

Supplementary Materials for “Excited-State Decay Mechanism of 2,4-Dithiothymine in Gas Phase, Microsolvated Surrounding, and Aqueous Solution”

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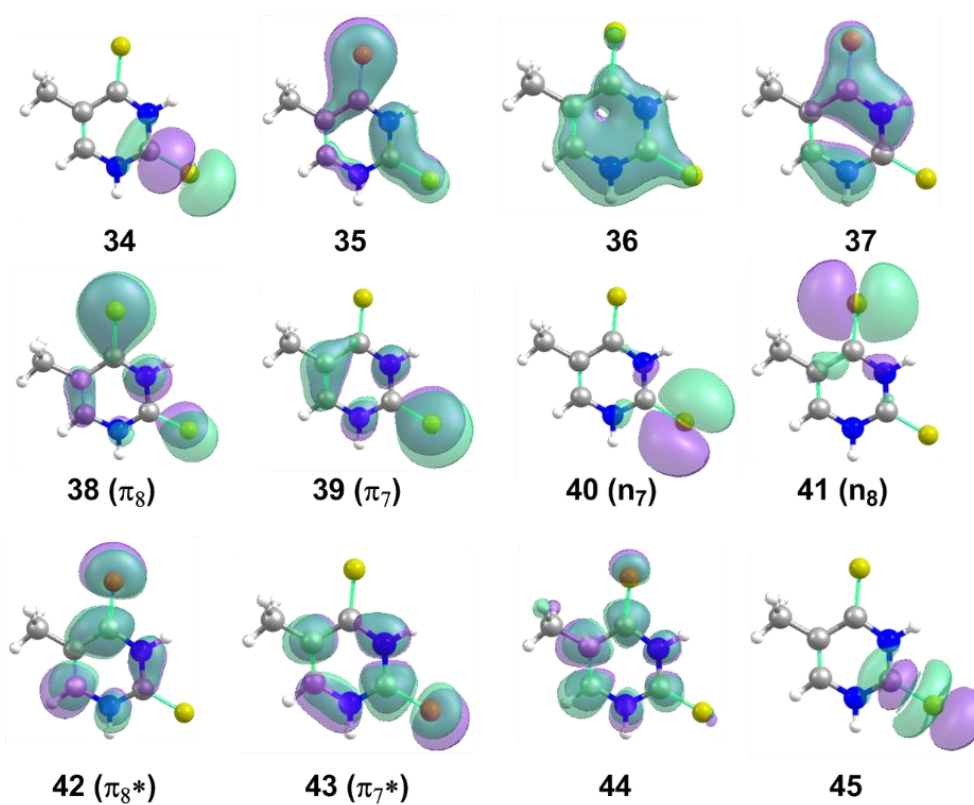
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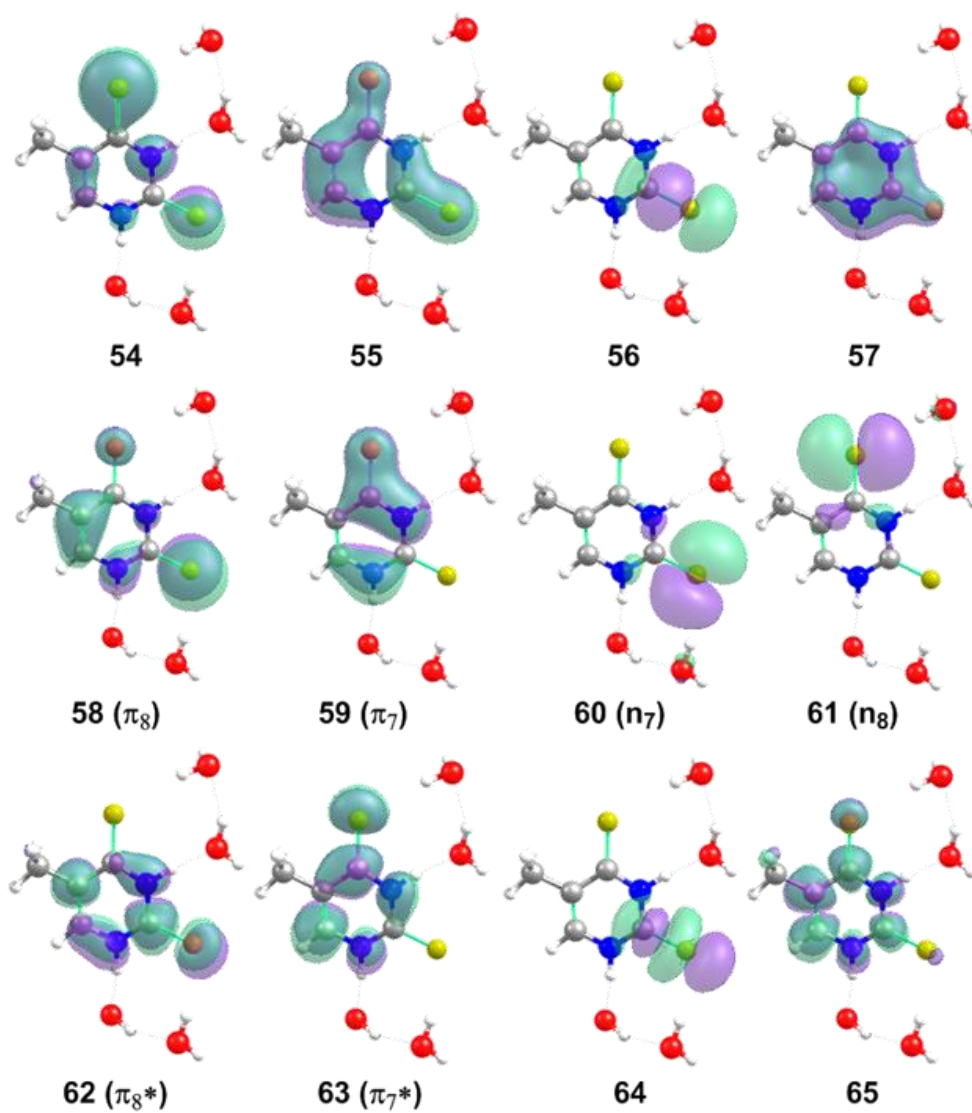
1. Active spaces of 2,4-dithiothymine used in CASSCF and CASPT2 calculations
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1. Active Spaces of 2,4-dtThy in CASSCF and CASPT2 calculations

(a) gas phase



(b) microsolvated surrounding



(c) aqueous solution

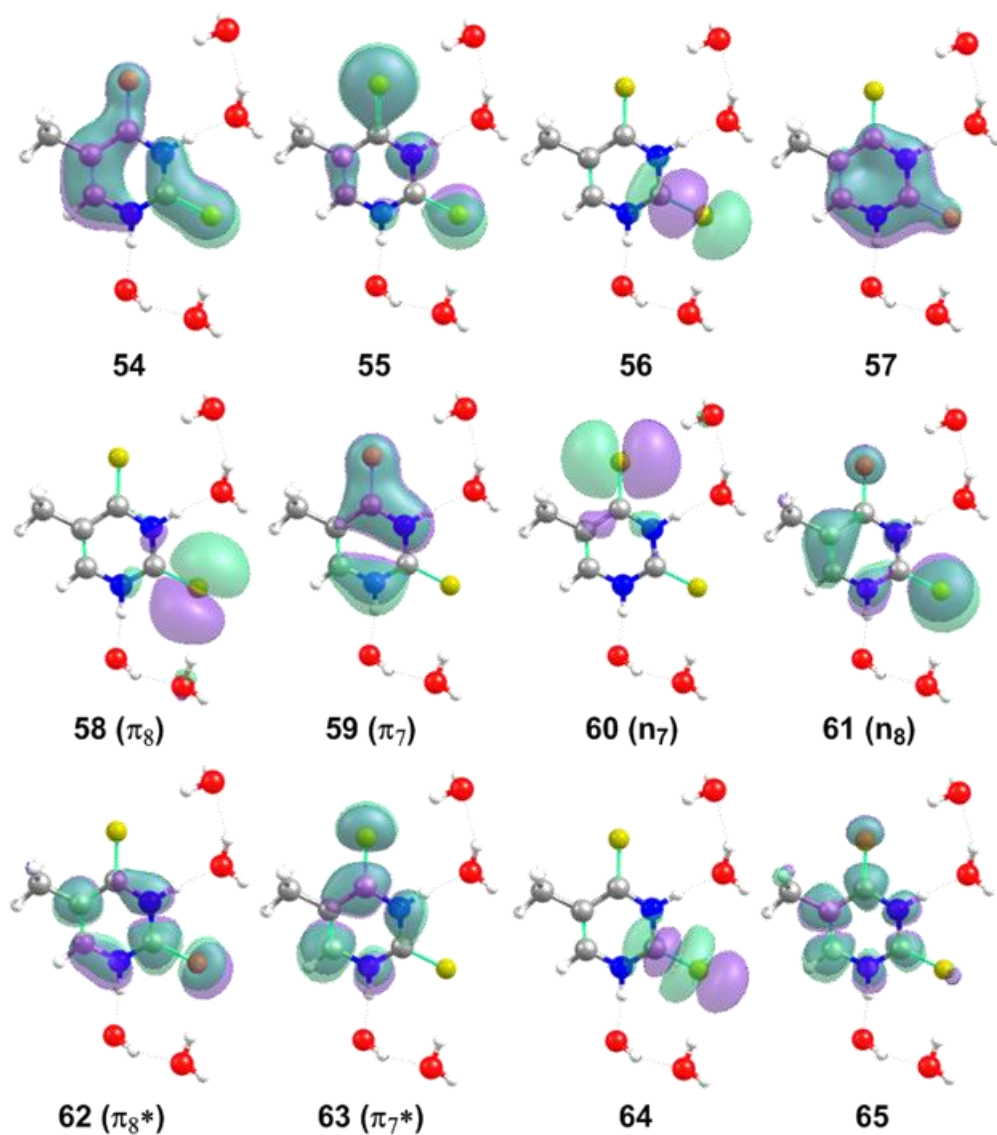


Figure S1: Active spaces of 2,4-dithiothymine in (a) gas phase, (b) microsolvated surrounding, and (c) aqueous solution.

2. Selection of microsolvated system and other computational details

In our 10 ps NVT MD simulations of aqueous 2,4-dithiothymine, we found a compact 4-water hydrogen-bond networks always around the two C=S bond. Thus, we adopted this minimally microsolvated model.

This situation is different from 7-water hydrogen-bonded network used in 4-thiothymine system recently by Martínez-Fernández et al. (ref. 47). This can be understandable. In terms of our previous QM/MM work on 4-thiothymidine, ref. 46, it is easily found that the hydrogen-bonding interaction is much stronger between the C=O group and water molecules than that between the C=S group and water molecules. Thus, more waters cluster around the C=O group and less waters around the C=S group. This has been observed in recent QM/MM work of Martínez-Fernández and coworkers (see Fig. S3 in their work). In 2,4-dithiothymine system, there is no C=O group, only the C=S groups; thus, the total number of water molecules that are compactly hydrogen-bonded with the two C=S groups is reduced, as observed in our 10 ps MD simulations.

All two-state minimum-energy conical intersections in Figs. 9-11 are directly optimized at CASSCF level using the penalty-function based method. Their single-point energies are refined by MS-CASPT2 method. Of course, at CASSCF level, they are truly degenerate points; but, at MS-CASPT2 level, a reasonably small energy gap, ca. 2-3 kcal/mol, turns out, as shown in Table 3. In addition, we have also identified some three- and four-state degenerate points based on MS-CASPT2 computed LIIC paths (Figs. S1-S6). The latter ones are not directly optimized.

3. Vertical excitation energies and adiabatic excitation energies of different snapshots in aqueous solution (QM/MM model)

Table S1: MS-CASPT2 computed vertical excitation energies (kcal/mol) to the lowest several excited singlet and triplet states of different snapshots in aqueous solution

states	snapshot1	snapshot2	snapshot3
$^1n_8\pi_8^*$	71.5	71.1	70.5
$^1\pi_7\pi_8^*$	85.6	83.6	82.9
$^1n_7\pi_7^*$	90.4	88.9	88.2
$^3\pi_8\pi_8^*$	64.3	63.0	63.6
$^3n_8\pi_8^*$	70.1	69.6	69.0
$^3\pi_7\pi_7^*$	76.1	75.1	74.9

Table S2: QM(MS-CASPT2)/MM computed single-point energies (kcal/mol) of all optimized excited-state minima relative to their S_0 minima of different snapshots in aqueous solution

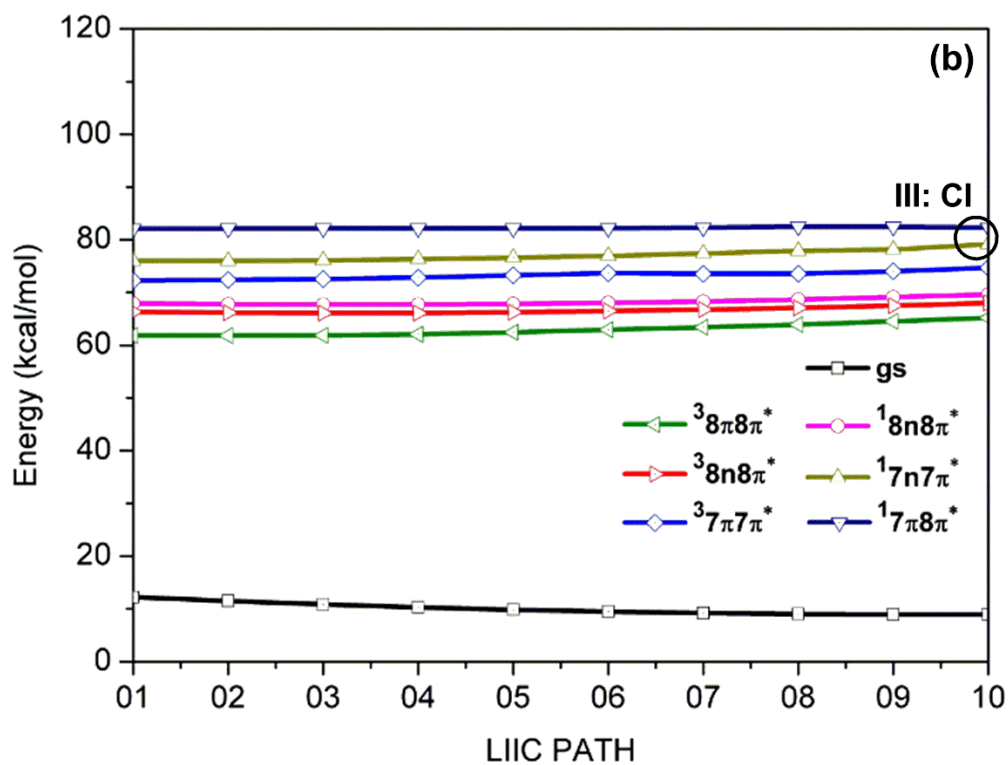
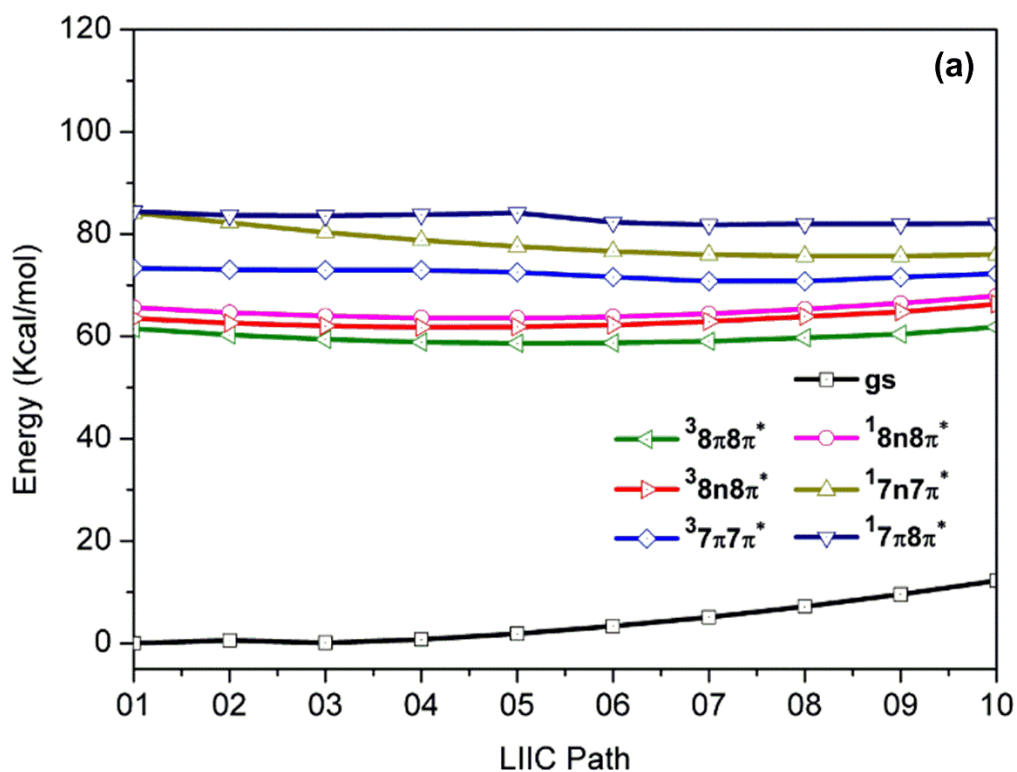
states	snapshot1	snapshot2	snapshot3
$^1n_8\pi_8^*$	64.1	65.5	65.1
$^1\pi_7\pi_8^*$	76.6	73.0	75.9
$^1n_7\pi_7^*$	80.9	81.2	81.5
$^3\pi_8\pi_8^*$	60.3	57.6	58.4
$^3n_8\pi_8^*$	63.4	61.0	62.6
$^3\pi_7\pi_7^*$	70.1	71.5	69.4

Table S3: Relative energies (in kcal/mol) of minimum energy conical intersections of different snapshots in aqueous solution (QM(CASPT2)/MM). The energy reference points are their corresponding S_0 minima.

	snapshot1	snapshot2	snapshot3
$^1\pi_7\pi_8^*/^1n_8\pi_8^*$	78.8/76.3	72.9/79.3	75.9/78.4
$^1n_8\pi_8^*/^1n_7\pi_7^*$	83.8/80.8	79.6/81.6	82.1/84.9
$^1\pi_7\pi_8^*/^1n_7\pi_7^*$	84.0/81.8	80.0/84.1	83.2/84.4
$^3n_8\pi_8^*/^3\pi_8\pi_8^*$	63.4/62.8	62.2/65.4	60.2/63.1
$^3n_8\pi_8^*/^3\pi_7\pi_7^*$	73.2/70.2	72.4/74.4	70.8/74.4

4. Linearly interpolated internal coordinate paths (QM/MM model)

gas phase



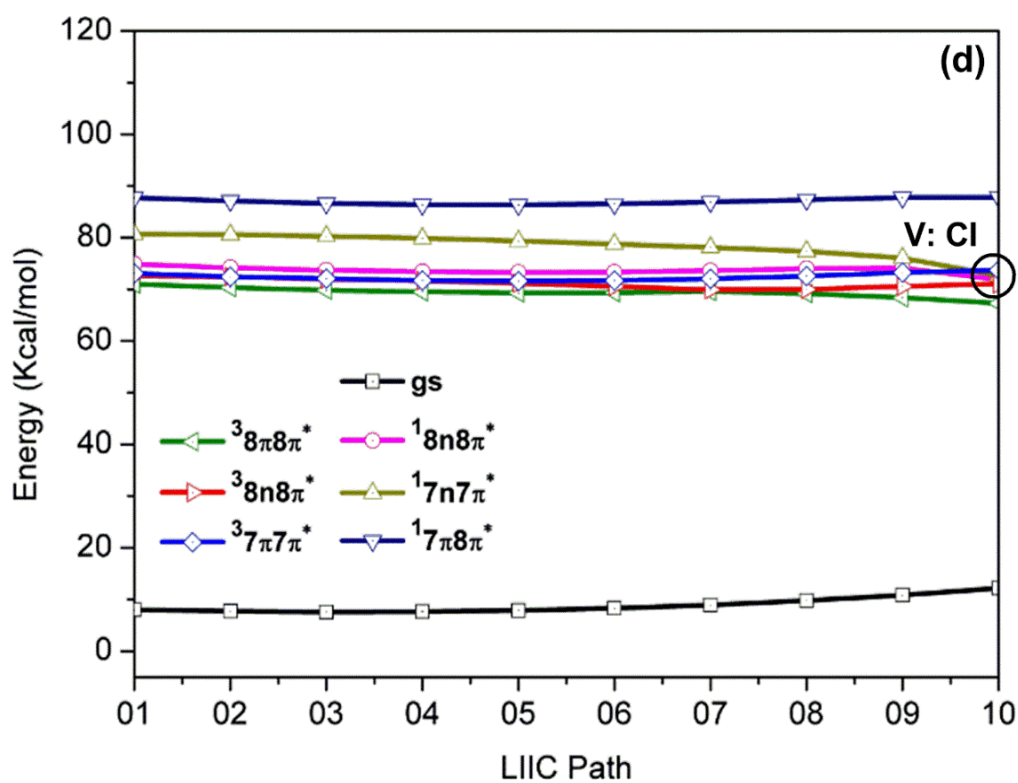
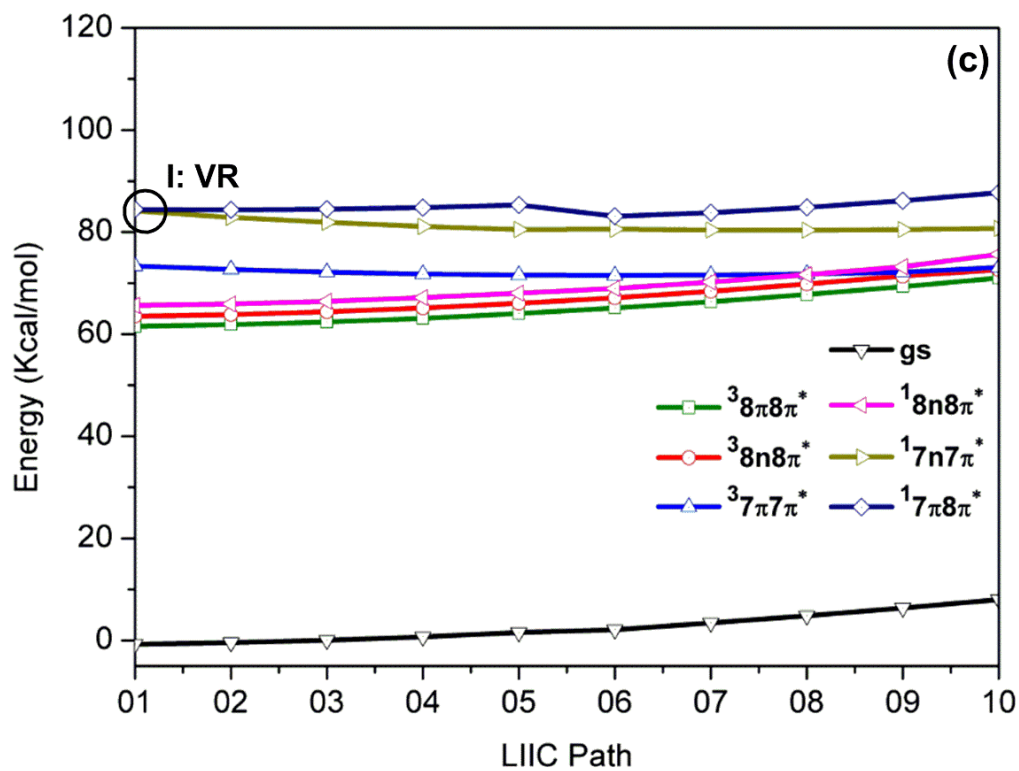
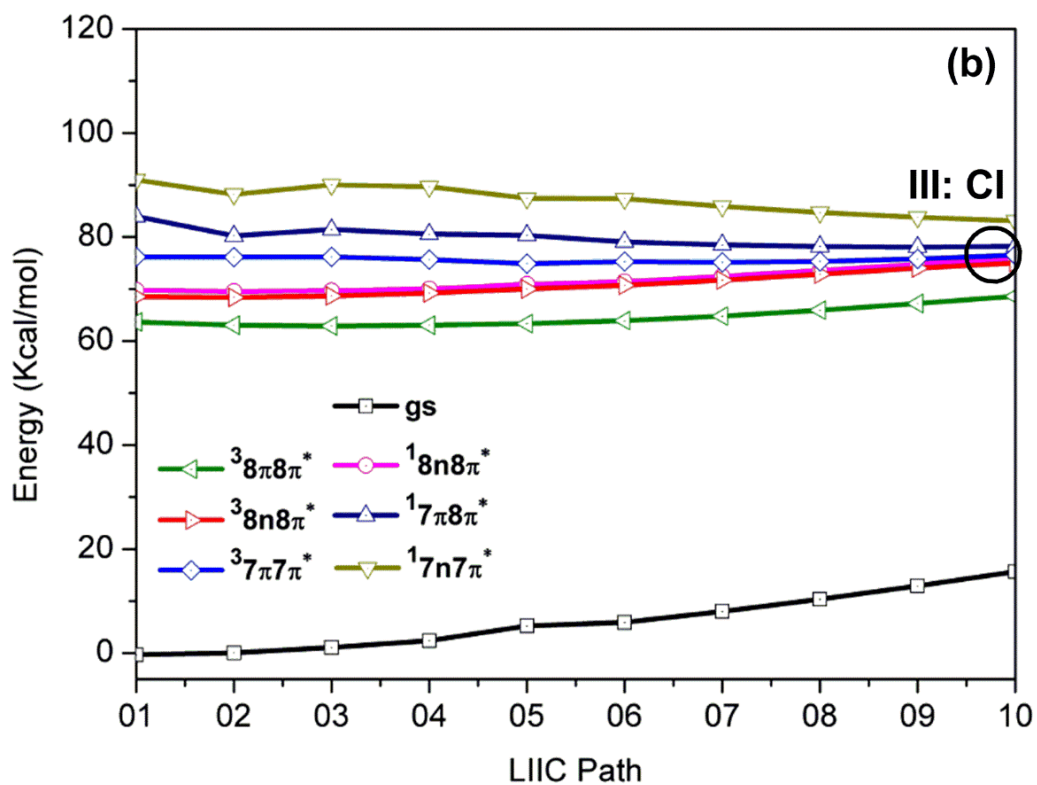
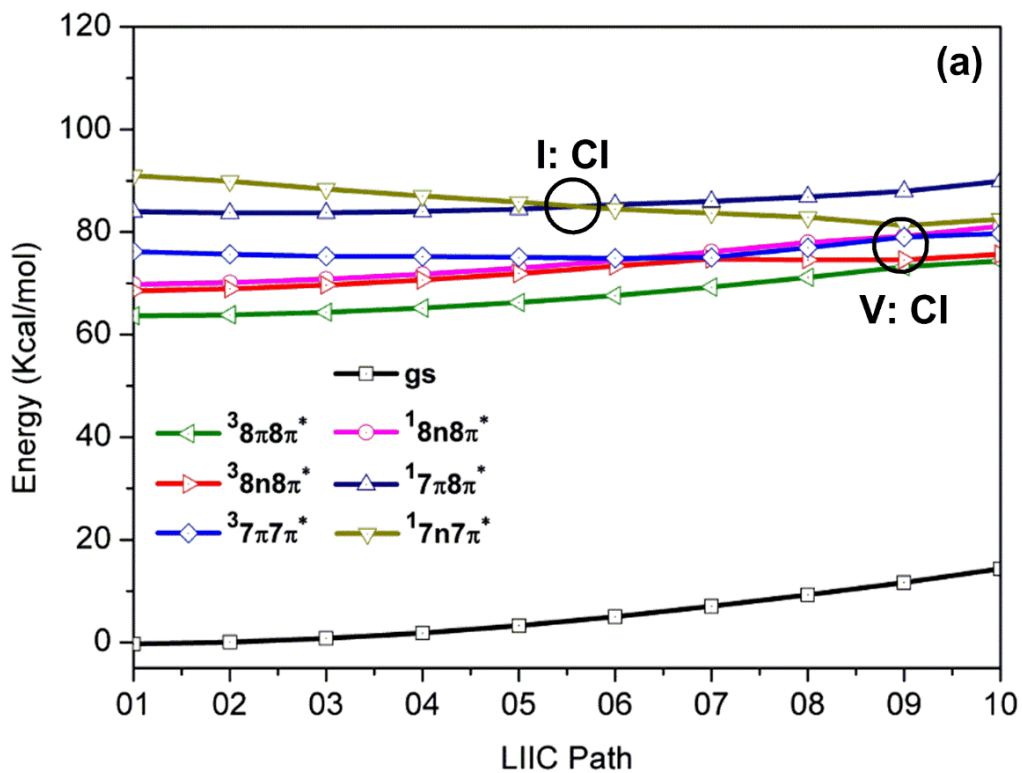


Figure S2: MS-CASPT2(16,12)/6-31G* computed LIIC paths of 2,4-dithiothymine in gas phase connecting (a) the Franck-Condon point to minimum ($^1\pi7\pi8^*$)_g; (b) minimum ($^1\pi7\pi8^*$)_g to the conical intersection ($^1n7\pi7^*/^1\pi7\pi8^*$)_g; (c) the Franck-Condon point to minimum ($^1n7\pi7^*$)_g; (d) minimum ($^1n7\pi7^*$)_g to the conical intersection ($^1n8\pi8^*/^1n7\pi7^*$)_g.

microsolvated surrounding



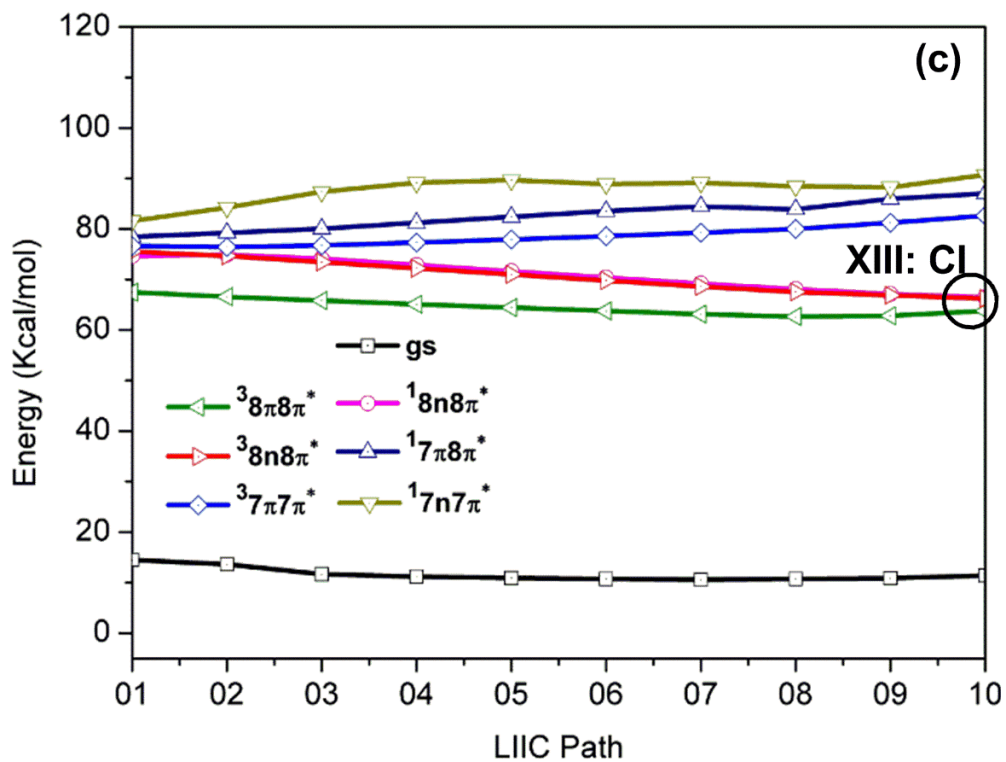
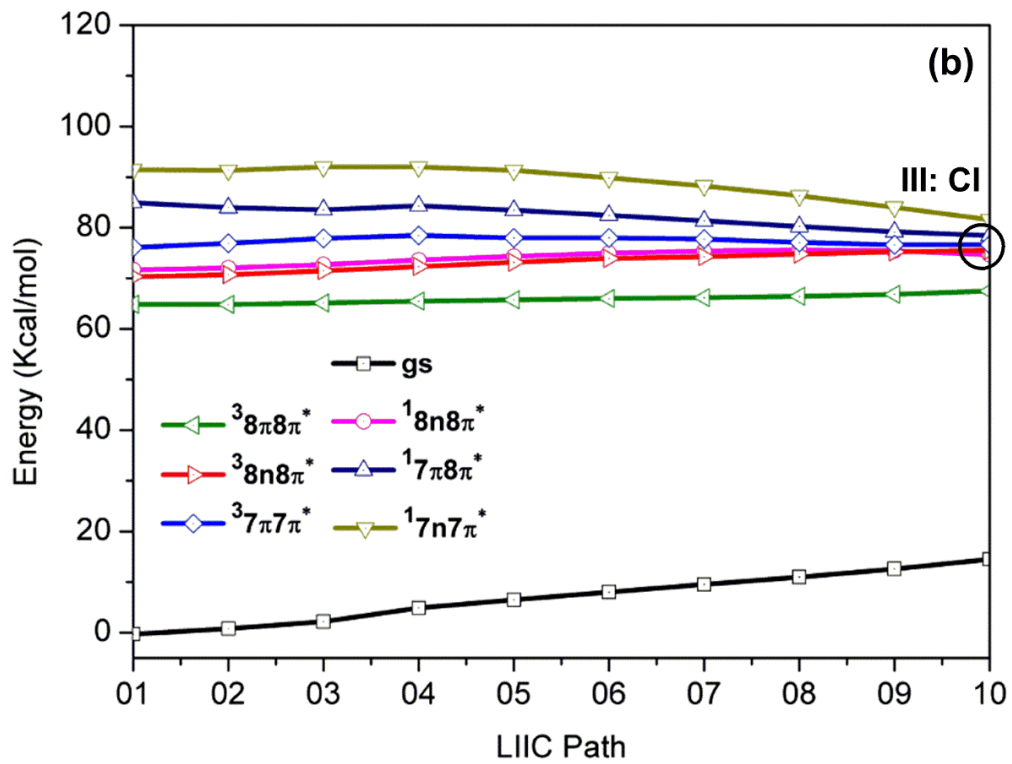
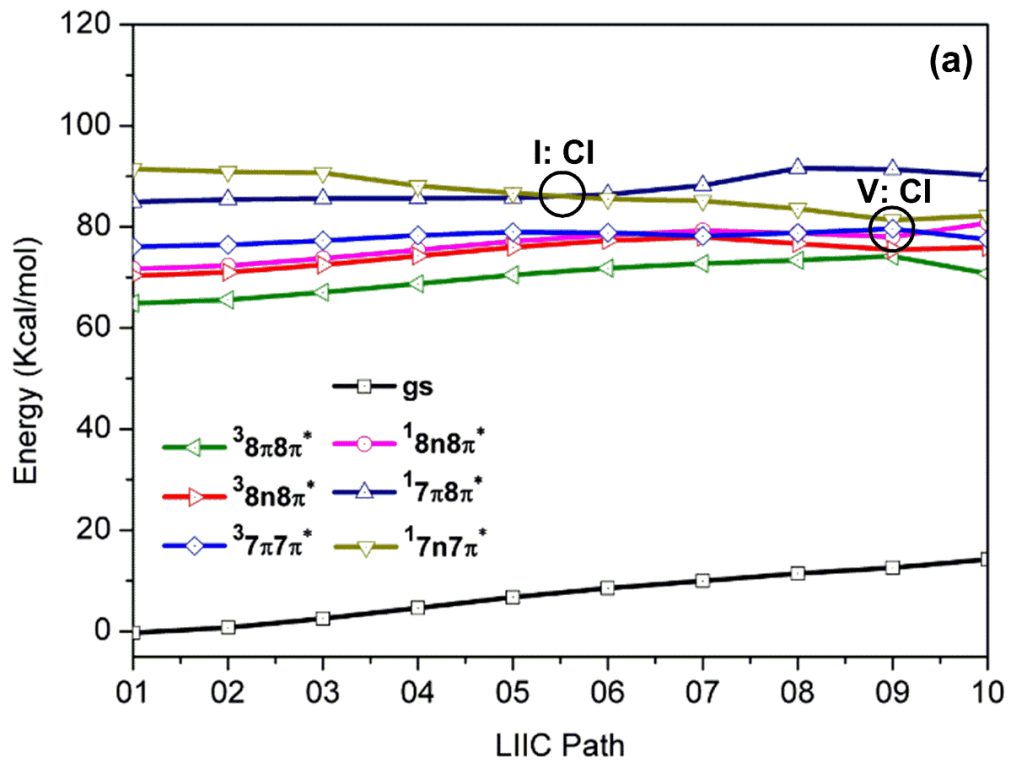


Figure S3: MS-CASPT2(16,12)/6-31G* computed LIIC paths of 2,4-dithiothymine in micro-solvated surrounding connecting (a) the Franck-Condon point to minimum ($^1n7\pi7^*$)_m; (b) the Franck-Condon point to minimum ($^1\pi7\pi8^*$)_m; (c) minimum ($^1\pi7\pi8^*$)_m to minimum ($^1n8\pi8^*$)_m.

