C	-3.4212119	1.4160775	-0.0700866
N	-4.0319424	0.1812414	-0.1057374
H	-1.5413589	2.4789802	0.0152593

H	-4.0860726	2.2825894	-0.0842971
Se	0.602497	0.2685894	0.0618167
O	-3.9046274	-2.1162377	-0.1317993
H	-5.0443648	0.0984704	-0.1560991
H	-1.4359393	-1.7446736	-0.0162783

Point4

C	-3.3503587	-1.0301973	-0.091445
N	-1.9649738	-0.8702433	-0.0200981
C	-1.2620001	0.3239492	0.0079557
C	-2.0377381	1.512454	-0.011919
C	-3.4276545	1.4199404	-0.0706414
N	-4.0322585	0.1808438	-0.1039327
H	-1.5393407	2.4810639	0.0125483
H	-4.0946443	2.2843642	-0.082147
Se	0.6128291	0.250327	0.0620124
O	-3.9024246	-2.1167711	-0.1346654
H	-5.0444518	0.0944372	-0.1569497
H	-1.4311758	-1.7399604	-0.0153111

Point5

C	-3.3496968	-1.0297397	-0.0917057
N	-1.9641662	-0.8681292	-0.017639
C	-1.2688786	0.3301911	0.0084751
C	-2.0361057	1.5146261	-0.0127896
C	-3.4341293	1.4238041	-0.071186
N	-4.0325386	0.1804652	-0.1021245

H	-1.5373725	2.4831498	0.0098284
H	-4.1032536	2.2861171	-0.0799827
Se	0.622857	0.231705	0.0622021
O	-3.9001002	-2.1172708	-0.137537
H	-5.0444802	0.0904006	-0.1578093
H	-1.4263272	-1.7351117	-0.0143248

Point6

C	-3.3489589	-1.0292348	-0.0919587
N	-1.9632944	-0.8659228	-0.0151715
C	-1.2757371	0.3364873	0.0089673
C	-2.0345087	1.5167964	-0.0136682
C	-3.4406356	1.4276678	-0.0717202
N	-4.0327819	0.1801054	-0.1003126
H	-1.5354539	2.4852375	0.007099
H	-4.1118999	2.2878468	-0.0778041
Se	0.6325739	0.2127276	0.0623875
O	-3.8976534	-2.1177366	-0.1404134
H	-5.0444487	0.0863605	-0.1586772
H	-1.4213933	-1.7301276	-0.0133208

Point7

C	-3.3481444	-1.0286828	-0.0922041
N	-1.9623578	-0.8636243	-0.012696
C	-1.2825749	0.3428369	0.009432
C	-2.0329465	1.5189644	-0.0145551
C	-3.4471728	1.4315306	-0.0722438

N	-4.0329876	0.179764	-0.0984967
H	-1.5335842	2.4873266	0.0043593
H	-4.1205825	2.2895525	-0.0756111
Se	0.6419732	0.193399	0.0625701
O	-3.8950837	-2.1181684	-0.1432944
H	-5.0443563	0.0823169	-0.1595528
H	-1.4163743	-1.7250078	-0.0123003

Point8

C	-3.3472528	-1.0280839	-0.092442
N	-1.961356	-0.8612341	-0.0102135
C	-1.2893914	0.3492388	0.0098691
C	-2.0314185	1.5211297	-0.0154509
C	-3.4537405	1.4353916	-0.0727565
N	-4.033155	0.179441	-0.0966766
H	-1.531763	2.4894167	0.0016086
H	-4.1293007	2.291233	-0.0734035
Se	0.6510484	0.1737234	0.0627516
O	-3.8923905	-2.1185661	-0.1461794
H	-5.0442019	0.0782699	-0.1604353
H	-1.41127	-1.7197524	-0.0112646

Point9

C	-3.3462834	-1.0274384	-0.0926722
N	-1.9602884	-0.8587525	-0.0077246
C	-1.296186	0.3556919	0.0102783
C	-2.0299242	1.5232918	-0.0163559

C	-3.4603382	1.4392499	-0.073258
N	-4.0332833	0.1791362	-0.0948523
H	-1.5299896	2.4915075	-0.0011538
H	-4.1380539	2.2928874	-0.0711811
Se	0.6597931	0.1537054	0.0629337
O	-3.8895732	-2.1189295	-0.149068
H	-5.0439845	0.0742193	-0.161324
H	-1.4060805	-1.7143613	-0.0102152

Point10

C	-3.3452356	-1.0267463	-0.092895
N	-1.9591545	-0.8561798	-0.00523
C	-1.3029581	0.3621953	0.0106594
C	-2.0284629	1.5254504	-0.0172706
C	-3.4669652	1.4431046	-0.0737481
N	-4.0333717	0.1788492	-0.0930233
H	-1.5282637	2.4935983	-0.0039284
H	-4.1468413	2.2945144	-0.0689438
Se	0.668201	0.1333494	0.063118
O	-3.8866313	-2.1192584	-0.1519598
H	-5.0437029	0.0701651	-0.1622181
H	-1.4008057	-1.7088345	-0.0091532

The S2 Minimum to S2S1 crossing point (4SeU)

Point1

C	-3.3464648	-1.0284589	-0.09307
N	-1.9573907	-0.8560177	-0.0080696

C	-1.3077204	0.3620431	0.0087978
C	-2.0332286	1.5278868	-0.0164288
C	-3.4651744	1.4410961	-0.0716157
N	-4.0321776	0.1785769	-0.0920525
H	-1.5331347	2.4958063	-0.0012058
H	-4.1463316	2.2916891	-0.0673648
Se	0.6747141	0.1362919	0.059134
O	-3.8864357	-2.1205558	-0.1514558
H	-5.0426754	0.0708497	-0.1587268
H	-1.3981722	-1.7089999	-0.0125351

Point2

C	-3.3485119	-1.0231181	-0.0895286
N	-1.9616127	-0.8454114	0.0038871
C	-1.3116923	0.3654498	0.0311448
C	-2.0500305	1.5324503	-0.0060165
C	-3.4721962	1.4391749	-0.0754237
N	-4.0393958	0.1788309	-0.0993235
H	-1.5563076	2.5019638	0.0172926
H	-4.154866	2.2873262	-0.080051
Se	0.7507504	0.0938169	0.020891
O	-3.8816931	-2.1154107	-0.1482297
H	-5.0471349	0.0707731	-0.1729891
H	-1.4015012	-1.6956379	-0.0062464