aqueous solution

snapshot1



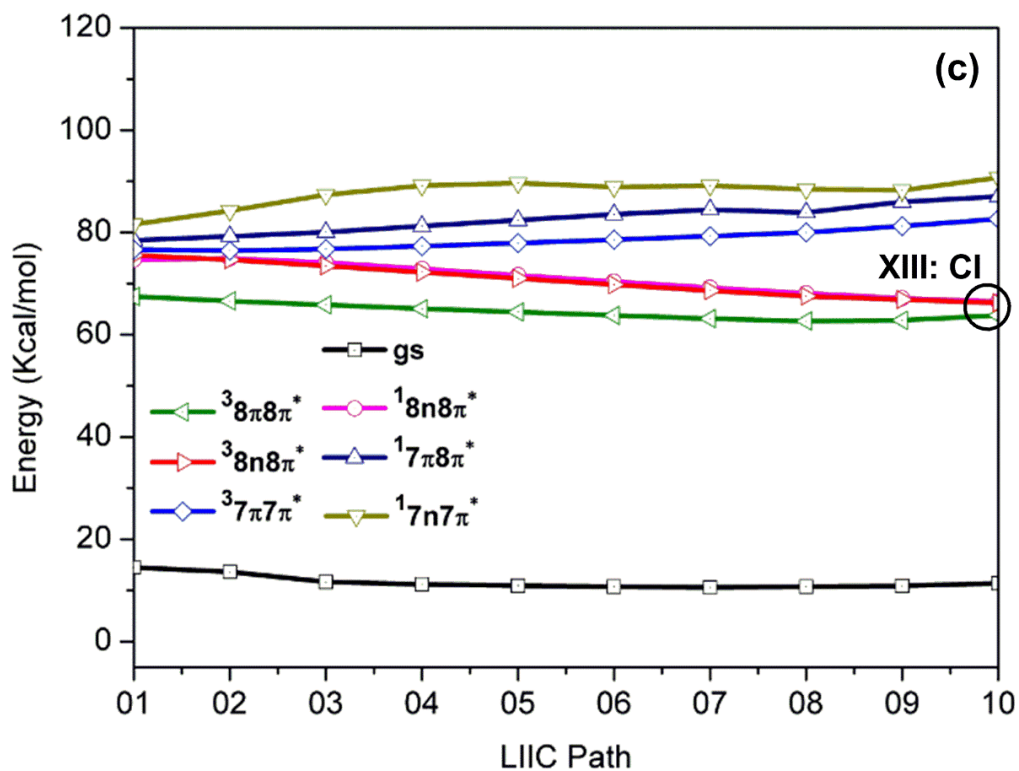
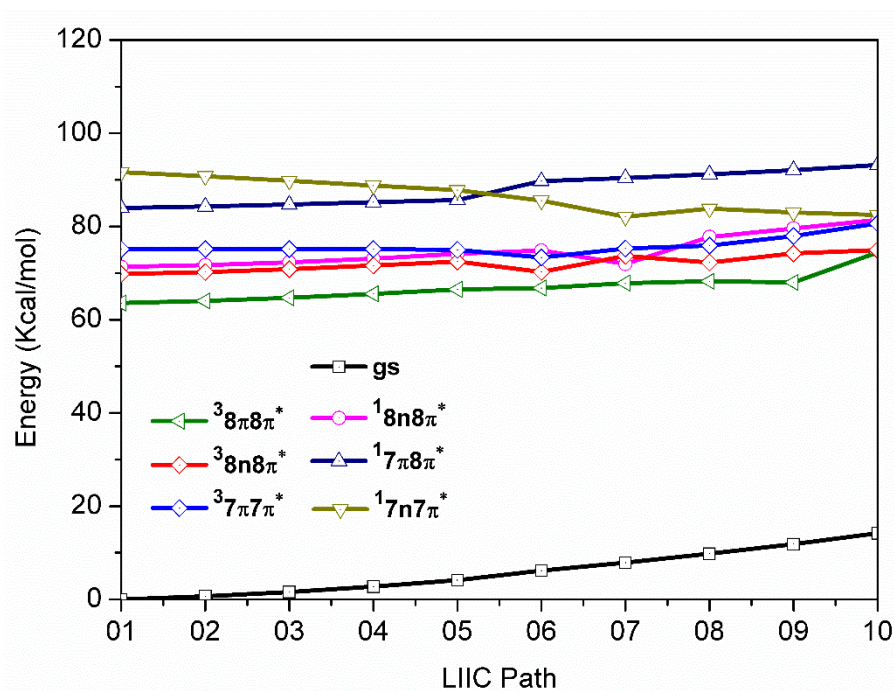


Figure S4: MS-CASPT2(16,12)/6-31G* computed LIIC paths of 2,4-dithiothymine in aqueous solution connecting (a) the Franck-Condon point to minimum ($1n7\pi7^*$)_w; (b) the Franck-Condon point to minimum ($1\pi7\pi8^*$)_w; (c) minimum ($1\pi7\pi8^*$)_w to minimum ($1n8\pi8^*$)_w.

snapshot2



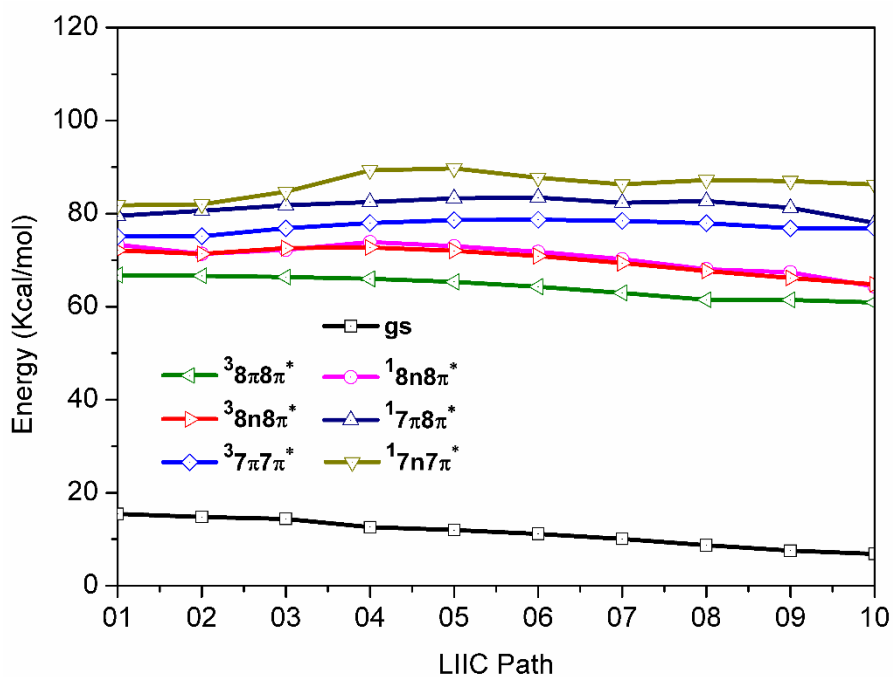
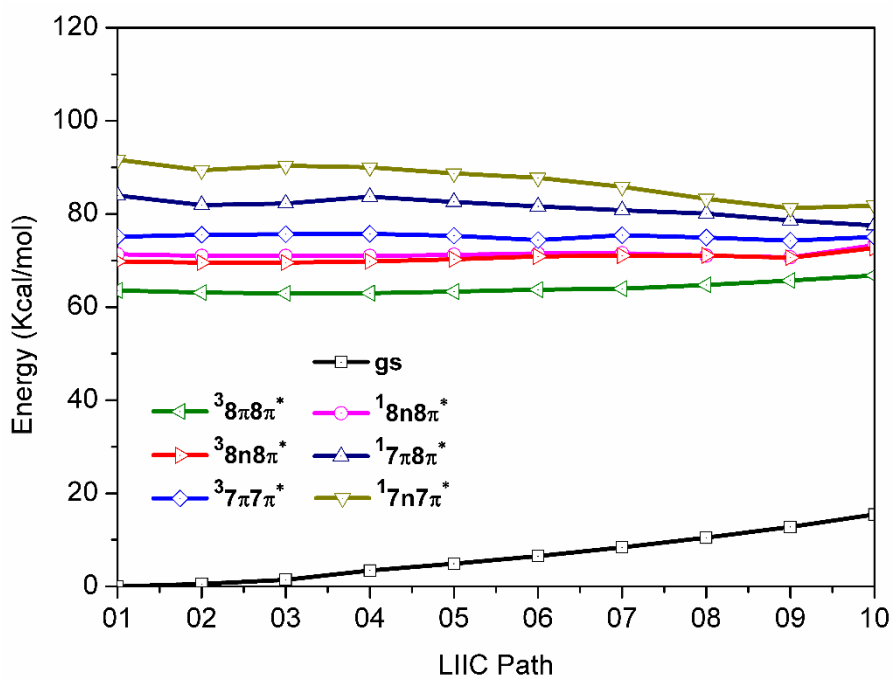
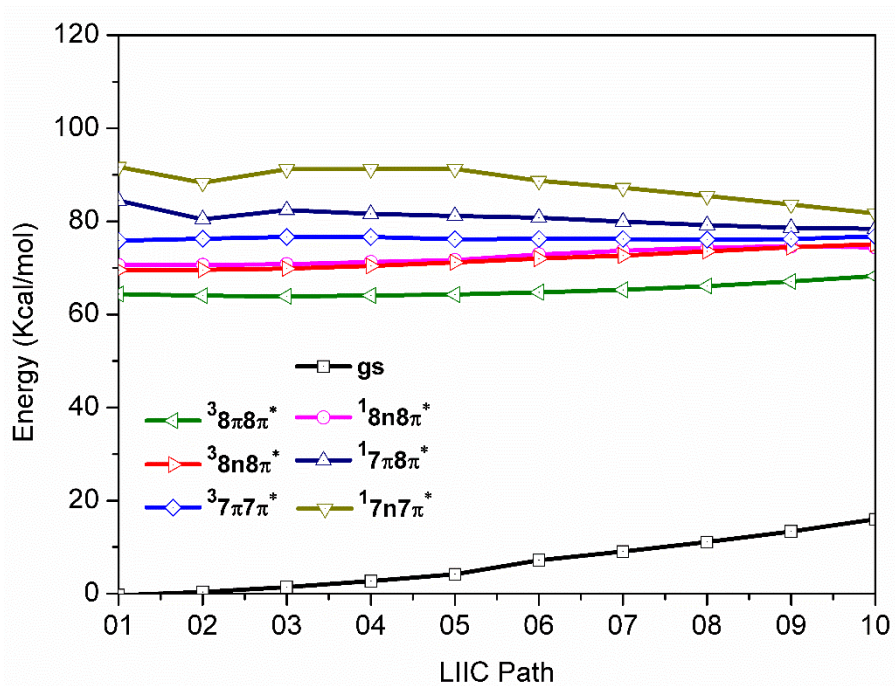
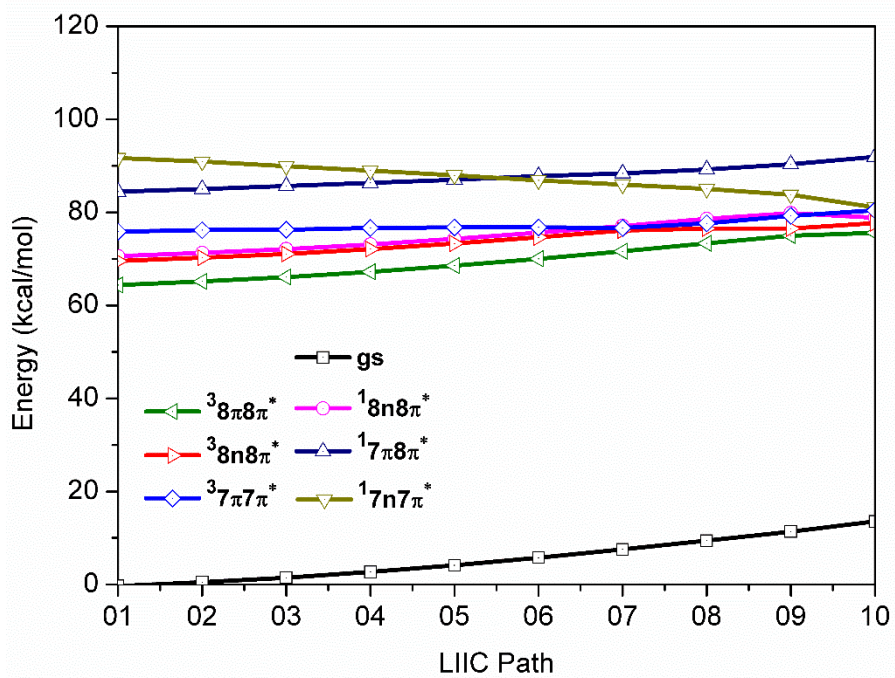


Figure S5: MS-CASPT2(16,12)/6-31G* computed LIIC paths of 2,4-dithiothymine in aqueous solution connecting (a) the Franck-Condon point to minimum ($^1n_7\pi_7^*$)_w; (b) the Franck-Condon point to minimum ($^1\pi_7\pi_8^*$)_w; (c) minimum ($^1\pi_7\pi_8^*$)_w to minimum ($^1n_8\pi_8^*$)_w.

snapshot3



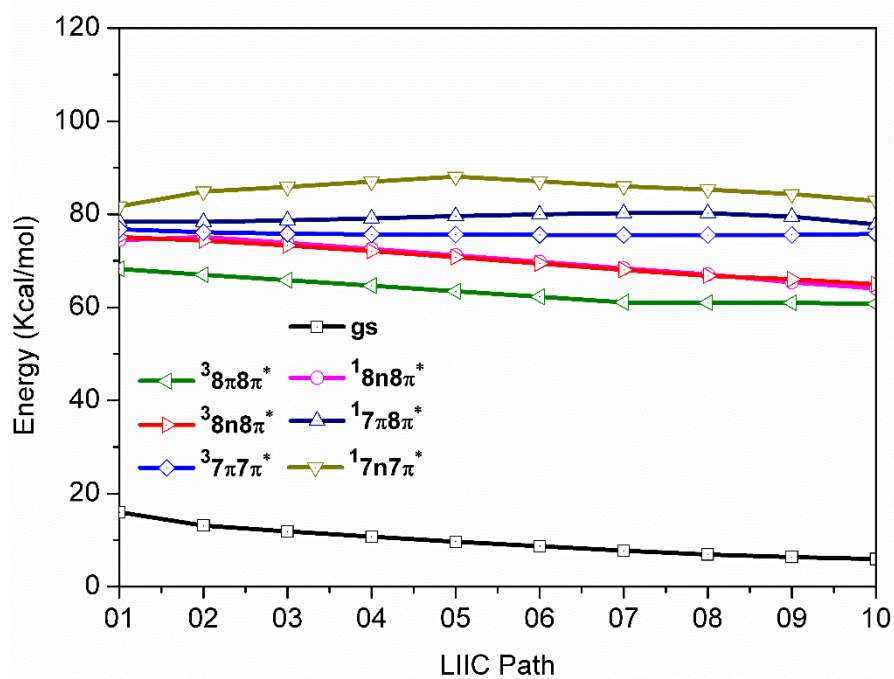
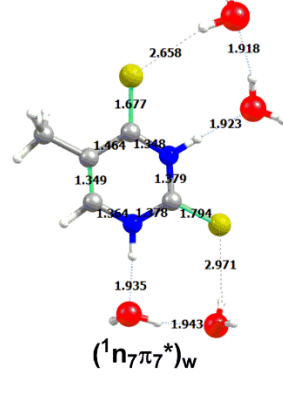
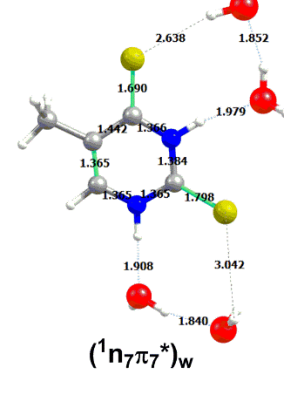
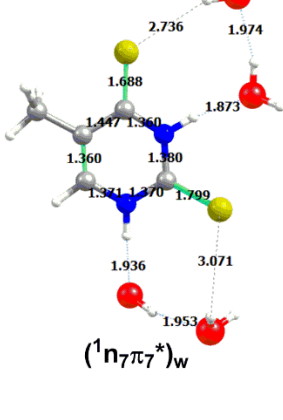
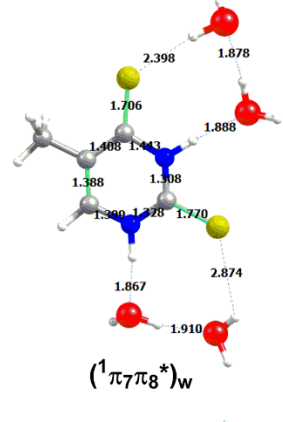
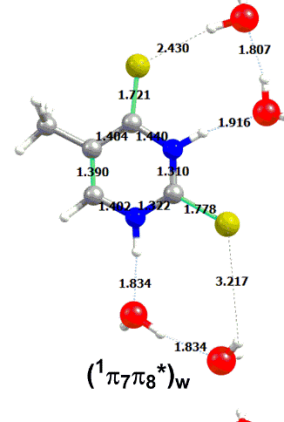
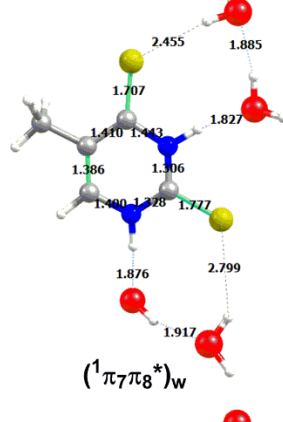
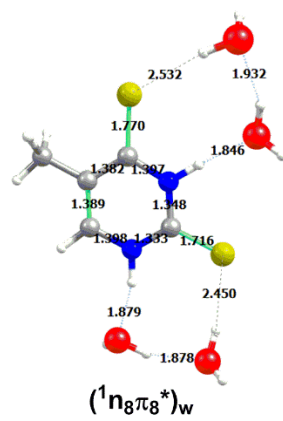
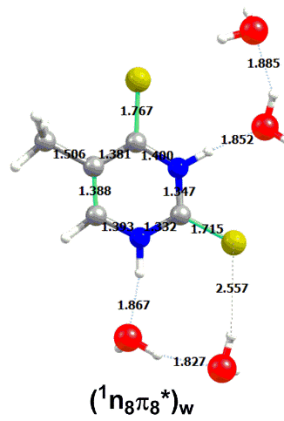
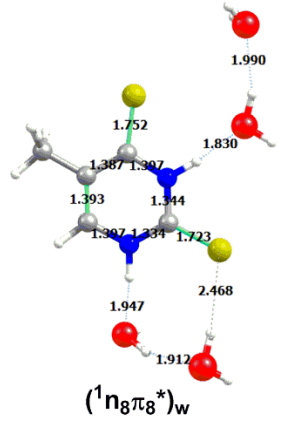
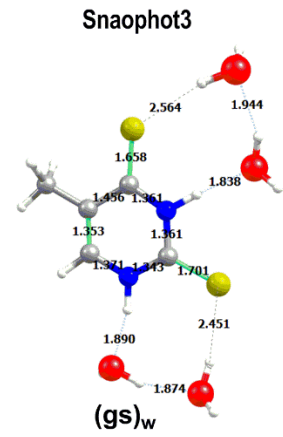
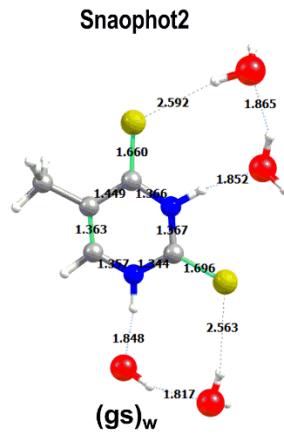
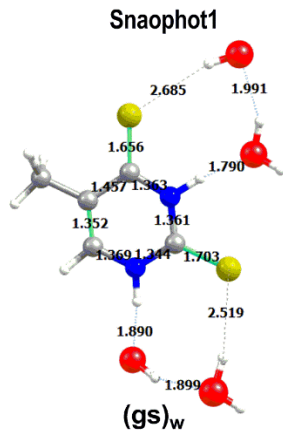
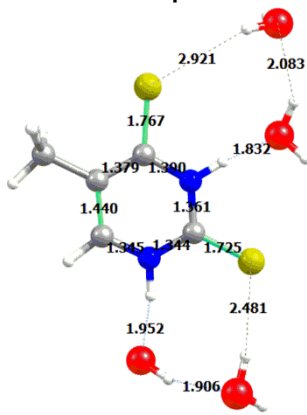


Figure S6: MS-CASPT2(16,12)/6-31G* computed LIIC paths of 2,4-dithiothymine in aqueous solution connecting (a) the Franck-Condon point to minimum ($^1n_7\pi_7^*$)_w; (b) the Franck-Condon point to minimum ($^1\pi_7\pi_8^*$)_w; (c) minimum ($^1\pi_7\pi_8^*$)_w to minimum ($^1n_8\pi_8^*$)_w.

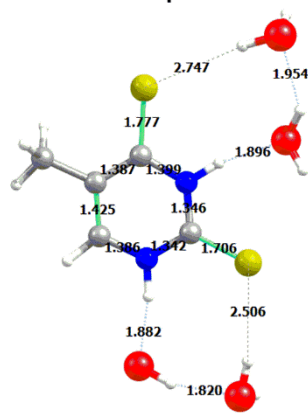
5. Minima and conical intersections optimized at CASSCF level of different snapshots in aqueous solution (QM/MM model)



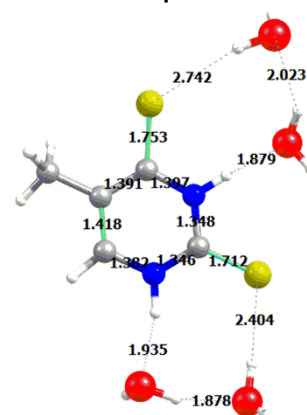
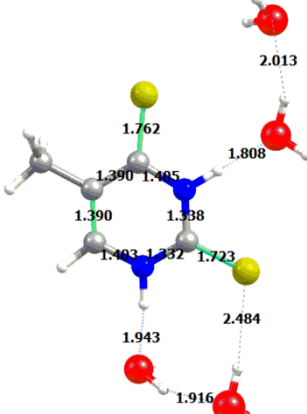
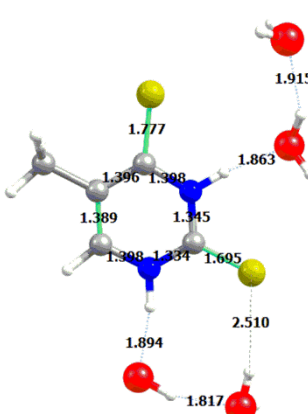
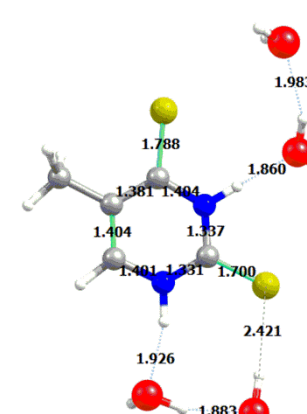
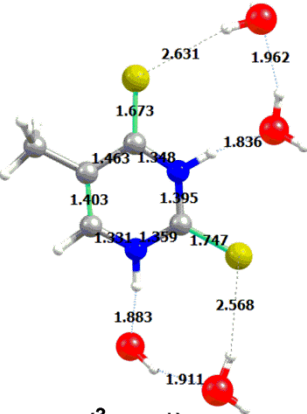
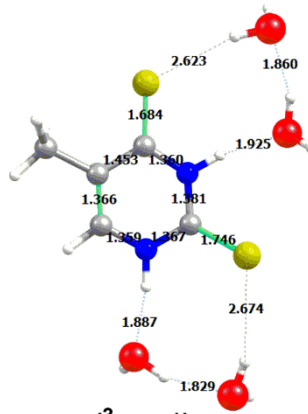
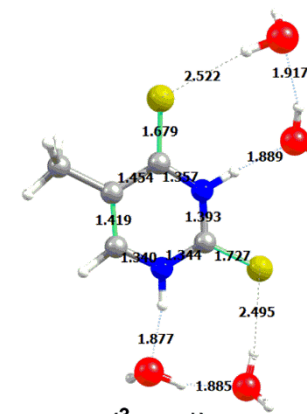
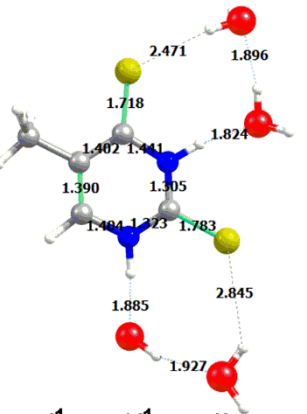
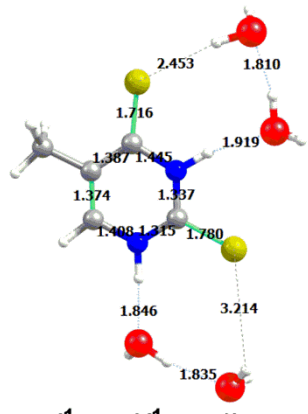
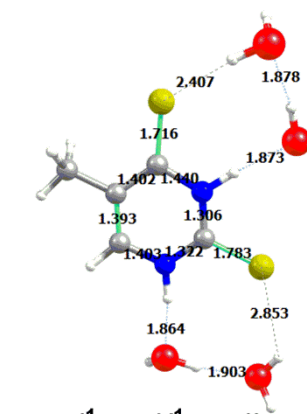
Snaophot1

 $(^3\pi_8\pi_8^*)_w$

Snaophot2

 $(^3\pi_8\pi_8^*)_w$

Snaophot3

 $(^3\pi_8\pi_8^*)_w$  $(^3n_8\pi_8^*)_w$  $(^3n_8\pi_8^*)_w$  $(^3n_8\pi_8^*)_w$  $(^3\pi_7\pi_7^*)_w$  $(^3\pi_7\pi_7^*)_w$  $(^3\pi_7\pi_7^*)_w$  $(^1\pi_7\pi_8^*/^1n_8\pi_8^*)_w$  $(^1\pi_7\pi_8^*/^1n_8\pi_8^*)_w$  $(^1\pi_7\pi_8^*/^1n_8\pi_8^*)_w$

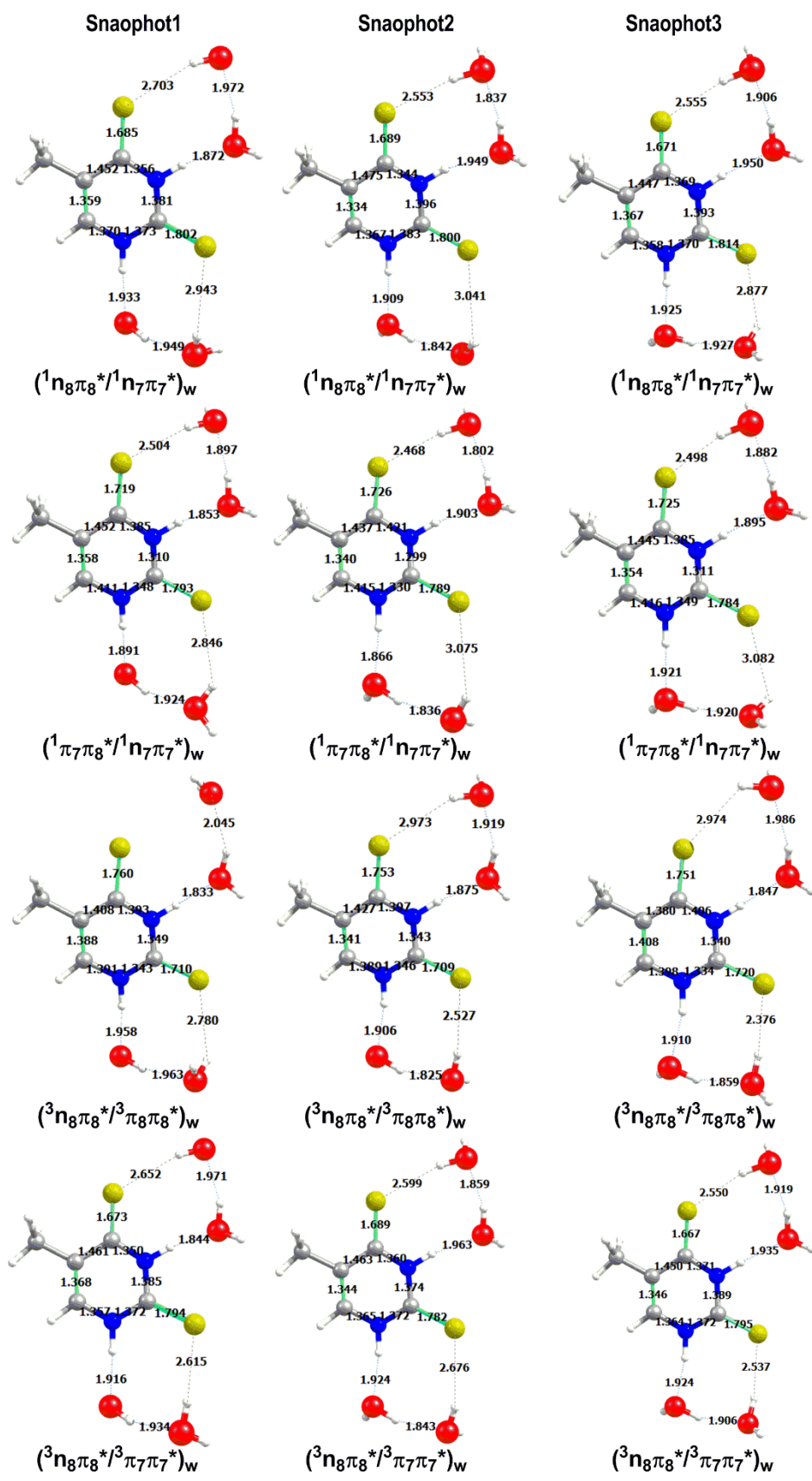


Figure S7: Minima and conical intersections optimized at CASSCF level of different snapshots in aqueous solution

6. Cartesian coordinates of all reported structures

Cartesian coordinates of optimized minimum structures

I. gas phase

gs

C	-0.62381240	-1.40786975	0.00333213
C	-1.03407674	-0.00169719	0.01376184
C	1.34066278	0.64641257	0.01435211
C	0.69925072	-1.67006952	-0.00152393
H	1.09030081	-2.66794996	-0.00943762
N	-0.00100328	0.89922249	0.01953390
H	-0.25133154	1.86611524	0.02629325
N	1.65147165	-0.67134968	0.00283579
H	2.61989942	-0.89914426	0.00017224
S	-2.59680793	0.52130500	0.01885195
S	2.49323539	1.87098403	0.02170996
C	-1.65159221	-2.50704426	-0.00156743
H	-2.28652295	-2.44836972	0.87402792
H	-2.29224002	-2.43538310	-0.87197784
H	-1.16564770	-3.47577691	-0.01036426

$^1n_8\pi_8^*$

C	-0.63839149	-1.40236250	0.00837063
C	-0.99801675	-0.06043941	0.02977822
C	1.33465439	0.64882750	0.02596324
C	0.72396639	-1.69960907	-0.00509810
H	1.12231142	-2.69091437	-0.02151829
N	0.00516490	0.92037108	0.03743799
H	-0.22559403	1.88715879	0.05521656

N	1.65412231	-0.65781518	0.00323520
H	2.62729709	-0.86251680	-0.00152743
S	-2.64523389	0.54363065	0.04589797
S	2.49963908	1.87746803	0.03914657
C	-1.66879096	-2.50400069	-0.00214647
H	-2.30418458	-2.46255386	0.87727332
H	-2.30654106	-2.44341197	-0.87877513
H	-1.18861680	-3.47444719	-0.01325426

${}^1\Pi_7\Pi_8^*$

N	0.12110662	-0.04596850	1.28204126
C	0.17350649	-0.03296606	-0.04294636
N	1.32601503	-0.01305971	-0.64765914
C	2.61974676	-0.00496086	0.00971631
C	2.53113718	-0.01976488	1.41244788
C	1.30201851	-0.03814909	2.05927140
S	-1.35415764	-0.04392644	-0.96878378
H	-0.77188415	-0.06427831	1.72062528
H	1.36252616	-0.00247158	-1.64716663
H	1.15724592	-0.05062148	3.11716794
C	3.79584215	-0.01254120	2.22712168
H	3.57798361	-0.02812233	3.28960836
H	4.40614986	-0.87269752	1.98015719
H	4.38270089	0.86945895	2.00102636
S	3.95825332	0.01617781	-1.03987017

${}^1\Pi_7\Pi_7^*$

C	-0.61852472	-1.39974668	0.00354272
C	-1.04014063	0.01656360	0.01437747
C	1.32667408	0.63447005	0.01424346

C	0.70629538	-1.67407583	-0.00186397
H	1.07492973	-2.68151772	-0.01008161
N	-0.03609131	0.92206811	0.01964491
H	-0.31778391	1.87762912	0.02538087
N	1.67903456	-0.70795961	0.00211566
H	2.63537059	-0.96901652	0.00023330
S	-2.62005056	0.51146674	0.01985520
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C	-1.64581314	-2.50090700	-0.00154123
H	-2.28334356	-2.44977270	0.87307390
H	-2.28817735	-2.43728620	-0.87177071
H	-1.15560939	-3.46866416	-0.00981993

${}^3\Pi_g\Pi_g^*$

C	-0.65758969	-1.38982055	0.00000549
C	-1.00321312	-0.04725365	0.00001836
C	1.34016617	0.65618261	-0.00000278
C	0.72482941	-1.69694248	-0.00001128
H	1.11662508	-2.69074524	-0.00001756
N	0.01291034	0.92337459	0.00001331
H	-0.23868497	1.88589607	0.00002150
N	1.65080493	-0.66215341	-0.00001460
H	2.62350355	-0.87096767	-0.00002511
S	-2.64834696	0.56737250	0.00003489
S	2.51402819	1.86920162	-0.00000638
C	-1.66875449	-2.51149005	-0.00000207
H	-2.30605758	-2.47201866	0.87509611
H	-2.30592420	-2.47212388	-0.87520364
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${}^3n_8\pi_8^*$

C	-0.07696304	-0.91097517	-0.16621250
C	-0.98515585	0.15911650	-0.15331839
C	0.81027209	1.79309084	0.11411625
C	1.26531485	-0.59092920	-0.03775953
H	-1.12677698	2.24506480	-0.00313295
N	1.65838726	0.74208091	0.09746035
H	2.05170902	-1.31541065	-0.03504163
N	-0.50310029	1.47077945	-0.01115242
H	2.62250118	0.96648029	0.18862982
S	-2.73367283	-0.01308598	-0.28965925
S	1.32828770	3.39156596	0.27755386
C	-0.52843929	-2.34341402	-0.31169334
H	-1.18280083	-2.64050314	0.50213868
H	-1.06069065	-2.50158048	-1.24465069
H	0.32412609	-3.01103291	-0.30528938

 ${}^3\pi_7\pi_7^*$

C	-0.63075185	-1.39166887	0.00000801
C	-1.04974182	0.00850487	0.00000768
C	1.33024937	0.62666778	-0.00000281
C	0.72836426	-1.67497343	-0.00000290
H	1.10541860	-2.67768804	-0.00000793
N	-0.03566695	0.92134482	0.00000427
H	-0.29357071	1.88351926	0.00000412
N	1.65437957	-0.69643876	-0.00000674
H	2.62235875	-0.92834029	-0.00001194
S	-2.62738014	0.51774043	0.00001031
S	2.56090599	1.88541394	0.00000207
C	-1.64587612	-2.49988138	0.00000086

H	-2.28746067	-2.44460999	0.87211505
H	-2.28741207	-2.44464161	-0.87215186
H	-1.15203023	-3.46556372	0.00003184

II. microsolvated surrounding

gs

C	-0.13678809	-0.79704746	-0.27973266
C	-1.10701568	0.28470821	-0.34850224
C	0.71827108	1.89134136	-0.16996165
C	1.16455232	-0.44844676	-0.16077322
H	-1.23736032	2.32535193	-0.41209409
N	1.57241050	0.86241947	-0.10516095
H	1.95859860	-1.16499384	-0.09451836
N	-0.59024625	1.55000398	-0.31204899
H	2.55901178	1.04988786	-0.02213908
S	-2.74773655	0.03663775	-0.45584821
S	1.21469224	3.52241005	-0.07782627
C	-0.57003473	-2.23751484	-0.32932146
H	-1.23282424	-2.47333192	0.49431465
H	-1.10438330	-2.45170128	-1.24688271
H	0.29382929	-2.88962963	-0.27358604
O	-4.70795052	3.00919358	0.51072054
H	-5.40741096	3.04288852	-0.12869872
H	-4.33283768	2.13838648	0.42922667
O	4.44359475	0.96836971	0.14997254
H	4.60321611	1.69953896	0.74837835
H	4.92016637	1.18016854	-0.64167295
O	4.30196674	3.36316599	1.63367204
H	3.41866038	3.54348165	1.32132596
H	4.77593365	4.18093466	1.56605429

O	-2.25212507	3.86286609	-0.65799219
H	-3.08316147	3.85151382	-0.18829321
H	-1.71724527	4.55320161	-0.28845357

¹n₈π₈*

C	-0.02861400	-1.04528600	-0.49594900
C	-0.97136400	-0.05914300	-0.77009700
C	0.63454900	1.69437900	-0.33758300
C	1.24912800	-0.62557100	-0.14514100
H	-1.28231300	2.01295200	-0.84135300
N	1.53420000	0.74738000	-0.09034800
H	2.05961500	-1.27783700	0.09762200
N	-0.60156300	1.29239900	-0.66675300
H	2.47445500	1.02273700	0.13135100
S	-2.64333000	-0.35445600	-1.27268200
S	1.01231600	3.37988200	-0.24840100
C	-0.36726100	-2.51272100	-0.58158900
H	-1.17888300	-2.77038500	0.09151200
H	-0.66721300	-2.78958800	-1.58739600
H	0.48947200	-3.11828700	-0.31327600
O	-4.21332400	4.01002100	1.14734400
H	-5.14141000	3.90152300	0.98628700
H	-4.02114300	3.51141400	1.93074600
O	4.36968100	1.14266500	0.55570000
H	4.37254000	1.92522200	1.10761800
H	4.87736900	1.37385500	-0.21057400
O	3.82413200	3.62824000	1.81612100
H	2.96156200	3.64217300	1.40629800
H	4.22533300	4.45704800	1.59191800
O	-2.46582800	3.46893700	-1.13003300

H	-3.03098300	3.69827800	-0.39582300
H	-1.75334100	4.09797400	-1.11536100
${}^1\Pi_{7\Pi_8}^*$			
N	1.33300164	0.79224674	0.00089963
C	0.48531733	1.79520122	-0.16575579
N	-0.79876071	1.57243786	-0.30610240
C	-1.38658995	0.25687305	-0.29470974
C	-0.47751773	-0.79304653	-0.09192691
C	0.87976383	-0.53386567	0.05894049
S	1.12883426	3.45345046	-0.17627310
H	2.32046040	0.97899213	0.07637090
H	-1.41220817	2.36947664	-0.42465107
H	1.63392701	-1.27078851	0.22955798
C	-0.96924057	-2.21495926	-0.04226094
H	-0.14837710	-2.90354573	0.12717819
H	-1.69756060	-2.33830318	0.75003193
H	-1.46032342	-2.47897453	-0.97125784
S	-3.08740344	0.15438257	-0.54628909
O	-4.91111856	2.90362850	0.23651735
H	-5.53954040	2.78651019	-0.46415228
H	-4.46728491	2.05817863	0.30528980
O	4.19524185	0.99996102	0.22501336
H	4.56938539	1.75878955	0.66977214
H	4.73794219	0.85246722	-0.53779664
O	5.25016522	3.40201077	1.39845812
H	4.70609644	4.17138367	1.29265490
H	5.63617642	3.46493847	2.26200280
O	-2.41330676	3.98185810	-0.52975995
H	-3.32192986	3.72640974	-0.35992499

H	-2.22354880	4.68058587	0.08098916
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¹n₇π₇*

C	-0.14255600	-0.82191900	-0.14657000
C	-1.08124100	0.27589700	-0.15425800
C	0.76671900	1.82025300	-0.51316100
C	1.17897600	-0.52042800	-0.30217300
H	-1.21146200	2.30897400	-0.36998100
N	1.62889300	0.76000500	-0.45919200
H	1.94286000	-1.27226800	-0.31544200
N	-0.57382000	1.53359700	-0.31948500
H	2.61326700	0.92313500	-0.56306700
S	-2.74693800	0.05470800	0.02335000
S	1.37733800	3.47034200	-0.13718900
C	-0.60144800	-2.24672000	0.02753000
H	-1.11387900	-2.38680800	0.97288000
H	-1.28577500	-2.54311800	-0.75970600
H	0.24949600	-2.91846700	0.00376400
O	-4.90058300	2.96698800	-0.05087900
H	-5.36572500	2.77001600	-0.85366500
H	-4.54424700	2.13611900	0.24442000
O	4.52511800	1.22895900	-0.43082500
H	4.64225700	1.71719600	0.38255200
H	4.95791700	1.73528200	-1.10477800
O	4.30923100	2.86653000	1.93567600
H	3.37412400	3.03385300	1.91175900
H	4.71691800	3.69246700	2.15928600
O	-2.25088600	3.97774600	-0.43551300
H	-3.18576900	3.79569500	-0.35529600
H	-2.06055700	4.66028500	0.19304200