Point3

C	-3.3502702	-1.0177222	-0.0860937
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N	-1.9656829	-0.8346705	0.016401
C	-1.3157066	0.3689868	0.0541984
C	-2.0667515	1.5369938	0.0047254
C	-3.478945	1.4372676	-0.0790101
N	-4.0462265	0.1790649	-0.1068388
H	-1.579554	2.5080724	0.0360071
H	-4.163036	2.2829476	-0.0926352
Se	0.8242035	0.0508283	-0.019153
O	-3.8765825	-2.1102018	-0.1453461
H	-5.0511193	0.0706423	-0.1878992
H	-1.4045208	-1.6820015	0.0010513

Point4

C	-3.3517433	-1.0122786	-0.0827604
N	-1.9696156	-0.8238088	0.0294455
C	-1.319782	0.3726392	0.0779348
C	-2.0833954	1.5415045	0.015768
C	-3.4854184	1.4353689	-0.0823958
N	-4.0526605	0.1792747	-0.1145993
H	-1.602873	2.5141168	0.0549159
H	-4.170831	2.2785508	-0.1051361
Se	0.8950974	0.0074309	-0.0608431
O	-3.8711108	-2.1049338	-0.1427858
H	-5.0546116	0.0704548	-0.20344
H	-1.4072477	-1.6681117	0.0093033

Point5

C	-3.3529353	-1.006794	-0.0795219
N	-1.9734263	-0.8128402	0.0430041
C	-1.3239384	0.3763911	0.1023444
C	-2.0999653	1.5459695	0.0270904
C	-3.4916132	1.4334735	-0.085602
N	-4.0586889	0.1794568	-0.1226087
H	-1.6262635	2.5200809	0.0740089
H	-4.1782395	2.2741336	-0.117578
Se	0.9634586	-0.0362727	-0.1040621
O	-3.8652849	-2.0996109	-0.1405317
H	-5.0575941	0.0702095	-0.2196037
H	-1.4097011	-1.6539893	0.0184672

Point6

C	-3.3538508	-1.001275	-0.0763699
N	-1.9771319	-0.8017801	0.0570713
C	-1.3281971	0.3802247	0.1274319
C	-2.1164634	1.5503745	0.0386801
C	-3.4975241	1.4315762	-0.0886511
N	-4.0643015	0.1796084	-0.1308742
H	-1.649724	2.5259476	0.0932868
H	-4.1852466	2.2696945	-0.1299916
Se	1.0293108	-0.0801771	-0.1487295
O	-3.859113	-2.0942366	-0.1385682
H	-5.0600475	0.0699069	-0.236393
H	-1.4119029	-1.6396563	0.0285147

Point7

C	-3.3544955	-0.9957282	-0.0732936
N	-1.9807514	-0.7906454	0.0716532
C	-1.3325812	0.3841193	0.1532183
C	-2.1328901	1.5547039	0.050532
C	-3.5031425	1.4296713	-0.0915678
N	-4.0694863	0.1797276	-0.1394077
H	-1.6732513	2.5316974	0.1127612
H	-4.1918321	2.2652326	-0.142416
Se	1.0926706	-0.1241699	-0.1948016
O	-3.8526044	-2.0888144	-0.136881
H	-5.0619494	0.0695497	-0.2538226
H	-1.4138782	-1.6251362	0.0394327

Point8

C	-3.3548763	-0.9901605	-0.0702797
N	-1.9843066	-0.779456	0.0867688
C	-1.3371164	0.38805	0.1797416
C	-2.1492433	1.5589393	0.0626488
C	-3.5084555	1.427753	-0.0943795
N	-4.074229	0.1798129	-0.1482257
H	-1.6968398	2.5373077	0.1324534
H	-4.1979684	2.2607479	-0.1548998
Se	1.1535433	-0.1681264	-0.2422703
O	-3.8457704	-2.0833471	-0.1354557
H	-5.0632733	0.0691427	-0.2719198
H	-1.4156563	-1.6104559	0.051225

Point9

C	-3.3550012	-0.9845795	-0.0673115
N	-1.9878224	-0.7682356	0.1024516
C	-1.3418315	0.3919866	0.2070586
C	-2.1655173	1.5630593	0.07504
C	-3.5134437	1.4258145	-0.0971174
N	-4.0785114	0.179864	-0.1573508
H	-1.7204806	2.5427524	0.1523945
H	-4.203618	2.2562409	-0.1675038
Se	1.2119181	-0.2119045	-0.2911641
O	-3.8386254	-2.0778379	-0.1342778
H	-5.0639872	0.068694	-0.2907265
H	-1.4172712	-1.5956466	0.0639143

Point10

C	-3.3548805	-0.978994	-0.0643683
N	-1.9913282	-0.7570125	0.118751
C	-1.3467601	0.3958924	0.2352464
C	-2.1817026	1.5670384	0.0877223
C	-3.5180802	1.4238483	-0.0998178
N	-4.0823105	0.1798808	-0.1668123
H	-1.7441609	2.5480001	0.1726239
H	-4.2087304	2.2517133	-0.1803032
Se	1.2677636	-0.2553386	-0.3415483
O	-3.8311874	-2.0722897	-0.1333306
H	-5.0640517	0.0682144	-0.3103007

H	-1.418763	-1.5807454	0.0775447
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The S1 Minimum to T1 Minimum (4SeU)

Point1

C	-3.3479377	-1.0305912	-0.0748237
N	-1.9633818	-0.8923193	0.029707
C	-1.2837362	0.3374512	-0.0061809
C	-2.0335544	1.5153933	-0.031632
C	-3.4262253	1.4363258	-0.0613411
N	-4.0315601	0.1724825	-0.0592038
H	-1.5406933	2.4891451	-0.0245746
H	-4.0918452	2.2984765	-0.0902134
Se	0.6385861	0.2701942	0.1143193
O	-3.8956957	-2.1205505	-0.1570297
H	-5.0383654	0.0794698	-0.1466217
H	-1.4597829	-1.7652698	-0.0969984

Point2

C	-3.3476256	-1.0309537	-0.0764513
N	-1.963487	-0.8921006	0.0245251
C	-1.2837171	0.3376469	-0.0050168
C	-2.0330615	1.5149632	-0.0296545
C	-3.4271527	1.4365528	-0.0615692
N	-4.031039	0.1730723	-0.0638389
H	-1.5389693	2.4879741	-0.0206121
H	-4.0929251	2.2985332	-0.08967
Se	0.6372721	0.2713312	0.1090317

O	-3.8971377	-2.1204051	-0.1546306
H	-5.0382199	0.0794644	-0.1470406
H	-1.4581292	-1.7658709	-0.0896656

Point3

C	-3.3473277	-1.0313272	-0.0780769
N	-1.9636189	-0.8918932	0.0193518
C	-1.2837099	0.3377888	-0.0038541
C	-2.0325651	1.5144902	-0.0276814
C	-3.4280765	1.4367557	-0.0617989
N	-4.0305132	0.1736524	-0.0684646
H	-1.5372308	2.4867484	-0.0166581
H	-4.0939945	2.2985704	-0.0891311
Se	0.6359262	0.2724632	0.1037476
O	-3.8985706	-2.1202642	-0.1522428
H	-5.0380558	0.079494	-0.1474503
H	-1.4564551	-1.7662709	-0.0823342

Point4

C	-3.3470444	-1.0317119	-0.0797012
N	-1.963778	-0.8916966	0.0141855
C	-1.2837148	0.3378771	-0.002693
C	-2.0320652	1.5139745	-0.0257115
C	-3.4289968	1.4369346	-0.0620304
N	-4.0299828	0.1742231	-0.0730822
H	-1.5354779	2.4854682	-0.0127103
H	-4.0950532	2.2985882	-0.0885965

Se	0.6345481	0.2735887	0.0984652
O	-3.8999952	-2.1201283	-0.1498652
H	-5.0378733	0.0795585	-0.1478514
H	-1.4547582	-1.7664685	-0.0750019

Point5

C	-3.3467766	-1.0321081	-0.081325
N	-1.9639651	-0.8915106	0.0090244
C	-1.2837318	0.3379118	-0.0015338
C	-2.0315618	1.5134162	-0.0237437
C	-3.4299136	1.4370897	-0.0622638
N	-4.0294481	0.1747844	-0.0776928
H	-1.5337105	2.4841337	-0.0087667
H	-4.0961015	2.2985867	-0.0880665
Se	0.6331377	0.2747059	0.0931826
O	-3.9014121	-2.119998	-0.1474964
H	-5.0376727	0.0796582	-0.1482447
H	-1.4530358	-1.7664622	-0.0676665

Point6

C	-3.3465247	-1.0325162	-0.082949
N	-1.9641809	-0.8913347	0.0038669
C	-1.283761	0.337893	-0.0003766
C	-2.0310549	1.5128155	-0.021777
C	-3.4308267	1.4372209	-0.0624991
N	-4.0289092	0.1753361	-0.0822977
H	-1.5319285	2.4827446	-0.004825

H	-4.0971393	2.298566	-0.0875409
Se	0.6316948	0.2758132	0.0878977
O	-3.9028218	-2.1198741	-0.1451354
H	-5.0374542	0.0797932	-0.1486311
H	-1.4512854	-1.7662499	-0.0603256

Point7

C	-3.3462895	-1.0329367	-0.0845739
N	-1.9644263	-0.8911686	-0.0012887
C	-1.2838025	0.3378207	0.0007782
C	-2.0305445	1.5121722	-0.0198102
C	-3.4317363	1.4373285	-0.0627365
N	-4.0283663	0.1758784	-0.0868982
H	-1.5301318	2.481301	-0.000883
H	-4.0981665	2.2985261	-0.0870198
Se	0.6302192	0.2769088	0.0826087
O	-3.904225	-2.1197572	-0.142781
H	-5.0372182	0.0799635	-0.1490114
H	-1.4495044	-1.765829	-0.052977

Point8

C	-3.3460716	-1.0333699	-0.0862005
N	-1.964702	-0.8910121	-0.006444
C	-1.2838565	0.3376947	0.0019305
C	-2.0300304	1.5114863	-0.0178422
C	-3.4326422	1.4374122	-0.0629762
N	-4.0278194	0.1764112	-0.0914954

H	-1.5283203	2.4798025	0.0030614
H	-4.0991831	2.2984671	-0.0865033
Se	0.6287107	0.2779907	0.0773134
O	-3.9056221	-2.1196481	-0.1404321
H	-5.0369648	0.0801696	-0.1493865
H	-1.4476901	-1.7651965	-0.0456181

Point9

C	-3.3458718	-1.0338163	-0.0878294
N	-1.965009	-0.8908648	-0.0116008
C	-1.2839231	0.3375147	0.00308
C	-2.0295128	1.5107578	-0.0158718
C	-3.4335444	1.4374722	-0.0632181
N	-4.0272688	0.1769345	-0.0960906
H	-1.5264937	2.4782489	0.0070107
H	-4.100189	2.2983889	-0.0859912
Se	0.6271689	0.279057	0.0720098
O	-3.9070139	-2.1195475	-0.1380874
H	-5.0366943	0.0804115	-0.1497574
H	-1.4458398	-1.7643489	-0.0382467

Point10

C	-3.345691	-1.0342765	-0.0894616
N	-1.9653484	-0.8907265	-0.0167607
C	-1.2840024	0.3372805	0.0042265
C	-2.0289915	1.5099862	-0.0138979
C	-3.4344429	1.4375082	-0.0634624

N	-4.0267147	0.1774481	-0.1006851
H	-1.524652	2.4766397	0.010967
H	-4.1011842	2.2982915	-0.0854837
Se	0.6255936	0.2801055	0.0666958
O	-3.9084009	-2.1194563	-0.1357459
H	-5.0364069	0.0806895	-0.1501248
H	-1.4439507	-1.7632822	-0.0308602

The T1 Minimum to T1S0 crossing point (4SeU)

Point1

C	-3.3457367	-1.0342344	-0.0899773
N	-1.9654061	-0.8907642	-0.0168922
C	-1.2840115	0.3372073	0.00459
C	-2.0289447	1.5099505	-0.0134116
C	-3.4343868	1.4375472	-0.0633479
N	-4.0267044	0.1775229	-0.1010518
H	-1.5245691	2.4765753	0.0118349
H	-4.1010848	2.2983655	-0.0853093
Se	0.6255662	0.279932	0.0675234
O	-3.9084825	-2.1193773	-0.1366893
H	-5.0363885	0.0808217	-0.1507704
H	-1.4440431	-1.763339	-0.0310913