³π₈π₈*

C	-0.39691431	-0.81577652	-0.34365234
C	-1.26923945	0.24452287	-0.52722721
C	0.53812368	1.84967120	-0.33193693
C	0.96015768	-0.51320907	-0.14479072
H	-1.38406264	2.33374825	-0.66415606
N	1.36949276	0.82424093	-0.15867564
H	1.73762485	-1.24025551	-0.05853199
N	-0.75998383	1.55940605	-0.50182288
H	2.34961815	1.01781893	-0.04256197
S	-3.02229223	0.09961344	-0.63013515
S	1.08560376	3.48416385	-0.33402761
C	-0.84855003	-2.25531091	-0.31919999
H	-1.30470451	-2.50726698	0.63239575
H	-1.57416375	-2.45144943	-1.09822117
H	-0.00330270	-2.91654203	-0.46572842
O	-4.30750491	3.29038301	1.16354212
H	-5.21553939	3.39999216	0.91375647
H	-4.11019827	2.37185314	1.02180439
O	4.26318597	1.04290167	0.20326543
H	4.34706772	1.74802841	0.84522462
H	4.68751546	1.36655465	-0.58025323
O	3.90259081	3.37399861	1.78082102
H	3.05776683	3.52601010	1.36429392
H	4.35018033	4.20915794	1.77439238
O	-2.41364235	3.92011388	-0.91429817
H	-3.01051605	3.99136580	-0.17341004
H	-1.68643568	4.50676894	-0.74320656

${}^3n_8\pi_8^*$

C	0.06728700	-1.17040900	-0.34398500
C	-0.93201500	-0.23037500	-0.57390300
C	0.64242700	1.59313900	-0.31555600
C	1.36056400	-0.69703900	-0.11869400
H	-1.30537500	1.82687300	-0.75188100
N	1.58977000	0.68665100	-0.09753600
H	2.20123700	-1.31136800	0.11952300
N	-0.59260400	1.13941000	-0.56862100
H	2.52939500	1.00286100	0.06541700
S	-2.61445300	-0.59981000	-0.94267700
S	0.97431600	3.28723700	-0.28953500
C	-0.20899200	-2.65336700	-0.35066700
H	-1.04794000	-2.89661100	0.29149900
H	-0.44222900	-3.00690900	-1.34959100
H	0.65580100	-3.20185900	0.00200000
O	-4.46061700	4.04014600	1.03371700
H	-5.33722300	4.05267300	0.67107600
H	-4.51171900	3.52933300	1.83182200
O	4.43468600	1.20125900	0.38711400
H	4.43969500	1.98262600	0.94037900
H	4.89350800	1.44999400	-0.40423500
O	3.85741000	3.66215300	1.68155200
H	2.98226800	3.65211700	1.30044500
H	4.21722600	4.51392400	1.47385200
O	-2.47796100	3.32479700	-1.00025000
H	-3.08084400	3.58381100	-0.30776800
H	-1.75482600	3.94041500	-0.96365200

${}^3\pi_7\pi_7^*$

C	-0.55246600	-0.68060900	-0.27693400
C	-1.44789800	0.47609100	-0.20197700
C	0.53154800	1.90132200	-0.17723800
C	0.82472600	-0.43962200	-0.32172800
H	1.54594700	-1.22932200	-0.39153000
N	-0.84949400	1.68688300	-0.18347000
H	-1.42767100	2.51364900	-0.19130800
N	1.32018500	0.79515700	-0.27135800
H	2.32281700	0.91275600	-0.29615200
S	-3.11301200	0.31598900	-0.14345700
S	1.23269300	3.50174200	-0.02404000
C	-1.08081500	-2.08653800	-0.32252300
H	-1.65923100	-2.32033200	0.56410300
H	-1.73134100	-2.23682900	-1.17692400
H	-0.26040300	-2.79368200	-0.39017100
O	-4.97000300	3.31251600	-0.02725900
H	-5.45171900	3.23366000	-0.84276200
H	-4.57211200	2.45433400	0.11247300
O	4.17798500	0.79214300	-0.33663700
H	4.46604500	1.30861300	0.41540400
H	4.57629500	1.20061600	-1.09496300
O	4.44829000	2.73416900	1.71810000
H	3.65995100	3.22743100	1.52098900
H	5.06804900	3.34656000	2.09307200
O	-2.32606000	4.23246400	-0.38174400
H	-3.26915500	4.12885700	-0.25981700
H	-2.04563100	4.91495900	0.21232400

III. aqueous solution

Snapshot1

gs

C	-0.14328801	-0.80692305	-0.15736001
C	-1.10271607	0.28906301	-0.15826501
C	0.74314605	1.85127613	0.15459601
C	1.16326208	-0.48284203	-0.02713000
H	-1.20671708	2.32394116	-0.03010500
N	1.59139611	0.80987506	0.11028401
H	1.94682113	-1.21446108	-0.03076100
N	-0.57210403	1.53307811	0.01057099
H	2.58307718	0.99361106	0.10442400
S	-2.73258319	0.06312100	-0.34568802
S	1.25232109	3.46025024	0.38143203
C	-0.59923504	-2.23200916	-0.29371802
H	-1.22796608	-2.52021018	0.54032504
H	-1.18153108	-2.36690616	-1.19541508
H	0.25418801	-2.89981020	-0.32779902
O	-4.86199935	2.94888321	-0.09742600
H	-5.26726737	2.91807520	-0.95386806
H	-4.44432932	2.10054315	0.01265199
O	4.43762031	1.11286807	-0.24261101
H	4.69241433	1.79984313	0.37503502
H	4.65090133	1.44909410	-1.10238008
O	4.50121832	3.32073523	1.49559110
H	3.56677525	3.46962624	1.37685909
H	4.92073235	4.15942330	1.36198710
O	-2.13281415	3.83257027	-0.29523502
H	-3.07795922	3.83053127	-0.16031501
H	-1.76123212	4.57097832	0.16596101

$^1n_8\pi_8^*$

C	-0.09747400	-0.85961006	-0.15461600
C	-0.96557906	0.22221601	-0.16382301
C	0.84611406	1.78666213	0.15356100
C	1.25655109	-0.58032904	0.01815900
H	-1.09145608	2.29424416	0.01440599
N	1.68022312	0.74553505	0.13661201
H	2.02892714	-1.31865309	0.02462400
N	-0.46426603	1.51170510	0.03325000
H	2.66775819	0.93113306	0.12538901
S	-2.69890519	0.12451501	-0.40224103
S	1.37271310	3.41850724	0.32546302
C	-0.58975604	-2.27444816	-0.30737102
H	-1.19850208	-2.57658118	0.53992103
H	-1.19015008	-2.39091917	-1.20372708
H	0.24147502	-2.96497521	-0.37828202
O	-5.23975237	2.95385921	0.10268700
H	-5.62514140	2.69623719	-0.72437205
H	-5.46635039	2.27413816	0.72333505
O	4.56484632	1.12398008	-0.26791501
H	4.77770134	1.80477413	0.37149402
H	4.62107233	1.54876211	-1.11296008
O	4.54432932	3.31992024	1.51438111
H	3.59965925	3.39300724	1.38974009
H	4.89846435	4.16494429	1.27370309
O	-2.40822817	3.54976325	-0.18162301
H	-3.34798924	3.55828325	-0.02144200
H	-2.05796214	4.39982831	0.04910000

${}^1\Pi_7\Pi_8^*$

C	-0.19731901	-0.84727806	-0.15628401
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C	-1.15285008	0.18958201	-0.17698101
C	0.68721605	1.74714712	0.12005500
C	1.15258908	-0.57139904	-0.00241600
H	-1.21879008	2.30141516	-0.03148800
N	1.57354611	0.75867905	0.11674101
H	1.93185813	-1.30200609	0.02161500
N	-0.59117204	1.50743910	-0.00199399
H	2.55934918	0.97091407	0.10410700
S	-2.84326220	0.06665700	-0.38069002
S	1.27823709	3.40855824	0.34296502
C	-0.64974204	-2.27317216	-0.29094702
H	-1.27826809	-2.55049518	0.54684803
H	-1.24575509	-2.39404817	-1.18532208
H	0.19677701	-2.95061721	-0.33303102
O	-4.69239733	2.86757220	-0.13089200
H	-5.13299537	2.75921820	-0.96341406
H	-4.26928830	2.02248814	0.02676900
O	4.39529731	1.22622308	-0.18236401
H	4.70923434	1.93573213	0.37482102
H	4.81364934	1.33532409	-1.02516907
O	4.66789133	3.51336725	1.46269210
H	3.81630927	3.92351328	1.40369810
H	5.27555138	4.18493130	1.74128712
O	-2.06741615	3.89966128	-0.28604802
H	-3.00405021	3.68894826	-0.29301302
H	-1.96359814	4.63978433	0.29319402

${}^1n_7\pi_7^*$

C	-0.16435175	-0.90630097	-0.12085476
C	-1.07595561	0.21634822	-0.16356483

C	0.82008135	1.72920350	-0.05163404
C	1.16303430	-0.62958172	-0.01003066
H	-1.14149232	2.25768188	-0.15044511
N	1.65500154	0.64875739	0.05934084
H	1.90875766	-1.39963010	0.01673966
N	-0.53355147	1.46049182	-0.07614363
H	2.64140706	0.79410035	-0.05057251
S	-2.74632719	0.03070576	-0.32277469
S	1.37213882	3.34031754	0.52721411
C	-0.67140503	-2.32107795	-0.18853329
H	-1.29730476	-2.56274741	0.66348833
H	-1.26398542	-2.48399381	-1.08034751
H	0.15914163	-3.01836748	-0.20338268
O	-4.77831005	2.96534698	-0.09701630
H	-5.16717510	2.85511724	-0.95479555
H	-4.47269973	2.10003461	0.15210163
O	4.53382564	1.15493473	-0.24346558
H	4.73732034	1.86818369	0.35942357
H	4.99078088	1.34621891	-1.05041435
O	4.60885421	3.43273823	1.52097625
H	3.95573087	3.25558659	2.18562188
H	4.24893368	4.14200745	1.00640356
O	-2.03682683	3.89918658	-0.26055155
H	-2.98346036	3.78016816	-0.19860357
H	-1.80990977	4.61321821	0.31699168

$^3\Pi_8\Pi_8^*$

C	-0.14774201	-0.86267106	-0.16092201
C	-1.00829807	0.21544301	-0.16383701
C	0.76338205	1.82270513	0.16861901

C	1.23695108	-0.51563403	0.02624500
H	-1.19245908	2.28892116	-0.01382099
N	1.60219811	0.77326205	0.14665201
H	2.01385614	-1.25505108	0.02977200
N	-0.55497404	1.51507811	0.03308400
H	2.59000418	0.99095507	0.14533501
S	-2.75410219	0.03934000	-0.37642502
S	1.26503909	3.46217025	0.36256002
C	-0.56556204	-2.29474416	-0.30879602
H	-1.11807808	-2.64211319	0.55676903
H	-1.18996908	-2.43386917	-1.18160508
H	0.30731902	-2.92836921	-0.41883102
O	-4.99496635	3.07759022	-0.05911300
H	-5.34381238	3.02630921	-0.93766106
H	-4.62367533	2.22775815	0.12188300
O	4.49878732	1.11762708	-0.24427001
H	4.71419334	1.81438313	0.37960403
H	4.60417833	1.50863610	-1.10055008
O	4.47908432	3.34379024	1.49241211
H	3.53020925	3.42355124	1.37384009
H	4.83436134	4.18808830	1.24992109
O	-2.18686915	3.80213127	-0.29303102
H	-3.10418422	3.94932728	-0.10608100
H	-1.67460712	4.50640832	0.08668100

$^3\text{p}_8\pi_8^*$

C	-0.10401013	-0.85928409	-0.16654091
C	-0.98511925	0.21605711	-0.17566698
C	0.82204577	1.78997035	0.14358208
C	1.24774433	-0.57409496	-0.01565869

H	-1.10736279	2.30105236	-0.05475494
N	1.66342349	0.75755340	0.13149583
H	2.02223923	-1.30934031	0.02158911
N	-0.47914718	1.51585195	-0.00723965
H	2.64994870	0.94869292	0.12887236
S	-2.73310969	0.09805882	-0.35878799
S	1.34524229	3.41979928	0.33891806
C	-0.58510325	-2.28003154	-0.30481438
H	-1.24571801	-2.54792560	0.51286304
H	-1.13040797	-2.42483080	-1.22996574
H	0.25050149	-2.96920203	-0.30209503
O	-5.09847649	3.01769606	-0.03750502
H	-5.14759673	2.52150901	-0.84447659
H	-5.34492980	2.41643523	0.65332326
O	4.54826131	1.11450678	-0.25259627
H	4.77290581	1.80049689	0.37670910
H	4.65401232	1.51113614	-1.10640518
O	4.54368667	3.33364598	1.50331569
H	3.59997889	3.41187927	1.38109893
H	4.90305336	4.17803625	1.26833245
O	-2.26601337	3.68127499	-0.19654398
H	-3.20719802	3.70772863	-0.04830156
H	-1.88487212	4.48671021	0.12382600

${}^3\Pi_7\Pi_7^*$

C	-0.17140101	-0.80984805	-0.14946800
C	-1.13879008	0.28751502	-0.15971901
C	0.72791605	1.82873213	0.13387700
C	1.18679308	-0.48134803	-0.02871900
H	-1.24698208	2.31831016	-0.07346200

N	1.59206811	0.78019105	0.10027200
H	1.96176014	-1.22077708	-0.05974800
N	-0.62574904	1.52490111	-0.00935500
H	2.58342418	0.97164206	0.09195600
S	-2.78183919	0.03795900	-0.35260802
S	1.26995509	3.46334724	0.42582603
C	-0.60666004	-2.23802716	-0.28311301
H	-1.22623808	-2.54206118	0.55344903
H	-1.19330808	-2.38507617	-1.18103308
H	0.25558501	-2.89516720	-0.32355202
O	-4.82027234	2.93022120	-0.10674501
H	-5.25117437	2.89123720	-0.95024206
H	-4.40511031	2.07875114	0.00074899
O	4.43018331	1.13008808	-0.23971201
H	4.71953733	1.81086513	0.36763902
H	4.69181733	1.41996310	-1.10289807
O	4.57031732	3.34385124	1.49932310
H	3.64102126	3.52474325	1.40920009
H	5.01389536	4.17569630	1.40603410
O	-2.12917515	3.91021328	-0.31322702
H	-3.07519122	3.82123227	-0.20672001
H	-1.84369313	4.63045133	0.22987601

Snapshot2

gs

C	-0.835150059	-0.585180040	0.169536013
C	-1.217628087	0.812085059	0.194543014
C	1.142136084	1.420091101	0.024356002
C	0.490234037	-0.862040063	0.010700001
N	-0.192011012	1.709814121	0.100210005

N	1.431826104	0.111937006	-0.075499004
H	0.868311062	-1.864146136	-0.024985003
H	-0.415859032	2.697959197	0.098544006
H	2.403708171	-0.161488010	-0.158931010
S	-2.791796203	1.319745093	0.338341026
S	2.319925167	2.639538192	0.073960003
C	-1.847529134	-1.681934121	0.353274027
H	-2.333214168	-1.595202113	1.317849093
H	-2.621317191	-1.634164116	-0.398435029
H	-1.369343098	-2.653302193	0.294759020
O	-3.056938220	4.747339341	1.124013081
H	-3.078247220	3.799280273	1.038388074
H	-3.780727271	5.067354367	0.602696045
O	5.525100397	1.317755095	0.207476016
H	4.726990338	1.813194130	0.376354029
H	5.928003429	1.741813125	-0.537617039
O	-0.550538039	4.543057328	0.022098003
H	0.220585017	4.907605354	0.434442033
H	-1.321703096	4.899187351	0.456910031
O	4.067882294	-0.955870068	-0.283429023
H	4.409274318	-1.337900095	-1.080179080
H	4.706648336	-0.287291022	-0.027859002
$^1n_8\pi_8^*$			
C	-0.815283057	-0.560651040	0.191026012
C	-1.156395082	0.776565057	0.231396019
C	1.166023081	1.440082105	0.021312000
C	0.524494036	-0.866488062	-0.006193999
N	-0.143770008	1.737923127	0.124527012
N	1.472156105	0.149911009	-0.107042006
H	0.904829065	-1.863724133	-0.070483007

H	-0.365117024	2.723065196	0.141796013
H	2.436968173	-0.119703011	-0.204213014
S	-2.831024203	1.306624095	0.426708033
S	2.348849170	2.681289193	0.067495002
C	-1.835985133	-1.652023118	0.374864025
H	-2.309838165	-1.586952113	1.348931097
H	-2.615034190	-1.603321116	-0.375041029
H	-1.369637099	-2.626313190	0.299571019
O	-3.208686231	4.760747343	0.941610070
H	-3.181302229	3.814708277	1.023371072
H	-3.967620287	4.947382354	0.405737030
O	5.549986402	1.351137099	0.208820015
H	4.741322342	1.832631133	0.373027028
H	5.941185430	1.774066129	-0.543116037
O	-0.630920047	4.552271325	0.025281004
H	0.109445010	5.048697365	0.366326025
H	-1.429613101	4.964718360	0.351470025
O	4.110414297	-0.940782066	-0.314597023
H	4.474079322	-1.319826094	-1.102731080
H	4.731892340	-0.262259017	-0.046494005
${}^1\Pi_7\Pi_8^*$			
C	-1.029748076	-0.606893045	0.242043017
C	-1.396203098	0.748345056	0.238763018
C	0.958089067	1.292025095	0.020858003
C	0.297022020	-0.981263073	0.066480003
N	-0.292698023	1.667019118	0.126664009
N	1.281588090	0.011595999	-0.033257001
H	0.661709045	-1.984369143	0.115847007
H	-0.483585036	2.661121189	0.142737011
H	2.250459160	-0.254800020	-0.120829010

S	-2.976595212	1.424547102	0.329090024
S	2.262764160	2.499634179	0.008899999
C	-2.067491151	-1.675742123	0.451976030
H	-2.554896186	-1.542188110	1.411072100
H	-2.836876204	-1.623488119	-0.303410020
H	-1.618840117	-2.662927192	0.421929028
O	-3.048661221	4.693070336	1.045919076
H	-3.065964222	3.735375267	1.073959078
H	-3.802842271	4.934530353	0.525037040
O	5.781151413	1.176219083	0.139068009
H	5.316527381	1.772190127	0.712333052
H	5.937938425	1.663132120	-0.659425048
O	-0.479553033	4.577178328	0.128273010
H	0.049571002	5.034408363	0.766884056
H	-1.389533099	4.797618345	0.338082026
O	3.966474285	-0.887842063	-0.258323018
H	4.293657307	-1.388682098	-0.992124071
H	4.654899336	-0.258505018	-0.047956006
${}^1n_{7\pi 7}^*$			
C	-0.944605070	-0.657892048	0.191170012
C	-1.275798092	0.745759051	0.183911013
C	1.069670075	1.271798094	-0.209497013
C	0.360463027	-0.994478073	-0.021988003
N	-0.254348018	1.628787120	-0.022010001
N	1.341915095	-0.065775007	-0.214927017
H	0.692213050	-2.013673143	-0.046602005
H	-0.451962033	2.613955187	-0.030931003
H	2.289763165	-0.372060026	-0.336709022
S	-2.850778204	1.318876094	0.404706029
S	2.362764172	2.442835177	0.226909019

C	-1.985806145	-1.716120125	0.447932031
H	-2.431737177	-1.604626114	1.430313102
H	-2.788796202	-1.675167119	-0.275525020
H	-1.537520110	-2.702139194	0.393471029
O	-3.010903218	4.773479343	1.063596078
H	-3.062101223	3.830965274	1.182078086
H	-3.766195270	5.005547358	0.539974037
O	5.679567411	1.256453091	0.162080012
H	5.231212377	1.675421119	0.886033065
H	5.506696396	1.813448130	-0.586088040
O	-0.425066028	4.589461331	0.088895004
H	0.182213015	4.976956356	0.703746050
H	-1.297714094	4.864562352	0.364791025
O	4.103921297	-0.960999071	-0.395933027
H	4.519103326	-1.407240100	-1.120883082
H	4.728192338	-0.294510021	-0.113441007
${}^3\Pi_g\Pi_g^*$			
C	-0.914942066	-0.635066045	0.133072007
C	-1.246141088	0.711325054	0.126551009
C	1.086940076	1.374386099	0.012583999
C	0.465857032	-0.956795070	-0.013460999
N	-0.226759018	1.665140120	0.031480003
N	1.397340099	0.069473003	-0.028345004
H	0.854774062	-1.950585139	0.034447005
H	-0.465542034	2.644657189	0.008254001
H	2.372128169	-0.181120015	-0.078040007
S	-2.905101207	1.316832094	0.322953023
S	2.277771162	2.595885186	0.050127003
C	-1.905507138	-1.751459127	0.338473024
H	-2.156088155	-1.854061134	1.388784102

H	-2.824904204	-1.578224112	-0.198554014
H	-1.485946109	-2.692324194	0.004183998
O	-2.933071209	4.884769351	1.263777090
H	-3.019221218	3.969475287	1.027670076
H	-3.563655255	5.347509386	0.728935051
O	5.458804394	1.363889096	0.227986016
H	4.629651332	1.805215132	0.404542031
H	5.791039418	1.778801128	-0.556221038
O	-0.534704040	4.538877325	-0.046614001
H	0.368188025	4.666138336	0.218128016
H	-1.102286079	4.966685359	0.585918041
O	4.076081293	-0.966623072	-0.228820016
H	4.398574317	-1.312349095	-1.049287078
H	4.691246336	-0.272158018	0.013422999
$^3\pi_8\pi_8^*$			
C	-0.842431061	-0.655840046	0.111189009
C	-1.187277083	0.696928051	0.080366006
C	1.131899081	1.369206100	-0.024169001
C	0.506984037	-0.957207066	-0.025176999
N	-0.180473011	1.661546118	-0.018374002
N	1.450278102	0.074541008	-0.063043002
H	0.908369065	-1.947049140	0.038743003
H	-0.413943029	2.641276190	-0.065840006
H	2.423856177	-0.173492010	-0.096225009
S	-2.840099206	1.333253093	0.225004018
S	2.291887166	2.604069188	0.027124001
C	-1.861291135	-1.747194128	0.307131020
H	-2.422164175	-1.595386113	1.223676091
H	-2.569081184	-1.794916131	-0.510563037
H	-1.371756099	-2.710737197	0.372092025

O	-3.000931217	4.777583345	1.359955097
H	-3.181087230	4.068955291	1.963027144
H	-3.642791263	4.704388337	0.665990047
O	5.477746394	1.367403097	0.216646018
H	4.644578332	1.805751130	0.383620030
H	5.815833421	1.782305128	-0.564891041
O	-0.633197044	4.491823323	-0.069531007
H	0.240014019	4.732245338	0.215121014
H	-1.260032092	4.825455349	0.563664043
O	4.132105298	-0.980340071	-0.229706017
H	4.453494322	-1.333294094	-1.047435074
H	4.744547344	-0.281446021	0.005743002
${}^3\Pi_7\Pi_7^*$			
C	-0.846114061	-0.567722038	0.168969010
C	-1.229273087	0.833703060	0.171661014
C	1.116665079	1.437353101	-0.111755006
C	0.478450032	-0.856771061	0.000100999
N	-0.220641015	1.737915126	0.054274006
N	1.428030104	0.106790006	-0.129837009
H	0.847387060	-1.863386132	-0.018859999
H	-0.443784033	2.721953194	0.044129001
H	2.385894171	-0.172401011	-0.252224017
S	-2.829916206	1.338745096	0.308991020
S	2.319219165	2.570885186	0.451181031
C	-1.859031135	-1.660954122	0.378695025
H	-2.353998171	-1.555781112	1.337714095
H	-2.627862187	-1.648099121	-0.381504030
H	-1.375409099	-2.631130190	0.351204023
O	-3.105261226	4.770637343	1.069674076
H	-3.152334225	3.820316275	1.094636081

H	-3.843700274	5.048404365	0.544455041
O	5.617858406	1.218245086	0.210524014
H	4.857923347	1.732189127	0.464227034
H	5.991176429	1.670036121	-0.533673038
O	-0.515035035	4.644955334	0.098020005
H	0.132077011	4.957943356	0.714691049
H	-1.368874099	4.927078352	0.421527028
O	4.081047293	-0.996191073	-0.353281028
H	4.437281321	-1.411344103	-1.126389081
H	4.740681339	-0.361049027	-0.075970004

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C	-0.123090010	-0.863976063	0.077826008
C	-0.622401045	0.503149036	0.055893003
C	1.675546121	1.304764095	-0.004853000
C	1.219111090	-1.031058075	0.066008004
N	0.325923025	1.479362107	0.021111002
N	2.089121150	0.027905003	0.031602000
H	1.688497120	-1.994276145	0.086527005
H	0.007439999	2.442232174	-0.032315002
H	3.074808224	-0.175153013	-0.007247998
S	-2.237731161	0.875130061	0.065581005
S	2.724139199	2.641781190	-0.092898008
C	-1.073317075	-2.026322146	0.116533006
H	-1.637798119	-2.038925148	1.040391074
H	-1.786082131	-1.972999140	-0.695394051
H	-0.526911037	-2.956963213	0.033345004
O	4.779843345	-0.984724072	-0.102911010
H	5.326061382	-0.195289017	-0.095789009
H	5.095322369	-1.507133107	-0.828361058

O	-0.476397036	4.213780304	-0.110109006
H	-1.262820088	4.425137316	0.388941029
H	0.231841014	4.745718339	0.221869018
O	5.907771427	1.578363116	-0.265245021
H	5.059229363	1.980889141	-0.436040032
H	6.193190447	1.954793141	0.556860040
O	-3.000182214	4.076262292	1.189449086
H	-3.713000267	4.292956306	0.603859045
H	-2.872739208	3.138293227	1.089142078
$^1n_{8\pi 8}^*$			
C	-0.153077013	-0.835762063	0.080317004
C	-0.614170042	0.466756035	0.059051006
C	1.666492121	1.308245092	-0.006467001
C	1.220322086	-1.045581075	0.066491005
N	0.331337021	1.494001108	0.021914002
N	2.092917150	0.045507005	0.028931004
H	1.682171119	-2.011619146	0.086237005
H	0.020796999	2.449391175	-0.029370004
H	3.083888223	-0.151513009	-0.011765002
S	-2.338851170	0.866621060	0.065963002
S	2.735600199	2.647380192	-0.097214009
C	-1.097975078	-1.999822145	0.119851011
H	-1.662467119	-2.011566144	1.043989077
H	-1.810629129	-1.947883139	-0.693385050
H	-0.553029040	-2.931142210	0.037891001
O	4.779280343	-0.956717070	-0.095723005
H	5.326883385	-0.168339014	-0.084234006
H	5.097180368	-1.484515108	-0.815417060
O	-0.485729035	4.223331302	-0.107331005
H	-1.286362094	4.423067318	0.368883025

H	0.200619017	4.777361345	0.238819015
O	5.924522427	1.604648117	-0.251550020
H	5.080430368	2.017509143	-0.425713032
H	6.212595446	1.974903141	0.571870042
O	-3.004224218	4.057671290	1.174215084
H	-3.732380267	4.267386308	0.604914044
H	-2.876200207	3.122038224	1.084121080
¹ π ₇ π ₈ *			
C	-0.219178014	-0.859912061	0.117161007
C	-0.714239053	0.458260031	0.083539006
C	1.591335113	1.217123088	0.068686006
C	1.145750084	-1.111162080	0.131736009
N	0.309129024	1.474862105	0.064670005
N	2.037858146	-0.033187002	0.110272008
H	1.594640116	-2.079618148	0.173252012
H	0.014680001	2.442768178	0.017011001
H	3.028660216	-0.217223017	0.067169003
S	-2.337387170	0.977772069	0.008429000
S	2.767801201	2.537506183	-0.005217000
C	-1.183587083	-2.010914145	0.137204008
H	-1.734293125	-2.026735147	1.069401078
H	-1.909199139	-1.910466137	-0.658058045
H	-0.663066046	-2.954584212	0.023590002
O	4.795730347	-0.780962054	-0.144599012
H	5.329133383	-0.000566998	-0.290013020
H	5.059777363	-1.410619104	-0.801464058
O	-0.414964029	4.279593306	-0.048062005
H	-1.323876094	4.292796310	0.259218020
H	0.021728002	4.979831360	0.415923031
O	6.118981440	1.715050123	-0.572504044

H	5.636179406	2.398829173	-0.129545009
H	7.034276504	1.861935133	-0.378714027
O	-2.956754214	4.005268291	1.142261081
H	-3.711944267	4.140349298	0.585096044
H	-2.802282200	3.060052222	1.102381077
${}^1n_{\pi\pi}^*$			
C	-0.192610014	-0.870524060	0.125774007
C	-0.637714048	0.523392040	0.079784006
C	1.670415118	1.235422090	0.194173014
C	1.138250081	-1.087557076	0.159165012
N	0.316096023	1.475433109	0.093152008
N	2.063057149	-0.085077006	0.176318012
H	1.547367109	-2.076210151	0.179427013
H	0.032435004	2.440889175	0.039541002
H	3.033223216	-0.322659022	0.151017011
S	-2.258058161	0.946579071	-0.010112000
S	2.831492202	2.526680179	-0.258264020
C	-1.185204084	-1.997313146	0.124292009
H	-1.782683130	-1.998568143	1.028003076
H	-1.867043133	-1.921668137	-0.713067052
H	-0.673390051	-2.950135212	0.057031004
O	4.865521348	-0.901415062	-0.075498004
H	5.390334388	-0.109769010	-0.178258013
H	5.196363372	-1.520337111	-0.711606052
O	-0.447777030	4.301163311	-0.042307001
H	-1.321877095	4.383918314	0.340644027
H	0.074127006	4.994820359	0.334481022
O	6.067861436	1.692353124	-0.437485030
H	5.626123403	2.099136152	-1.171621083
H	5.788783414	2.181925155	0.325262024

O	-3.020356218	4.094695293	1.182496083
H	-3.738564269	4.175174299	0.568392040
H	-2.913461207	3.157875230	1.310680096
${}^3\Pi_u\Pi_g^*$			
C	-0.178953264	-0.897712526	0.067572302
C	-0.605094295	0.426339567	0.030022302
C	1.662403870	1.275442627	0.028454302
C	1.224688838	-1.096232540	0.113494309
N	0.327526773	1.465804643	0.042338299
N	2.072604896	-0.005264462	0.082250303
H	1.691701868	-2.057009611	0.136951307
H	0.007322747	2.417056709	-0.033503707
H	3.058970968	-0.191788478	0.054484304
S	-2.294850916	0.892980528	0.006067703
S	2.726269944	2.614212727	-0.060849708
C	-1.114225330	-2.077344612	0.090303306
H	-1.521658363	-2.251716623	1.080499378
H	-1.945441390	-1.945083601	-0.589818742
H	-0.583305294	-2.972776675	-0.205685717
O	4.813899095	-0.997706537	-0.068342705
H	5.329720132	-0.188852476	-0.073044709
H	5.101912115	-1.484391572	-0.828181760
O	-0.489829287	4.225238843	-0.158186714
H	-1.149611334	4.547270864	0.448123331
H	0.345770773	4.603709867	0.083489303
O	5.881057171	1.597315652	-0.254351720
H	5.010553108	1.955946678	-0.419353732
H	6.129507191	1.961299676	0.584239340
O	-2.969199214	4.225353304	1.270928089
H	-3.664397263	4.445036318	0.665286045

H	-2.873567206	3.284178234	1.216254089
${}^3n_8\pi_8^*$			
C	-0.166096012	-0.855054061	0.070432005
C	-0.588915042	0.459018035	0.026771003
C	1.683688122	1.278421091	-0.007386002
C	1.218289087	-1.086789081	0.062353003
N	0.363482026	1.489532105	-0.028246000
N	2.087546149	0.011395001	0.054121005
H	1.676753121	-2.047548149	0.146429012
H	0.053400006	2.444735177	-0.129501008
H	3.073611219	-0.181977013	0.042779001
S	-2.296845165	0.987763073	-0.009107003
S	2.755844197	2.595787188	-0.076215007
C	-1.130061079	-2.011287146	0.127306007
H	-1.687363120	-2.005696145	1.056088074
H	-1.843510134	-1.978501144	-0.686101047
H	-0.595467045	-2.949200214	0.058277005
O	4.812388349	-1.003292071	-0.070000006
H	5.345791385	-0.206358013	-0.085278004
H	5.091728366	-1.509954108	-0.820217058
O	-0.504912038	4.219409305	-0.145348009
H	-1.224838090	4.410140317	0.449144032
H	0.254595017	4.702546339	0.151478009
O	5.918894426	1.577774115	-0.267094019
H	5.056386364	1.943397139	-0.451401031
H	6.151549442	1.937510138	0.578010043
O	-3.066034221	4.188196304	1.152409081
H	-3.528424253	3.973636287	0.353086026
H	-3.314717238	3.523947255	1.779504129

${}^3\pi_7\pi_7^*$

C	-0.158842013	-0.861949060	0.083200004
C	-0.651398048	0.505770035	0.062203002
C	1.668616122	1.262789089	0.019331004
C	1.245608090	-1.064323078	0.076059006
N	0.292737023	1.479673104	0.039796002
N	2.079931151	-0.016116003	0.040429004
H	1.699931122	-2.032420146	0.102448006
H	-0.007138003	2.444554178	-0.004762003
H	3.069851219	-0.211102013	0.002878999
S	-2.282597163	0.903428063	0.060838005
S	2.743093195	2.608333187	-0.114505008
C	-1.104095082	-2.020576143	0.122831009
H	-1.649247118	-2.053588146	1.060145075
H	-1.841244133	-1.951277139	-0.667641048
H	-0.565430039	-2.953259210	0.008751999
O	4.790198343	-0.953260071	-0.112977009
H	5.358037388	-0.181313012	-0.130983011
H	5.086546366	-1.510365110	-0.820170061
O	-0.475139034	4.272565308	-0.082850006
H	-1.320558094	4.411747317	0.341735026
H	0.135645010	4.879079351	0.312786025
O	5.978029428	1.590353114	-0.307058020
H	5.143910370	2.022991144	-0.458254035
H	6.310393455	1.960583139	0.499890035
O	-3.016547216	4.063937294	1.164797083
H	-3.750847272	4.235942305	0.590324040
H	-2.870556209	3.124557225	1.101271080

Cartesian coordinates of optimized conical intersection structures

I. gas phase

${}^1n_8\pi_8^*/{}^1n_7\pi_7^*$

C	-0.62015700	-1.39686500	0.01152600
C	-1.02591900	-0.00212200	0.05364400
C	1.34171600	0.64982200	0.16720700
C	0.70848700	-1.67248400	0.03495600
H	1.08553900	-2.67545200	0.01140500
N	-0.01566600	0.92362100	0.12142200
H	-0.29186100	1.88057000	0.15748700
N	1.67090200	-0.68858400	0.10333400
H	2.63063300	-0.94549200	0.11965000
S	-2.62162200	0.51743400	0.03632900
S	2.50580600	1.87842400	-0.44637200
C	-1.64666400	-2.49828900	-0.05521600
H	-2.30960200	-2.47147600	0.80220500
H	-2.26147900	-2.41362300	-0.94402700
H	-1.15832600	-3.46610300	-0.07355000

${}^1\pi_7\pi_8^*/{}^1n_7\pi_7^*$

C	-0.61249000	-1.41505200	-0.00272900
C	-1.05192200	-0.02585300	-0.00787700
C	1.28448000	0.62104200	0.01647500
C	0.70757900	-1.70811700	0.00015900
H	1.11095400	-2.70104400	0.00520600
N	0.00007400	0.88745600	0.02238800
H	-0.29317500	1.84478700	0.06064700
N	1.68381700	-0.67353600	-0.00119600
H	2.64856000	-0.89262200	-0.04798700
S	-2.63007500	0.59191700	-0.01324200
S	2.53038800	1.91769900	0.04491000
C	-1.64536700	-2.50437000	0.00585800

H	-2.28589400	-2.42483100	0.87671400
H	-2.28272100	-2.41843800	-0.86450500
H	-1.17242100	-3.47965200	0.00517800

${}^3\pi_8\pi_8^*/{}^3n_8\pi_7^*$

C	-0.60376207	-1.43007061	0.01900146
C	-1.00024524	-0.04754125	0.07914243
C	1.33809165	0.65210075	-0.00324898
C	0.72082654	-1.70129552	-0.03078526
H	1.13164315	-2.69057450	-0.04059718
N	0.00349011	0.93235238	0.02423849
H	-0.21586467	1.89652289	0.11807792
N	1.66225748	-0.65674220	-0.03154968
H	2.63213006	-0.86479826	-0.05738824
S	-2.65543929	0.45353445	-0.22803991
S	2.49306258	1.88187486	0.00885423
C	-1.66891378	-2.48777803	0.03010196
H	-2.30872132	-2.43939715	0.90467619
H	-2.31198975	-2.40372680	-0.84452909
H	-1.22477942	-3.47507602	0.05204567

${}^3n_8\pi_8^*/{}^3\pi_7\pi_7^*$

C	-0.62570193	-1.39252494	0.01239206
C	-1.03445073	-0.00188974	0.05321450
C	1.33607684	0.64685255	0.18964565
C	0.70953936	-1.67003503	0.02054769
H	1.08931139	-2.67289356	-0.00996651
N	-0.01735730	0.91843561	0.09211616
H	-0.28303204	1.87742503	0.12007490
N	1.66014314	-0.68418596	0.06691984

H	2.62149008	-0.92649177	0.13869037
S	-2.62649573	0.52294511	0.04439011
S	2.52529959	1.85825642	-0.39542421
C	-1.64406670	-2.50035928	-0.04680436
H	-2.30345132	-2.47466336	0.81194147
H	-2.26203660	-2.41428709	-0.93193641
H	-1.15348407	-3.46719699	-0.06580125

II. microsolvated surrounding

${}^1n_8\pi_8^*/{}^1\pi_7\pi_8^*$

N	1.32832800	0.80313300	-0.00103900
C	0.47738900	1.80361300	-0.16786100
N	-0.80652900	1.57527100	-0.30621200
C	-1.38869900	0.25779400	-0.29187400
C	-0.47619800	-0.78904500	-0.08837900
C	0.88002600	-0.52446400	0.06019600
S	1.11455700	3.46333000	-0.18065900
H	2.31534100	0.99262900	0.07104500
H	-1.42264900	2.37023800	-0.42496100
H	1.63703400	-1.25844300	0.23102500
C	-0.96303700	-2.21260200	-0.03555100
H	-0.13861400	-2.89795800	0.12999100
H	-1.68775700	-2.33619900	0.76063400
H	-1.45704200	-2.48087600	-0.96145700
S	-3.08966300	0.14831800	-0.54100400
O	-4.92626200	2.89792500	0.22785200
H	-5.54843900	2.77529700	-0.47714200
H	-4.47733700	2.05593100	0.30232400
O	4.19105000	1.01064100	0.21257700
H	4.57340500	1.76540700	0.65738000

H	4.73281600	0.85552400	-0.54932300
O	5.28821800	3.38145300	1.41194900
H	4.77156900	4.16768200	1.29518800
H	5.63946500	3.42190700	2.29164000
O	-2.42861700	3.97896600	-0.53464300
H	-3.33759000	3.72426700	-0.36628400
H	-2.23916100	4.67656100	0.07740400