Point2

C	-3.3395462	-1.0267993	-0.0965069
N	-1.9574051	-0.8869899	-0.0135839
C	-1.2827996	0.3475422	0.042232

C	-2.0417969	1.5201754	0.0037727
C	-3.4391259	1.4410943	-0.0641941
N	-4.0266001	0.1800451	-0.1137566
H	-1.5440332	2.4901269	0.0364109
H	-4.1085118	2.3002014	-0.0906184
Se	0.6278578	0.2225975	-0.0046565
O	-3.8923945	-2.1182218	-0.1397284
H	-5.0351639	0.0797241	-0.1736815
H	-1.4346725	-1.7592883	0.0097177

Point3

C	-3.3326185	-1.0201156	-0.1033109
N	-1.9481238	-0.8853355	-0.0094325
C	-1.281305	0.3557436	0.0794913
C	-2.0531599	1.5285647	0.0204114
C	-3.4421948	1.4438379	-0.063596
N	-4.0250955	0.1821304	-0.1261465
H	-1.5614476	2.5014805	0.0596191
H	-4.1137271	2.3016552	-0.093575
Se	0.6229832	0.1749014	-0.0781425
O	-3.8808075	-2.1143704	-0.1453921
H	-5.0324165	0.0787389	-0.1971566
H	-1.426279	-1.7570235	0.0526375

Point4

C	-3.3252914	-1.0141537	-0.1100097
N	-1.9384308	-0.8845369	-0.0040277

C	-1.2793335	0.3624499	0.1173737
C	-2.0630763	1.5356601	0.0380101
C	-3.4436737	1.4459218	-0.0625085
N	-4.0224522	0.1838669	-0.1388504
H	-1.5770467	2.5112621	0.0838539
H	-4.1170046	2.3026988	-0.0960965
Se	0.6115103	0.1339834	-0.1554892
O	-3.8711772	-2.1096655	-0.1521277
H	-5.0283773	0.0779804	-0.2219303
H	-1.4198384	-1.7552597	0.0972093

Point5

C	-3.3177733	-1.0090168	-0.1160058
N	-1.9288977	-0.8838175	0.0035377
C	-1.2765827	0.3679493	0.1571487
C	-2.0714282	1.5417157	0.0582614
C	-3.4433288	1.447352	-0.0618141
N	-4.0186547	0.1852512	-0.1525054
H	-1.5909011	2.5197797	0.1116609
H	-4.1181904	2.3032297	-0.1001481
Se	0.5925804	0.0987318	-0.240223
O	-3.8620659	-2.1052074	-0.1588538
H	-5.0229619	0.0775445	-0.2491364
H	-1.4159876	-1.7533044	0.1434851

Point6

C	-3.3101978	-1.0049657	-0.1207448
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N	-1.9200473	-0.882509	0.0147439
C	-1.2725484	0.3723897	0.2003005
C	-2.0778901	1.5468376	0.0827162
C	-3.4406126	1.4480159	-0.062141
N	-4.013452	0.1861827	-0.1677203
H	-1.6029196	2.5271963	0.145224
H	-4.1167754	2.3030349	-0.107374
Se	0.5637888	0.0690214	-0.3364301
O	-3.8524773	-2.1018672	-0.1651513
H	-5.0157884	0.0775248	-0.2802283
H	-1.4152718	-1.7506538	0.1922123

Point7

C	-3.3025659	-1.0024769	-0.1238838
N	-1.912458	-0.8798597	0.0320112
C	-1.2663921	0.3759273	0.2485882
C	-2.0818327	1.5510383	0.1125627
C	-3.4346061	1.4476391	-0.06363
N	-4.0062919	0.1864131	-0.1850528
H	-1.6128008	2.5336233	0.18593
H	-4.1118843	2.3017025	-0.1187221
Se	0.5205353	0.0454176	-0.448751
O	-3.8415938	-2.1004342	-0.1717376
H	-5.0060463	0.07798	-0.3171443
H	-1.4182554	-1.7467627	0.2452365

Point8

C	-3.2945941	-1.0023678	-0.1252847
N	-1.9068889	-0.8748461	0.059407
C	-1.2566902	0.3788334	0.3044012
C	-2.0820789	1.5542562	0.1487717
C	-3.4238137	1.4456825	-0.0658476
N	-3.9960992	0.1854432	-0.2051305
H	-1.6198304	2.5391808	0.2344275
H	-4.1021084	2.2984667	-0.1344503
Se	0.4541849	0.0292396	-0.583106
O	-3.8285273	-2.1016976	-0.1809516
H	-4.9921149	0.0788688	-0.3628683
H	-1.4256308	-1.740852	0.3060387

Point9

C	-3.2853638	-1.0060818	-0.1248075
N	-1.9045875	-0.8658905	0.1039311
C	-1.2409324	0.3814281	0.3716769
C	-2.0762639	1.5562533	0.1926387
C	-3.405521	1.4411076	-0.0679377
N	-3.9806648	0.1823059	-0.229026
H	-1.6222425	2.543916	0.2912084
H	-4.084838	2.2919242	-0.154751
Se	0.3469998	0.0236152	-0.7481116
O	-3.8117604	-2.1065818	-0.1973265
H	-4.9705599	0.0799347	-0.4226408
H	-1.4384573	-1.7317233	0.3805531

Point10

C	-3.2724608	-1.0163517	-0.1218241
N	-1.9080589	-0.8506485	0.177476
C	-1.2146663	0.3831485	0.4578259
C	-2.0590794	1.5558951	0.2462132
C	-3.3738822	1.4317538	-0.0693886
N	-3.9550204	0.1750541	-0.2590507
H	-1.6151194	2.5469603	0.3569626
H	-4.0539341	2.2795068	-0.1816727
Se	0.1581413	0.0386769	-0.9549912
O	-3.7877814	-2.1163417	-0.2282242
H	-4.933525	0.0804321	-0.506045
H	-1.4588053	-1.717878	0.4781258

Franck-Condon Point to the S2 Minimum (24SeU)

Point1

C	-4.4320506	-0.4926929	0.0257602
N	-3.0650609	-0.3530777	0.0854706
C	-2.4255243	0.8719762	0.080168
C	-3.1406088	2.0362257	0.0145215
C	-4.5823309	1.9914553	-0.0469079
N	-5.116096	0.6962204	-0.0443969
H	-1.3351276	0.8370377	0.1321573
H	-2.6400171	3.0039868	0.010381
Se	-5.2597088	-2.113743	0.0408498
Se	-5.6649687	3.4501057	-0.1197267
H	-2.5342924	-1.2196425	0.1374624

H	-6.1339832	0.6127021	-0.0871682
Point2			
C	-4.432052	-0.493367	0.0258721
N	-3.0649715	-0.3517324	0.0852656
C	-2.4196244	0.8682597	0.080565
C	-3.1397245	2.0395552	0.0148102
C	-4.5732027	1.9886069	-0.0464333
N	-5.1161049	0.6988791	-0.0439409
H	-1.3296029	0.83054	0.1324678
H	-2.6393746	3.0073494	0.0107077
Se	-5.2610285	-2.1138862	0.0407426
Se	-5.6833481	3.4472991	-0.1214419
H	-2.5365962	-1.2204249	0.1368553
H	-6.134139	0.6194753	-0.0868991
Point3			
C	-4.4320396	-0.4939598	0.0259821
N	-3.0648673	-0.3503609	0.0850631
C	-2.4137184	0.8645223	0.080962
C	-3.1388357	2.0428588	0.0151027
C	-4.564045	1.9858012	-0.0459487
N	-5.1160521	0.7016484	-0.0434766
H	-1.3240801	0.8239967	0.1327754
H	-2.6387252	3.0106849	0.0110345
Se	-5.2623994	-2.1139136	0.0406207
Se	-5.7018587	3.4440764	-0.1231685

H	-2.5389286	-1.2211961	0.1362462
H	-6.1342193	0.6263956	-0.0866216

Point4

C	-4.432014	-0.4944709	0.0260902
N	-3.0647485	-0.3489629	0.0848631
C	-2.407807	0.8607643	0.0813589
C	-3.137943	2.046137	0.0153989
C	-4.5548589	1.9830388	-0.0454543
N	-5.115938	0.7045288	-0.0430042
H	-1.3185601	0.8174079	0.13308
H	-2.6380692	3.0139934	0.0113612
Se	-5.2638221	-2.1138245	0.0404841
Se	-5.7204946	3.4404341	-0.1249058
H	-2.5412901	-1.2219552	0.1356351
H	-6.1342238	0.6334632	-0.0863361

Point5

C	-4.4319756	-0.4948998	0.0261962
N	-3.0646155	-0.3475379	0.0846656
C	-2.401891	0.8569859	0.0817559
C	-3.137047	2.0493898	0.0156988
C	-4.5456454	1.9803199	-0.0449501
N	-5.1157629	0.7075204	-0.042524
H	-1.3130439	0.8107736	0.1333817
H	-2.6374074	3.0172752	0.0116878
Se	-5.2652971	-2.1136184	0.0403327

Se	-5.7392498	3.4363686	-0.1266529
H	-2.5436814	-1.2227015	0.1350222
H	-6.1341525	0.6406782	-0.0860426

Point6

C	-4.4319252	-0.4952462	0.0263
N	-3.0644686	-0.3460857	0.0844706
C	-2.3959712	0.8531871	0.0821527
C	-3.1361483	2.0526176	0.0160021
C	-4.5364055	1.977645	-0.0444362
N	-5.1155271	0.7106235	-0.0420363
H	-1.3075324	0.8040941	0.1336805
H	-2.6367401	3.0205306	0.012014
Se	-5.2668249	-2.1132948	0.0401666
Se	-5.7581183	3.4318764	-0.1284088
H	-2.5461028	-1.2234345	0.1344075
H	-6.1340051	0.6480408	-0.0857414

Point7

C	-4.4318632	-0.4955098	0.0264015
N	-3.0643081	-0.3446059	0.0842781
C	-2.3900484	0.8493682	0.0825493
C	-3.1352475	2.0558207	0.0163088
C	-4.5271402	1.9750144	-0.0439128
N	-5.1152308	0.7138385	-0.0415411
H	-1.3020266	0.7973695	0.1339763
H	-2.6360679	3.0237595	0.0123396

Se	-5.268406	-2.112853	0.0399858
Se	-5.7770939	3.4269542	-0.1301728
H	-2.5485552	-1.2241534	0.1337912
H	-6.1337815	0.6555511	-0.0854328

Point8

C	-4.4317902	-0.4956902	0.0265007
N	-3.0641344	-0.3430981	0.0840882
C	-2.3841234	0.8455292	0.0829458
C	-3.1343453	2.0589991	0.0166186
C	-4.5178507	1.9724286	-0.0433798
N	-5.1148744	0.7171655	-0.0410387
H	-1.2965277	0.7905997	0.1342691
H	-2.6353914	3.0269624	0.0126645
Se	-5.2700409	-2.1122925	0.0397904
Se	-5.7961705	3.4215986	-0.131944
H	-2.5510389	-1.2248575	0.1331732
H	-6.1334815	0.6632091	-0.0851169

Point9

C	-4.4317068	-0.495787	0.0265973
N	-3.0639478	-0.3415622	0.0839009
C	-2.3781971	0.8416703	0.083342
C	-3.1334424	2.0621532	0.0169315
C	-4.5085379	1.9698879	-0.0428375
N	-5.1144582	0.7206047	-0.0405294
H	-1.2910366	0.783785	0.1345591

H	-2.6347111	3.0301393	0.0129885
Se	-5.2717301	-2.1116127	0.0395803
Se	-5.8153417	3.4158066	-0.1337213
H	-2.5535547	-1.2255461	0.1325538
H	-6.1331051	0.671015	-0.084794

Point10

C	-4.4316135	-0.4958001	0.0266914
N	-3.0637487	-0.3399977	0.083716
C	-2.3722701	0.8377917	0.083738
C	-3.1325392	2.0652832	0.0172473
C	-4.4992029	1.9673926	-0.0422858
N	-5.1139824	0.7241564	-0.0400134
H	-1.2855544	0.7769254	0.1348461
H	-2.6340275	3.0332905	0.0133113
Se	-5.2734741	-2.1108132	0.0393556
Se	-5.8346015	3.409575	-0.1355039
H	-2.5561032	-1.2262186	0.1319329
H	-6.1326519	0.6789686	-0.0844644

The S2 Minimum to S2S1 crossing point (24SeU)

Point1

C	-4.4326793	-0.4953167	0.0274533
N	-3.0645516	-0.3407059	0.0813294
C	-2.3720704	0.8364938	0.080262
C	-3.1314465	2.064663	0.0161221
C	-4.4983295	1.9679641	-0.0402388

N	-5.1141623	0.7252512	-0.0370876
H	-1.2852897	0.7746782	0.1287842
H	-2.6321199	3.0322469	0.0114551
Se	-5.275885	-2.1096176	0.041361
Se	-5.8327131	3.4113263	-0.1296543
H	-2.5575502	-1.227381	0.1279461
H	-6.1329718	0.6809517	-0.0791613