${}^1n_8\pi_8^*/{}^1n_7\pi_7^*$

C	-0.12062000	-0.76379000	-0.15257200
C	-1.05957500	0.32744700	-0.15219100
C	0.78231000	1.88269300	-0.52287700
C	1.19867000	-0.46247600	-0.30798400
H	-1.18559800	2.36866400	-0.33541400
N	1.64723700	0.82465700	-0.46924600
H	1.95761200	-1.21855000	-0.32079500
N	-0.54938700	1.59144900	-0.30454300
H	2.63134300	0.99376300	-0.58254700
S	-2.72772000	0.11175400	0.01597900
S	1.38977700	3.53571900	-0.11880300
C	-0.57151900	-2.19069600	0.01641400
H	-1.08160400	-2.32554600	0.96376900
H	-1.25628200	-2.47660000	-0.77438600
H	0.27153900	-2.87424600	-0.00842600
O	-4.87826600	3.01188200	-0.02769200
H	-5.34731100	2.81083300	-0.82730500
H	-4.53485400	2.17989500	0.27799000
O	4.54564400	1.30320200	-0.45448700
H	4.65474300	1.77678500	0.36855500
H	4.96714600	1.83039000	-1.11921900

O	4.31749900	2.88340600	1.94754100
H	3.38288700	3.04917100	1.92071700
H	4.72200900	3.69941200	2.20806700
O	-2.23406300	4.01747100	-0.42549800
H	-3.17100200	3.85431100	-0.33998800
H	-2.03282900	4.71281200	0.18510000

${}^1\pi_7\pi_8^*/{}^1n_7\pi_7^*$

C	-0.18166300	-0.83247500	-0.22466200
C	-1.13122900	0.26050500	-0.28052500
C	0.71722100	1.78731200	-0.41389200
C	1.14073200	-0.55712900	-0.26987000
H	-1.19767000	2.31497000	-0.42382000
N	1.60853300	0.77909600	-0.34534800
H	1.91300400	-1.29703000	-0.24123200
N	-0.56619900	1.52692400	-0.36904100
H	2.59290200	0.96153300	-0.38298400
S	-2.85082100	0.10902700	-0.23330500
S	1.32971800	3.47621300	-0.43801400
C	-0.67570600	-2.24943800	-0.11370100
H	-1.26165200	-2.38267400	0.78765500
H	-1.31448100	-2.49929300	-0.95330000
H	0.15608100	-2.94477100	-0.09208800
O	-4.68525100	2.99398200	0.19427000
H	-5.28628600	2.82497500	-0.51961700
H	-4.29726300	2.14536800	0.39459800
O	4.46657400	1.32806900	-0.27285500
H	4.62664700	1.90746500	0.46974200
H	5.01651600	1.63812100	-0.97896800
O	4.39628700	3.23353100	1.88131200

H	3.47591500	3.44029100	1.98513000
H	4.87937600	3.99440100	2.17406300
O	-2.12786200	3.99431000	-0.45467000
H	-3.05196100	3.76715200	-0.33592300
H	-1.97367700	4.73337800	0.11720100

${}^3\pi_8\pi_8^*/{}^3\pi_8\pi_7^*$

C	-0.05757682	-0.82624827	-0.22238540
C	-0.93543147	0.25009245	-0.24215511
C	0.89490144	1.83143010	-0.26124497
C	1.30432817	-0.54168190	-0.25273174
H	-1.04897366	2.34035693	-0.35079099
N	1.72867143	0.79273844	-0.25719852
H	2.07831369	-1.27785158	-0.23038012
N	-0.41808360	1.55886130	-0.28242170
H	2.71609754	0.97996996	-0.24635112
S	-2.69513717	0.13424344	-0.14863598
S	1.45592371	3.46179116	-0.24689626
C	-0.54477936	-2.25240617	-0.16793973
H	-1.13628751	-2.42326887	0.72560725
H	-1.16080970	-2.49748143	-1.02651134
H	0.29152095	-2.94004760	-0.16044319
O	-5.13170339	3.30031746	0.11483758
H	-5.44908171	2.98277656	-0.72635724
H	-5.25926680	2.58033982	0.71969476
O	4.64271637	1.16514654	-0.22129884
H	4.73895362	1.71001959	0.55904482
H	4.82753166	1.74440258	-0.94844825
O	4.25337441	3.08680963	1.85268879
H	3.40329358	3.29144512	1.47047093

H	4.67955786	3.91987541	2.00006589
O	-2.31906488	3.74897065	-0.44586685
H	-3.23412934	3.77867324	-0.17666465
H	-1.90707383	4.55453944	-0.16752922

${}^3\Pi_8\Pi_8^*/{}^3\Pi_7\Pi_7^*$

C	-0.30728700	-0.78582300	-0.27916800
C	-1.29892400	0.30219100	-0.40627700
C	0.55469200	1.87289800	-0.17564900
C	1.03396500	-0.44022100	-0.11328800
H	-1.44189900	2.31550200	-0.42550900
N	1.43806300	0.83100400	-0.07295800
H	1.80210400	-1.17827600	-0.01258600
N	-0.80303700	1.53800700	-0.34444000
H	2.42560900	1.01516600	0.02100700
S	-2.91114900	-0.01787300	-0.61992000
S	1.11241000	3.56416900	-0.02467500
C	-0.71540200	-2.22953000	-0.32456800
H	-1.41651300	-2.46989500	0.46560900
H	-1.19883300	-2.46738100	-1.26495500
H	0.15581100	-2.86631300	-0.20769000
O	-4.92848900	2.63913900	0.16636300
H	-5.58039500	2.56434500	-0.51926300
H	-4.42725700	1.82405700	0.12846900
O	4.29832300	1.04584800	0.22410500
H	4.53465500	1.85313100	0.67096300
H	4.81689200	1.04774700	-0.57057200
O	4.73635200	3.60175800	1.36542100
H	3.94378700	4.11290600	1.21115300
H	5.46165500	4.21943700	1.41717600

O	-2.49370700	3.93775400	-0.46383700
H	-3.39565300	3.66599500	-0.29130400
H	-2.28567600	4.58300300	0.19881300

II. aqueous solution

Snapshot1

${}^1n_8\pi_8^*/{}^1\pi_7\pi_8^*$

C	-0.19636301	-0.88026406	-0.16616101
C	-1.13820608	0.15850801	-0.19533801
C	0.69970705	1.70869812	0.10738000
C	1.15826008	-0.60878504	-0.00926299
H	-1.20561708	2.26831016	-0.03592200
N	1.58401311	0.72523205	0.09811200
H	1.93298913	-1.34302109	0.01768200
N	-0.57778704	1.47350210	-0.01638300
H	2.56943518	0.93829606	0.07265800
S	-2.84113420	0.04768900	-0.39366702
S	1.28780309	3.37794524	0.32213502
C	-0.65695705	-2.30460616	-0.29518802
H	-1.28213809	-2.57906218	0.54670803
H	-1.25598009	-2.42478417	-1.18790808
H	0.18793101	-2.98390921	-0.34059202
O	-4.68980533	2.86317020	-0.11850800
H	-5.10996336	2.75704519	-0.96133606
H	-4.26397730	2.02033514	0.04102800
O	4.41241831	1.22212608	-0.20021501
H	4.68914933	1.96384214	0.33509202
H	4.79867034	1.34795409	-1.05845207
O	4.66942633	3.57318325	1.39522609
H	3.81964227	3.97445128	1.47431910

H	5.29051438	4.17958130	1.76958212
O	-2.04551214	3.86805927	-0.28864502
H	-2.98534621	3.67572326	-0.28949901
H	-1.91888513	4.58588933	0.31327202

${}^1n_8\pi_8^*/{}^1n_7\pi_7^*$

C	-0.20243701	-0.87566606	-0.15868601
C	-1.10969307	0.25660701	-0.20162401
C	0.80171105	1.74991512	-0.12251201
C	1.12625308	-0.61035304	-0.05977600
H	-1.15743908	2.29441416	-0.19961701
N	1.63208111	0.66219604	-0.00788800
H	1.86476613	-1.38809809	-0.02986200
N	-0.55547504	1.49192710	-0.12575801
H	2.61928818	0.79923205	-0.11996500
S	-2.77854619	0.07649900	-0.35300902
S	1.37450110	3.35828024	0.45248003
C	-0.72039905	-2.28748816	-0.21305701
H	-1.34651509	-2.51720818	0.64187404
H	-1.31621509	-2.45337217	-1.10223507
H	0.10626801	-2.99005921	-0.22350501
O	-4.77628334	3.01170621	-0.14717901
H	-5.17038437	2.90220121	-1.00258307
H	-4.45561232	2.14857615	0.09141000
O	4.50883332	1.15463108	-0.32259402
H	4.71956634	1.84584513	0.30292502
H	4.91355835	1.40300310	-1.14174108
O	4.60795933	3.36814824	1.51521911
H	3.83719127	3.25847523	2.06016514
H	4.48272532	4.19280129	1.06320007

O	-2.03393914	3.94472928	-0.31167802
H	-2.98055921	3.81889527	-0.25662102
H	-1.81741512	4.66153433	0.26628601

${}^1\pi_7\pi_8^*/{}^1n_7\pi_7^*$

C	-0.20121401	-0.88787206	-0.14867901
C	-1.15653708	0.20482001	-0.17669401
C	0.68367305	1.72156412	0.10907100
C	1.12015508	-0.61611404	0.00544700
H	-1.22197608	2.25334616	-0.02515600
N	1.57983511	0.71421204	0.10881800
H	1.88719813	-1.35990809	0.04409100
N	-0.59495804	1.45938810	-0.00814100
H	2.56542518	0.90747806	0.06413700
S	-2.85628120	0.07016000	-0.39667502
S	1.28046209	3.39954524	0.31841102
C	-0.68162104	-2.30586616	-0.27797902
H	-1.31794709	-2.57311018	0.55925403
H	-1.27176909	-2.42908917	-1.17485608
H	0.15421500	-2.99745021	-0.31060302
O	-4.67207533	2.90806120	-0.14396100
H	-5.12328036	2.80242120	-0.97112006
H	-4.32860931	2.04412614	0.05634700
O	4.40497231	1.27037808	-0.18407501
H	4.70258734	1.98635014	0.37209802
H	4.78195234	1.41626010	-1.04086707
O	4.64626033	3.56853625	1.46517210
H	3.80829727	4.00487228	1.47720710
H	5.28464937	4.21464230	1.73647312
O	-2.01937814	3.90989028	-0.25422002

H	-2.96180121	3.71879426	-0.27872701
H	-1.91273213	4.64659333	0.32884002

${}^3\pi_8\pi_8^*/{}^3\pi_8\pi_7^*$

C	-0.11521700	-0.90295106	-0.14761501
C	-0.96436007	0.21964701	-0.15606101
C	0.87781806	1.74742812	0.16809101
C	1.23915809	-0.62871504	-0.02233800
H	-1.02150207	2.30889616	-0.13713200
N	1.68674212	0.67589204	0.15701501
H	1.99469114	-1.38547709	0.01628800
N	-0.43573703	1.50132410	-0.01627700
H	2.67407919	0.85407506	0.10814800
S	-2.71288719	0.13703000	-0.33815902
S	1.42018110	3.35120324	0.40508103
C	-0.65065604	-2.30915816	-0.23259101
H	-1.30540009	-2.53520318	0.60410104
H	-1.21041608	-2.47847118	-1.14655208
H	0.15965001	-3.02820121	-0.21457501
O	-4.92966135	2.97278421	-0.10426600
H	-5.24529637	2.80569420	-0.98367607
H	-5.20699937	2.22874616	0.42818403
O	4.59596833	1.07840707	-0.18874301
H	4.76306034	1.82183512	0.39078902
H	4.90153635	1.34692609	-1.04517507
O	4.60642533	3.43927724	1.49192110
H	3.93777128	3.14890122	2.10217615
H	4.09857829	3.94043428	0.86226606
O	-2.13148815	3.76101027	-0.27289201
H	-3.06122322	3.80465727	-0.07450100

H	-1.67536112	4.44019632	0.20675701
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${}^3n_8\pi_8^*/{}^3\pi_7\pi_7^*$

C	-0.17419701	-0.83401105	-0.16561301
C	-1.12279807	0.27642501	-0.18932501
C	0.77065005	1.80078613	-0.07902600
C	1.15869408	-0.54107303	-0.06463800
H	-1.20116608	2.30689116	-0.16255701
N	1.62518711	0.73104405	0.01380700
H	1.91573213	-1.30163709	-0.05276800
N	-0.58404404	1.51137210	-0.09823701
H	2.61624319	0.89289506	-0.05315500
S	-2.77439219	0.05248500	-0.33358902
S	1.30172109	3.41126224	0.50656203
C	-0.65447004	-2.25584316	-0.24408201
H	-1.28768409	-2.50687518	0.59880304
H	-1.24015308	-2.41907217	-1.14007608
H	0.18837501	-2.93937421	-0.25013301
O	-4.81387934	2.96316721	-0.15495401
H	-5.22452337	2.89745120	-1.00732807
H	-4.41730731	2.10723015	0.00068199
O	4.50237332	1.12288208	-0.30216802
H	4.75974134	1.80567313	0.31732402
H	4.86845235	1.37036009	-1.13962008
O	4.63178933	3.30989623	1.52629611
H	3.67882426	3.33769524	1.59470411
H	4.88400235	4.16636629	1.20493908
O	-2.09282715	3.91204028	-0.33337902
H	-3.04015022	3.81774527	-0.24221801
H	-1.81246913	4.60676933	0.24517801

Snapshot2

${}^1\pi_7\pi_8^*/{}^1n_8\pi_8^*$

C	-1.018316074	-0.596912043	0.239787018
C	-1.378282098	0.742461054	0.248592020
C	0.996889074	1.277247090	0.005393999
C	0.288209023	-0.981985071	0.061993004
N	-0.277152017	1.668714120	0.116241006
N	1.293544093	-0.002534002	-0.046535006
H	0.633402047	-1.992667145	0.057758003
H	-0.456276034	2.663657192	0.131822011
H	2.256299165	-0.288332019	-0.127573009
S	-2.944832210	1.427903101	0.389579026
S	2.293178162	2.496786179	-0.029189004
C	-2.062185149	-1.661217118	0.443265032
H	-2.522033183	-1.550075110	1.418373101
H	-2.849677203	-1.572643112	-0.290033022
H	-1.624604116	-2.650190192	0.371488027
O	-3.011988216	4.720713338	1.063113077
H	-3.032585219	3.765916272	1.126670080
H	-3.767671272	4.947028356	0.537342041
O	5.778894414	1.214303086	0.138823010
H	5.326736384	1.778933126	0.752325056
H	5.882840421	1.728924124	-0.650855049
O	-0.440929032	4.582936332	0.144538008
H	0.088415009	5.051463364	0.775122054
H	-1.350337099	4.807822348	0.351319024
O	3.999433286	-0.877193064	-0.276102019
H	4.336846310	-1.380871098	-1.003391074
H	4.681299338	-0.242002017	-0.063123003

${}^1n_7\pi_7^*/{}^1n_8\pi_8^*$

C	-0.901952066	-0.588920043	0.201037014
C	-1.279699091	0.837016059	0.209300016
C	1.076417080	1.365727098	-0.081369008
C	0.379822029	-0.899497065	-0.002097002
N	-0.266975018	1.710332122	0.076371003
N	1.373543099	0.019299999	-0.192554012
H	0.714345052	-1.919027140	-0.024763003
H	-0.464548033	2.697815192	0.094658009
H	2.319398165	-0.287687021	-0.308247023
S	-2.876956206	1.363250098	0.362625028
S	2.392674175	2.581487184	0.088385004
C	-1.938610138	-1.654467118	0.435556030
H	-2.406684174	-1.543506110	1.407486099
H	-2.728740199	-1.613922118	-0.301561022
H	-1.482100107	-2.637937188	0.388431029
O	-3.032729218	4.764611343	0.991553072
H	-3.076879222	3.812562273	1.054552074
H	-3.786386271	5.015591359	0.474426036
O	5.700404411	1.312425095	0.167398010
H	5.238583377	1.809272128	0.829469060
H	5.697699410	1.856033135	-0.609076044
O	-0.406930028	4.645315333	0.151632010
H	0.134968012	5.134164370	0.754958057
H	-1.312784094	4.883851350	0.358620024
O	4.123180295	-0.910087066	-0.361449027
H	4.513625325	-1.353013096	-1.102237077
H	4.757255340	-0.248305020	-0.093531005

${}^1n_7\pi_7^*/{}^1\pi_7\pi_8^*$

C	-0.911639063	-0.584451040	0.188573011
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C	-1.297314095	0.799220056	0.208054015
C	1.031208076	1.370883099	-0.001404002
C	0.376719029	-0.912476068	0.019961000
N	-0.215551018	1.715316125	0.114796008
N	1.370794097	0.088408008	-0.095190007
H	0.749604053	-1.912761137	-0.000415002
H	-0.420402029	2.702271192	0.152756009
H	2.335392166	-0.187371012	-0.169154011
S	-2.894668207	1.426507100	0.388782027
S	2.338381166	2.592228185	-0.006738998
C	-1.944951142	-1.655402121	0.384992028
H	-2.413970172	-1.547615113	1.355657098
H	-2.727555196	-1.574235116	-0.355458026
H	-1.497807109	-2.640441191	0.318014021
O	-3.019599219	4.743066341	1.014577072
H	-3.027297219	3.790734272	1.082834079
H	-3.774001270	4.955446359	0.481534035
O	5.779341416	1.264318089	0.177081012
H	5.246891380	1.867696132	0.679200047
H	6.069423435	1.749182125	-0.584780040
O	-0.446873031	4.605016332	0.121336009
H	0.093372008	5.146291372	0.685081048
H	-1.355217098	4.830657347	0.330308025
O	4.068649294	-0.869807062	-0.285907022
H	4.390767318	-1.345172097	-1.038836076
H	4.752507345	-0.238735019	-0.064930006
${}^3\Pi_8\Pi_8^*/{}^3\Pi_8\Pi_8^*$			
C	-0.788758058	-0.647744047	0.147186011
C	-1.159193086	0.729687054	0.177210015
C	1.156903082	1.407926099	0.021162999

C	0.516906036	-0.907857065	-0.015577999
N	-0.153378009	1.694932122	0.086141007
N	1.467604106	0.102679008	-0.089463007
H	0.914790065	-1.900210137	-0.057303006
H	-0.393087027	2.672804190	0.079218004
H	2.434312174	-0.161565011	-0.154496013
S	-2.781152200	1.333688098	0.458623031
S	2.339594167	2.639542188	0.079878004
C	-1.800855130	-1.742726125	0.325454025
H	-2.295530165	-1.661282122	1.288755092
H	-2.570098183	-1.710523123	-0.436378033
H	-1.322212096	-2.713034197	0.274622021
O	-3.212243234	5.048794364	1.007427072
H	-3.358050240	4.143544301	1.241235091
H	-3.931407281	5.290616381	0.439172031
O	5.527427396	1.352243095	0.203104012
H	4.701495340	1.796367130	0.386134029
H	5.864675422	1.778441129	-0.572638042
O	-0.649734045	4.528952325	0.020554001
H	0.146739010	4.912928354	0.363851026
H	-1.394025100	4.986214360	0.397878028
O	4.151819299	-0.978230072	-0.284980020
H	4.488041325	-1.330126095	-1.097109080
H	4.768593343	-0.290882019	-0.030217000
${}^3\Pi_8\Pi_8^*/{}^3\Pi_7\Pi_7^*$			
C	-0.860355062	-0.582399044	0.176530011
C	-1.240877087	0.830256058	0.191597016
C	1.101453080	1.420112104	-0.123657007
C	0.435037029	-0.869979060	-0.036058000
N	-0.223968016	1.724637122	0.069047005

N	1.393966102	0.082932008	-0.221405015
H	0.794304057	-1.879667138	-0.062648003
H	-0.436561033	2.710486193	0.093041008
H	2.348770169	-0.204346012	-0.341450027
S	-2.840484204	1.356347098	0.325223024
S	2.345001168	2.591428186	0.384228028
C	-1.880997135	-1.662000120	0.409167030
H	-2.347415169	-1.554619113	1.384474101
H	-2.671237190	-1.628317115	-0.326218025
H	-1.416141100	-2.639876188	0.359645025
O	-3.154433228	4.793802347	0.969206071
H	-3.191740229	3.843259279	0.993108070
H	-3.929893283	5.074812363	0.504002038
O	5.632335404	1.233024091	0.222255016
H	4.875050349	1.730166124	0.517433038
H	5.955926430	1.696125120	-0.537987039
O	-0.522156035	4.670925337	0.143301009
H	0.057255005	5.003960361	0.826095058
H	-1.401280099	4.960165356	0.373642028
O	4.102470293	-0.993385073	-0.390509029
H	4.497159324	-1.418950100	-1.138816084
H	4.743529339	-0.350063027	-0.092868009

Snapshot3

${}^1\pi_7\pi_8^*/{}^1n_8\pi_8^*$

C	-0.228664014	-0.864500060	0.118316011
C	-0.720228053	0.448473030	0.081186008
C	1.582466113	1.204125087	0.069001004
C	1.140717084	-1.121072083	0.135211010
N	0.302006023	1.462357107	0.070626007

N	2.032550144	-0.038633003	0.102647009
H	1.591499116	-2.088151152	0.179393014
H	0.003757000	2.432504177	0.032989005
H	3.023456218	-0.220061015	0.053311004
S	-2.350387171	0.978011072	-0.005978999
S	2.753134196	2.546994183	0.002718003
C	-1.195602084	-2.014428146	0.133681011
H	-1.750703128	-2.030420147	1.064684077
H	-1.917000138	-1.913702136	-0.661926045
H	-0.675878047	-2.959365212	0.019575002
O	4.792242343	-0.773859056	-0.142152011
H	5.318251382	0.012821002	-0.291556021
H	5.060060362	-1.397266099	-0.803866057
O	-0.415219029	4.256850305	-0.042654004
H	-1.325305095	4.280850308	0.266063018
H	0.042141004	4.940819355	0.434040033
O	6.138529443	1.699205123	-0.614792042
H	5.581122403	2.415750176	-0.349713024
H	6.986045501	1.866435135	-0.237698017
O	-2.954493214	3.998217290	1.156625084
H	-3.714827267	4.145989301	0.612763044
H	-2.821147205	3.050041220	1.125227082
${}^1n_7\pi_7^*/{}^1n_8\pi_8^*$			
C	-0.223089015	-0.878660065	0.099311007
C	-0.683070047	0.492670036	0.069199006
C	1.646156119	1.209257085	0.208880013
C	1.124473079	-1.105628082	0.120237009
N	0.281023018	1.464107107	0.099906008
N	2.039278146	-0.102026009	0.148451009
H	1.540613109	-2.093524153	0.128675010

H	-0.023836001	2.418533172	0.054470003
H	3.013325215	-0.341543025	0.105070005
S	-2.301225165	0.902243066	-0.000394999
S	2.803026202	2.547087186	-0.196222014
C	-1.208785085	-2.018719144	0.108550007
H	-1.787394130	-2.038264147	1.024398072
H	-1.911336136	-1.948124142	-0.711250053
H	-0.682753049	-2.962677216	0.023257001
O	4.842623346	-0.898939063	-0.119278007
H	5.335952382	-0.090975004	-0.245104017
H	5.150695370	-1.500088106	-0.783973057
O	-0.413495028	4.326863312	-0.044215003
H	-1.294307093	4.394862319	0.325703025
H	0.090161008	5.030999360	0.341197022
O	6.070043435	1.685316120	-0.382720026
H	5.592177402	2.345615167	-0.871784063
H	6.180649444	2.030736145	0.497335035
O	-2.982641216	4.063617295	1.144986084
H	-3.733060270	4.225479307	0.587650044
H	-2.874210204	3.117243222	1.136945083

${}^1\pi_7\pi_8^*/{}^1n_7\pi_7^*$

C	-0.255147018	-0.906145066	0.114610008
C	-0.704797049	0.466080032	0.074626004
C	1.586438112	1.172386083	0.056268004
C	1.074617078	-1.158942081	0.137156012
N	0.298831023	1.419673104	0.030188001
N	2.017604146	-0.102975009	0.144799009
H	1.500783107	-2.140411152	0.151365008
H	0.015611999	2.388606172	-0.035560002
H	2.995734214	-0.321873025	0.115927008

S	-2.345779169	0.990979074	-0.008288001
S	2.774243198	2.496486178	-0.075709008
C	-1.263162090	-2.019274145	0.125878012
H	-1.831595131	-2.010210143	1.047540073
H	-1.967924140	-1.912647136	-0.689176049
H	-0.772400056	-2.980585214	0.035439000
O	4.832382348	-0.828637061	-0.131788011
H	5.318202385	-0.026140001	-0.316607023
H	5.161952372	-1.486488108	-0.726261050
O	-0.367487024	4.244056307	-0.023270003
H	-1.255233089	4.306988309	0.330014025
H	0.105350009	4.988613358	0.317531025
O	6.025219433	1.753536126	-0.450205032
H	5.712077410	2.456590177	-1.005392073
H	6.102691438	2.114341150	0.423010032
O	-2.916378212	4.060505294	1.180118082
H	-3.659724263	4.211654302	0.611733043
H	-2.830658202	3.111259223	1.219624085
${}^3\pi_8\pi_8^*/{}^3n_8\pi_8^*$			
C	-0.143534011	-0.853325064	0.075244004
C	-0.567973043	0.459602035	0.047349002
C	1.708785125	1.276965092	-0.023643999
C	1.244413092	-1.086790076	0.028974000
N	0.385897027	1.488546105	-0.043559003
N	2.115446152	0.007217999	0.019950003
H	1.702737121	-2.049405148	0.088401007
H	0.066302004	2.440749176	-0.141484010
H	3.099912223	-0.193305015	-0.000541999
S	-2.238138162	0.977483070	-0.037353003
S	2.789435200	2.612698190	-0.099333010

C	-1.101579077	-2.013312143	0.138147007
H	-1.702155122	-1.979242140	1.037325074
H	-1.777867130	-2.013048147	-0.707945050
H	-0.557784042	-2.947725212	0.139553010
O	4.817212345	-1.026792076	-0.074057007
H	5.357202383	-0.233996015	-0.084700005
H	5.096395365	-1.541080113	-0.815969061
O	-0.528236038	4.188981301	-0.085350004
H	-1.319312093	4.366129312	0.418320029
H	0.154386012	4.778639345	0.200782014
O	5.917834426	1.524553108	-0.303671021
H	5.051432365	1.927027136	-0.345365023
H	6.363316456	1.939133140	0.419195029
O	-3.131370223	4.162111299	1.206060087
H	-3.835221277	4.358258314	0.600268042
H	-3.311497237	3.283778234	1.503808106
${}^3\pi_7\pi_7^*/{}^3n_8\pi_8^*$			
C	-0.148250012	-0.842190058	0.116310011
C	-0.637994046	0.522166037	0.106341010
C	1.674926121	1.297803091	0.245100016
C	1.184108084	-1.032611073	0.110121008
N	0.307333023	1.514997109	0.138072012
N	2.084163151	-0.008034001	0.142068010
H	1.620177115	-2.012506143	0.099307006
H	-0.004791001	2.471152177	0.085494009
H	3.062257219	-0.233789016	0.123036007
S	-2.259122162	0.909819064	0.072374006
S	2.753614197	2.592412185	-0.372238025
C	-1.105862079	-2.001765146	0.122944010
H	-1.671850120	-2.045722149	1.047835073

H	-1.818595130	-1.935988139	-0.688646051
H	-0.557413041	-2.930943213	0.025829004
O	4.826346346	-0.981960073	-0.046201005
H	5.386721388	-0.209247014	-0.107156006
H	5.111294367	-1.571133116	-0.731982054
O	-0.512951039	4.332733311	-0.052376006
H	-1.377206101	4.421427318	0.348295025
H	0.020232002	5.016403361	0.329415023
O	6.021425434	1.576431111	-0.307748025
H	5.204398373	1.983699141	-0.619728044
H	6.187166447	1.953587140	0.574661039
O	-3.073432220	4.048310293	1.163918083
H	-3.808881274	4.183398301	0.570401040
H	-2.936054213	3.091896225	1.205233089

Cartesian coordinates of LIIC paths

I. gas phase

FC point to minimum ${}^1n_7\pi_7^*$

point 1

C	-0.6238126	-1.4078701	0.0033321
C	-1.0340770	-0.0016972	0.0137618
C	1.3406632	0.6464128	0.0143521
C	0.6992509	-1.6700700	-0.0015239
H	1.0903011	-2.6679507	-0.0094376
N	-0.0010033	0.8992227	0.0195339
H	-0.2513316	1.8661158	0.0262933
N	1.6514721	-0.6713499	0.0028358
H	2.6199002	-0.8991445	0.0001722
S	-2.5968087	0.5213051	0.0188520
S	2.4932361	1.8709846	0.0217100

C	-1.6515927	-2.5070450	-0.0015674
H	-2.2865236	-2.4483704	0.8740282
H	-2.2922407	-2.4353838	-0.8719781
H	-1.1656480	-3.4757779	-0.0103643

point 2

C	-0.6232413	-1.4070052	0.0033556
C	-1.0347427	0.0003022	0.0138304
C	1.3391693	0.6451452	0.0143406
C	0.7000198	-1.6705470	-0.0015618
H	1.0885932	-2.6695140	-0.0095103
N	-0.0048900	0.9017594	0.0195473
H	-0.2587170	1.8674463	0.0261914
N	1.6545527	-0.6754137	0.0027568
H	2.6216992	-0.9069099	0.0001823
S	-2.5994010	0.5202259	0.0189624
S	2.5023245	1.8794531	0.0218053
C	-1.6509809	-2.5063876	-0.0015642
H	-2.2862030	-2.4485430	0.8739239
H	-2.2918226	-2.4356115	-0.8719557
H	-1.1645748	-3.4750190	-0.0103041

point 3

C	-0.6226658	-1.4061309	0.0033791
C	-1.0354105	0.0023089	0.0138989
C	1.3376602	0.6438630	0.0143289
C	0.7007923	-1.6710158	-0.0015996
H	1.0868855	-2.6710631	-0.0095825
N	-0.0087800	0.9042966	0.0195602
H	-0.2661026	1.8687641	0.0260894

N	1.6576289	-0.6794782	0.0026775
H	2.6234785	-0.9146746	0.0001917
S	-2.6019912	0.5191428	0.0190730
S	2.5114120	1.8878926	0.0219015
C	-1.6503612	-2.5057243	-0.0015609
H	-2.2858740	-2.4487116	0.8738193
H	-2.2913960	-2.4358356	-0.8719329
H	-1.1634906	-3.4742524	-0.0102436

point 4

C	-0.6220862	-1.4052472	0.0034027
C	-1.0360805	0.0043229	0.0139672
C	1.3361357	0.6425662	0.0143168
C	0.7015684	-1.6714765	-0.0016372
H	1.0851782	-2.6725981	-0.0096542
N	-0.0126734	0.9068343	0.0195727
H	-0.2734883	1.8700692	0.0259873
N	1.6607007	-0.6835434	0.0025980
H	2.6252379	-0.9224386	0.0002002
S	-2.6045793	0.5180557	0.0191836
S	2.5204986	1.8963030	0.0219986
C	-1.6497337	-2.5050552	-0.0015575
H	-2.2855366	-2.4488765	0.8737145
H	-2.2909607	-2.4360562	-0.8719099
H	-1.1623954	-3.4734781	-0.0101827

point 5

C	-0.6215025	-1.4043543	0.0034263
C	-1.0367527	0.0063441	0.0140354
C	1.3345958	0.6412549	0.0143045

C	0.7023481	-1.6719292	-0.0016748
H	1.0834712	-2.6741190	-0.0097254
N	-0.0165702	0.9093725	0.0195848
H	-0.2808742	1.8713614	0.0258850
N	1.6637680	-0.6876093	0.0025182
H	2.6269774	-0.9302016	0.0002080
S	-2.6071653	0.5169648	0.0192944
S	2.5295844	1.9046842	0.0220967
C	-1.6490982	-2.5043802	-0.0015540
H	-2.2851907	-2.4490374	0.8736093
H	-2.2905168	-2.4362731	-0.8718867
H	-1.1612891	-3.4726962	-0.0101216

point 6

C	-0.6209145	-1.4034520	0.0034499
C	-1.0374271	0.0083725	0.0141034
C	1.3330405	0.6399290	0.0142919
C	0.7031315	-1.6723737	-0.0017122
H	1.0817646	-2.6756256	-0.0097962
N	-0.0204702	0.9119111	0.0195964
H	-0.2882600	1.8726407	0.0257825
N	1.6668307	-0.6916759	0.0024382
H	2.6286968	-0.9379636	0.0002150
S	-2.6097490	0.5158699	0.0194052
S	2.5386692	1.9130363	0.0221956
C	-1.6484549	-2.5036994	-0.0015505
H	-2.2848363	-2.4491945	0.8735039
H	-2.2900642	-2.4364865	-0.8718631
H	-1.1601717	-3.4719067	-0.0100601

point 7

C	-0.6203224	-1.4025405	0.0034735
C	-1.0381037	0.0104081	0.0141713
C	1.3314698	0.6385885	0.0142790
C	0.7039185	-1.6728101	-0.0017494
H	1.0800584	-2.6771181	-0.0098665
N	-0.0243735	0.9144501	0.0196076
H	-0.2956458	1.8739071	0.0256798
N	1.6698888	-0.6957430	0.0023580
H	2.6303961	-0.9457245	0.0002212
S	-2.6123304	0.5147710	0.0195162
S	2.5477530	1.9213592	0.0222955
C	-1.6478036	-2.5030127	-0.0015469
H	-2.2844734	-2.4493478	0.8733982
H	-2.2896029	-2.4366963	-0.8718392
H	-1.1590434	-3.4711095	-0.0099982

point 8

C	-0.6197262	-1.4016197	0.0034972
C	-1.0387825	0.0124508	0.0142391
C	1.3298836	0.6372335	0.0142659
C	0.7047091	-1.6732384	-0.0017866
H	1.0783526	-2.6785964	-0.0099363
N	-0.0282801	0.9169895	0.0196184
H	-0.3030315	1.8751606	0.0255770
N	1.6729421	-0.6998107	0.0022775
H	2.6320752	-0.9534839	0.0002265
S	-2.6149094	0.5136682	0.0196272
S	2.5568358	1.9296528	0.0223963
C	-1.6471445	-2.5023202	-0.0015432

H	-2.2841020	-2.4494972	0.8732922
H	-2.2891330	-2.4369026	-0.8718150
H	-1.1579039	-3.4703046	-0.0099360

point 9

C	-0.6191257	-1.4006896	0.0035209
C	-1.0394634	0.0145006	0.0143067
C	1.3282819	0.6358640	0.0142524
C	0.7055034	-1.6736586	-0.0018237
H	1.0766473	-2.6800605	-0.0100056
N	-0.0321900	0.9195291	0.0196287
H	-0.3104169	1.8764011	0.0254740
N	1.6759906	-0.7038789	0.0021968
H	2.6337340	-0.9612419	0.0002311
S	-2.6174861	0.5125613	0.0197383
S	2.5659176	1.9379173	0.0224980
C	-1.6464774	-2.5016219	-0.0015395
H	-2.2837221	-2.4496428	0.8731859
H	-2.2886543	-2.4371053	-0.8717905
H	-1.1567535	-3.4694921	-0.0098735

point 10

C	-0.6185210	-1.3997503	0.0035447
C	-1.0401466	0.0165576	0.0143741
C	1.3266647	0.6344800	0.0142386
C	0.7063013	-1.6740707	-0.0018606
H	1.0749425	-2.6815104	-0.0100744
N	-0.0361030	0.9220691	0.0196385
H	-0.3178021	1.8776285	0.0253709
N	1.6790342	-0.7079477	0.0021158

H	2.6353723	-0.9689983	0.0002347
S	-2.6200602	0.5114503	0.0198495
S	2.5749984	1.9461525	0.0226007
C	-1.6458024	-2.5009178	-0.0015356
H	-2.2833336	-2.4497846	0.8730794
H	-2.2881669	-2.4373045	-0.8717658
H	-1.1555920	-3.4686720	-0.0098106

FC point and minimum ${}^1\Pi_7\Pi_8^*$

point 1

C	-0.6238126	-1.4078701	0.0033321
C	-1.0340770	-0.0016972	0.0137618
C	1.3406632	0.6464128	0.0143521
C	0.6992509	-1.6700700	-0.0015239
H	1.0903011	-2.6679507	-0.0094376
N	-0.0010033	0.8992227	0.0195339
H	-0.2513316	1.8661158	0.0262933
N	1.6514721	-0.6713499	0.0028358
H	2.6199002	-0.8991445	0.0001722
S	-2.5968087	0.5213051	0.0188520
S	2.4932361	1.8709846	0.0217100
C	-1.6515927	-2.5070450	-0.0015674
H	-2.2865236	-2.4483704	0.8740282
H	-2.2922407	-2.4353838	-0.8719781
H	-1.1656480	-3.4757779	-0.0103643

point 2

C	-0.6244509	-1.4068371	0.0033800
C	-1.0381980	-0.0085221	0.0137691
C	1.3342942	0.6418462	0.0142274

C	0.7019810	-1.6749906	-0.0017439
H	1.0947403	-2.6717267	-0.0095781
N	0.0007157	0.8993324	0.0193185
H	-0.2538818	1.8652749	0.0260883
N	1.6537079	-0.6706453	0.0028636
H	2.6229196	-0.8951782	0.0005022
S	-2.6013764	0.5314994	0.0197173
S	2.4967945	1.8730422	0.0216631
C	-1.6511946	-2.5069132	-0.0016269
H	-2.2865911	-2.4465983	0.8735250
H	-2.2916476	-2.4340529	-0.8720985
H	-1.1660274	-3.4761495	-0.0100071

point 3

C	-0.6251110	-1.4058011	0.0034280
C	-1.0423124	-0.0153641	0.0137762
C	1.3279060	0.6372906	0.0141030
C	0.7046732	-1.6798868	-0.0019676
H	1.0991769	-2.6754603	-0.0097228
N	0.0024370	0.8994201	0.0190998
H	-0.2564131	1.8643968	0.0258788
N	1.6558586	-0.6698822	0.0028928
H	2.6258415	-0.8911569	0.0008348
S	-2.6057646	0.5417034	0.0205832
S	2.5003899	1.8750518	0.0216215
C	-1.6507957	-2.5067977	-0.0016845
H	-2.2866576	-2.4448544	0.8730212
H	-2.2910549	-2.4327503	-0.8722156
H	-1.1663884	-3.4765274	-0.0096486

point 4

C	-0.6257930	-1.4047622	0.0034760
C	-1.0464203	-0.0222231	0.0137832
C	1.3214989	0.6327467	0.0139789
C	0.7073279	-1.6847584	-0.0021949
H	1.1036109	-2.6791510	-0.0098718
N	0.0041606	0.8994859	0.0188778
H	-0.2589254	1.8634815	0.0256648
N	1.6579240	-0.6690606	0.0029232
H	2.6286656	-0.8870806	0.0011701
S	-2.6099730	0.5519153	0.0214492
S	2.5040228	1.8770132	0.0215853
C	-1.6503963	-2.5066985	-0.0017403
H	-2.2867234	-2.4431390	0.8725167
H	-2.2904630	-2.4314757	-0.8723292
H	-1.1667309	-3.4769118	-0.0092889

point 5

C	-0.6264975	-1.4037203	0.0035241
C	-1.0505216	-0.0290988	0.0137901
C	1.3150731	0.6282152	0.0138549
C	0.7099451	-1.6896050	-0.0024260
H	1.1080423	-2.6827984	-0.0100251
N	0.0058869	0.8995297	0.0186527
H	-0.2614186	1.8625293	0.0254464
N	1.6599040	-0.6681804	0.0029548
H	2.6313919	-0.8829498	0.0015080
S	-2.6140017	0.5621330	0.0223150
S	2.5076940	1.8789265	0.0215547
C	-1.6499965	-2.5066155	-0.0017941

H	-2.2867886	-2.4414519	0.8720118
H	-2.2898720	-2.4302294	-0.8724394
H	-1.1670553	-3.4773026	-0.0089279

point 6

C	-0.6272247	-1.4026754	0.0035724
C	-1.0546162	-0.0359912	0.0137971
C	1.3086289	0.6236969	0.0137311
C	0.7125250	-1.6944261	-0.0026609
H	1.1124709	-2.6864018	-0.0101828
N	0.0076159	0.8995517	0.0184245
H	-0.2638927	1.8615404	0.0252236
N	1.6617986	-0.6672416	0.0029877
H	2.6340203	-0.8787644	0.0018484
S	-2.6178507	0.5723547	0.0231802
S	2.5114040	1.8807917	0.0215296
C	-1.6495966	-2.5065489	-0.0018459
H	-2.2868535	-2.4397934	0.8715064
H	-2.2892824	-2.4290113	-0.8725459
H	-1.1673614	-3.4776997	-0.0085656

point 7

C	-0.6279749	-1.4016274	0.0036207
C	-1.0587040	-0.0429000	0.0138043
C	1.3021664	0.6191926	0.0136075
C	0.7150677	-1.6992214	-0.0028995
H	1.1168967	-2.6899608	-0.0103449
N	0.0093479	0.8995519	0.0181933
H	-0.2663476	1.8605150	0.0249966
N	1.6636077	-0.6662442	0.0030217

H	2.6365507	-0.8745247	0.0021913
S	-2.6215199	0.5825784	0.0240446
S	2.5151535	1.8826085	0.0215104
C	-1.6491966	-2.5064984	-0.0018958
H	-2.2869184	-2.4381635	0.8710007
H	-2.2886944	-2.4278215	-0.8726487
H	-1.1676494	-3.4781031	-0.0082019

point 8

C	-0.6287485	-1.4005763	0.0036691
C	-1.0627851	-0.0498250	0.0138116
C	1.2956861	0.6147031	0.0134839
C	0.7175736	-1.7039906	-0.0031421
H	1.1213195	-2.6934747	-0.0105115
N	0.0110830	0.8995304	0.0179592
H	-0.2687832	1.8594532	0.0247655
N	1.6653312	-0.6651881	0.0030568
H	2.6389832	-0.8702310	0.0025366
S	-2.6250094	0.5928023	0.0249076
S	2.5189433	1.8843771	0.0214969
C	-1.6487969	-2.5064641	-0.0019435
H	-2.2869834	-2.4365622	0.8704947
H	-2.2881084	-2.4266598	-0.8727477
H	-1.1679194	-3.4785128	-0.0078370

point 9

C	-0.6295459	-1.3995220	0.0037175
C	-1.0668592	-0.0567662	0.0138191
C	1.2891881	0.6102291	0.0133605
C	0.7200426	-1.7087332	-0.0033885

H	1.1257393	-2.6969432	-0.0106827
N	0.0128213	0.8994873	0.0177223
H	-0.2711995	1.8583553	0.0245302
N	1.6669689	-0.6640733	0.0030930
H	2.6413176	-0.8658834	0.0028842
S	-2.6283193	0.6030245	0.0257689
S	2.5227738	1.8860972	0.0214895
C	-1.6483975	-2.5064459	-0.0019891
H	-2.2870489	-2.4349895	0.8699885
H	-2.2875245	-2.4255264	-0.8728428
H	-1.1681713	-3.4789288	-0.0074706

point 10

C	-0.6303673	-1.3984645	0.0037661
C	-1.0709265	-0.0637232	0.0138270
C	1.2826727	0.6057715	0.0132371
C	0.7224750	-1.7134488	-0.0036389
H	1.1301560	-2.7003655	-0.0108585
N	0.0145632	0.8994226	0.0174826
H	-0.2735964	1.8572215	0.0242910
N	1.6685210	-0.6628999	0.0031302
H	2.6435539	-0.8614821	0.0032341
S	-2.6314498	0.6132430	0.0266283
S	2.5266458	1.8877689	0.0214881
C	-1.6479987	-2.5064439	-0.0020326
H	-2.2871149	-2.4334457	0.8694824
H	-2.2869433	-2.4244213	-0.8729340
H	-1.1684052	-3.4793509	-0.0071029

${}^1\pi_7\pi_8^*$ to ${}^1\pi_7\pi_8^*$ / ${}^1n_7\pi_7^*$

point 1

N	0.1211067	-0.0459685	1.2820416
C	0.1735065	-0.0329661	-0.0429464
N	1.3260154	-0.0130597	-0.6476593
C	2.6197475	-0.0049609	0.0097163
C	2.5311379	-0.0197649	1.4124483
C	1.3020189	-0.0381491	2.0592720
S	-1.3541580	-0.0439265	-0.9687841
H	-0.7718844	-0.0642783	1.7206258
H	1.3625265	-0.0024716	-1.6471671
H	1.1572462	-0.0506215	3.1171688
C	3.7958432	-0.0125412	2.2271223
H	3.5779846	-0.0281223	3.2896093
H	4.4061511	-0.8726978	1.9801577
H	4.3827021	0.8694592	2.0010269
S	3.9582544	0.0161778	-1.0398705

point 2

N	0.1197167	-0.0455667	1.2836312
C	0.1728464	-0.0332935	-0.0445210
N	1.3279034	-0.0136930	-0.6467938
C	2.6166594	-0.0025811	0.0061998
C	2.5296725	-0.0190947	1.4147473
C	1.3034688	-0.0385832	2.0582909
S	-1.3554176	-0.0463017	-0.9719410
H	-0.7717958	-0.0586354	1.7242529
H	1.3650188	-0.0065359	-1.6465012
H	1.1593666	-0.0524018	3.1167001
C	3.7955390	-0.0133863	2.2269646
H	3.5784667	-0.0294240	3.2895197

H	4.4058202	-0.8734515	1.9792721
H	4.3821008	0.8685619	2.0004607
S	3.9588328	0.0204956	-1.0375205

point 3

N	0.1183368	-0.0451510	1.2852180
C	0.1721961	-0.0336238	-0.0460995
N	1.3297933	-0.0143058	-0.6459279
C	2.6135590	-0.0001907	0.0026894
C	2.5282086	-0.0184261	1.4170470
C	1.3049201	-0.0390024	2.0573051
S	-1.3566664	-0.0487230	-0.9750970
H	-0.7716628	-0.0529857	1.7278700
H	1.3675133	-0.0105946	-1.6458228
H	1.1614823	-0.0541668	3.1162236
C	3.7952300	-0.0142413	2.2268054
H	3.5789431	-0.0307378	3.2894278
H	4.4054796	-0.8742172	1.9783822
H	4.3814990	0.8676525	1.9998974
S	3.9593667	0.0248225	-1.0351569

point 4

N	0.1169673	-0.0447212	1.2868022
C	0.1715557	-0.0339572	-0.0476818
N	1.3316850	-0.0148980	-0.6450617
C	2.6104463	0.0022102	-0.0008146
C	2.5267460	-0.0177593	1.4193473
C	1.3063727	-0.0394066	2.0563146
S	-1.3579043	-0.0511902	-0.9782520
H	-0.7714855	-0.0473296	1.7314769

H	1.3700102	-0.0146475	-1.6451319
H	1.1635932	-0.0559168	3.1157394
C	3.7949162	-0.0151064	2.2266449
H	3.5794137	-0.0320636	3.2893334
H	4.4051295	-0.8749948	1.9774881
H	4.3808965	0.8667311	1.9993368
S	3.9598561	0.0291584	-1.0327798

point 5

N	0.1156079	-0.0442776	1.2883836
C	0.1709252	-0.0342934	-0.0492678
N	1.3335785	-0.0154695	-0.6441953
C	2.6073213	0.0046213	-0.0043124
C	2.5252848	-0.0170944	1.4216481
C	1.3078268	-0.0397959	2.0553196
S	-1.3591311	-0.0537026	-0.9814057
H	-0.7712640	-0.0416673	1.7350735
H	1.3725098	-0.0186945	-1.6444284
H	1.1656994	-0.0576520	3.1152477
C	3.7945974	-0.0159812	2.2264829
H	3.5798785	-0.0334010	3.2892366
H	4.4047698	-0.8757841	1.9765899
H	4.3802932	0.8657980	1.9987788
S	3.9603012	0.0335030	-1.0303892

point 6

N	0.1142587	-0.0438201	1.2899624
C	0.1703046	-0.0346326	-0.0508577
N	1.3354740	-0.0160202	-0.6433287
C	2.6041840	0.0070423	-0.0078039

C	2.5238249	-0.0164315	1.4239495
C	1.3092823	-0.0401705	2.0543201
S	-1.3603468	-0.0562602	-0.9845581
H	-0.7709983	-0.0359989	1.7386597
H	1.3750120	-0.0227355	-1.6437121
H	1.1678006	-0.0593724	3.1147485
C	3.7942737	-0.0168659	2.2263193
H	3.5803375	-0.0347501	3.2891372
H	4.4044006	-0.8765851	1.9756876
H	4.3796890	0.8648532	1.9982232
S	3.9607019	0.0378560	-1.0279852

point 7

N	0.1129198	-0.0433488	1.2915385
C	0.1696939	-0.0349746	-0.0524512
N	1.3373713	-0.0165500	-0.6424620
C	2.6010344	0.0094730	-0.0112890
C	2.5223662	-0.0157708	1.4262514
C	1.3107391	-0.0405305	2.0533163
S	-1.3615513	-0.0588623	-0.9877090
H	-0.7706885	-0.0303246	1.7422353
H	1.3775172	-0.0267703	-1.6429830
H	1.1698970	-0.0610783	3.1142419
C	3.7939449	-0.0177602	2.2261541
H	3.5807907	-0.0361105	3.2890353
H	4.4040218	-0.8773975	1.9747811
H	4.3790837	0.8638968	1.9976698
S	3.9610584	0.0422173	-1.0255678

point 8

N	0.1115911	-0.0428637	1.2931119
C	0.1690931	-0.0353195	-0.0540485
N	1.3392705	-0.0170589	-0.6415952
C	2.5978723	0.0119132	-0.0147677
C	2.5209087	-0.0151124	1.4285538
C	1.3121974	-0.0408759	2.0523082
S	-1.3627445	-0.0615088	-0.9908583
H	-0.7703346	-0.0246447	1.7458003
H	1.3800255	-0.0307986	-1.6422408
H	1.1719885	-0.0627698	3.1137281
C	3.7936112	-0.0186642	2.2259873
H	3.5812380	-0.0374821	3.2889308
H	4.4036336	-0.8782214	1.9738706
H	4.3784772	0.8629290	1.9971184
S	3.9613708	0.0465865	-1.0231371

point 9

N	0.1102726	-0.0423648	1.2946826
C	0.1685021	-0.0356672	-0.0556495
N	1.3411716	-0.0175468	-0.6407283
C	2.5946978	0.0143625	-0.0182400
C	2.5194524	-0.0144564	1.4308567
C	1.3136571	-0.0412068	2.0512959
S	-1.3639262	-0.0641992	-0.9940059
H	-0.7699368	-0.0189592	1.7493545
H	1.3825370	-0.0348205	-1.6414856
H	1.1740750	-0.0644472	3.1132071
C	3.7932723	-0.0195776	2.2258188
H	3.5816795	-0.0388649	3.2888236
H	4.4032360	-0.8790566	1.9729561

H	4.3778694	0.8619498	1.9965689
S	3.9616390	0.0509634	-1.0206931

point 10

N	0.1089644	-0.0418522	1.2962507
C	0.1679211	-0.0360176	-0.0572541
N	1.3430747	-0.0180136	-0.6398614
C	2.5915109	0.0168207	-0.0217060
C	2.5179971	-0.0138030	1.4331601
C	1.3151182	-0.0415233	2.0502795
S	-1.3650965	-0.0669331	-0.9971516
H	-0.7694951	-0.0132685	1.7528978
H	1.3850518	-0.0388356	-1.6407172
H	1.1761566	-0.0661105	3.1126790
C	3.7929282	-0.0205005	2.2256485
H	3.5821150	-0.0402585	3.2887137
H	4.4028289	-0.8799029	1.9720375
H	4.3772601	0.8609594	1.9960211
S	3.9618632	0.0553479	-1.0182359

${}^1n_7\pi_7^*$ to ${}^1n_8\pi_8^*$ / ${}^1n_7\pi_7^*$

point 1

C	-0.6185249	-1.3997471	0.0035427
C	-1.0401409	0.0165636	0.0143775
C	1.3266745	0.6344702	0.0142435
C	0.7062956	-1.6740763	-0.0018640
H	1.0749300	-2.6815185	-0.0100816
N	-0.0360913	0.9220684	0.0196449
H	-0.3177840	1.8776296	0.0253809
N	1.6790350	-0.7079598	0.0021157

H	2.6353713	-0.9690168	0.0002333
S	-2.6200513	0.5114669	0.0198552
S	2.5750169	1.9461343	0.0226100
C	-1.6458136	-2.5009077	-0.0015412
H	-2.2833442	-2.4497734	0.8730741
H	-2.2881780	-2.4372869	-0.8717710
H	-1.1556097	-3.4686651	-0.0098199

point 2

C	-0.6190686	-1.4002439	0.0043556
C	-1.0382243	0.0139159	0.0186698
C	1.3291943	0.6347600	0.0315490
C	0.7060903	-1.6752837	0.0024056
H	1.0751850	-2.6824189	-0.0075129
N	-0.0329716	0.9213141	0.0310664
H	-0.3135733	1.8772199	0.0401614
N	1.6782476	-0.7075306	0.0137276
H	2.6348646	-0.9685476	0.0140038
S	-2.6197050	0.5122319	0.0212792
S	2.5692669	1.9512736	-0.0291809
C	-1.6468534	-2.5010576	-0.0078374
H	-2.2873865	-2.4524005	0.8648101
H	-2.2859804	-2.4347995	-0.8803258
H	-1.1573003	-3.4690516	-0.0171713

point 3

C	-0.6195237	-1.4005408	0.0051689
C	-1.0363913	0.0114072	0.0229044
C	1.3315031	0.6353894	0.0487659
C	0.7059924	-1.6761559	0.0066847

H	1.0756632	-2.6829392	-0.0048828
N	-0.0300617	0.9207820	0.0424357
H	-0.3096899	1.8769851	0.0548785
N	1.6774292	-0.7066844	0.0252859
H	2.6343502	-0.9675587	0.0276591
S	-2.6194828	0.5129762	0.0226484
S	2.5630507	1.9533329	-0.0807662
C	-1.6476603	-2.5010967	-0.0140893
H	-2.2911947	-2.4549446	0.8565707
H	-2.2835483	-2.4322989	-0.8888195
H	-1.1586506	-3.4692720	-0.0244443

point 4

C	-0.6198913	-1.4006397	0.0059798
C	-1.0346407	0.0090369	0.0271005
C	1.3336023	0.6363560	0.0659297
C	0.7060007	-1.6766963	0.0109624
H	1.0763616	-2.6830828	-0.0022212
N	-0.0273600	0.9204711	0.0537717
H	-0.3061312	1.8769247	0.0695555
N	1.6765793	-0.7054251	0.0368067
H	2.6338275	-0.9660553	0.0412420
S	-2.6193840	0.5137003	0.0239897
S	2.5563796	1.9523384	-0.1322090
C	-1.6482371	-2.5010264	-0.0203133
H	-2.2947683	-2.4574202	0.8483425
H	-2.2808879	-2.4297719	-0.8972659
H	-1.1596648	-3.4693281	-0.0316710

point 5

C	-0.6201718	-1.4005400	0.0067852
C	-1.0329723	0.0068060	0.0312777
C	1.3354907	0.6376619	0.0830777
C	0.7061151	-1.6769032	0.0152279
H	1.0772805	-2.6828479	0.0004416
N	-0.0248672	0.9203831	0.0650937
H	-0.3028985	1.8770408	0.0842166
N	1.6756973	-0.7037516	0.0483070
H	2.6332958	-0.9640358	0.0547968
S	-2.6194098	0.5144040	0.0253307
S	2.5492584	1.9482760	-0.1835766
C	-1.6485839	-2.5008465	-0.0265263
H	-2.2981040	-2.4598415	0.8401113
H	-2.2780024	-2.4272041	-0.9056790
H	-1.1603425	-3.4692197	-0.0388844

point 6

C	-0.6203642	-1.4002382	0.0075821
C	-1.0313871	0.0047175	0.0354562
C	1.3371648	0.6393137	0.1002478
C	0.7063375	-1.6767705	0.0194698
H	1.0784236	-2.6822268	0.0030739
N	-0.0225866	0.9205230	0.0764220
H	-0.2999966	1.8773381	0.0988873
N	1.6747822	-0.7016569	0.0598039
H	2.6327541	-0.9614924	0.0683688
S	-2.6195631	0.5150864	0.0267000
S	2.5416857	1.9410899	-0.2349377
C	-1.6486977	-2.5005552	-0.0327455
H	-2.3011958	-2.4622229	0.8318627

H -2.2748926 -2.4245804 -0.9140731

H -1.1606788 -3.4689440 -0.0461183

point 7

C -0.6204664 -1.3997281 0.0083670

C -1.0298874 0.0027760 0.0396568

C 1.3386186 0.6413230 0.1174783

C 0.7066711 -1.6762870 0.0236754

H 1.0797978 -2.6812062 0.0056421

N -0.0205240 0.9208989 0.0877770

H -0.2974346 1.8778237 0.1135935

N 1.6738329 -0.6991280 0.0713139

H 2.6322011 -0.9584105 0.0820032

S -2.6198494 0.5157459 0.0281279

S 2.5336539 1.9306815 -0.2863585

C -1.6485729 -2.5001492 -0.0389884

H -2.3040339 -2.4645785 0.8235820

H -2.2715570 -2.4218843 -0.9224622

H -1.1606643 -3.4684956 -0.0534079

point 8

C -0.6204754 -1.3990006 0.0091362

C -1.0284768 0.0009881 0.0439005

C 1.3398432 0.6437061 0.1348071

C 0.7071209 -1.6754362 0.0278301

H 1.0814137 -2.6797668 0.0081097

N -0.0186879 0.9215222 0.0991789

H -0.2952255 1.8785079 0.1283613

N 1.6728479 -0.6961462 0.0828520

H 2.6316351 -0.9547686 0.0957441

S	-2.6202761	0.5163801	0.0296467
S	2.5251485	1.9169066	-0.3378996
C	-1.6482004	-2.4996238	-0.0452727
H	-2.3066048	-2.4669225	0.8152550
H	-2.2679922	-2.4190984	-0.9308599
H	-1.1602848	-3.4678665	-0.0607894

point 9

C	-0.6203867	-1.3980432	0.0098850
C	-1.0271602	-0.0006373	0.0482089
C	1.3408270	0.6464849	0.1522710
C	0.7076939	-1.6741964	0.0319167
H	1.0832855	-2.6778824	0.0104366
N	-0.0170893	0.9224081	0.1106470
H	-0.2933865	1.8794036	0.1432164
N	1.6718256	-0.6926860	0.0944308
H	2.6310543	-0.9505377	0.1096337
S	-2.6208528	0.5169859	0.0312913
S	2.5161477	1.8995728	-0.3896103
C	-1.6475683	-2.4989721	-0.0516162
H	-2.3088909	-2.4692689	0.8068682
H	-2.2641928	-2.4162038	-0.9392788
H	-1.1595209	-3.4670460	-0.0683002

point 10

C	-0.6201947	-1.3968403	0.0106077
C	-1.0259438	-0.0020895	0.0526037
C	1.3415559	0.6496869	0.1699043
C	0.7083986	-1.6725397	0.0359144
H	1.0854313	-2.6755203	0.0125776

N	-0.0157423	0.9235755	0.1221994
H	-0.2919391	1.8805273	0.1581839
N	1.6707643	-0.6887153	0.1060591
H	2.6304565	-0.9456811	0.1237108
S	-2.6215918	0.5175593	0.0330997
S	2.5066215	1.8784371	-0.4415239
C	-1.6466611	-2.4981858	-0.0580366
H	-2.3108694	-2.4716319	0.7984092
H	-2.2601521	-2.4131805	-0.9477300
H	-1.1583484	-3.4660203	-0.0759791

II. microsolvated surrounding

FC point to ${}^1n_7\pi_7^*$

point 1

C	-0.1369756	-0.7979745	-0.2804768
C	-1.1072190	0.2836126	-0.3502994
C	0.7180212	1.8905201	-0.1743053
C	1.1644186	-0.4491934	-0.1621704
H	-1.2375985	2.3242509	-0.4170036
N	1.5722092	0.8616931	-0.1083468
H	1.9584765	-1.1656713	-0.0952674
N	-0.5904525	1.5490391	-0.3157664
H	2.5587399	1.0495271	-0.0250813
S	-2.7478895	0.0355883	-0.4566094
S	1.2148427	3.5216966	-0.0841780
C	-0.5701262	-2.2385187	-0.3283219
H	-1.2328249	-2.4734327	0.4956489
H	-1.1045395	-2.4538154	-1.2455945
H	0.2937917	-2.8905177	-0.2719127
O	-4.7009097	3.0119143	0.5179796

H	-5.4048421	3.0468914	-0.1164509
H	-4.3281112	2.1403360	0.4340712
O	4.4434653	0.9709123	0.1489821
H	4.6010477	1.7004935	0.7498347
H	4.9194976	1.1867963	-0.6418916
O	4.2955142	3.3622311	1.6395437
H	3.4132093	3.5425540	1.3243966
H	4.7692384	4.1803645	1.5746753
O	-2.2507491	3.8615259	-0.6638647
H	-3.0795478	3.8518343	-0.1901612
H	-1.7129014	4.5511565	-0.2972711

point 2

C	-0.1403849	-0.7888926	-0.2680882
C	-1.1070625	0.2947238	-0.3318508
C	0.7278147	1.8967887	-0.2310266
C	1.1664058	-0.4446088	-0.1869535
H	-1.2352993	2.3345943	-0.4254817
N	1.5820535	0.8638043	-0.1632680
H	1.9576641	-1.1650049	-0.1290520
N	-0.5886681	1.5598374	-0.3285890
H	2.5702197	1.0500336	-0.1079572
S	-2.7532414	0.0494168	-0.3989666
S	1.2408339	3.5325019	-0.1223129
C	-0.5795894	-2.2285487	-0.2827635
H	-1.2235814	-2.4487650	0.5600601
H	-1.1354338	-2.4575558	-1.1839937
H	0.2832236	-2.8828611	-0.2357571
O	-4.7116957	2.9904706	0.4770455
H	-5.4035596	2.9847829	-0.1714758

H	-4.3175791	2.1254023	0.4338087
O	4.4598469	0.9938283	0.0773588
H	4.6084548	1.6925073	0.7155140
H	4.9455621	1.2480830	-0.6960691
O	4.2955910	3.3035336	1.7028030
H	3.4107521	3.5034700	1.4085776
H	4.7689991	4.1242751	1.6860860
O	-2.2532126	3.8855803	-0.6579305
H	-3.0999204	3.8514207	-0.2186448
H	-1.7504075	4.5849963	-0.2609142

point 3

C	-0.1417747	-0.7810101	-0.2555188
C	-1.1047601	0.3047319	-0.3126364
C	0.7376416	1.9006591	-0.2832422
C	1.1694322	-0.4418227	-0.2101173
H	-1.2314080	2.3436534	-0.4301976
N	1.5921180	0.8636439	-0.2147829
H	1.9576295	-1.1662939	-0.1614615
N	-0.5855034	1.5691176	-0.3382754
H	2.5812347	1.0476108	-0.1858682
S	-2.7555487	0.0626592	-0.3421233
S	1.2662686	3.5405625	-0.1532054
C	-0.5861633	-2.2192834	-0.2392709
H	-1.2116387	-2.4258237	0.6209527
H	-1.1623888	-2.4604721	-1.1245389
H	0.2753424	-2.8760394	-0.2018319
O	-4.7247919	2.9751119	0.4325912
H	-5.4005745	2.9324622	-0.2313578
H	-4.3142814	2.1166881	0.4309722

O	4.4758292	1.0204557	0.0078839
H	4.6148116	1.6887406	0.6794028
H	4.9677780	1.3117931	-0.7483471
O	4.2914455	3.2452982	1.7575394
H	3.4025104	3.4585477	1.4873730
H	4.7613063	4.0678098	1.7851677
O	-2.2534537	3.9088555	-0.6464483
H	-3.1167784	3.8510086	-0.2437319
H	-1.7864972	4.6151498	-0.2187684

point 4

C	-0.1414869	-0.7744937	-0.2427355
C	-1.1007010	0.3134135	-0.2926678
C	0.7472457	1.9022827	-0.3306525
C	1.1732262	-0.4408121	-0.2314687
H	-1.2262844	2.3513200	-0.4310881
N	1.6021430	0.8613599	-0.2625983
H	1.9581426	-1.1694538	-0.1922672
N	-0.5812992	1.5768049	-0.3447169
H	2.5916176	1.0425725	-0.2583434
S	-2.7552826	0.0748832	-0.2862880
S	1.2908211	3.5459246	-0.1761138
C	-0.5902240	-2.2110363	-0.1979361
H	-1.1975123	-2.4050485	0.6782565
H	-1.1857057	-2.4629276	-1.0675013
H	0.2698126	-2.8703014	-0.1701734
O	-4.7405048	2.9655000	0.3840054
H	-5.3964424	2.8897173	-0.2967103
H	-4.3189201	2.1135085	0.4247755
O	4.4910253	1.0504855	-0.0594019

H	4.6205989	1.6891862	0.6417078
H	4.9855835	1.3774876	-0.7991585
O	4.2855140	3.1886209	1.8040669
H	3.3910704	3.4092398	1.5608450
H	4.7492497	4.0122943	1.8720041
O	-2.2518588	3.9311658	-0.6293263
H	-3.1304557	3.8506431	-0.2654763
H	-1.8215875	4.6414773	-0.1708781

point 5

C	-0.1398536	-0.7694800	-0.2296692
C	-1.0952802	0.3205634	-0.2719313
C	0.7563674	1.9018354	-0.3730685
C	1.1775339	-0.4415140	-0.2508329
H	-1.2203185	2.3574844	-0.4281485
N	1.6118794	0.8571402	-0.3064923
H	1.9590026	-1.1743504	-0.2212537
N	-0.5764110	1.5828369	-0.3478514
H	2.6012140	1.0352877	-0.3250637
S	-2.7529281	0.0856626	-0.2315825
S	1.3141272	3.5486399	-0.1904897
C	-0.5921288	-2.2040863	-0.1587451
H	-1.1816770	-2.3868096	0.7320350
H	-1.2056943	-2.4652942	-1.0130186
H	0.2663280	-2.8658512	-0.1407136
O	-4.7589526	2.9613727	0.3306571
H	-5.3914917	2.8563630	-0.3681133
H	-4.3320041	2.1152812	0.4143361
O	4.5050488	1.0837080	-0.1247315
H	4.6262210	1.6938074	0.6024864

H	4.9984548	1.4449511	-0.8491316
O	4.2800566	3.1343127	1.8429263
H	3.3789549	3.3567600	1.6294311
H	4.7357032	3.9587443	1.9470850
O	-2.2488848	3.9522897	-0.6065599
H	-3.1413156	3.8503395	-0.2839671
H	-1.8561662	4.6638197	-0.1174338

point 6

C	-0.1371911	-0.7660547	-0.2162259
C	-1.0888983	0.3260100	-0.2503983
C	0.7647226	1.8995336	-0.4103686
C	1.1821180	-0.4438014	-0.2680413
H	-1.2139469	2.3620487	-0.4214121
N	1.6210754	0.8512350	-0.3462821
H	1.9600417	-1.1807729	-0.2482056
N	-0.5712227	1.5871788	-0.3476465
H	2.6098622	1.0261980	-0.3857987
S	-2.7489770	0.0945882	-0.1780798
S	1.3357425	3.5487837	-0.1959025
C	-0.5921967	-2.1986572	-0.1216148
H	-1.1645541	-2.3713996	0.7824327
H	-1.2226371	-2.4679202	-0.9611396
H	0.2646355	-2.8628239	-0.1133134
O	-4.7800845	2.9625010	0.2719022
H	-5.3858348	2.8322057	-0.4461118
H	-4.3538450	2.1214996	0.3986575
O	4.5174953	1.1199471	-0.1884763
H	4.6320088	1.7025048	0.5617049
H	5.0059018	1.5140422	-0.8989382

O	4.2772005	3.0829286	1.8747514
H	3.3686626	3.3021157	1.6937766
H	4.7233980	3.9078589	2.0111139
O	-2.2450849	3.9719807	-0.5782028
H	-3.1497837	3.8500742	-0.2993033
H	-1.8908229	4.6820092	-0.0587189

point 7

C	-0.1337994	-0.7642461	-0.2023002
C	-1.0819626	0.3296230	-0.2280344
C	0.7719945	1.8956382	-0.4424725
C	1.1867551	-0.4474784	-0.2829306
H	-1.2076573	2.3649346	-0.4109354
N	1.6294715	0.8439621	-0.3818084
H	1.9611228	-1.1884294	-0.2729102
N	-0.5661505	1.5898295	-0.3440893
H	2.6173847	1.0158171	-0.4403698
S	-2.7439261	0.1012754	-0.1258294
S	1.3551262	3.5464571	-0.1919901
C	-0.5907042	-2.1949089	-0.0864257
H	-1.1465131	-2.3590340	0.8296337
H	-1.2367773	-2.4711127	-0.9118617
H	0.2645388	-2.8612776	-0.0877959
O	-4.8036779	2.9686625	0.2071083
H	-5.3793610	2.8170272	-0.5311950
H	-4.3845326	2.1317151	0.3766346
O	4.5279384	1.1590036	-0.2510379
H	4.6382181	1.7150953	0.5192917
H	5.0074855	1.5845797	-0.9491772
O	4.2789411	3.0348195	1.9001735

H	3.3626640	3.2461667	1.7545931
H	4.7149392	3.8600618	2.0648676
O	-2.2411161	3.9899774	-0.5443415
H	-3.1563592	3.8497815	-0.3115714
H	-1.9262573	4.6958740	0.0049327

point 8

C	-0.1299652	-0.7640257	-0.1877883
C	-1.0748862	0.3313157	-0.2048080
C	0.7778358	1.8904511	-0.4693286
C	1.1912327	-0.4522852	-0.2953498
H	-1.2019832	2.3660888	-0.3967884
N	1.6368000	0.8356997	-0.4129327
H	1.9621344	-1.1969548	-0.2951670
N	-0.5616408	1.5908231	-0.3371816
H	2.6235876	1.0047187	-0.4886350
S	-2.7382744	0.1053726	-0.0748725
S	1.3716408	3.5417782	-0.1784344
C	-0.5878901	-2.1929377	-0.0530482
H	-1.1278784	-2.3498555	0.8738312
H	-1.2483213	-2.4751285	-0.8651608
H	0.2658913	-2.8611962	-0.0639747
O	-4.8293243	2.9796245	0.1356941
H	-5.3717202	2.8105783	-0.6237581
H	-4.4238968	2.1455263	0.3470804
O	4.5359387	1.2006108	-0.3127659
H	4.6450272	1.7312996	0.4751831
H	5.0028482	1.6562675	-1.0002890
O	4.2871084	2.9901862	1.9197537
H	3.3633558	3.1896875	1.8125397

H	4.7127778	3.8155616	2.1090965
O	-2.2377329	4.0060127	-0.5050772
H	-3.1616106	3.8493561	-0.3208278
H	-1.9632690	4.7052385	0.0731680

point 9

C	-0.1259630	-0.7653118	-0.1726003
C	-1.0680833	0.3310472	-0.1806965
C	0.7818773	1.8843075	-0.4909127
C	1.1953471	-0.4579084	-0.3051707
H	-1.1974901	2.3654858	-0.3790518
N	1.6427885	0.8268746	-0.4395434
H	1.9629846	-1.2059261	-0.3148033
N	-0.5581603	1.5902287	-0.3269408
H	2.6282639	0.9935183	-0.5304881
S	-2.7325179	0.1065708	-0.0252497
S	1.3845652	3.5348664	-0.1549573
C	-0.5839630	-2.1927773	-0.0213604
H	-1.1089353	-2.3439370	0.9152086
H	-1.2574470	-2.4801677	-0.8210092
H	0.2685853	-2.8624952	-0.0416753
O	-4.8564108	2.9951356	0.0571800
H	-5.3623089	2.8125798	-0.7240497
H	-4.4714619	2.1625712	0.3087729
O	4.5410631	1.2444074	-0.3739000
H	4.6525348	1.7507372	0.4293580
H	4.9917516	1.7286599	-1.0525005
O	4.3033080	2.9491221	1.9339381
H	3.3729805	3.1334153	1.8681271
H	4.7191451	3.7744090	2.1444543

O	-2.2357704	4.0198203	-0.4605160
H	-3.1661628	3.8486588	-0.3270876
H	-2.0027349	4.7099220	0.1456330

point 10

C	-0.1220549	-0.7679740	-0.1566685
C	-1.0619617	0.3288232	-0.1556916
C	0.7837407	1.8775666	-0.5072347
C	1.1989037	-0.4639932	-0.3122997
H	-1.1947569	2.3631311	-0.3578184
N	1.6471662	0.8179466	-0.4615674
H	1.9635958	-1.2148787	-0.3316872
N	-0.5561828	1.5881487	-0.3134047
H	2.6311994	0.9828533	-0.5658684
S	-2.7271397	0.1046145	0.0229985
S	1.3931147	3.5258232	-0.1213338
C	-0.5791069	-2.1944011	0.0087426
H	-1.0899323	-2.3412824	0.9539308
H	-1.2643135	-2.4863702	-0.7793833
H	0.2725406	-2.8650293	-0.0207471
O	-4.8841090	3.0149210	-0.0287567
H	-5.3502644	2.8227222	-0.8321119
H	-4.5264036	2.1825224	0.2605184
O	4.5429129	1.2899286	-0.4345337
H	4.6607607	1.7729287	0.3818622
H	4.9741186	1.8011608	-1.1057970
O	4.3288495	2.9116383	1.9430306
H	3.3935226	3.0780738	1.9216440
H	4.7359675	3.7365385	2.1714538
O	-2.2361214	4.0311404	-0.4107692

H	-3.1706790	3.8475241	-0.3303259
H	-2.0455816	4.7097369	0.2219771

FC point to ${}^1\pi_7\pi_8^*$

point 1

C	-0.1369756	-0.7979745	-0.2804768
C	-1.1072190	0.2836126	-0.3502994
C	0.7180212	1.8905201	-0.1743053
C	1.1644186	-0.4491934	-0.1621704
H	-1.2375985	2.3242509	-0.4170036
N	1.5722092	0.8616931	-0.1083468
H	1.9584765	-1.1656713	-0.0952674
N	-0.5904525	1.5490391	-0.3157664
H	2.5587399	1.0495271	-0.0250813
S	-2.7478895	0.0355883	-0.4566094
S	1.2148427	3.5216966	-0.0841780
C	-0.5701262	-2.2385187	-0.3283219
H	-1.2328249	-2.4734327	0.4956489
H	-1.1045395	-2.4538154	-1.2455945
H	0.2937917	-2.8905177	-0.2719127
O	-4.7009097	3.0119143	0.5179796
H	-5.4048421	3.0468914	-0.1164509
H	-4.3281112	2.1403360	0.4340712
O	4.4434653	0.9709123	0.1489821
H	4.6010477	1.7004935	0.7498347
H	4.9194976	1.1867963	-0.6418916
O	4.2955142	3.3622311	1.6395437
H	3.4132093	3.5425540	1.3243966
H	4.7692384	4.1803645	1.5746753
O	-2.2507491	3.8615259	-0.6638647

H	-3.0795478	3.8518343	-0.1901612
H	-1.7129014	4.5511565	-0.2972711

point 2

C	-0.1615945	-0.7991935	-0.2861655
C	-1.1280778	0.2772585	-0.3687867
C	0.6964771	1.8810115	-0.1743157
C	1.1446224	-0.4572150	-0.1542069
H	-1.2531491	2.3263641	-0.4270512
N	1.5528554	0.8568210	-0.0996535
H	1.9361797	-1.1747898	-0.0765449
N	-0.6078773	1.5498852	-0.3259611
H	2.5383130	1.0471154	-0.0093168
S	-2.7753083	0.0415481	-0.5020950
S	1.2033280	3.5171098	-0.0790050
C	-0.5963906	-2.2391873	-0.3369953
H	-1.2711336	-2.4701841	0.4782774
H	-1.1196084	-2.4540765	-1.2608293
H	0.2647396	-2.8938073	-0.2679287
O	-4.7024158	2.9639466	0.5020427
H	-5.4094423	2.9754370	-0.1298313
H	-4.3079141	2.1009000	0.4221955
O	4.4213062	0.9842191	0.1737706
H	4.5994401	1.7169931	0.7647303
H	4.9116397	1.1663324	-0.6166523
O	4.4156968	3.4082780	1.6349107
H	3.5441304	3.6681418	1.3487217
H	4.9576961	4.1821718	1.5612278
O	-2.2628272	3.8748245	-0.6524680
H	-3.1091273	3.8325696	-0.2133368