Point2

C	-4.4347717	-0.4963619	-0.0010025
N	-3.0634127	-0.3378474	0.0778538
C	-2.378456	0.8338374	0.0798737
C	-3.1334804	2.0626928	0.0039159
C	-4.5013333	1.9636943	-0.0434979
N	-5.1164524	0.7288187	-0.0408916
H	-1.2934179	0.7763189	0.1456658
H	-2.6334711	3.028	0.0049307
Se	-5.2655717	-2.1233154	0.0532073
Se	-5.8199803	3.4220695	-0.1129109
H	-2.5561885	-1.2216147	0.1363171
H	-6.1332335	0.6842618	-0.0748901

Point3

C	-4.4361708	-0.4972131	-0.0296092
N	-3.0620584	-0.334949	0.0744569
C	-2.3847111	0.8312516	0.0795254
C	-3.1355797	2.060571	-0.0083368

C	-4.5043513	1.9590988	-0.0467991
N	-5.1183641	0.7318745	-0.0446175
H	-1.3017055	0.7782012	0.1626403
H	-2.6352437	3.0237506	-0.0016957
Se	-5.2564772	-2.1347106	0.064787
Se	-5.8070775	3.4320574	-0.096208
H	-2.5549954	-1.2158677	0.1447243
H	-6.1330346	0.6864892	-0.0702966

Point4

C	-4.4368663	-0.4978587	-0.0584289
N	-3.0604904	-0.3320048	0.0711172
C	-2.3908345	0.82874	0.0791976
C	-3.1377416	2.0583037	-0.0206296
C	-4.5073801	1.9541821	-0.0501164
N	-5.1198918	0.7344194	-0.0482907
H	-1.3101575	0.7803268	0.1796885
H	-2.6374338	3.0195063	-0.0083976
Se	-5.2486286	-2.1438445	0.0762186
Se	-5.7940088	3.4412954	-0.0794828
H	-2.5539765	-1.2101353	0.1531789
H	-6.1323596	0.6876235	-0.0654835

Point5

C	-4.4368382	-0.4982891	-0.0875282
N	-3.0587043	-0.3290099	0.0678114
C	-2.3968211	0.8263061	0.0788698

C	-3.1399645	2.0558952	-0.0329557
C	-4.5104165	1.9489407	-0.0534228
N	-5.1210258	0.736445	-0.0519385
H	-1.3187758	0.7826991	0.1967905
H	-2.640043	3.015274	-0.0151461
Se	-5.2420726	-2.1507112	0.0876295
Se	-5.7807827	3.4497751	-0.0626678
H	-2.5531345	-1.2044134	0.161689
H	-6.1311904	0.6876423	-0.06056

Point6

C	-4.4360557	-0.4984958	-0.1169785
N	-3.0566899	-0.3259604	0.0645151
C	-2.4026621	0.8239535	0.0785205
C	-3.1422483	2.0533478	-0.0453073
C	-4.5134575	1.9433632	-0.0566904
N	-5.1217523	0.7379322	-0.0555899
H	-1.3275588	0.7853236	0.2139263
H	-2.6430786	3.0110603	-0.0219105
Se	-5.2368782	-2.1552559	0.0991561
Se	-5.7674135	3.4574739	-0.0456899
H	-2.552469	-1.1986988	0.1702604
H	-6.1295056	0.6865105	-0.0556409

Point7

C	-4.4344762	-0.4984724	-0.1468553
N	-3.05443	-0.3228536	0.0612017

C	-2.4083444	0.8216862	0.0781274
C	-3.144594	2.0506618	-0.0576763
C	-4.5165006	1.9374289	-0.0598903
N	-5.1220524	0.7388513	-0.0592755
H	-1.336501	0.7882078	0.2310751
H	-2.6465542	3.0068708	-0.0286578
Se	-5.2331386	-2.1573712	0.1109436
Se	-5.7539214	3.4643535	-0.0284705
H	-2.5519756	-1.1929884	0.1788962
H	-6.1272809	0.6841793	-0.050847

Point8

C	-4.4320446	-0.4982138	-0.1772386
N	-3.0519	-0.3196876	0.0578423
C	-2.4138501	0.8195078	0.0776666
C	-3.1470045	2.0478356	-0.0700538
C	-4.5195431	1.9311072	-0.0629925
N	-5.1219022	0.73916	-0.0630277
H	-1.3455929	0.7913612	0.2482153
H	-2.6504901	3.002711	-0.0353532
Se	-5.2309748	-2.1568904	0.1231458
Se	-5.7403339	3.4703582	-0.0109252
H	-2.5516457	-1.1872801	0.1875967
H	-6.1244876	0.6805846	-0.0463046

Point9

C	-4.4286909	-0.4977173	-0.2082124
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N	-3.0490668	-0.316462	0.0544053
C	-2.4191559	0.8174226	0.0771132
C	-3.1494839	2.0448647	-0.0824307
C	-4.5225826	1.9243559	-0.0659657
N	-5.1212716	0.7388019	-0.0668799
H	-1.3548207	0.7947961	0.265325
H	-2.6549143	2.9985853	-0.0419596
Se	-5.2305385	-2.1535792	0.1359247
Se	-5.7266863	3.4754131	0.007037
H	-2.5514651	-1.1815722	0.1963593
H	-6.1210928	0.675645	-0.042145

Point10

C	-4.4243298	-0.4969831	-0.2398641
N	-3.0458874	-0.313178	0.0508558
C	-2.4242327	0.8154344	0.0764405
C	-3.1520388	2.0417415	-0.0947976
C	-4.525617	1.9171189	-0.0687776
N	-5.1201239	0.7377044	-0.0708665
H	-1.3641654	0.7985274	0.2823814
H	-2.659864	2.9944969	-0.048438
Se	-5.2320159	-2.1471243	0.1494491
Se	-5.7130239	3.4794206	0.0255135
H	-2.5514131	-1.1758638	0.2051783
H	-6.1170574	0.6692591	-0.0385037

The S1 Minimum to T1 Minimum (24SeU)