H -1.7637729 4.5713401 -0.2445737

point 3

C -0.1842488 -0.7996238 -0.2905324

C -1.1475167 0.2710974 -0.3852111

C 0.6754003 1.8728127 -0.1745697

C 1.1265504 -0.4636704 -0.1461968

H -1.2686326 2.3285533 -0.4353677

N 1.5345241 0.8537722 -0.0917316

H 1.9159907 -1.1818250 -0.0583906

N -0.6246695 1.5512177 -0.3348690

H 2.5188444 1.0471097 0.0045655

S -2.8008013 0.0468049 -0.5439928

S 1.1914687 3.5140881 -0.0749639

C -0.6198840 -2.2393326 -0.3435547

H -1.3056128 -2.4665835 0.4635795

H -1.1326148 -2.4543809 -1.2732476

H 0.2387371 -2.8960324 -0.2625488

O -4.7093822 2.9207651 0.4821883

H -5.4161702 2.9103945 -0.1500011

H -4.2958157 2.0654074 0.4088946

O 4.4001363 1.0011313 0.1948320

H 4.5984987 1.7365929 0.7756186

H 4.9038071 1.1496058 -0.5940977

O 4.5337538 3.4459035 1.6304122

H 3.6811864 3.7837925 1.3719796

H 5.1387111 4.1711887 1.5514760

O -2.2772937 3.8864201 -0.6383129

H -3.1387488 3.8114994 -0.2345293

H -1.8184326 4.5871055 -0.1912699

point 4

C	-0.2048606	-0.7992823	-0.2935681
C	-1.1653887	0.2652011	-0.3995040
C	0.6551495	1.8658299	-0.1750163
C	1.1103632	-0.4686855	-0.1381801
H	-1.2837049	2.3309118	-0.4418433
N	1.5174969	0.8523804	-0.0846020
H	1.8980376	-1.1869745	-0.0408862
N	-0.6405500	1.5530686	-0.3424239
H	2.5006518	1.0492507	0.0165165
S	-2.8243404	0.0515593	-0.5821602
S	1.1797867	3.5125043	-0.0720110
C	-0.6406719	-2.2389326	-0.3480097
H	-1.3363487	-2.4625903	0.4515957
H	-1.1436965	-2.4546219	-1.2828766
H	0.2157000	-2.8972485	-0.2558233
O	-4.7215893	2.8820757	0.4585472
H	-5.4249994	2.8517143	-0.1767872
H	-4.2915936	2.0334308	0.3941908
O	4.3802646	1.0212063	0.2120453
H	4.5985569	1.7589098	0.7823458
H	4.8961626	1.1362925	-0.5744745
O	4.6484417	3.4758266	1.6258919
H	3.8222702	3.8887079	1.3944521
H	5.3105813	4.1491764	1.5449399
O	-2.2937175	3.8964531	-0.6212791
H	-3.1679509	3.7888602	-0.2535638
H	-1.8762652	4.5987897	-0.1373573

point 5

C	-0.2234231	-0.7981715	-0.2952487
C	-1.1816065	0.2596717	-0.4115437
C	0.6360372	1.8599659	-0.1755099
C	1.0961495	-0.4723967	-0.1301806
H	-1.2980547	2.3335593	-0.4462453
N	1.5019985	0.8524607	-0.0782286
H	1.8823671	-1.1904598	-0.0241244
N	-0.6552815	1.5554885	-0.3484678
H	2.4839963	1.0532443	0.0265461
S	-2.8459554	0.0560751	-0.6163970
S	1.1687784	3.5122128	-0.0699588
C	-0.6589063	-2.2379419	-0.3503983
H	-1.3635103	-2.4581492	0.4423343
H	-1.1530837	-2.4546383	-1.2897744
H	0.1954478	-2.8975018	-0.2478565
O	-4.7387552	2.8474226	0.4310131
H	-5.4357226	2.7992135	-0.2103190
H	-4.2949583	2.0044303	0.3777642
O	4.3619450	1.0439358	0.2253398
H	4.5999182	1.7834726	0.7848177
H	4.8888264	1.1260010	-0.5579942
O	4.7588143	3.4988640	1.6210990
H	3.9653757	3.9824825	1.4163281
H	5.4721166	4.1179761	1.5409671
O	-2.3117111	3.9050677	-0.6010912
H	-3.1963217	3.7648543	-0.2701046
H	-1.9366950	4.6066746	-0.0826077

point 6

C	-0.2400061	-0.7962644	-0.2955293
C	-1.1961520	0.2546536	-0.4211525
C	0.6183160	1.8551403	-0.1758148
C	1.0839205	-0.4749327	-0.1222028
H	-1.3114200	2.3366532	-0.4482215
N	1.4881863	0.8538312	-0.0725191
H	1.8689418	-1.1925061	-0.0082051
N	-0.6686816	1.5585613	-0.3527530
H	2.4690721	1.0587866	0.0347208
S	-2.8657425	0.0606887	-0.6464393
S	1.1588951	3.5130718	-0.0684853
C	-0.6748264	-2.2362792	-0.3507760
H	-1.3873478	-2.4531775	0.4357841
H	-1.1611001	-2.4542064	-1.2940181
H	0.1777063	-2.8968149	-0.2387947
O	-4.7605061	2.8161549	0.3992423
H	-5.4479235	2.7525230	-0.2510192
H	-4.3054962	1.9777267	0.3589571
O	4.3453672	1.0687775	0.2346955
H	4.6028429	1.8097525	0.7830002
H	4.8818679	1.1182975	-0.5448308
O	4.8642432	3.5158670	1.6157101
H	4.1087127	4.0650616	1.4376915
H	5.6226479	4.0793949	1.5387764
O	-2.3309628	3.9124107	-0.5773479
H	-3.2235300	3.7396488	-0.2837069
H	-1.9992396	4.6109937	-0.0266031

point 7

C	-0.2547597	-0.7934896	-0.2943379
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C	-1.2090848	0.2503469	-0.4280909
C	0.6021663	1.8513091	-0.1756095
C	1.0736055	-0.4763947	-0.1142322
H	-1.3236033	2.3403993	-0.4472967
N	1.4761424	0.8563344	-0.0673289
H	1.8576382	-1.1933208	0.0067641
N	-0.6806339	1.5624192	-0.3549401
H	2.4559984	1.0655893	0.0411567
S	-2.8838734	0.0658176	-0.6719437
S	1.1505272	3.5149649	-0.0671445
C	-0.6887580	-2.2338148	-0.3492033
H	-1.4081886	-2.4475525	0.4319302
H	-1.1681668	-2.4530304	-1.2956895
H	0.1621100	-2.8951722	-0.2288155
O	-4.7863302	2.7873947	0.3626548
H	-5.4609247	2.7110405	-0.2995845
H	-4.3225903	1.9524774	0.3367760
O	4.3306499	1.0951882	0.2401319
H	4.6075381	1.8371952	0.7769076
H	4.8752975	1.1127353	-0.5351292
O	4.9644140	3.5276623	1.6093504
H	4.2507931	4.1366749	1.4585194
H	5.7619975	4.0351046	1.5375029
O	-2.3512675	3.9186290	-0.5495493
H	-3.2493489	3.7133714	-0.2938661
H	-2.0635629	4.6119352	0.0312264

point 8

C	-0.2679172	-0.7897196	-0.2915693
C	-1.2205487	0.2470160	-0.4320476

C	0.5876864	1.8484808	-0.1744893
C	1.0650488	-0.4768405	-0.1062388
H	-1.3344855	2.3450585	-0.4428634
N	1.4658667	0.8598565	-0.0624682
H	1.8482475	-1.1930754	0.0206600
N	-0.6910983	1.5672532	-0.3545933
H	2.4448120	1.0734022	0.0460075
S	-2.9006034	0.0719647	-0.6924651
S	1.1439892	3.5178201	-0.0653731
C	-0.7011128	-2.2303607	-0.3457361
H	-1.4264304	-2.4411039	0.4307692
H	-1.1748057	-2.4507352	-1.2948613
H	0.1482068	-2.8925075	-0.2181224
O	-4.8155150	2.7600173	0.3204416
H	-5.4737175	2.6739015	-0.3569499
H	-4.3453211	1.9276644	0.3099008
O	4.3178350	1.1226545	0.2416886
H	4.6141491	1.8652514	0.7665838
H	4.8690566	1.1088860	-0.5290229
O	5.0592971	3.5349994	1.6016132
H	4.3904799	4.1977552	1.4786896
H	5.8904150	3.9865607	1.5362393
O	-2.3725545	3.9238678	-0.5171264
H	-3.2736707	3.6861070	-0.3000671
H	-2.1295239	4.6096396	0.0915595

point 9

C	-0.2797942	-0.7847683	-0.2870829
C	-1.2307769	0.2449871	-0.4326301
C	0.5748820	1.8467244	-0.1719681

C	1.0580103	-0.4762752	-0.0981853
H	-1.3440407	2.3509410	-0.4341674
N	1.4572714	0.8643391	-0.0577098
H	1.8404796	-1.1918920	0.0333294
N	-0.7001204	1.5733138	-0.3511733
H	2.4354611	1.0820312	0.0494508
S	-2.9162767	0.0797077	-0.7074328
S	1.1395021	3.5216199	-0.0624939
C	-0.7123798	-2.2256713	-0.3404214
H	-1.4425264	-2.4336203	0.4323187
H	-1.1816381	-2.4468672	-1.2915900
H	0.1354693	-2.8887009	-0.2069476
O	-4.8470740	2.7326656	0.2715840
H	-5.4848826	2.6399902	-0.4242280
H	-4.3723570	1.9021138	0.2767183
O	4.3068809	1.1507214	0.2394014
H	4.6227484	1.8934047	0.7520787
H	4.8630067	1.1063728	-0.5266582
O	5.1490933	3.5385155	1.5920762
H	4.5269911	4.2488543	1.4979977
H	6.0084825	3.9349534	1.5340714
O	-2.3949048	3.9282625	-0.4794732
H	-3.2965087	3.6578992	-0.3018385
H	-2.1972130	4.6041917	0.1551325

point 10

C	-0.2907793	-0.7784094	-0.2807071
C	-1.2400913	0.2446206	-0.4293617
C	0.5636524	1.8461582	-0.1674816
C	1.0521719	-0.4746567	-0.0900394

H	-1.3523531	2.3583736	-0.4202980
N	1.4501754	0.8697774	-0.0528002
H	1.8339761	-1.1898420	0.0445700
N	-0.7078423	1.5808879	-0.3440337
H	2.4277970	1.0913461	0.0516723
S	-2.9313270	0.0896568	-0.7161349
S	1.1371659	3.5263955	-0.0577189
C	-0.7231053	-2.2194654	-0.3333022
H	-1.4569585	-2.4248809	0.4366156
H	-1.1893669	-2.4409168	-1.2859177
H	0.1233220	-2.8835923	-0.1955636
O	-4.8796670	2.7038331	0.2148957
H	-5.4925174	2.6080301	-0.5026112
H	-4.4018529	1.8745764	0.2354009
O	4.2976518	1.1790203	0.2332798
H	4.6333167	1.9212014	0.7334268
H	4.8569153	1.1049096	-0.5282159
O	5.2341506	3.5387231	1.5803168
H	4.6598496	4.2905742	1.5161795
H	6.1169897	3.8812003	1.5301068
O	-2.4185491	3.9319247	-0.4359848
H	-3.3179797	3.6287618	-0.2988075
H	-2.2669593	4.5956065	0.2226728

$1\pi_7\pi_8^*$ to $1n_8\pi_8^*$

point 1

C	-0.2907794	-0.7784096	-0.2807072
C	-1.2400916	0.2446207	-0.4293618
C	0.5636526	1.8461587	-0.1674816
C	1.0521722	-0.4746568	-0.0900394

H	-1.3523535	2.3583743	-0.4202981
N	1.4501758	0.8697776	-0.0528002
H	1.8339766	-1.1898423	0.0445700
N	-0.7078425	1.5808883	-0.3440338
H	2.4277977	1.0913464	0.0516723
S	-2.9313278	0.0896568	-0.7161351
S	1.1371662	3.5263965	-0.0577189
C	-0.7231055	-2.2194660	-0.3333023
H	-1.4569589	-2.4248816	0.4366157
H	-1.1893672	-2.4409175	-1.2859181
H	0.1233220	-2.8835931	-0.1955637
O	-4.8796684	2.7038339	0.2148958
H	-5.4925189	2.6080308	-0.5026113
H	-4.4018541	1.8745769	0.2354010
O	4.2976530	1.1790206	0.2332799
H	4.6333180	1.9212019	0.7334270
H	4.8569167	1.1049099	-0.5282160
O	5.2341521	3.5387241	1.5803172
H	4.6598509	4.2905754	1.5161799
H	6.1169914	3.8812014	1.5301072
O	-2.4185498	3.9319258	-0.4359849
H	-3.3179806	3.6287628	-0.2988076
H	-2.2669599	4.5956078	0.2226729

point 2

C	-0.2746579	-0.7990895	-0.3011104
C	-1.2168961	0.2256463	-0.4692484
C	0.5774614	1.8336509	-0.1930990
C	1.0645740	-0.4906177	-0.0927871
H	-1.3374742	2.3367848	-0.4772158

N	1.4595198	0.8548924	-0.0586760
H	1.8454690	-1.2037362	0.0573201
N	-0.6935438	1.5612738	-0.3863789
H	2.4353624	1.0762324	0.0585990
S	-2.9088686	0.0656478	-0.7801563
S	1.1402248	3.5122524	-0.0913573
C	-0.7068460	-2.2406107	-0.3515672
H	-1.4520187	-2.4429068	0.4085783
H	-1.1563176	-2.4700687	-1.3105889
H	0.1371886	-2.9035023	-0.1958343
O	-4.8522168	2.7848818	0.3661473
H	-5.5037046	2.7287710	-0.3210957
H	-4.4061304	1.9389757	0.3490250
O	4.3101012	1.1552634	0.2672101
H	4.6182175	1.9050707	0.7740963
H	4.8694085	1.1062886	-0.4962432
O	5.1356561	3.5587531	1.6065800
H	4.5101772	4.2648447	1.5024309
H	5.9936344	3.9565339	1.5377270
O	-2.4056636	3.9077742	-0.5313509
H	-3.2942514	3.6399066	-0.2932142
H	-2.1706185	4.5909107	0.0823683

point 3

C	-0.2562370	-0.8231896	-0.3210302
C	-1.1926330	0.2019274	-0.5074554
C	0.5900807	1.8187669	-0.2174186
C	1.0786979	-0.5081789	-0.0957116
H	-1.3241513	2.3101126	-0.5314582
N	1.4688020	0.8388990	-0.0643102

H	1.8595236	-1.2181508	0.0690831
N	-0.6798917	1.5375105	-0.4268231
H	2.4424403	1.0613679	0.0653487
S	-2.8849274	0.0345760	-0.8417104
S	1.1400529	3.4962914	-0.1233428
C	-0.6863536	-2.2657318	-0.3698945
H	-1.4420220	-2.4664088	0.3805976
H	-1.1191086	-2.5033199	-1.3348578
H	0.1560010	-2.9262022	-0.1970187
O	-4.8126284	2.8862253	0.5159124
H	-5.4969005	2.8721479	-0.1411787
H	-4.4091659	2.0210771	0.4708489
O	4.3216278	1.1343280	0.3002959
H	4.6004198	1.8917671	0.8131969
H	4.8798405	1.1122033	-0.4651781
O	5.0249220	3.5797712	1.6297306
H	4.3491799	4.2314538	1.4857166
H	5.8523283	4.0342284	1.5411620
O	-2.3964586	3.8762333	-0.6224228
H	-3.2654784	3.6522167	-0.2888408
H	-2.0801734	4.5739020	-0.0630818

point 4

C	-0.2355706	-0.8502657	-0.3403538
C	-1.1675178	0.1739354	-0.5434260
C	0.6012407	1.8019754	-0.2399624
C	1.0945288	-0.5268931	-0.0989565
H	-1.3127796	2.2788041	-0.5819768
N	1.4779043	0.8222513	-0.0696519
H	1.8762337	-1.2326418	0.0793731

N	-0.6671811	1.5100503	-0.4646374
H	2.4489472	1.0472208	0.0717752
S	-2.8598020	-0.0031030	-0.8998554
S	1.1362741	3.4789629	-0.1529594
C	-0.6615784	-2.2944016	-0.3883696
H	-1.4267357	-2.4951997	0.3527620
H	-1.0778989	-2.5399919	-1.3587936
H	0.1799242	-2.9512770	-0.1995498
O	-4.7597076	3.0068623	0.6622166
H	-5.4699405	3.0359414	0.0335464
H	-4.4078055	2.1213761	0.6003682
O	4.3322696	1.1167471	0.3319037
H	4.5799884	1.8815499	0.8502066
H	4.8878441	1.1233802	-0.4357621
O	4.9014798	3.6004584	1.6496760
H	4.1775335	4.1885384	1.4665266
H	5.6918915	4.1124531	1.5402790
O	-2.3915552	3.8377198	-0.7075389
H	-3.2326762	3.6652247	-0.2853440
H	-1.9975239	4.5441459	-0.2113371

point 5

C	-0.2126835	-0.8797882	-0.3589364
C	-1.1417470	0.1422325	-0.5765783
C	0.6107003	1.7838134	-0.2602670
C	1.1120905	-0.5462415	-0.1026515
H	-1.3037395	2.2433900	-0.6277240
N	1.4867482	0.8054656	-0.0746604
H	1.8957393	-1.2466969	0.0877190
N	-0.6556868	1.4794264	-0.4990891

H	2.4548462	1.0343102	0.0777046
S	-2.8337863	-0.0468278	-0.9535980
S	1.1285387	3.4607781	-0.1795327
C	-0.6324440	-2.3260963	-0.4070165
H	-1.4058871	-2.5289687	0.3252455
H	-1.0328448	-2.5793213	-1.3824126
H	0.2091597	-2.9782210	-0.2037984
O	-4.6925926	3.1455908	0.8028937
H	-5.4215559	3.2173694	0.1993454
H	-4.3990431	2.2402593	0.7365386
O	4.3421299	1.1030847	0.3613297
H	4.5570720	1.8746836	0.8845585
H	4.8930871	1.1405347	-0.4087738
O	4.7650775	3.6192274	1.6664427
H	3.9963759	4.1341666	1.4454468
H	5.5113556	4.1889446	1.5351859
O	-2.3915803	3.7927422	-0.7850455
H	-3.1969684	3.6784279	-0.2822564
H	-1.9245748	4.5015381	-0.3599110

point 6

C	-0.1875826	-0.9111407	-0.3766112
C	-1.1154995	0.1074674	-0.6063245
C	0.6182502	1.7648785	-0.2778960
C	1.1314339	-0.5656328	-0.1069157
H	-1.2973870	2.2044751	-0.6676784
N	1.4952887	0.7891167	-0.0793087
H	1.9182091	-1.2597322	0.0936680
N	-0.6456587	1.4462458	-0.5294607
H	2.4601411	1.0232025	0.0829380

S	-2.8071691	-0.0959356	-1.0019221
S	1.1165344	3.4422965	-0.2024440
C	-0.5988656	-2.3601904	-0.4258068
H	-1.3791830	-2.5672699	0.2982923
H	-0.9841152	-2.6204621	-1.4056863
H	0.2439219	-3.0064306	-0.2100753
O	-4.6108267	3.3010286	0.9355888
H	-5.3514735	3.4131174	0.3524968
H	-4.3801087	2.3779444	0.8778055
O	4.3513694	1.0939330	0.3878143
H	4.5318995	1.8714374	0.9156570
H	4.8952705	1.1643540	-0.3850053
O	4.6157671	3.6342158	1.6802046
H	3.8074024	4.0664138	1.4231447
H	5.3100970	4.2609774	1.5262800
O	-2.3971469	3.7418809	-0.8533315
H	-3.1595863	3.6913166	-0.2790216
H	-1.8631957	4.4463164	-0.5062433

point 7

C	-0.1602691	-0.9436285	-0.3932017
C	-1.0889403	0.0703621	-0.6320874
C	0.6237120	1.7458130	-0.2924447
C	1.1526209	-0.5844106	-0.1118623
H	-1.2940451	2.1627180	-0.7008589
N	1.5035057	0.7738278	-0.0835846
H	1.9438177	-1.2710955	0.0967843
N	-0.6373201	1.4111729	-0.5550623
H	2.4648647	1.0145023	0.0872560
S	-2.7802324	-0.1496778	-1.0438148

S	1.0999918	3.4241062	-0.2211291
C	-0.5607691	-2.3959612	-0.4446771
H	-1.3463308	-2.6095232	0.2721901
H	-0.9319082	-2.6624943	-1.4285569
H	0.2844118	-3.0352045	-0.2186447
O	-4.5144247	3.4716548	1.0577456
H	-5.2604866	3.6194195	0.4894299
H	-4.3485488	2.5344640	1.0221289
O	4.3601869	1.0899050	0.4105591
H	4.5047682	1.8720796	0.9428970
H	4.8941195	1.1954786	-0.3652352
O	4.4540045	3.6432932	1.6913085
H	3.6129483	3.9834687	1.4003452
H	5.0879954	4.3253613	1.5142897
O	-2.4088317	3.6857583	-0.9108446
H	-3.1218717	3.7033883	-0.2750179
H	-1.8151818	4.3790458	-0.6477535

point 8

C	-0.1307546	-0.9764946	-0.4085394
C	-1.0622252	0.0316913	-0.6533172
C	0.6269347	1.7272815	-0.3035370
C	1.1757047	-0.6018682	-0.1176070
H	-1.2939951	2.1188051	-0.7263295
N	1.5113900	0.7602514	-0.0874884
H	1.9727175	-1.2800791	0.0966400
N	-0.6308667	1.3749057	-0.5752363
H	2.4690619	1.0088337	0.0904287
S	-2.7532485	-0.2072417	-1.0782928
S	1.0786889	3.4067959	-0.2350622

C	-0.5181140	-2.4326016	-0.4635578
H	-1.3070619	-2.6550278	0.2472305
H	-0.8764699	-2.7044366	-1.4509644
H	0.3307870	-3.0637533	-0.2297527
O	-4.4039322	3.6558648	1.1665763
H	-5.1504936	3.8321747	0.6068494
H	-4.3022912	2.7096956	1.1670041
O	4.3687936	1.0916190	0.4287486
H	4.4760260	1.8768614	0.9656903
H	4.8893725	1.2344792	-0.3501957
O	4.2807581	3.6440888	1.7002954
H	3.4160441	3.8837673	1.3777970
H	4.8456147	4.3784725	1.5003091
O	-2.4271530	3.6250038	-0.9560895
H	-3.0852839	3.7141443	-0.2695655
H	-1.7822168	4.3005907	-0.7818752

point 9

C	-0.0990791	-1.0089443	-0.4224882
C	-1.0355065	-0.0077437	-0.6695080
C	0.6277901	1.7099393	-0.3108112
C	1.2007063	-0.6172754	-0.1242795
H	-1.2974682	2.0734200	-0.7431913
N	1.5189265	0.7490406	-0.0910249
H	2.0050056	-1.2859451	0.0928002
N	-0.6264662	1.3381472	-0.5893560
H	2.4727689	1.0068114	0.0922323
S	-2.7264771	-0.2677751	-1.1044325
S	1.0524535	3.3909214	-0.2437178
C	-0.4709180	-2.4692416	-0.4824180

H	-1.2611588	-2.7029885	0.2236499
H	-0.8181140	-2.7452612	-1.4728899
H	0.3831261	-3.0912199	-0.2436750
O	-4.2804688	3.8520341	1.2590067
H	-5.0244982	4.0470738	0.7018526
H	-4.2396743	2.9034482	1.3094695
O	4.3773804	1.0996696	0.4415814
H	4.4460480	1.8859871	0.9835036
H	4.8807680	1.2818270	-0.3405298
O	4.0976194	3.6340427	1.7079169
H	3.2204234	3.7661524	1.3562298
H	4.5843959	4.4163336	1.4858214
O	-2.4525432	3.5602166	-0.9876045
H	-3.0514098	3.7230686	-0.2619085
H	-1.7658431	4.2120847	-0.9060703

point 10

C	-0.0653303	-1.0401780	-0.4349753
C	-1.0089386	-0.0471474	-0.6802155
C	0.6261675	1.6943952	-0.3138908
C	1.2275887	-0.6299144	-0.1320378
H	-1.3046349	2.0272099	-0.7505613
N	1.5260761	0.7408110	-0.0941885
H	2.0406886	-1.2879636	0.0848006
N	-0.6242584	1.3015710	-0.5968130
H	2.4759900	1.0090000	0.0924765
S	-2.7001607	-0.3304126	-1.1214050
S	1.0211662	3.3769636	-0.2465056
C	-0.4192841	-2.5049784	-0.5013290
H	-1.2084836	-2.7525561	0.2015491

H	-0.7572420	-2.7839105	-1.4944197
H	0.4413932	-3.1167116	-0.2607876
O	-4.1457428	4.0585885	1.3315804
H	-4.8865627	4.2597200	0.7720443
H	-4.1594103	3.1156214	1.4460882
O	4.3860809	1.1145845	0.4483140
H	4.4152106	1.8995663	0.9959116
H	4.8680326	1.3378582	-0.3367340
O	3.9068954	3.6104856	1.7151451
H	3.0304613	3.6300442	1.3363055
H	4.3068352	4.4347486	1.4727081
O	-2.4853193	3.4919302	-1.0039148
H	-3.0219795	3.7295832	-0.2511582
H	-1.7674523	4.1149151	-1.0178287

III. aqueous solution

Snapshot1

FC point to ${}^1n_7\pi_7^*$

point 1

C	-0.143000013	-0.807000057	-0.157000010
C	-1.103000082	0.289000021	-0.158000013
C	0.743000053	1.851001135	0.155000012
C	1.163000082	-0.483000036	-0.027000004
H	-1.207000086	2.324001166	-0.030000000
N	1.591000112	0.810000058	0.110000006
H	1.947000138	-1.214000090	-0.031000002
N	-0.572000039	1.533000111	0.011000002
H	2.583001186	0.994000073	0.104000009
S	-2.733001198	0.063000007	-0.346000025
S	1.252000091	3.460001249	0.381000026

C	-0.599000044	-2.232001161	-0.294000021
H	-1.228000088	-2.520001179	0.540000040
H	-1.182000085	-2.367001172	-1.195000087
H	0.254000021	-2.900001208	-0.328000024
O	-4.862001351	2.949001212	-0.097000005
H	-5.267002380	2.918001209	-0.954000067
H	-4.444001321	2.101001153	0.013000001
O	4.438001319	1.113000082	-0.243000018
H	4.692001340	1.800000127	0.375000029
H	4.651001337	1.449000102	-1.102000080
O	4.501001326	3.321001239	1.496000106
H	3.567001259	3.470001249	1.377000097
H	4.921001355	4.159001298	1.362000097
O	-2.133001152	3.833001278	-0.295000023
H	-3.078001221	3.831001274	-0.160000012
H	-1.761000129	4.571001332	0.166000014

point 2

C	-0.149382012	-0.814342058	-0.157221011
C	-1.103149077	0.285284022	-0.162836010
C	0.749726055	1.840458130	0.124663010
C	1.159347082	-0.496600034	-0.030675003
H	-1.201388087	2.321076165	-0.048340003
N	1.595394114	0.794417058	0.096941007
H	1.938520141	-1.232417088	-0.031230004
N	-0.569885040	1.528963108	-0.003883002
H	2.586973185	0.973190072	0.079530006
S	-2.737860198	0.065048002	-0.346938024
S	1.265536091	3.449560248	0.388100028
C	-0.612236042	-2.237800160	-0.285032022

H	-1.240795091	-2.519393181	0.551379039
H	-1.196650088	-2.376292170	-1.184636087
H	0.237729016	-2.909642209	-0.316495023
O	-4.854348348	2.956623211	-0.102401005
H	-5.258083378	2.916096208	-0.959136071
H	-4.448293319	2.107051151	0.023416003
O	4.445590319	1.116866082	-0.252301018
H	4.694655338	1.804055128	0.366888027
H	4.678380338	1.444625103	-1.107261081
O	4.513100323	3.323100237	1.499900106
H	3.570052257	3.449338248	1.445739105
H	4.896690354	4.172518300	1.332100096
O	-2.123274154	3.844572279	-0.297167020
H	-3.068517222	3.830226278	-0.170762011
H	-1.767316130	4.580525331	0.176016011

point 3

C	-0.155764011	-0.821683058	-0.157441011
C	-1.103297077	0.281568023	-0.167673013
C	0.756452056	1.829916131	0.094326009
C	1.155693081	-0.510200037	-0.034350001
H	-1.195776088	2.318150169	-0.066680006
N	1.599787116	0.778834058	0.083882008
H	1.930039139	-1.250834091	-0.031461000
N	-0.567769040	1.524925109	-0.018766001
H	2.590945184	0.952379070	0.055060004
S	-2.742720199	0.067097003	-0.347876028
S	1.279072090	3.439119248	0.395199026
C	-0.625471046	-2.243600160	-0.276064018
H	-1.253590089	-2.518785183	0.562758038

H	-1.211299085	-2.385584173	-1.174271087
H	0.221457017	-2.919284210	-0.304989021
O	-4.846694349	2.964246216	-0.107802010
H	-5.249165376	2.914191207	-0.964272070
H	-4.452584322	2.113102150	0.033832000
O	4.453178318	1.120731081	-0.261602017
H	4.697309337	1.808110128	0.358777026
H	4.705759340	1.440249103	-1.112522081
O	4.525300325	3.325200240	1.503900109
H	3.578800255	3.426800245	1.517600111
H	4.873800353	4.183000302	1.300500091
O	-2.113547151	3.856144279	-0.299333022
H	-3.059034222	3.829451277	-0.181524016
H	-1.773632130	4.590048331	0.186032013

point 4

C	-0.162145010	-0.829024059	-0.157662011
C	-1.103445078	0.277853018	-0.172510010
C	0.763178053	1.819374132	0.063989002
C	1.152039080	-0.523801036	-0.038025005
H	-1.190163084	2.315225168	-0.085020009
N	1.604181113	0.763251053	0.070823003
H	1.921558137	-1.269250089	-0.031691002
N	-0.565654040	1.520888111	-0.033649000
H	2.594917189	0.931569069	0.030590001
S	-2.747579200	0.069145003	-0.348814026
S	1.292609095	3.428679247	0.402299029
C	-0.638706044	-2.249400159	-0.267095020
H	-1.266385092	-2.518178180	0.574137042
H	-1.225949087	-2.394876171	-1.163907081

H	0.205185012	-2.928925211	-0.293483020
O	-4.839041351	2.971868215	-0.113204010
H	-5.240246380	2.912285211	-0.969409068
H	-4.456875320	2.119152154	0.044248002
O	4.460767323	1.124597081	-0.270903021
H	4.699963341	1.812165129	0.350665024
H	4.733137341	1.435874104	-1.117784082
O	4.537400328	3.327300237	1.507800108
H	3.592100257	3.403100243	1.591400112
H	4.845300348	4.191100301	1.267500090
O	-2.103821154	3.867716280	-0.301500024
H	-3.049550218	3.828676276	-0.192286015
H	-1.779947130	4.599572331	0.196047015

point 5

C	-0.168527010	-0.836366060	-0.157883012
C	-1.103593078	0.274137019	-0.177346013
C	0.769903054	1.808831132	0.033651000
C	1.148385085	-0.537401039	-0.041700003
H	-1.184551085	2.312300168	-0.103360006
N	1.608574115	0.747668053	0.057765004
H	1.913077140	-1.287667093	-0.031921004
N	-0.563538040	1.516850108	-0.048532004
H	2.598889188	0.910758068	0.006118998
S	-2.752439196	0.071194004	-0.349752024
S	1.306145095	3.418238247	0.409398032
C	-0.651941047	-2.255200164	-0.258127021
H	-1.279180090	-2.517570181	0.585515041
H	-1.240598089	-2.404168174	-1.153542081
H	0.188914013	-2.938566212	-0.281978019

O	-4.831387347	2.979491214	-0.118605010
H	-5.231328378	2.910380210	-0.974545072
H	-4.461167323	2.125203153	0.054665005
O	4.468356323	1.128462080	-0.280204021
H	4.702617339	1.816220130	0.342553023
H	4.760516342	1.431499104	-1.123045083
O	4.549600329	3.329400240	1.511700107
H	3.610500258	3.378400244	1.666300119
H	4.807500344	4.193500300	1.235800086
O	-2.094094151	3.879287280	-0.303666020
H	-3.040067219	3.827901274	-0.203048015
H	-1.786263130	4.609095331	0.206063012

point 6

C	-0.174909014	-0.843707061	-0.158103012
C	-1.103741078	0.270421020	-0.182182011
C	0.776629056	1.798289128	0.003313999
C	1.144731084	-0.551001037	-0.045375002
H	-1.178938086	2.309375167	-0.121700009
N	1.612968117	0.732085053	0.044706005
H	1.904596138	-1.306084096	-0.032152000
N	-0.561423040	1.512812110	-0.063415003
H	2.602862187	0.889948067	-0.018350999
S	-2.757299197	0.073243005	-0.350690023
S	1.319681094	3.407797246	0.416498029
C	-0.665177046	-2.260999164	-0.249159017
H	-1.291975093	-2.516963183	0.596894045
H	-1.255248091	-2.413459172	-1.143177081
H	0.172642014	-2.948208213	-0.270472017
O	-4.823733348	2.987113213	-0.124006010

H	-5.222410376	2.908475209	-0.979681071
H	-4.465458321	2.131254152	0.065081007
O	4.475944323	1.132328080	-0.289505020
H	4.705271338	1.820274130	0.334442022
H	4.787895343	1.427123105	-1.128306079
O	4.561700327	3.331500238	1.515700111
H	3.636900260	3.353100242	1.740400127
H	4.769800344	4.195700301	1.203800087
O	-2.084367148	3.890858280	-0.305833022
H	-3.030583219	3.827126273	-0.213810014
H	-1.792579131	4.618619330	0.216079015

point 7

C	-0.181291014	-0.851048062	-0.158324012
C	-1.103890079	0.266705021	-0.187019013
C	0.783355057	1.787747129	-0.027023002
C	1.141077084	-0.564601041	-0.049050005
H	-1.173326082	2.306450166	-0.140040012
N	1.617361114	0.716502053	0.031647001
H	1.896116136	-1.324500094	-0.032382002
N	-0.559307040	1.508775107	-0.078298008
H	2.606834186	0.869137060	-0.042821002
S	-2.762158197	0.075291006	-0.351628027
S	1.333217093	3.397356246	0.423597032
C	-0.678412049	-2.266799163	-0.240191019
H	-1.304770096	-2.516355180	0.608273044
H	-1.269897093	-2.422751175	-1.132813081
H	0.156371009	-2.957849214	-0.258966021
O	-4.816080344	2.994736218	-0.129408010
H	-5.213492374	2.906570208	-0.984817069

H	-4.469749324	2.137304151	0.075497004
O	4.483533322	1.136193079	-0.298806019
H	4.707925336	1.824329131	0.326330025
H	4.815273349	1.422748100	-1.133567080
O	4.573900329	3.333600240	1.519600110
H	3.669200266	3.327800241	1.812600129
H	4.725500339	4.197600302	1.173500086
O	-2.074641151	3.902430281	-0.307999024
H	-3.021100215	3.826351277	-0.224573014
H	-1.798894131	4.628142335	0.226095017

point 8

C	-0.187673013	-0.858390063	-0.158545012
C	-1.104038079	0.262989017	-0.191855016
C	0.790081059	1.777205129	-0.057360004
C	1.137424083	-0.578201039	-0.052725004
H	-1.167714083	2.303525165	-0.158380009
N	1.621754116	0.700919053	0.018588002
H	1.887635134	-1.342917098	-0.032612003
N	-0.557192041	1.504737109	-0.093182007
H	2.610806186	0.848326059	-0.067291004
S	-2.767018198	0.077340006	-0.352566025
S	1.346753098	3.386915245	0.430697030
C	-0.691648047	-2.272599163	-0.231223015
H	-1.317565094	-2.515748182	0.619652043
H	-1.284547090	-2.432043173	-1.122448081
H	0.140099010	-2.967490215	-0.247461020
O	-4.808426346	3.002358217	-0.134809010
H	-5.204573377	2.904665207	-0.989953073
H	-4.474041322	2.143355155	0.085913006

O	4.491121322	1.140059084	-0.308107024
H	4.710579340	1.828384131	0.318218024
H	4.842652350	1.418372101	-1.138828080
O	4.586000331	3.335700238	1.523600108
H	3.702900268	3.303000238	1.883000134
H	4.679200336	4.195100304	1.146800083
O	-2.064914148	3.914001281	-0.310166021
H	-3.011616215	3.825576276	-0.235335018
H	-1.805210131	4.637666335	0.236111014

point 9

C	-0.194055012	-0.865731064	-0.158765012
C	-1.104186079	0.259274018	-0.196692014
C	0.796806055	1.766662125	-0.087697005
C	1.133770083	-0.591802043	-0.056400002
H	-1.162101084	2.300600164	-0.176720012
N	1.626148118	0.685336048	0.005529003
H	1.879154137	-1.361334096	-0.032843005
N	-0.555077041	1.500700111	-0.108065006
H	2.614778190	0.827516058	-0.091761007
S	-2.771877199	0.079388007	-0.353504023
S	1.360289098	3.376475245	0.437796032
C	-0.704883051	-2.278399163	-0.222254016
H	-1.330360097	-2.515140178	0.631030047
H	-1.299196092	-2.441334176	-1.112084081
H	0.123828011	-2.977132216	-0.235955018
O	-4.800772347	3.009981217	-0.140210010
H	-5.195655375	2.902760211	-0.995089072
H	-4.478332320	2.149405154	0.096329008
O	4.498710322	1.143924084	-0.317408023

H	4.713233338	1.832438132	0.310106023
H	4.870031351	1.413997101	-1.144089081
O	4.598100329	3.337700242	1.527500112
H	3.744900267	3.279400234	1.948000140
H	4.623100335	4.191000303	1.126800083
O	-2.055188146	3.925573281	-0.312333023
H	-3.002133216	3.824801275	-0.246097018
H	-1.811526132	4.647189335	0.246126017

point 10

C	-0.200436017	-0.873072064	-0.158986013
C	-1.104334079	0.255558019	-0.201528016
C	0.803532057	1.756120125	-0.118035007
C	1.130116082	-0.605402046	-0.060075006
H	-1.156489085	2.297674163	-0.195060015
N	1.630541115	0.669753048	-0.007530002
H	1.870673135	-1.379750099	-0.033073001
N	-0.552961041	1.496662107	-0.122948010
H	2.618750189	0.806705056	-0.116231010
S	-2.776737200	0.081436008	-0.354442027
S	1.373825097	3.366034244	0.444896030
C	-0.718118054	-2.284198162	-0.213286017
H	-1.343155095	-2.514533180	0.642409046
H	-1.313846095	-2.450626174	-1.101719081
H	0.107556006	-2.986773217	-0.224449017
O	-4.793119344	3.017603216	-0.145611010
H	-5.186737373	2.900854210	-1.000225070
H	-4.482623323	2.155456153	0.106745010
O	4.506298327	1.147790083	-0.326709022
H	4.715887337	1.836493132	0.301995021

H	4.897410353	1.409622102	-1.149350082
O	4.610288334	3.339839240	1.531428110
H	3.792351274	3.257206234	2.006956142
H	4.568689330	4.189183304	1.107968077
O	-2.045461148	3.937144282	-0.314499025
H	-2.992649217	3.824026273	-0.256859017
H	-1.817841132	4.656713335	0.256142019

FC point to ${}^1\pi_7\pi_8^*$

point 1

C	-0.143000013	-0.807000057	-0.157000010
C	-1.103000082	0.289000021	-0.158000013
C	0.743000053	1.851001135	0.155000012
C	1.163000082	-0.483000036	-0.027000004
H	-1.207000086	2.324001166	-0.030000000
N	1.591000112	0.810000058	0.110000006
H	1.947000138	-1.214000090	-0.031000002
N	-0.572000039	1.533000111	0.011000002
H	2.583001186	0.994000073	0.104000009
S	-2.733001198	0.063000007	-0.346000025
S	1.252000091	3.460001249	0.381000026
C	-0.599000044	-2.232001161	-0.294000021
H	-1.228000088	-2.520001179	0.540000040
H	-1.182000085	-2.367001172	-1.195000087
H	0.254000021	-2.900001208	-0.328000024
O	-4.862001351	2.949001212	-0.097000005
H	-5.267002380	2.918001209	-0.954000067
H	-4.444001321	2.101001153	0.013000001
O	4.438001319	1.113000082	-0.243000018
H	4.692001340	1.800000127	0.375000029