Point1

C	-4.4318033	-0.4905938	0.0271925
N	-3.0718924	-0.3558131	0.0838421
C	-2.3901932	0.8746334	0.0789121
C	-3.1386052	2.0499562	0.0140856
C	-4.5318754	1.9750812	-0.0461196
N	-5.1292393	0.694192	-0.040309
H	-1.303475	0.8296732	0.1268996
H	-2.6341739	3.0180229	0.0124215
Se	-5.2739029	-2.106644	0.0370786
Se	-5.7262408	3.4776425	-0.1168236
H	-2.5590589	-1.2314738	0.1366737
H	-6.1393091	0.5858773	-0.0852822

Point2

C	-4.4321099	-0.4906248	0.0270979
N	-3.0717062	-0.3555428	0.083763
C	-2.3893616	0.8738421	0.0788898
C	-3.1395524	2.0499295	0.0141657
C	-4.5322025	1.9751856	-0.0460666
N	-5.1288391	0.693933	-0.0402816
H	-1.3026625	0.8287656	0.1272388
H	-2.6366168	3.0187318	0.0124088
Se	-5.2729788	-2.1080341	0.0371298
Se	-5.7251386	3.4777564	-0.1172981
H	-2.559309	-1.2316326	0.1363082
H	-6.1392919	0.5882441	-0.0847846

Point3

C	-4.4324169	-0.4906549	0.0270033
N	-3.0715203	-0.3552716	0.0836839
C	-2.3885305	0.873051	0.0788673
C	-3.1405007	2.0499016	0.014246
C	-4.5325306	1.9752898	-0.0460138
N	-5.1284398	0.6936743	-0.0402547
H	-1.3018509	0.8278575	0.1275775
H	-2.6390609	3.0194369	0.0123966
Se	-5.2720534	-2.1094223	0.0371815
Se	-5.7240368	3.4778696	-0.1177722
H	-2.5595598	-1.2317902	0.135943
H	-6.1392686	0.5906122	-0.084287

Point4

C	-4.4327243	-0.4906842	0.0269087
N	-3.0713348	-0.3549995	0.083605
C	-2.3877002	0.8722601	0.0788445
C	-3.1414501	2.0498727	0.0143263
C	-4.5328597	1.9753937	-0.0459614
N	-5.1280414	0.6934159	-0.0402285
H	-1.30104	0.8269489	0.1279157
H	-2.6415064	3.0201381	0.0123849
Se	-5.2711268	-2.1108087	0.0372336
Se	-5.7229354	3.477982	-0.1182459
H	-2.5598113	-1.2319466	0.1355779

H	-6.139239	0.5929816	-0.0837895
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Point5

C	-4.4330321	-0.4907127	0.0268141
N	-3.0711495	-0.3547266	0.0835261
C	-2.3868704	0.8714694	0.0788216
C	-3.1424006	2.0498426	0.0144066
C	-4.5331899	1.9754974	-0.0459092
N	-5.1276438	0.6931578	-0.0402028
H	-1.3002299	0.8260399	0.1282534
H	-2.6439531	3.0208354	0.0123738
Se	-5.2701989	-2.1121934	0.0372861
Se	-5.7218343	3.4780937	-0.1187193
H	-2.5600636	-1.232102	0.135213
H	-6.1392033	0.5953523	-0.0832922

Point6

C	-4.4333402	-0.4907403	0.0267195
N	-3.0709646	-0.3544527	0.0834474
C	-2.3860413	0.870679	0.0787984
C	-3.1433523	2.0498115	0.0144871
C	-4.5335211	1.9756008	-0.0458573
N	-5.127247	0.6929	-0.0401778
H	-1.2994206	0.8251304	0.1285906
H	-2.646401	3.0215289	0.0123632
Se	-5.2692697	-2.1135761	0.0373391
Se	-5.7207336	3.4782046	-0.1191924

H	-2.5603166	-1.2322562	0.1348483
H	-6.1391613	0.5977243	-0.0827949

Point7

C	-4.4336486	-0.4907672	0.0266249
N	-3.07078	-0.354178	0.0833687
C	-2.3852129	0.8698888	0.078775
C	-3.144305	2.0497792	0.0145676
C	-4.5338533	1.975704	-0.0458057
N	-5.1268511	0.6926424	-0.0401533
H	-1.2986121	0.8242204	0.1289273
H	-2.6488502	3.0222184	0.0123532
Se	-5.2683393	-2.1149571	0.0373925
Se	-5.7196332	3.4783148	-0.119665
H	-2.5605703	-1.2324093	0.1344837
H	-6.1391131	0.6000975	-0.0822977

Point8

C	-4.4339575	-0.4907932	0.0265303
N	-3.0705957	-0.3539025	0.0832901
C	-2.3843851	0.8690988	0.0787514
C	-3.1452589	2.0497459	0.0146482
C	-4.5341866	1.975807	-0.0457544
N	-5.126456	0.6923852	-0.0401294
H	-1.2978044	0.82331	0.1292635
H	-2.6513007	3.0229041	0.0123436
Se	-5.2674077	-2.1163362	0.0374464

Se	-5.7185333	3.4784243	-0.1201373
H	-2.5608248	-1.2325612	0.1341194
H	-6.1390586	0.602472	-0.0818007

Point9

C	-4.4342667	-0.4908184	0.0264357
N	-3.0704117	-0.353626	0.0832116
C	-2.383558	0.868309	0.0787276
C	-3.1462139	2.0497115	0.0147289
C	-4.5345209	1.9759097	-0.0457033
N	-5.1260618	0.6921282	-0.040106
H	-1.2969975	0.8223991	0.1295992
H	-2.6537524	3.0235859	0.0123346
Se	-5.2664748	-2.1177135	0.0375007
Se	-5.7174337	3.478533	-0.1206092
H	-2.56108	-1.232712	0.1337552
H	-6.138998	0.6048476	-0.0813039

Point10

C	-4.4345763	-0.4908428	0.0263411
N	-3.070228	-0.3533487	0.0831332
C	-2.3827315	0.8675194	0.0787036
C	-3.14717	2.0496759	0.0148096
C	-4.5348562	1.9760122	-0.0456525
N	-5.1256684	0.6918716	-0.0400832
H	-1.2961914	0.8214878	0.1299345
H	-2.6562054	3.0242639	0.0123261

Se	-5.2655406	-2.119089	0.0375555
Se	-5.7163344	3.4786409	-0.1210808
H	-2.5613359	-1.2328617	0.1333913
H	-6.1389311	0.6072245	-0.0808072

The T1 Minimum to T1S0 crossing point (24SeU)