H	4.651001337	1.449000102	-1.102000080
O	4.501001326	3.321001239	1.496000106
H	3.567001259	3.470001249	1.377000097
H	4.921001355	4.159001298	1.362000097
O	-2.133001152	3.833001278	-0.295000023
H	-3.078001221	3.831001274	-0.160000012
H	-1.761000129	4.571001332	0.166000014

point 2

C	-0.149928012	-0.811305057	-0.156993009
C	-1.109461082	0.278160021	-0.160228013
C	0.735902051	1.839565133	0.151023012
C	1.160965083	-0.492668035	-0.024306000
H	-1.209196087	2.321607168	-0.030227001
N	1.588214116	0.804435061	0.110702007
H	1.944393141	-1.223685087	-0.025184000
N	-0.574991039	1.530259110	0.009447999
H	2.579441183	0.991525074	0.103939006
S	-2.746128196	0.063641004	-0.350032023
S	1.254045091	3.454441247	0.376701027
C	-0.605624041	-2.236407159	-0.293780021
H	-1.234531088	-2.523172184	0.540655040
H	-1.190057084	-2.369837171	-1.194011086
H	0.246696020	-2.905536212	-0.328657024
O	-4.843961350	2.940237211	-0.100945005
H	-5.252951380	2.900581208	-0.955174068
H	-4.425426316	2.092450151	0.014394002
O	4.432340318	1.125597083	-0.236255019
H	4.693014338	1.815145133	0.374973025
H	4.668244335	1.436366101	-1.093471081

O	4.518698325	3.342367242	1.492308106
H	3.593819258	3.520497252	1.379962098
H	4.959598358	4.161909302	1.404096100
O	-2.126491155	3.840625278	-0.294127023
H	-3.070607223	3.815424275	-0.174919010
H	-1.784373126	4.578845331	0.179987015

point 3

C	-0.156856011	-0.815610056	-0.156986014
C	-1.115922082	0.267320020	-0.162457013
C	0.728803053	1.828130132	0.147047012
C	1.158929085	-0.502335035	-0.021612001
H	-1.211391087	2.319212164	-0.030454003
N	1.585427114	0.798869058	0.111404008
H	1.941786138	-1.233369088	-0.019368004
N	-0.577982039	1.527518110	0.007897002
H	2.575882186	0.989049069	0.103879007
S	-2.759255200	0.064283002	-0.354064025
S	1.256090092	3.448882250	0.372402028
C	-0.612247044	-2.240813163	-0.293559020
H	-1.241062087	-2.526343184	0.541311040
H	-1.198115088	-2.372674169	-1.193022086
H	0.239392019	-2.911072210	-0.329313024
O	-4.825920348	2.931474210	-0.104890006
H	-5.238900375	2.883161206	-0.956348069
H	-4.406850316	2.083899149	0.015787003
O	4.426679318	1.138193084	-0.229510015
H	4.694027337	1.830289132	0.374946026
H	4.685487337	1.423732100	-1.084942078
O	4.536395325	3.363733244	1.488615105

H	3.620637262	3.570992255	1.382924099
H	4.998194361	4.164817300	1.446191102
O	-2.119982153	3.848250278	-0.293253024
H	-3.063213220	3.799846276	-0.189837015
H	-1.807745128	4.586689331	0.193974016

point 4

C	-0.163784010	-0.819915061	-0.156979013
C	-1.122383082	0.256481020	-0.164685014
C	0.721704050	1.816694130	0.143070012
C	1.156894086	-0.512003034	-0.018917002
H	-1.213587088	2.316818166	-0.030681004
N	1.582641112	0.793303055	0.112106010
H	1.939179141	-1.243053090	-0.013552002
N	-0.580973044	1.524777109	0.006344999
H	2.572322183	0.986573070	0.103818009
S	-2.772383198	0.064924005	-0.358095028
S	1.258135092	3.443322248	0.368103029
C	-0.618871046	-2.245219162	-0.293338020
H	-1.247593087	-2.529515183	0.541966040
H	-1.206172087	-2.375510173	-1.192033085
H	0.232088018	-2.916607208	-0.329969024
O	-4.807880346	2.922710210	-0.108835006
H	-5.224850375	2.865742204	-0.957522070
H	-4.388275316	2.075349148	0.017180999
O	4.421019317	1.150789084	-0.222765016
H	4.695040336	1.845433132	0.374919028
H	4.702731340	1.411098099	-1.076412079
O	4.554093330	3.385099241	1.484923109
H	3.647455262	3.621488259	1.385886100

H	5.036790364	4.167726299	1.488286110
O	-2.113472151	3.855875277	-0.292380019
H	-3.055819222	3.784268271	-0.204756013
H	-1.831117131	4.594533330	0.207961013

point 5

C	-0.170713014	-0.824220061	-0.156972012
C	-1.128844083	0.245641015	-0.166914014
C	0.714606053	1.805259128	0.139093012
C	1.154858082	-0.521670039	-0.016223003
H	-1.215782089	2.314424169	-0.030908005
N	1.579854115	0.787738058	0.112809006
H	1.936571139	-1.252738092	-0.007736000
N	-0.583963044	1.522036109	0.004793002
H	2.568763185	0.984097071	0.103758006
S	-2.785510202	0.065565003	-0.362127025
S	1.260180092	3.437763247	0.363804025
C	-0.625494044	-2.249625160	-0.293118020
H	-1.254124092	-2.532686183	0.542621039
H	-1.214229086	-2.378347172	-1.191043084
H	0.224783018	-2.922142212	-0.330626024
O	-4.789840344	2.913947209	-0.112780007
H	-5.210799375	2.848322203	-0.958696071
H	-4.369700316	2.066798146	0.018575000
O	4.415358317	1.163385085	-0.216020017
H	4.696052340	1.860578132	0.374891029
H	4.719974342	1.398464103	-1.067883075
O	4.571790330	3.406465244	1.481230108
H	3.674273266	3.671983262	1.388848101
H	5.075386367	4.170634302	1.530381112

O	-2.106963149	3.863499277	-0.291506019
H	-3.048425219	3.768691272	-0.219675018
H	-1.854489133	4.602376330	0.221948014

point 6

C	-0.177641014	-0.828525061	-0.156966011
C	-1.135305083	0.234801015	-0.169142014
C	0.707507050	1.793824131	0.135117007
C	1.152822083	-0.531338038	-0.013528998
H	-1.217978090	2.312030165	-0.031134001
N	1.577068114	0.782172055	0.113511007
H	1.933964137	-1.262422089	-0.001918998
N	-0.586954043	1.519295108	0.003240999
H	2.565203183	0.981622072	0.103697007
S	-2.798637200	0.066207006	-0.366159027
S	1.262225092	3.432203245	0.359504026
C	-0.632118046	-2.254031164	-0.292897020
H	-1.260655092	-2.535857182	0.543277039
H	-1.222286090	-2.381184170	-1.190054084
H	0.217479017	-2.927678210	-0.331282024
O	-4.771799343	2.905183208	-0.116725007
H	-5.196748375	2.830902206	-0.959870072
H	-4.351124311	2.058247150	0.019968001
O	4.409697316	1.175981086	-0.209275013
H	4.697065338	1.875722137	0.374864025
H	4.737217340	1.385830102	-1.059354077
O	4.589487329	3.427831246	1.477538107
H	3.701091265	3.722479266	1.391809101
H	5.113983370	4.173542301	1.572476115
O	-2.100453152	3.871123276	-0.290633019

H	-3.041031221	3.753113268	-0.234594017
H	-1.877861135	4.610220330	0.235935015

point 7

C	-0.184569013	-0.832830061	-0.156959010
C	-1.141766083	0.223961015	-0.171371015
C	0.700409053	1.782388129	0.131140007
C	1.150787084	-0.541005038	-0.010834999
H	-1.220173085	2.309636168	-0.031361002
N	1.574281112	0.776606058	0.114213008
H	1.931357140	-1.272106091	0.003896999
N	-0.589945043	1.516554107	0.001690002
H	2.561644185	0.979146073	0.103636009
S	-2.811764204	0.066848004	-0.370191025
S	1.264270092	3.426644248	0.355205027
C	-0.638741044	-2.258437163	-0.292677019
H	-1.267186092	-2.539029181	0.543932039
H	-1.230343089	-2.384020174	-1.189065083
H	0.210175016	-2.933213214	-0.331938024
O	-4.753758341	2.896419207	-0.120670008
H	-5.182698375	2.813482204	-0.961044067
H	-4.332549311	2.049697148	0.021362002
O	4.404036315	1.188577087	-0.202530014
H	4.698078337	1.890866137	0.374837026
H	4.754460342	1.373196101	-1.050825073
O	4.607184334	3.449197248	1.473845106
H	3.727909270	3.772975269	1.394771102
H	5.152579373	4.176450299	1.614572117
O	-2.093944151	3.878748281	-0.289760020
H	-3.033637218	3.737536269	-0.249512015

H	-1.901233137	4.618064335	0.249922017
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point 8

C	-0.191497012	-0.837135061	-0.156952009
C	-1.148227083	0.213121015	-0.173599015
C	0.693310050	1.770953128	0.127163007
C	1.148751085	-0.550673037	-0.008141000
H	-1.222369086	2.307242164	-0.031588003
N	1.571495115	0.771041055	0.114915010
H	1.928749137	-1.281791093	0.009713001
N	-0.592936043	1.513813107	0.000137999
H	2.558084182	0.976670068	0.103576006
S	-2.824892203	0.067489007	-0.374222027
S	1.266315092	3.421084247	0.350906028
C	-0.645365046	-2.262843161	-0.292456019
H	-1.273717092	-2.542200181	0.544587039
H	-1.238400088	-2.386857173	-1.188075088
H	0.202871015	-2.938748212	-0.332595024
O	-4.735718339	2.887656207	-0.124615008
H	-5.168647370	2.796063203	-0.962218068
H	-4.313973311	2.041146147	0.022755003
O	4.398375315	1.201173087	-0.195785014
H	4.699091336	1.906010137	0.374810028
H	4.771703345	1.360562100	-1.042295074
O	4.624881333	3.470563251	1.470153105
H	3.754726269	3.823470278	1.397733103
H	5.191175371	4.179358303	1.656667119
O	-2.087434149	3.886372281	-0.288886020
H	-3.026243220	3.721958269	-0.264431020
H	-1.924606140	4.625908334	0.263909018

point 9

C	-0.198425016	-0.841439060	-0.156945013
C	-1.154689084	0.202282015	-0.175827015
C	0.686211047	1.759517126	0.123187008
C	1.146715081	-0.560340042	-0.005446001
H	-1.224564087	2.304848167	-0.031815004
N	1.568708113	0.765475058	0.115617011
H	1.926142140	-1.291475095	0.015529003
N	-0.595927043	1.511072106	-0.001413999
H	2.554524185	0.974194069	0.103515008
S	-2.838019206	0.068130004	-0.378254030
S	1.268360093	3.415525245	0.346607023
C	-0.651988049	-2.267249165	-0.292235019
H	-1.280248091	-2.545371186	0.545242038
H	-1.246457092	-2.389693171	-1.187086087
H	0.195567015	-2.944284210	-0.333251024
O	-4.717677337	2.878892206	-0.128560009
H	-5.154597370	2.778643201	-0.963392069
H	-4.295398311	2.032595145	0.024149004
O	4.392714314	1.213769088	-0.189040015
H	4.700103340	1.921155137	0.374783029
H	4.788946347	1.347928099	-1.033766076
O	4.642578333	3.491929253	1.466460104
H	3.781544273	3.873966281	1.400695099
H	5.229772374	4.182266301	1.698762122
O	-2.080925152	3.893997280	-0.288013021
H	-3.018849216	3.706381265	-0.279350019
H	-1.947978142	4.633751334	0.277896019

point 10

C	-0.205353015	-0.845744060	-0.156938012
C	-1.161150084	0.191442014	-0.178056010
C	0.679113050	1.748082124	0.119210008
C	1.144680082	-0.570008042	-0.002752002
H	-1.226760088	2.302453163	-0.032042000
N	1.565922111	0.759910055	0.116319007
H	1.923535138	-1.301159091	0.021344999
N	-0.598917042	1.508331111	-0.002966001
H	2.550965182	0.971719070	0.103455009
S	-2.851146205	0.068772008	-0.382286027
S	1.270405093	3.409965243	0.342308025
C	-0.658612046	-2.271655164	-0.292015019
H	-1.286779091	-2.548543185	0.545898038
H	-1.254515091	-2.392530170	-1.186097087
H	0.188262014	-2.949819214	-0.333908024
O	-4.699637336	2.870129205	-0.132505009
H	-5.140546370	2.761223199	-0.964566070
H	-4.276822306	2.024045144	0.025543000
O	4.387054314	1.226366089	-0.182294011
H	4.701116338	1.936299142	0.374756025
H	4.806189344	1.335293098	-1.025237072
O	4.660275338	3.513295250	1.462768103
H	3.808362272	3.924462284	1.403657100
H	5.268368377	4.185175299	1.740857124
O	-2.074415150	3.901621280	-0.287139021
H	-3.011455219	3.690803266	-0.294268023
H	-1.971350144	4.641595333	0.291883021

${}^1\Pi_7\Pi_8^*$ to ${}^1\Pi_8\Pi_8^*$

point 1

C	-0.205353015	-0.845745060	-0.156938012
C	-1.161150084	0.191442014	-0.178056010
C	0.679113050	1.748082124	0.119210008
C	1.144680082	-0.570008042	-0.002752002
H	-1.226760088	2.302454163	-0.032042000
N	1.565922111	0.759910055	0.116319007
H	1.923535138	-1.301160091	0.021344999
N	-0.598918043	1.508331111	-0.002966001
H	2.550966182	0.971719070	0.103455009
S	-2.851147205	0.068772008	-0.382286027
S	1.270406093	3.409966243	0.342308025
C	-0.658612046	-2.271656164	-0.292015019
H	-1.286779091	-2.548543185	0.545898038
H	-1.254515091	-2.392531170	-1.186097087
H	0.188263014	-2.949820214	-0.333908024
O	-4.699638336	2.870129205	-0.132505009
H	-5.140547370	2.761224199	-0.964567070
H	-4.276824306	2.024045144	0.025543000
O	4.387055314	1.226366089	-0.182295011
H	4.701117339	1.936299142	0.374756025
H	4.806190344	1.335294098	-1.025237072
O	4.660276333	3.513297251	1.462768103
H	3.808364273	3.924463285	1.403657100
H	5.268369377	4.185176300	1.740858124
O	-2.074416150	3.901622280	-0.287139021
H	-3.011456219	3.690804266	-0.294268023
H	-1.971351144	4.641597334	0.291883021

point 2

C	-0.194675012	-0.847123059	-0.156690013
C	-1.140792085	0.195072012	-0.176464012
C	0.696381051	1.752581126	0.123113008
C	1.155808082	-0.570957042	-0.000409001
H	-1.212934089	2.301753168	-0.026895000
N	1.577288114	0.758512053	0.118657007
H	1.933877140	-1.303006094	0.021791001
N	-0.585210045	1.508957107	0.001064001
H	2.562666185	0.967309071	0.105892008
S	-2.835570206	0.075311003	-0.384452029
S	1.280583092	3.411127248	0.340426027
C	-0.652396044	-2.271694164	-0.293650023
H	-1.278446095	-2.551464185	0.545270037
H	-1.248754091	-2.392118173	-1.188059086
H	0.192693016	-2.951312213	-0.338775026
O	-4.760915341	2.879824209	-0.106321007
H	-5.213385374	2.789815202	-0.932155069
H	-4.343331313	2.030959146	0.039167001
O	4.405531315	1.215045088	-0.191767014
H	4.708385339	1.921756139	0.374390025
H	4.821329349	1.338302095	-1.033603074
O	4.646127334	3.491871250	1.468513105
H	3.783986273	3.865494280	1.402189098
H	5.224905378	4.185863299	1.733372124
O	-2.112697150	3.862835276	-0.275429022
H	-3.050066219	3.676361267	-0.263881019
H	-1.976062145	4.598021328	0.295148023

point 3

C	-0.183997014	-0.848500063	-0.156442009
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C	-1.120434080	0.198702014	-0.174872014
C	0.713649052	1.757080127	0.127017007
C	1.166935087	-0.571906042	0.001934000
H	-1.199107084	2.301053167	-0.021746999
N	1.588654116	0.757113057	0.120995007
H	1.944218142	-1.304853092	0.022236002
N	-0.571503041	1.509583107	0.005093003
H	2.574367183	0.962900072	0.108330007
S	-2.819992201	0.081851004	-0.386618025
S	1.290761092	3.412288247	0.338544024
C	-0.646179048	-2.271732164	-0.295285022
H	-1.270113093	-2.554384185	0.544642041
H	-1.242994087	-2.391705172	-1.190021084
H	0.197123013	-2.952803213	-0.343642022
O	-4.822192347	2.889518207	-0.080136004
H	-5.286223379	2.818406204	-0.899743063
H	-4.409838315	2.037872148	0.052792003
O	4.424008317	1.203723087	-0.201239017
H	4.715652340	1.907212136	0.374025025
H	4.836468348	1.341309097	-1.041970075
O	4.631979331	3.470446250	1.474257108
H	3.759608273	3.806526276	1.400720102
H	5.181441373	4.186551303	1.725886123
O	-2.150977155	3.824048277	-0.263719017
H	-3.088676224	3.661918263	-0.233493016
H	-1.980773140	4.554445328	0.298413020

point 4

C	-0.173319011	-0.849878062	-0.156194010
C	-1.100076081	0.202332017	-0.173280011

C	0.730917053	1.761579128	0.130920007
C	1.178063086	-0.572855042	0.004278001
H	-1.185280085	2.300352165	-0.016599999
N	1.600021113	0.755715055	0.123333008
H	1.954560139	-1.306699095	0.022682003
N	-0.557796038	1.510208108	0.009122000
H	2.586068186	0.958490067	0.110767006
S	-2.804415202	0.088390005	-0.388785027
S	1.300938096	3.413449246	0.336662026
C	-0.639963046	-2.271771165	-0.296921021
H	-1.261780091	-2.557304185	0.544014040
H	-1.237234088	-2.391292170	-1.191982088
H	0.201553015	-2.954295212	-0.348509024
O	-4.883469353	2.899212210	-0.053951002
H	-5.359060388	2.846997206	-0.867331063
H	-4.476345323	2.044785145	0.066416005
O	4.442484318	1.192402086	-0.210712015
H	4.722920341	1.892668134	0.373659025
H	4.851607347	1.344317094	-1.050336076
O	4.617830332	3.449020249	1.480002104
H	3.735230268	3.747558272	1.399251101
H	5.137976367	4.187239302	1.718400122
O	-2.189258160	3.785261272	-0.252009018
H	-3.127286223	3.647475264	-0.203105012
H	-1.985484140	4.510870323	0.301678023

point 5

C	-0.162641013	-0.851256060	-0.155947011
C	-1.079719077	0.205962014	-0.171688013
C	0.748185054	1.766078125	0.134824012

C	1.189190086	-0.573804042	0.006621002
H	-1.171454086	2.299651164	-0.011452999
N	1.611387116	0.754317054	0.125670008
H	1.964901140	-1.308546093	0.023128004
N	-0.544089041	1.510834109	0.013151002
H	2.597769184	0.954081068	0.113205010
S	-2.788838203	0.094930006	-0.390951029
S	1.311116096	3.414610245	0.334780023
C	-0.633746044	-2.271809165	-0.298556020
H	-1.253447089	-2.560224186	0.543386039
H	-1.231473089	-2.390879174	-1.193944087
H	0.205983017	-2.955787211	-0.353376026
O	-4.944745358	2.908906208	-0.027766004
H	-5.431898393	2.875588208	-0.834919062
H	-4.542853325	2.051699148	0.080041006
O	4.460960320	1.181080084	-0.220184017
H	4.730187341	1.878124136	0.373293025
H	4.866745351	1.347325097	-1.058702077
O	4.603681329	3.427595249	1.485746107
H	3.710852268	3.688589268	1.397783100
H	5.094512367	4.187926301	1.710915122
O	-2.227539159	3.746475268	-0.240299018
H	-3.165896228	3.633032260	-0.172717014
H	-1.990196141	4.467294323	0.304943020

point 6

C	-0.151963010	-0.852634059	-0.155699012
C	-1.059361078	0.209592016	-0.170096010
C	0.765453054	1.770577126	0.138727012
C	1.200318085	-0.574753042	0.008963998

H	-1.157627081	2.298951163	-0.006305999
N	1.622753118	0.752918052	0.128008008
H	1.975243142	-1.310392097	0.023573000
N	-0.530382037	1.511459110	0.017180999
H	2.609469187	0.949671069	0.115642009
S	-2.773260198	0.101469007	-0.393118026
S	1.321293095	3.415771244	0.332898025
C	-0.627530043	-2.271847165	-0.300192019
H	-1.245114088	-2.563144186	0.542758038
H	-1.225713090	-2.390467172	-1.195906086
H	0.210413014	-2.957279211	-0.358243028
O	-5.006022358	2.918600212	-0.001582002
H	-5.504736397	2.904180211	-0.802507056
H	-4.609360332	2.058612150	0.093665008
O	4.479437321	1.169759083	-0.229657015
H	4.737455342	1.863581134	0.372928025
H	4.881884350	1.350333099	-1.067068079
O	4.589532330	3.406169243	1.491491109
H	3.686474268	3.629621263	1.396314098
H	5.051048362	4.188614301	1.703429121
O	-2.265820164	3.707688269	-0.228589019
H	-3.204506228	3.618589262	-0.142330011
H	-1.994907141	4.423719317	0.308208022

point 7

C	-0.141285013	-0.854012063	-0.155451013
C	-1.039003073	0.213222013	-0.168504012
C	0.782721055	1.775076128	0.142630012
C	1.211445085	-0.575702042	0.011306999
H	-1.143801082	2.298250168	-0.001157999

N	1.634119115	0.751520056	0.130346009
H	1.985584144	-1.312239094	0.024019001
N	-0.516675040	1.512085110	0.021210001
H	2.621170191	0.945261070	0.118080008
S	-2.757683199	0.108008008	-0.395284028
S	1.331471094	3.416933248	0.331015022
C	-0.621314046	-2.271885165	-0.301827023
H	-1.236781091	-2.566064186	0.542130037
H	-1.219952090	-2.390054170	-1.197868084
H	0.214843016	-2.958770215	-0.363111025
O	-5.067299364	2.928294210	0.024603001
H	-5.577573401	2.932771213	-0.770095055
H	-4.675867334	2.065525147	0.107290010
O	4.497913323	1.158437082	-0.239129018
H	4.744722343	1.849037131	0.372562024
H	4.897023355	1.353341096	-1.075434080
O	4.575384327	3.384744243	1.497235106
H	3.662096263	3.570653259	1.394845102
H	5.007583362	4.189302300	1.695943121
O	-2.304100164	3.668901265	-0.216879014
H	-3.243116233	3.604146258	-0.111942007
H	-1.999618142	4.380143317	0.311473025

point 8

C	-0.130606009	-0.855390062	-0.155203009
C	-1.018645074	0.216852016	-0.166911014
C	0.799989056	1.779575129	0.146534012
C	1.222573089	-0.576651042	0.013650000
H	-1.129974082	2.297549167	0.003989002
N	1.645485117	0.750122054	0.132684009

H	1.995926141	-1.314085092	0.024465002
N	-0.502967036	1.512711111	0.025239003
H	2.632871189	0.940852066	0.120517007
S	-2.742106195	0.114548009	-0.397450030
S	1.341648099	3.418093247	0.329133024
C	-0.615097044	-2.271923166	-0.303462022
H	-1.228447089	-2.568985186	0.541502041
H	-1.214192086	-2.389641174	-1.199830088
H	0.219273018	-2.960262215	-0.367978027
O	-5.128576370	2.937989213	0.050788003
H	-5.650411406	2.961362215	-0.737683055
H	-4.742374341	2.072438149	0.120914006
O	4.516390324	1.147116081	-0.248602016
H	4.751989344	1.834493133	0.372196024
H	4.912162354	1.356348098	-1.083801076
O	4.561235328	3.363318242	1.502980108
H	3.637718263	3.511685255	1.393377101
H	4.964119357	4.189989299	1.688457120
O	-2.342381169	3.630114261	-0.205169015
H	-3.281726238	3.589703259	-0.081554004
H	-2.004329142	4.336568312	0.314738022

point 9

C	-0.119928006	-0.856768060	-0.154955010
C	-0.998287070	0.220481018	-0.165319010
C	0.817257057	1.784074131	0.150438011
C	1.233700089	-0.577600042	0.015994001
H	-1.116147078	2.296848165	0.009136002
N	1.656851120	0.748724052	0.135022009
H	2.006267143	-1.315931095	0.024910003

N	-0.489260033	1.513336107	0.029268000
H	2.644572192	0.936442067	0.122955011
S	-2.726528196	0.121087010	-0.399616026
S	1.351826098	3.419255246	0.327251021
C	-0.608881043	-2.271961166	-0.305098021
H	-1.220114087	-2.571905186	0.540874040
H	-1.208432087	-2.389228172	-1.201791087
H	0.223703014	-2.961754214	-0.372845028
O	-5.189852375	2.947683211	0.076973006
H	-5.723249410	2.989953218	-0.705271049
H	-4.808881348	2.079352151	0.134539008
O	4.534866325	1.135795080	-0.258074019
H	4.759257344	1.819949131	0.371831024
H	4.927301353	1.359356100	-1.092167077
O	4.547086325	3.341893242	1.508724110
H	3.613341258	3.452716251	1.391908100
H	4.920655352	4.190677303	1.680972119
O	-2.380662174	3.591327256	-0.193459016
H	-3.320336238	3.575260255	-0.051166005
H	-2.009041143	4.292992306	0.318004025

point 10

C	-0.109250008	-0.858146059	-0.154708012
C	-0.977929071	0.224111015	-0.163727012
C	0.834525058	1.788573127	0.154341011
C	1.244828088	-0.578549042	0.018337002
H	-1.102321079	2.296148164	0.014283002
N	1.668217122	0.747325056	0.137360010
H	2.016609145	-1.317778093	0.025356004
N	-0.475553035	1.513962107	0.033298002

H	2.656273190	0.932033068	0.125392010
S	-2.710951197	0.127627011	-0.401783028
S	1.362003098	3.420416245	0.325369024
C	-0.602665041	-2.272000166	-0.306733020
H	-1.211781086	-2.574825186	0.540246039
H	-1.202671088	-2.388815171	-1.203753086
H	0.228133016	-2.963245213	-0.377712025
O	-5.251129375	2.957377214	0.103157009
H	-5.796087415	3.018544215	-0.672860048
H	-4.875388350	2.086265148	0.148163010
O	4.553343327	1.124473079	-0.267547022
H	4.766524345	1.805406128	0.371465024
H	4.942439357	1.362364097	-1.100533079
O	4.532937326	3.320467241	1.514469107
H	3.588963258	3.393748246	1.390439099
H	4.877191352	4.191364302	1.673486119
O	-2.418943174	3.552540257	-0.181749011
H	-3.358946243	3.560817256	-0.020779002
H	-2.013752143	4.249416306	0.321269022

Snapshot2

FC point to ${}^1\pi_7\pi_8^*$

point01

C	-1.577921	-1.105490	0.321253
C	-2.301686	1.534458	0.368497
C	2.158067	2.683411	0.045353
C	0.925966	-1.628944	0.020787
N	-0.362827	3.231434	0.188973
N	2.706088	0.211649	-0.141729
H	1.640282	-3.522450	-0.047243

H	-0.786126	5.098483	0.187083
H	4.542903	-0.304246	-0.300466
S	-5.276117	2.494438	0.638727
S	4.384167	4.988879	0.139840
C	-3.492214	-3.178521	0.667073
H	-4.408733	-3.014113	2.490659
H	-4.952974	-3.087812	-0.752111
H	-2.587035	-5.013445	0.557469
O	-5.776895	8.970532	2.124052
H	-5.816579	7.179071	1.961536
H	-7.145056	9.575244	1.139505
O	10.440741	2.490659	0.391173
H	8.932737	3.426075	0.710537
H	11.202300	3.291905	-1.016673
O	-1.041239	8.585028	0.041574
H	0.417629	9.274778	0.820141
H	-2.498218	9.257770	0.863605
O	7.687408	-1.806578	-0.534792
H	8.331804	-2.528454	-2.040904
H	8.894943	-0.542351	-0.052912

point02

C	-1.619047	-1.109838	0.336415
C	-2.339371	1.521256	0.377739
C	2.119077	2.656987	0.044752
C	0.885297	-1.653541	0.032411
N	-0.384427	3.222741	0.194640
N	2.674357	0.191133	-0.132844
H	1.596977	-3.547222	-0.017531
H	-0.800890	5.091034	0.196292
H	4.510359	-0.323415	-0.292399

S	-5.315335	2.516577	0.636798
S	4.371728	4.960055	0.126211
C	-3.538284	-3.177081	0.687915
H	-4.455458	-3.002828	2.510229
H	-4.998405	-3.085416	-0.732123
H	-2.639520	-5.015324	0.584222
O	-5.775906	8.959295	2.107553
H	-5.814661	7.165734	1.968996
H	-7.150382	9.547546	1.122987
O	10.494216	2.461746	0.377000
H	9.038785	3.429866	0.786088
H	11.208688	3.281602	-1.051374
O	-1.026996	8.592486	0.063754
H	0.381007	9.301619	0.889980
H	-2.513186	9.236804	0.838521
O	7.665844	-1.791576	-0.529411
H	8.307569	-2.538426	-2.022277
H	8.883814	-0.535677	-0.056985
point03			
C	-1.660174	-1.114188	0.351578
C	-2.377054	1.508054	0.386982
C	2.080086	2.630561	0.044150
C	0.844630	-1.678135	0.044033
N	-0.406027	3.214048	0.200309
N	2.642627	0.170616	-0.123960
H	1.553672	-3.571991	0.012181
H	-0.815655	5.083582	0.205502
H	4.477814	-0.342583	-0.284332
S	-5.354552	2.538715	0.634871
S	4.359292	4.931233	0.112582

C	-3.584353	-3.175643	0.708755
H	-4.502186	-2.991542	2.529799
H	-5.043836	-3.083018	-0.712136
H	-2.692006	-5.017204	0.610973
O	-5.774916	8.948059	2.091052
H	-5.812743	7.152398	1.976457
H	-7.155705	9.519849	1.106469
O	10.547506	2.432833	0.362827
H	9.145163	3.435282	0.864244
H	11.211834	3.268251	-1.080651
O	-1.012753	8.599945	0.085932
H	0.344384	9.328461	0.959820
H	-2.528153	9.215835	0.813436
O	7.644279	-1.776571	-0.524030
H	8.283335	-2.548396	-2.003650
H	8.872686	-0.529002	-0.061055

point04

C	-1.701300	-1.118536	0.366739
C	-2.414737	1.494853	0.396225
C	2.041097	2.604137	0.043549
C	0.803961	-1.702732	0.055656
N	-0.427628	3.205357	0.205976
N	2.610897	0.150099	-0.115075
H	1.510367	-3.596763	0.041893
H	-0.830419	5.076133	0.214711
H	4.445269	-0.361752	-0.276265
S	-5.393770	2.560851	0.632941
S	4.346854	4.902409	0.098954
C	-3.630421	-3.174203	0.729597
H	-4.548913	-2.980257	2.549369

H	-5.089269	-3.080620	-0.692150
H	-2.744491	-5.019084	0.637726
O	-5.773928	8.936823	2.074553
H	-5.810825	7.139060	1.983918
H	-7.161030	9.492151	1.089951
O	10.600986	2.403921	0.348654
H	9.258326	3.437306	0.942176
H	11.214156	3.254222	-1.108702
O	-0.998510	8.607402	0.108111
H	0.307761	9.355301	1.029659
H	-2.543120	9.194869	0.788352
O	7.622715	-1.761569	-0.518649
H	8.259099	-2.558366	-1.985021
H	8.861559	-0.522328	-0.065128

point05

C	-1.742426	-1.122885	0.381900
C	-2.452420	1.481651	0.405467
C	2.002106	2.577711	0.042948
C	0.763293	-1.727329	0.067280
N	-0.449228	3.196664	0.211644
N	2.579164	0.129582	-0.106191
H	1.467062	-3.621532	0.071604
H	-0.845182	5.068684	0.223919
H	4.412724	-0.380922	-0.268197
S	-5.432989	2.582989	0.631014
S	4.334418	4.873587	0.085325
C	-3.676491	-3.172765	0.750437
H	-4.595640	-2.968970	2.568939
H	-5.134700	-3.078222	-0.672162
H	-2.796976	-5.020963	0.664479

O	-5.772939	8.925587	2.058053
H	-5.808907	7.125724	1.991378
H	-7.166354	9.464453	1.073432
O	10.654276	2.375008	0.334482
H	9.377915	3.435628	1.019228
H	11.215748	3.239401	-1.135368
O	-0.984270	8.614861	0.130291
H	0.271138	9.382143	1.099499
H	-2.558086	9.173900	0.763268
O	7.601149	-1.746564	-0.513267
H	8.234863	-2.568338	-1.966394
H	8.850430	-0.515653	-0.069200

point06

C	-1.783552	-1.127233	0.397062
C	-2.490103	1.468449	0.414710
C	1.963116	2.551287	0.042347
C	0.722624	-1.751924	0.078904
N	-0.470827	3.187972	0.217313
N	2.547434	0.109066	-0.097306
H	1.423757	-3.646304	0.101316
H	-0.859946	5.061235	0.233130
H	4.380181	-0.400089	-0.260130
S	-5.472207	2.605127	0.629084
S	4.321979	4.844765	0.071696
C	-3.722558	-3.171325	0.771278
H	-4.642365	-2.957684	2.588509
H	-5.180130	-3.075826	-0.652175
H	-2.849461	-5.022843	0.691230
O	-5.771949	8.914350	2.041552
H	-5.806989	7.112387	1.998839

H	-7.171679	9.436756	1.056914
O	10.707755	2.346095	0.320309
H	9.503247	3.429483	1.093819
H	11.216963	3.223776	-1.160658
O	-0.970027	8.622320	0.152471
H	0.234513	9.408984	1.169338
H	-2.573055	9.152932	0.738184
O	7.579586	-1.731562	-0.507885
H	8.210628	-2.578308	-1.947767
H	8.839302	-0.508979	-0.073270

point07

C	-1.824678	-1.131581	0.412225
C	-2.527786	1.455248	0.423953
C	1.924125	2.524861	0.041744
C	0.681957	-1.776520	0.090527
N	-0.492427	3.179281	0.222980
N	2.515702	0.088549	-0.088422
H	1.380452	-3.671073	0.131028
H	-0.874711	5.053785	0.242338
H	4.347636	-0.419258	-0.252063
S	-5.511424	2.627264	0.627157
S	4.309543	4.815941	0.058068
C	-3.768628	-3.169887	0.792118
H	-4.689093	-2.946399	2.608079
H	-5.225563	-3.073428	-0.632187
H	-2.901947	-5.024721	0.717983
O	-5.770961	8.903114	2.025053
H	-5.805070	7.099049	2.006298
H	-7.177002	9.409058	1.040394
O	10.761234	2.317182	0.306136

H	9.633425	3.418736	1.164922
H	11.217622	3.207415	-1.184528
O	-0.955784	8.629776	0.174648
H	0.197890	9.435824	1.239177
H	-2.588021	9.131965	0.713099
O	7.558020	-1.716557	-0.502503
H	8.186392	-2.588278	-1.929140
H	8.828173	-0.502306	-0.077343

point08

C	-1.865804	-1.135931	0.427386
C	-2.565471	1.442046	0.433195
C	1.885134	2.498437	0.041143
C	0.641288	-1.801117	0.102149
N	-0.514026	3.170588	0.228647
N	2.483971	0.068030	-0.079537
H	1.337148	-3.695843	0.160740
H	-0.889475	5.046334	0.251547
H	4.315091	-0.438428	-0.243996
S	-5.550642	2.649402	0.625227
S	4.297105	4.787118	0.044439
C	-3.814696	-3.168449	0.812960
H	-4.735820	-2.935113	2.627649
H	-5.270994	-3.071030	-0.612201
H	-2.954432	-5.026602	0.744735
O	-5.769973	8.891878	2.008552
H	-5.803152	7.085713	2.013758
H	-7.182327	9.381362	1.023876
O	10.814525	2.288269	0.291963
H	9.767535	3.403514	1.231606
H	11.217957	3.190083	-1.206991

O	-0.941541	8.637235	0.196828
H	0.161267	9.462666	1.309017
H	-2.602988	9.110997	0.688015
O	7.536455	-1.701555	-0.497123
H	8.162156	-2.598249	-1.910511
H	8.817044	-0.495632	-0.081415

point09

C	-1.906930	-1.140280	0.442547
C	-2.603154	1.428845	0.442438
C	1.846143	2.472011	0.040542
C	0.600619	-1.825712	0.113773
N	-0.535626	3.161897	0.234315
N	2.452241	0.047513	-0.070651
H	1.293843	-3.720614	0.190452
H	-0.904240	5.038885	0.260756
H	4.282546	-0.457595	-0.235929
S	-5.589859	2.671540	0.623298
S	4.284669	4.758294	0.030810
C	-3.860765	-3.167009	0.833802
H	-4.782547	-2.923828	2.647219
H	-5.316425	-3.068632	-0.592214
H	-3.006917	-5.028480	0.771488
O	-5.768984	8.880641	1.992053
H	-5.801236	7.072376	2.021219
H	-7.187651	9.353662	1.007358
O	10.868004	2.259357	0.277790
H	9.904100	3.383398	1.292830
H	11.218182	3.171875	-1.228056
O	-0.927298	8.644694	0.219008
H	0.124644	9.489505	1.378856