Point1

C	-4.434549	-0.4908538	0.0265653
N	-3.0702082	-0.3533177	0.0834334
C	-2.3827381	0.8675645	0.0787982
C	-3.1471976	2.0496907	0.014595
C	-4.5348776	1.9759836	-0.0459584
N	-5.125662	0.6918313	-0.0401627
H	-1.2962009	0.8215676	0.1301225
H	-2.6562542	3.0242889	0.011943
Se	-5.2654784	-2.1191159	0.0380605
Se	-5.716383	3.4785704	-0.1217958
H	-2.5613006	-1.2328089	0.1339169
H	-6.1389197	0.6071533	-0.0809468

Point2

C	-4.4337194	-0.485227	0.027121
N	-3.0695309	-0.3482389	0.0917315
C	-2.3802265	0.8706086	0.0806283
C	-3.1392627	2.0469956	-0.0043071
C	-4.5322649	1.968206	-0.0872554
N	-5.1347756	0.6940393	-0.054875

H	-1.293984	0.8203857	0.1445083
H	-2.6466409	3.0210293	-0.0132573
Se	-5.2672431	-2.1121174	0.0470604
Se	-5.7236404	3.4626628	-0.0432047
H	-2.5609913	-1.2270499	0.1572025
H	-6.1474898	0.6092598	-0.1167811

Point3

C	-4.4332647	-0.4794616	0.0275347
N	-3.0694651	-0.3430755	0.1003301
C	-2.3786744	0.8738945	0.0821826
C	-3.1318047	2.0446509	-0.0242823
C	-4.5300033	1.9622227	-0.1298306
N	-5.1425505	0.6967791	-0.0712391
H	-1.2929012	0.820026	0.1592133
H	-2.6371827	3.0179189	-0.0391333
Se	-5.2696259	-2.1047937	0.0566188
Se	-5.7285467	3.4424265	0.0398745
H	-2.5615539	-1.2210207	0.1816552
H	-6.1541964	0.6109869	-0.1543528

Point4

C	-4.4332974	-0.473556	0.0276188
N	-3.0701876	-0.3377833	0.109491
C	-2.3782622	0.8774772	0.0835583
C	-3.1247571	2.0427906	-0.0461604
C	-4.5280672	1.9584636	-0.1744303

N	-5.1487548	0.7001338	-0.0899037
H	-1.2931812	0.8206366	0.1747801
H	-2.6276759	3.015027	-0.0664762
Se	-5.2727649	-2.0971099	0.0668081
Se	-5.7307837	3.4167158	0.1293605
H	-2.5632221	-1.2146073	0.2080229
H	-6.1588152	0.6123657	-0.1940979

Point5

C	-4.4340009	-0.4674973	0.027296
N	-3.0719565	-0.332293	0.1194495
C	-2.3792575	0.8814501	0.0847177
C	-3.1180837	2.0415947	-0.0706397
C	-4.5264652	1.9575654	-0.2218332
N	-5.1530097	0.7042313	-0.1116661
H	-1.2951546	0.8224538	0.1915248
H	-2.6179327	3.0124639	-0.0957862
Se	-5.276891	-2.0889939	0.0780113
Se	-5.7297078	3.3837506	0.2271433
H	-2.5663322	-1.2076367	0.2370423
H	-6.1609776	0.6134652	-0.2366887

Point6

C	-4.4356558	-0.4612369	0.0266352
N	-3.075133	-0.326504	0.1304234
C	-2.382023	0.8859406	0.0854544
C	-3.1117854	2.0413109	-0.0982648

C	-4.5252303	1.9604486	-0.2728654
N	-5.1547327	0.709258	-0.1375259
H	-1.2992556	0.8257946	0.2094702
H	-2.6077983	3.0104105	-0.1272096
Se	-5.2823885	-2.0802804	0.0910332
Se	-5.7243065	3.3408671	0.3350506
H	-2.5713574	-1.1998631	0.2694646
H	-6.1601027	0.6144081	-0.2830946

Point7

C	-4.4386728	-0.4546469	0.0258711
N	-3.0802165	-0.3202684	0.142649
C	-2.3870434	0.8911101	0.0853883
C	-3.1059217	2.0422853	-0.129473
C	-4.5244239	1.968439	-0.3284433
N	-5.153048	0.715476	-0.1687226
H	-1.3060447	0.8310639	0.2283381
H	-2.5971829	3.0091549	-0.1605755
Se	-5.2898801	-2.0706169	0.1071732
Se	-5.7130684	3.2841142	0.4548354
H	-2.5789657	-1.1909405	0.3061247
H	-6.1553013	0.6153833	-0.3345941

Point8

C	-4.4436314	-0.4474453	0.0254187
N	-3.0878972	-0.3133586	0.15645
C	-2.3949949	0.8971657	0.0839924

C	-3.1006739	2.0449952	-0.1646809
C	-4.5241818	1.9834562	-0.3896412
N	-5.1466459	0.7232377	-0.2067356
H	-1.3162721	0.8387972	0.2475931
H	-2.5861488	3.0091313	-0.1954999
Se	-5.3003441	-2.0593092	0.1282674
Se	-5.6936321	3.2076139	0.5880796
H	-2.5901127	-1.1803743	0.3480486
H	-6.1452346	0.6166442	-0.3927208

Point9

C	-4.4513187	-0.439073	0.0258985
N	-3.0991363	-0.3054117	0.1723558
C	-2.4068971	0.9043947	0.0806718
C	-3.0965205	2.0500651	-0.2043635
C	-4.5248553	2.0083044	-0.4577805
N	-5.1335665	0.7329886	-0.2531998
H	-1.331025	0.8497772	0.2665428
H	-2.5751512	3.0109531	-0.2315213
Se	-5.3152703	-2.0450737	0.156682
Se	-5.66194	3.1026126	0.7357974
H	-2.6061842	-1.1674452	0.3965931
H	-6.1279043	0.6184618	-0.4591051

Point10

C	-4.4627413	-0.4285181	0.0281576
N	-3.1152862	-0.2958522	0.1913293

C	-2.4244596	0.9132324	0.0749861
C	-3.0946989	2.0582149	-0.2490542
C	-4.5273735	2.0471383	-0.5345961
N	-5.1108516	0.7452368	-0.3096588
H	-1.3520722	0.8653069	0.2846001
H	-2.5656677	3.0154257	-0.268229
Se	-5.3368461	-2.0256794	0.1951454
Se	-5.6102341	2.9561986	0.8973496
H	-2.6292249	-1.1511198	0.4536635
H	-6.1003134	0.6209699	-0.5351222