H -2.617957 9.090031 0.662929

O 7.514891 -1.686550 -0.491741

H 8.137920 -2.608221 -1.891884

H 8.805916 -0.488957 -0.085486

point10

C -1.948056 -1.144628 0.457709

C -2.640837 1.415643 0.451679

C 1.807153 2.445587 0.039941

C 0.559950 -1.850308 0.125397

N -0.557225 3.153205 0.239984

N 2.420511 0.026997 -0.061768

H 1.250538 -3.745384 0.220163

H -0.919004 5.031435 0.269966

H 4.250004 -0.476765 -0.227861

S -5.629078 2.693676 0.621370

S 4.272230 4.729472 0.017181

C -3.906833 -3.165571 0.854642

H -4.829274 -2.912540 2.666789

H -5.361858 -3.066234 -0.572226

H -3.059400 -5.030360 0.798239

O -5.767994 8.869405 1.975554

H -5.799318 7.059038 2.028680

H -7.192976 9.325965 0.990840

O 10.921385 2.230466 0.263660

H 10.043964 3.356482 1.346271

H 11.217777 3.150714 -1.244428

O -0.913055 8.652151 0.241186

H 0.088022 9.516347 1.448696

H -2.632923 9.069062 0.637845

O 7.493327 -1.671548 -0.486359

H 8.113687 -2.618191 -1.873257

H 8.794787 -0.482283 -0.089558

FC point to 'n₇π₇'*

point01

C -1.577921 -1.105490 0.321253

C -2.301686 1.534458 0.368497

C 2.158067 2.683411 0.045353

C 0.925966 -1.628944 0.020787

N -0.362827 3.231434 0.188973

N 2.706088 0.211649 -0.141729

H 1.640282 -3.522450 -0.047243

H -0.786126 5.098483 0.187083

H 4.542903 -0.304246 -0.300466

S -5.276117 2.494438 0.638727

S 4.384167 4.988879 0.139840

C -3.492214 -3.178521 0.667073

H -4.408733 -3.014113 2.490659

H -4.952974 -3.087812 -0.752111

H -2.587035 -5.013445 0.557469

O -5.776895 8.970532 2.124052

H -5.816579 7.179071 1.961536

H -7.145056 9.575244 1.139505

O 10.440741 2.490659 0.391173

H 8.932737 3.426075 0.710537

H 11.202300 3.291905 -1.016673

O -1.041239 8.585028 0.041574

H 0.417629 9.274778 0.820141

H -2.498218 9.257770 0.863605

O 7.687408 -1.806578 -0.534792

H 8.331804 -2.528454 -2.040904

H 8.894943 -0.542351 -0.052912

point02

C -1.600275 -1.120831 0.325702

C -2.313255 1.520555 0.366168

C 2.143518 2.652503 -0.003553

C 0.899451 -1.656555 0.013939

N -0.375315 3.214471 0.163329

N 2.687888 0.174467 -0.171056

H 1.604207 -3.553809 -0.051737

H -0.793248 5.080873 0.159720

H 4.519696 -0.348273 -0.337739

S -5.287954 2.494044 0.652721

S 4.393642 4.947819 0.171969

C -3.520352 -3.185761 0.687074

H -4.428713 -3.016324 2.514216

H -4.987397 -3.096626 -0.726460

H -2.621587 -5.023795 0.578147

O -5.767030 8.975814 2.111253

H -5.812926 7.185612 1.991603

H -7.141712 9.562167 1.126050

O 10.473807 2.478187 0.381914

H 9.009492 3.416721 0.826685

H 11.128886 3.326118 -1.058490

O -1.014537 8.594720 0.055505

H 0.409636 9.289380 0.876697

H -2.492966 9.250591 0.844122

O 7.695753 -1.807179 -0.558355

H 8.355747 -2.542479 -2.049325

H 8.900070 -0.543512 -0.070606

point03

C	-1.622627	-1.136169	0.330152
C	-2.324824	1.506654	0.363840
C	2.128969	2.621592	-0.052461
C	0.872936	-1.684167	0.007092
N	-0.387802	3.197509	0.137687
N	2.669688	0.137283	-0.200381
H	1.568131	-3.585170	-0.056231
H	-0.800371	5.063260	0.132358
H	4.496486	-0.392298	-0.375010
S	-5.299792	2.493647	0.666716
S	4.403117	4.906761	0.204096
C	-3.548488	-3.193002	0.707077
H	-4.448693	-3.018533	2.537774
H	-5.021821	-3.105442	-0.700809
H	-2.656137	-5.034145	0.598822
O	-5.757166	8.981093	2.098454
H	-5.809273	7.192152	2.021669
H	-7.138367	9.549090	1.112595
O	10.506877	2.465904	0.372465
H	9.089785	3.406239	0.947365
H	11.046387	3.355606	-1.090491
O	-0.987837	8.604412	0.069436
H	0.401641	9.303982	0.933251
H	-2.487715	9.243414	0.824639
O	7.704098	-1.807780	-0.581917
H	8.379688	-2.556505	-2.057744
H	8.905195	-0.544674	-0.088297
point04			
C	-1.644980	-1.151510	0.334601
C	-2.336391	1.492751	0.361514

C	2.114420	2.590682	-0.101367
C	0.846420	-1.711778	0.000244
N	-0.400291	3.180549	0.112044
N	2.651486	0.100101	-0.229706
H	1.532056	-3.616530	-0.060726
H	-0.807493	5.045650	0.104995
H	4.473278	-0.436323	-0.412283
S	-5.311631	2.493250	0.680710
S	4.412592	4.865701	0.236225
C	-3.576624	-3.200244	0.727078
H	-4.468673	-3.020742	2.561331
H	-5.056244	-3.114255	-0.675158
H	-2.690687	-5.044495	0.619499
O	-5.747302	8.986375	2.085653
H	-5.805620	7.198692	2.051736
H	-7.135022	9.536013	1.099140
O	10.540136	2.453431	0.363205
H	9.180800	3.389893	1.068990
H	10.958170	3.381672	-1.115477
O	-0.961135	8.614105	0.083367
H	0.393645	9.318583	0.989806
H	-2.482463	9.236235	0.805156
O	7.712443	-1.808381	-0.605480
H	8.403629	-2.570530	-2.066162
H	8.910319	-0.545834	-0.105991
point05			
C	-1.667332	-1.166851	0.339051
C	-2.347960	1.478851	0.359186
C	2.099871	2.559774	-0.150275
C	0.819905	-1.739389	-0.006605

N	-0.412779	3.163587	0.086400
N	2.633286	0.062917	-0.259032
H	1.495979	-3.647890	-0.065220
H	-0.814616	5.028040	0.077634
H	4.450071	-0.480349	-0.449556
S	-5.323468	2.492853	0.694703
S	4.422069	4.824643	0.268354
C	-3.604762	-3.207485	0.747079
H	-4.488655	-3.022951	2.584886
H	-5.090667	-3.123069	-0.649508
H	-2.725236	-5.054845	0.640177
O	-5.737437	8.991655	2.072854
H	-5.801969	7.205231	2.081804
H	-7.131677	9.522935	1.085685
O	10.573207	2.441148	0.353946
H	9.281634	3.367343	1.188745
H	10.865870	3.403418	-1.133087
O	-0.934434	8.623797	0.097298
H	0.385652	9.333185	1.046360
H	-2.477212	9.229056	0.785671
O	7.720788	-1.808982	-0.629041
H	8.427572	-2.584556	-2.074581
H	8.915444	-0.546996	-0.123684
point06			
C	-1.689685	-1.182190	0.343499
C	-2.359529	1.464948	0.356858
C	2.085322	2.528864	-0.199181
C	0.793390	-1.767000	-0.013451
N	-0.425266	3.146625	0.060758
N	2.615084	0.025734	-0.288357

H	1.459904	-3.679250	-0.069714
H	-0.821738	5.010429	0.050270
H	4.426863	-0.524374	-0.486827
S	-5.335305	2.492456	0.708696
S	4.431544	4.783583	0.300482
C	-3.632898	-3.214726	0.767080
H	-4.508635	-3.025162	2.608444
H	-5.125090	-3.131883	-0.623857
H	-2.759788	-5.065195	0.660852
O	-5.727573	8.996937	2.060055
H	-5.798317	7.211771	2.111869
H	-7.128332	9.509858	1.072231
O	10.606277	2.428676	0.344497
H	9.391790	3.338485	1.303745
H	10.771409	3.420274	-1.142899
O	-0.907732	8.633490	0.111231
H	0.377656	9.347785	1.102916
H	-2.471958	9.221877	0.766188
O	7.729133	-1.809583	-0.652604
H	8.451513	-2.598581	-2.083000
H	8.920569	-0.548157	-0.141376
point07			
C	-1.712039	-1.197531	0.347948
C	-2.371096	1.451045	0.354530
C	2.070773	2.497953	-0.248089
C	0.766875	-1.794612	-0.020299
N	-0.437755	3.129664	0.035115
N	2.596884	-0.011448	-0.317684
H	1.423827	-3.710610	-0.074208
H	-0.828860	4.992819	0.022907

H	4.403655	-0.568401	-0.524100
S	-5.347144	2.492059	0.722692
S	4.441019	4.742523	0.332611
C	-3.661034	-3.221968	0.787082
H	-4.528615	-3.027371	2.632001
H	-5.159514	-3.140696	-0.598206
H	-2.794338	-5.075545	0.681530
O	-5.717708	9.002217	2.047254
H	-5.794664	7.218312	2.141937
H	-7.124987	9.496781	1.058776
O	10.639347	2.416204	0.335237
H	9.509667	3.303767	1.411778
H	10.676786	3.431650	-1.144745
O	-0.881032	8.643182	0.125162
H	0.369663	9.362387	1.159470
H	-2.466707	9.214698	0.746704
O	7.737478	-1.810184	-0.676167
H	8.475454	-2.612607	-2.091418
H	8.925696	-0.549319	-0.159070
point08			
C	-1.734391	-1.212870	0.352398
C	-2.382665	1.437142	0.352203
C	2.056224	2.467043	-0.296995
C	0.740359	-1.822223	-0.027148
N	-0.450242	3.112702	0.009471
N	2.578682	-0.048632	-0.347009
H	1.387751	-3.741970	-0.078701
H	-0.835983	4.975209	-0.004454
H	4.380446	-0.612426	-0.561371
S	-5.358982	2.491662	0.736685

S	4.450496	4.701465	0.364740
C	-3.689171	-3.229209	0.807083
H	-4.548595	-3.029581	2.655557
H	-5.193937	-3.149510	-0.572555
H	-2.828888	-5.085896	0.702207
O	-5.707844	9.007499	2.034455
H	-5.791011	7.224852	2.172004
H	-7.121643	9.483704	1.045321
O	10.672417	2.403921	0.325789
H	9.633319	3.263686	1.510679
H	10.584006	3.437588	-1.139339
O	-0.854330	8.652875	0.139093
H	0.361667	9.376989	1.216026
H	-2.461455	9.207519	0.727221
O	7.745823	-1.810785	-0.699728
H	8.499397	-2.626632	-2.099837
H	8.930821	-0.550479	-0.176763
point09			
C	-1.756744	-1.228210	0.356846
C	-2.394232	1.423242	0.349875
C	2.041673	2.436135	-0.345903
C	0.713844	-1.849834	-0.033996
N	-0.462730	3.095740	-0.016170
N	2.560483	-0.085814	-0.376335
H	1.351676	-3.773330	-0.083195
H	-0.843105	4.957598	-0.031817
H	4.357238	-0.656453	-0.598644
S	-5.370819	2.491266	0.750679
S	4.459971	4.660405	0.396867
C	-3.717309	-3.236451	0.827084

H	-4.568577	-3.031790	2.679114
H	-5.228360	-3.158324	-0.546904
H	-2.863438	-5.096246	0.722883
O	-5.697980	9.012779	2.021655
H	-5.787358	7.231392	2.202070
H	-7.118298	9.470625	1.031866
O	10.705676	2.391448	0.316529
H	9.760466	3.219113	1.598884
H	10.494893	3.437837	-1.126912
O	-0.827628	8.662567	0.153024
H	0.353674	9.391591	1.272581
H	-2.456204	9.200340	0.707738
O	7.754168	-1.811386	-0.723291
H	8.523338	-2.640658	-2.108258
H	8.935946	-0.551641	-0.194455
point10			
C	-1.779096	-1.243549	0.361295
C	-2.405801	1.409339	0.347547
C	2.027124	2.405225	-0.394809
C	0.687329	-1.877445	-0.040843
N	-0.475217	3.078780	-0.041814
N	2.542283	-0.122998	-0.405660
H	1.315599	-3.804690	-0.087691
H	-0.850227	4.939986	-0.059179
H	4.334030	-0.700478	-0.635916
S	-5.382658	2.490871	0.764672
S	4.469446	4.619347	0.428996
C	-3.745445	-3.243692	0.847085
H	-4.588557	-3.033999	2.702671
H	-5.262783	-3.167138	-0.521253

H	-2.897988	-5.106596	0.743560
O	-5.688115	9.018060	2.008856
H	-5.783705	7.237933	2.232137
H	-7.114953	9.457548	1.018411
O	10.738703	2.379071	0.307220
H	9.889708	3.170713	1.675155
H	10.411454	3.431259	-1.106510
O	-0.800926	8.672259	0.166955
H	0.345678	9.406193	1.329135
H	-2.450952	9.193162	0.688253
O	7.762511	-1.811987	-0.746852
H	8.547278	-2.654682	-2.116677
H	8.941071	-0.552802	-0.212148

${}^1\pi_7\pi_8^*$ to ${}^1n_8\pi_8^*$

point01

C	-1.946418	-1.147064	0.457314
C	-2.638058	1.413515	0.451645
C	1.810358	2.441526	0.039684
C	0.561249	-1.853821	0.124722
N	-0.553690	3.150175	0.239995
N	2.422629	0.022677	-0.062361
H	1.250999	-3.749219	0.219208
H	-0.914627	5.028563	0.270231
H	4.251886	-0.481880	-0.228657
S	-5.625717	2.692860	0.621720
S	4.276452	4.724317	0.017008
C	-3.906066	-3.167183	0.854156
H	-4.828252	-2.913958	2.666404
H	-5.361155	-3.067027	-0.572587
H	-3.059468	-5.032343	0.797464

O	-5.761777	8.868487	1.976654
H	-5.793902	7.058129	2.029566
H	-7.186630	9.325800	0.992106
O	10.924511	2.222318	0.262672
H	10.047676	3.348597	1.345485
H	11.221198	3.142616	-1.245330
O	-0.907069	8.649278	0.241885
H	0.094486	9.512883	1.449420
H	-2.626719	9.066908	0.638727
O	7.494656	-1.678077	-0.487549
H	8.114486	-2.624830	-1.874608
H	8.796677	-0.489439	-0.090707

point02

C	-1.901335	-1.137332	0.446610
C	-2.587747	1.419513	0.450048
C	1.854037	2.472620	0.039750
C	0.609015	-1.829778	0.109564
N	-0.522356	3.165066	0.239476
N	2.462557	0.051635	-0.077908
H	1.301985	-3.723962	0.180053
H	-0.889666	5.041595	0.269978
H	4.291143	-0.453472	-0.246129
S	-5.595065	2.668004	0.642237
S	4.294476	4.762382	0.029289
C	-3.857558	-3.162147	0.837959
H	-4.776774	-2.923397	2.653372
H	-5.314549	-3.062895	-0.587714
H	-3.007108	-5.024638	0.771758
O	-5.795306	8.882712	1.954735
H	-5.818111	7.074864	2.018936

H	-7.221195	9.328401	0.967065
O	10.876003	2.259092	0.277332
H	9.926801	3.361326	1.274312
H	11.221865	3.165936	-1.220997
O	-0.938757	8.644087	0.220317
H	0.106968	9.515969	1.365291
H	-2.635038	9.101913	0.641556
O	7.524978	-1.689160	-0.499434
H	8.152297	-2.610305	-1.897860
H	8.812823	-0.490123	-0.090391

point03

C	-1.856250	-1.127600	0.435909
C	-2.537439	1.425511	0.448451
C	1.897716	2.503711	0.039815
C	0.656782	-1.805733	0.094405
N	-0.491023	3.179957	0.238956
N	2.502483	0.080591	-0.093455
H	1.352972	-3.698708	0.140896
H	-0.864705	5.054626	0.269726
H	4.330400	-0.425064	-0.263602
S	-5.564416	2.643149	0.662752
S	4.312502	4.800447	0.041572
C	-3.809053	-3.157113	0.821764
H	-4.725298	-2.932836	2.640339
H	-5.267942	-3.058762	-0.602840
H	-2.954749	-5.016936	0.746053
O	-5.828834	8.896936	1.932816
H	-5.842321	7.091602	2.008305
H	-7.255760	9.331001	0.942023
O	10.827498	2.295866	0.291993

H	9.805927	3.374057	1.203138
H	11.222534	3.189257	-1.196665
O	-0.970446	8.638894	0.198750
H	0.119450	9.519055	1.281161
H	-2.643355	9.136918	0.644383
O	7.555301	-1.700241	-0.511316
H	8.190107	-2.595781	-1.921109
H	8.828967	-0.490807	-0.090074
point04			
C	-1.811166	-1.117867	0.425205
C	-2.487129	1.431509	0.446854
C	1.941393	2.534805	0.039881
C	0.704550	-1.781689	0.079246
N	-0.459689	3.194848	0.238438
N	2.542411	0.109547	-0.109001
H	1.403959	-3.673454	0.101741
H	-0.839741	5.067658	0.269473
H	4.369657	-0.396655	-0.281074
S	-5.533764	2.618293	0.683266
S	4.330529	4.838511	0.053853
C	-3.760546	-3.152078	0.805568
H	-4.673822	-2.942273	2.627307
H	-5.221336	-3.054631	-0.617967
H	-2.902391	-5.009231	0.720345
O	-5.862363	8.911160	1.910897
H	-5.866532	7.108337	1.997675
H	-7.290325	9.333599	0.916982
O	10.778990	2.332638	0.306652
H	9.685050	3.386788	1.131963
H	11.223203	3.212576	-1.172333

O	-1.002135	8.633701	0.177181
H	0.131931	9.522141	1.197032
H	-2.651673	9.171926	0.647212
O	7.585623	-1.711325	-0.523201
H	8.227919	-2.581256	-1.944358
H	8.845111	-0.491491	-0.089758

point05

C	-1.766081	-1.108137	0.414502
C	-2.436819	1.437507	0.445259
C	1.985072	2.565897	0.039947
C	0.752317	-1.757646	0.064088
N	-0.428356	3.209740	0.237918
N	2.582337	0.138506	-0.124548
H	1.454946	-3.648199	0.062586
H	-0.814780	5.080689	0.269220
H	4.408914	-0.368247	-0.298545
S	-5.503113	2.593439	0.703783
S	4.348553	4.876576	0.066137
C	-3.712040	-3.147044	0.789371
H	-4.622344	-2.951713	2.614274
H	-5.174730	-3.050498	-0.633092
H	-2.850032	-5.001529	0.694639
O	-5.895893	8.925384	1.888978
H	-5.890741	7.125073	1.987043
H	-7.324890	9.336199	0.891939
O	10.730485	2.369412	0.321312
H	9.564176	3.399517	1.060790
H	11.223871	3.235897	-1.148001
O	-1.033824	8.628508	0.155613
H	0.144413	9.525227	1.112903

H -2.659990 9.206929 0.650039

O 7.615946 -1.722408 -0.535084

H 8.265730 -2.566732 -1.967609

H 8.861256 -0.492177 -0.089443

point06

C -1.720998 -1.098405 0.403799

C -2.386509 1.443503 0.443662

C 2.028749 2.596990 0.040013

C 0.800084 -1.733601 0.048929

N -0.397020 3.224632 0.237399

N 2.622263 0.167462 -0.140095

H 1.505932 -3.622945 0.023429

H -0.789819 5.093721 0.268967

H 4.448172 -0.339839 -0.316017

S -5.472464 2.568584 0.724298

S 4.366579 4.914643 0.078418

C -3.663535 -3.142010 0.773174

H -4.570868 -2.961152 2.601240

H -5.128123 -3.046365 -0.648220

H -2.797673 -4.993826 0.668933

O -5.929420 8.939610 1.867059

H -5.914950 7.141810 1.976414

H -7.359455 9.338800 0.866899

O 10.681979 2.406186 0.335973

H 9.443300 3.412248 0.989616

H 11.224539 3.259218 -1.123669

O -1.065513 8.623315 0.134046

H 0.156895 9.528311 1.028773

H -2.668308 9.241936 0.652868

O 7.646268 -1.733489 -0.546968

H	8.303540	-2.552207	-1.990859
H	8.877400	-0.492861	-0.089125
point07			
C	-1.675913	-1.088673	0.393095
C	-2.336198	1.449501	0.442066
C	2.072429	2.628084	0.040077
C	0.847850	-1.709558	0.033771
N	-0.365687	3.239523	0.236879
N	2.662191	0.196420	-0.155640
H	1.556919	-3.597691	-0.015726
H	-0.764857	5.106752	0.268715
H	4.487431	-0.311431	-0.333489
S	-5.441812	2.543728	0.744815
S	4.384605	4.952708	0.090701
C	-3.615027	-3.136974	0.756979
H	-4.519392	-2.970589	2.588209
H	-5.081517	-3.042234	-0.663345
H	-2.745315	-4.986122	0.643225
O	-5.962950	8.953834	1.845140
H	-5.939160	7.158545	1.965782
H	-7.394020	9.341398	0.841858
O	10.633472	2.442959	0.350633
H	9.322425	3.424979	0.918441
H	11.225208	3.282537	-1.099337
O	-1.097201	8.618122	0.112478
H	0.169376	9.531397	0.944644
H	-2.676625	9.276941	0.655697
O	7.676591	-1.744572	-0.558851
H	8.341351	-2.537683	-2.014110
H	8.893546	-0.493545	-0.088810

point08

C	-1.630830	-1.078941	0.382394
C	-2.285888	1.455499	0.440469
C	2.116106	2.659175	0.040143
C	0.895617	-1.685513	0.018612
N	-0.334353	3.254415	0.236361
N	2.702117	0.225376	-0.171187
H	1.607906	-3.572437	-0.054883
H	-0.739894	5.119784	0.268462
H	4.526688	-0.283022	-0.350962
S	-5.411161	2.518873	0.765330
S	4.402629	4.990772	0.102983
C	-3.566522	-3.131939	0.740782
H	-4.467913	-2.980028	2.575175
H	-5.034911	-3.038101	-0.678472
H	-2.692956	-4.978419	0.617519
O	-5.996479	8.968058	1.823223
H	-5.963371	7.175281	1.955152
H	-7.428585	9.343998	0.816815
O	10.584966	2.479733	0.365294
H	9.201551	3.437710	0.847266
H	11.225876	3.305859	-1.075005
O	-1.128890	8.612929	0.090909
H	0.181858	9.534483	0.860513
H	-2.684942	9.311947	0.658524
O	7.706912	-1.755656	-0.570735
H	8.379163	-2.523159	-2.037359
H	8.909690	-0.494230	-0.088494

point09

C	-1.585745	-1.069209	0.371690
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C	-2.235580	1.461497	0.438872
C	2.159785	2.690269	0.040210
C	0.943383	-1.661470	0.003454
N	-0.303019	3.269306	0.235842
N	2.742046	0.254334	-0.186733
H	1.658892	-3.547182	-0.094038
H	-0.714933	5.132816	0.268209
H	4.565945	-0.254614	-0.368434
S	-5.380511	2.494017	0.785844
S	4.420655	5.028837	0.115266
C	-3.518014	-3.126905	0.724585
H	-4.416437	-2.989467	2.562142
H	-4.988304	-3.033970	-0.693599
H	-2.640597	-4.970715	0.591813
O	-6.030008	8.982284	1.801304
H	-5.987580	7.192018	1.944521
H	-7.463150	9.346599	0.791774
O	10.536461	2.516507	0.379954
H	9.080674	3.450440	0.776094
H	11.226544	3.329180	-1.050673
O	-1.160577	8.607738	0.069342
H	0.194339	9.537569	0.776385
H	-2.693260	9.346952	0.661353
O	7.737234	-1.766737	-0.582618
H	8.416972	-2.508634	-2.060608
H	8.925834	-0.494914	-0.088178
point10			
C	-1.540662	-1.059477	0.360987
C	-2.185270	1.467495	0.437275
C	2.203464	2.721361	0.040274

C	0.991150	-1.637425	-0.011705
N	-0.271686	3.284199	0.235322
N	2.781972	0.283291	-0.202280
H	1.709879	-3.521928	-0.133194
H	-0.689971	5.145847	0.267956
H	4.605202	-0.226206	-0.385907
S	-5.349860	2.469162	0.806361
S	4.438681	5.066902	0.127547
C	-3.469509	-3.121871	0.708390
H	-4.364961	-2.998905	2.549110
H	-4.941698	-3.029838	-0.708725
H	-2.588239	-4.963012	0.566107
O	-6.063538	8.996508	1.779385
H	-6.011789	7.208753	1.933891
H	-7.497715	9.349197	0.766732
O	10.487954	2.553279	0.394613
H	8.959800	3.463171	0.704919
H	11.227213	3.352499	-1.026340
O	-1.192266	8.602545	0.047774
H	0.206821	9.540655	0.692256
H	-2.701577	9.381957	0.664182
O	7.767557	-1.777820	-0.594502
H	8.454784	-2.494110	-2.083860
H	8.941980	-0.495598	-0.087861

Snapshot3

FC point to ${}^1\pi_7\pi_8^*$

point01

C	-0.232436	-1.632723	0.147399
C	-1.175410	0.950532	0.105825

C	3.167183	2.466093	-0.009449
C	2.303576	-1.948308	0.124722
N	0.616051	2.794905	0.039684
N	3.947640	0.052912	0.060471
H	3.189860	-3.768116	0.164406
H	0.013228	4.614713	-0.060471
H	5.810910	-0.330702	-0.013228
S	-4.229209	1.653510	0.124722
S	5.147616	4.992658	-0.175745
C	-2.027676	-3.828587	0.221098
H	-3.095371	-3.853153	1.965315
H	-3.375053	-3.728432	-1.313360
H	-0.995886	-5.587922	0.062361
O	9.032893	-1.861380	-0.194642
H	10.064685	-0.368497	-0.181414
H	9.628156	-2.847817	-1.564693
O	-0.899510	7.963308	-0.207870
H	-2.386724	8.362040	0.735103
H	0.438416	8.968642	0.419519
O	11.164506	2.981988	-0.500777
H	9.560126	3.743549	-0.823921
H	11.703078	3.694415	1.052577
O	-5.669180	7.702526	2.246884
H	-7.016555	8.112596	1.141395
H	-5.429185	5.929962	2.057912
point02			
C	-0.254161	-1.628364	0.154716
C	-1.196454	0.944544	0.110795
C	3.147515	2.451355	0.005119
C	2.286712	-1.961419	0.137695

N	0.610631	2.797649	0.047963
N	3.935264	0.043898	0.075914
H	3.168914	-3.782429	0.181605
H	0.012939	4.618468	-0.051170
H	5.799605	-0.335608	0.001364
S	-4.251786	1.678398	0.111643
S	5.154872	4.974700	-0.158300
C	-2.052411	-3.822032	0.224481
H	-3.116939	-3.847263	1.970597
H	-3.402329	-3.711913	-1.306400
H	-1.025755	-5.584039	0.059678
O	9.034673	-1.814426	-0.204414
H	10.063636	-0.323582	-0.223137
H	9.619294	-2.823531	-1.559961
O	-0.888895	7.980657	-0.195895
H	-2.401723	8.337715	0.706778
H	0.392052	9.021335	0.459179
O	11.206832	3.015058	-0.566540
H	9.638469	3.857545	-0.766004
H	11.911127	3.712409	0.925773
O	-5.662292	7.690841	2.236022
H	-7.018511	8.083583	1.136419
H	-5.416303	5.916825	2.059679
point03			
C	-0.275883	-1.624002	0.162033
C	-1.217498	0.938555	0.115767
C	3.127848	2.436617	0.019685
C	2.269850	-1.974529	0.150670
N	0.605211	2.800393	0.056244
N	3.922888	0.034884	0.091355

H	3.147968	-3.796743	0.198803
H	0.012650	4.622223	-0.041869
H	5.788301	-0.340514	0.015959
S	-4.274364	1.703284	0.098564
S	5.162131	4.956742	-0.140858
C	-2.077143	-3.815478	0.227863
H	-3.138506	-3.841375	1.975879
H	-3.429607	-3.695395	-1.299440
H	-1.055626	-5.580153	0.056996
O	9.036451	-1.767472	-0.214185
H	10.062589	-0.278668	-0.264858
H	9.610431	-2.799244	-1.555228
O	-0.878279	7.998007	-0.183919
H	-2.416720	8.313391	0.678453
H	0.345688	9.074028	0.498840
O	11.249351	3.048128	-0.632302
H	9.718485	3.976057	-0.701088
H	12.126922	3.721277	0.776976
O	-5.655404	7.679157	2.225160
H	-7.020467	8.054570	1.131443
H	-5.403422	5.903688	2.061444
point04			
C	-0.297607	-1.619643	0.169352
C	-1.238542	0.932565	0.120736
C	3.108182	2.421877	0.034253
C	2.252986	-1.987640	0.163643
N	0.599790	2.803135	0.064523
N	3.910512	0.025870	0.106798
H	3.127024	-3.811058	0.216003
H	0.012361	4.625980	-0.032568

H	5.776997	-0.345419	0.030551
S	-4.296942	1.728172	0.085486
S	5.169389	4.938784	-0.123416
C	-2.101876	-3.808924	0.231246
H	-3.160074	-3.835485	1.981161
H	-3.456885	-3.678877	-1.292480
H	-1.085495	-5.576270	0.054313
O	9.038231	-1.720518	-0.223959
H	10.061541	-0.233753	-0.306582
H	9.601568	-2.774957	-1.550496
O	-0.867664	8.015357	-0.171944
H	-2.431718	8.289066	0.650128
H	0.299323	9.126721	0.538500
O	11.291681	3.081009	-0.697876
H	9.813408	4.090650	-0.629562
H	12.343593	3.719807	0.603947
O	-5.648516	7.667471	2.214300
H	-7.022423	8.025559	1.126468
H	-5.390540	5.890552	2.063211
point05			
C	-0.319332	-1.615281	0.176669
C	-1.259588	0.926576	0.125708
C	3.088515	2.407139	0.048819
C	2.236122	-2.000751	0.176616
N	0.594370	2.805879	0.072802
N	3.898137	0.016858	0.122241
H	3.106079	-3.825373	0.233202
H	0.012072	4.629735	-0.023266
H	5.765692	-0.350325	0.045144
S	-4.319521	1.753059	0.072409

S	5.176646	4.920826	-0.105972
C	-2.126609	-3.802371	0.234628
H	-3.181639	-3.829596	1.986440
H	-3.484162	-3.662361	-1.285520
H	-1.115364	-5.572387	0.051629
O	9.040009	-1.673564	-0.233731
H	10.060494	-0.188840	-0.348303
H	9.592703	-2.750668	-1.545762
O	-0.857049	8.032704	-0.159969
H	-2.446715	8.264742	0.621803
H	0.252961	9.179415	0.578162
O	11.334199	3.114080	-0.763638
H	9.923681	4.198524	-0.554474
H	12.553056	3.707433	0.407535
O	-5.641628	7.655787	2.203438
H	-7.024378	7.996546	1.121494
H	-5.377660	5.877415	2.064976

point06

C	-0.341054	-1.610920	0.183986
C	-1.280631	0.920588	0.130678
C	3.068847	2.392401	0.063387
C	2.219258	-2.013860	0.189589
N	0.588950	2.808621	0.081082
N	3.885761	0.007844	0.137684
H	3.085135	-3.839687	0.250400
H	0.011782	4.633491	-0.013965
H	5.754388	-0.355229	0.059738
S	-4.342099	1.777945	0.059330
S	5.183904	4.902868	-0.088528
C	-2.151342	-3.795815	0.238009

H	-3.203207	-3.823708	1.991722
H	-3.511440	-3.645843	-1.278560
H	-1.145234	-5.568503	0.048946
O	9.041788	-1.626610	-0.243503
H	10.059447	-0.143925	-0.390026
H	9.583841	-2.726382	-1.541028
O	-0.846433	8.050054	-0.147994
H	-2.461714	8.240417	0.593478
H	0.206596	9.232108	0.617821
O	11.376529	3.147150	-0.829401
H	10.048108	4.297020	-0.479501
H	12.746802	3.685548	0.191289
O	-5.634740	7.644103	2.192576
H	-7.026334	7.967533	1.116518
H	-5.364778	5.864277	2.066742
point07			
C	-0.362778	-1.606560	0.191303
C	-1.301675	0.914599	0.135650
C	3.049181	2.377661	0.077955
C	2.202395	-2.026971	0.202564
N	0.583530	2.811364	0.089361
N	3.873385	-0.001170	0.153126
H	3.064189	-3.854002	0.267598
H	0.011493	4.637246	-0.004664
H	5.743086	-0.360135	0.074330
S	-4.364678	1.802833	0.046251
S	5.191161	4.884910	-0.071086
C	-2.176076	-3.789262	0.241392
H	-3.224774	-3.817819	1.997004
H	-3.538718	-3.629325	-1.271600

H	-1.175104	-5.564618	0.046264
O	9.043568	-1.579654	-0.253274
H	10.058400	-0.099010	-0.431750
H	9.574978	-2.702095	-1.536296
O	-0.835818	8.067403	-0.136019
H	-2.476711	8.216093	0.565153
H	0.160232	9.284801	0.657481
O	11.419048	3.180220	-0.895163
H	10.184503	4.383966	-0.409135
H	12.918020	3.656556	-0.037543
O	-5.627852	7.632419	2.181713
H	-7.028290	7.938520	1.111543
H	-5.351897	5.851140	2.068507

point08

C	-0.384503	-1.602199	0.198622
C	-1.322719	0.908609	0.140620
C	3.029514	2.362923	0.092521
C	2.185531	-2.040082	0.215536
N	0.578109	2.814108	0.097642
N	3.861011	-0.010184	0.168567
H	3.043245	-3.868317	0.284797
H	0.011204	4.641003	0.004637
H	5.731781	-0.365040	0.088923
S	-4.387256	1.827719	0.033172
S	5.198419	4.866954	-0.053642
C	-2.200809	-3.782708	0.244774
H	-3.246342	-3.811929	2.002286
H	-3.565994	-3.612809	-1.264641
H	-1.204973	-5.560735	0.043581
O	9.045346	-1.532700	-0.263048

H	10.057351	-0.054097	-0.473471
H	9.566115	-2.677806	-1.531563
O	-0.825204	8.084753	-0.124044
H	-2.491710	8.191768	0.536828
H	0.113867	9.337492	0.697143
O	11.461378	3.213290	-0.960926
H	10.329721	4.458794	-0.346591
H	13.063208	3.623565	-0.271620
O	-5.620964	7.620734	2.170851
H	-7.030246	7.909507	1.106567
H	-5.339017	5.838005	2.070272

point09

C	-0.406225	-1.597837	0.205939
C	-1.343763	0.902620	0.145592
C	3.009846	2.348185	0.107089
C	2.168667	-2.053193	0.228509
N	0.572689	2.816850	0.105921
N	3.848635	-0.019198	0.184010
H	3.022299	-3.882631	0.301995
H	0.010915	4.644758	0.013939
H	5.720477	-0.369946	0.103517
S	-4.409835	1.852606	0.020093
S	5.205678	4.848996	-0.036200
C	-2.225542	-3.776155	0.248157
H	-3.267907	-3.806041	2.007566
H	-3.593273	-3.596291	-1.257681
H	-1.234843	-5.556851	0.040897
O	9.047126	-1.485746	-0.272820
H	10.056304	-0.009182	-0.515194
H	9.557250	-2.653519	-1.526831

O	-0.814587	8.102102	-0.112068
H	-2.506707	8.167444	0.508503
H	0.067503	9.390185	0.736802
O	11.503897	3.246172	-1.026688
H	10.480189	4.521117	-0.294657
H	13.182204	3.590017	-0.502873
O	-5.614076	7.609048	2.159989
H	-7.032202	7.880494	1.101591
H	-5.326135	5.824867	2.072039

point10

C	-0.427949	-1.593478	0.213256
C	-1.364807	0.896632	0.150562
C	2.990180	2.333445	0.121655
C	2.151803	-2.066304	0.241484
N	0.567269	2.819594	0.114200
N	3.836259	-0.028212	0.199453
H	3.001356	-3.896946	0.319196
H	0.010626	4.648513	0.023240
H	5.709173	-0.374852	0.118110
S	-4.432413	1.877492	0.007015
S	5.212934	4.831038	-0.018756
C	-2.250275	-3.769601	0.251540
H	-3.289475	-3.800150	2.012847
H	-3.620551	-3.579772	-1.250721
H	-1.264712	-5.552968	0.038216
O	9.048904	-1.438792	-0.282592
H	10.055257	0.035733	-0.556917
H	9.548387	-2.629233	-1.522097
O	-0.803973	8.119452	-0.100093
H	-2.521705	8.143119	0.480178

H	0.021140	9.442878	0.776464
O	11.546227	3.279278	-1.092347
H	10.632805	4.571459	-0.255338
H	13.275192	3.558128	-0.725916
O	-5.607188	7.597364	2.149127
H	-7.034158	7.851483	1.096616
H	-5.313254	5.811730	2.073806

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point01

C	-0.232436	-1.632723	0.147399
C	-1.175410	0.950532	0.105825
C	3.167183	2.466093	-0.009449
C	2.303576	-1.948308	0.124722
N	0.616051	2.794905	0.039684
N	3.947640	0.052912	0.060471
H	3.189860	-3.768116	0.164406
H	0.013228	4.614713	-0.060471
H	5.810910	-0.330702	-0.013228
S	-4.229209	1.653510	0.124722
S	5.147616	4.992658	-0.175745
C	-2.027676	-3.828587	0.221098
H	-3.095371	-3.853153	1.965315
H	-3.375053	-3.728432	-1.313360
H	-0.995886	-5.587922	0.062361
O	9.032893	-1.861380	-0.194642
H	10.064685	-0.368497	-0.181414
H	9.628156	-2.847817	-1.564693
O	-0.899510	7.963308	-0.207870
H	-2.386724	8.362040	0.735103
H	0.438416	8.968642	0.419519

O	11.164506	2.981988	-0.500777
H	9.560126	3.743549	-0.823921
H	11.703078	3.694415	1.052577
O	-5.669180	7.702526	2.246884
H	-7.016555	8.112596	1.141395
H	-5.429185	5.929962	2.057912

point02

C	-0.248612	-1.630289	0.157095
C	-1.180391	0.958588	0.110449
C	3.164229	2.455493	0.031872
C	2.285114	-1.956235	0.143857
N	0.612232	2.798021	0.054349
N	3.940621	0.033323	0.090276
H	3.158900	-3.781247	0.183354
H	0.016658	4.618426	-0.045830
H	5.800558	-0.357542	0.019511
S	-4.235075	1.672317	0.108355
S	5.168250	4.972716	-0.210901
C	-2.052554	-3.818696	0.222228
H	-3.127170	-3.840989	1.962464
H	-3.393438	-3.714015	-1.317474
H	-1.027805	-5.582599	0.067082
O	9.049473	-1.839325	-0.189203
H	10.076562	-0.346179	-0.199100
H	9.647944	-2.846113	-1.540764
O	-0.895643	7.985448	-0.194115
H	-2.401129	8.357225	0.724510
H	0.403162	9.024861	0.442487
O	11.196438	3.010523	-0.537438
H	9.643499	3.789889	-0.988945

H	11.625325	3.761991	1.035532
O	-5.675356	7.710156	2.244928
H	-7.024006	8.091371	1.133354
H	-5.439461	5.937818	2.104063
point03			
C	-0.264788	-1.627855	0.166791
C	-1.185372	0.966644	0.115071
C	3.161276	2.444892	0.073195
C	2.266651	-1.964161	0.162993
N	0.608412	2.801137	0.069013
N	3.933605	0.013735	0.120083
H	3.127941	-3.794381	0.202303
H	0.020088	4.622142	-0.031190
H	5.790204	-0.384380	0.052253
S	-4.240940	1.691122	0.091988
S	5.188886	4.952774	-0.246057
C	-2.077433	-3.808803	0.223358
H	-3.158966	-3.828825	1.959612
H	-3.411825	-3.699596	-1.321586
H	-1.059726	-5.577277	0.071802
O	9.066054	-1.817268	-0.183765
H	10.088441	-0.323861	-0.216786
H	9.667729	-2.844406	-1.516834
O	-0.891775	8.007588	-0.180359
H	-2.415533	8.352410	0.713916
H	0.367907	9.081081	0.465457
O	11.228186	3.038869	-0.574099
H	9.730090	3.836497	-1.159235
H	11.540590	3.825949	1.008870
O	-5.681532	7.717789	2.242971

H	-7.031457	8.070145	1.125315
H	-5.449740	5.945674	2.150214
point04			
C	-0.280963	-1.625421	0.176487
C	-1.190354	0.974702	0.119695
C	3.158322	2.434292	0.114516
C	2.248188	-1.972088	0.182128
N	0.604593	2.804252	0.083677
N	3.926586	-0.005854	0.149887
H	3.096981	-3.807515	0.221251
H	0.023518	4.625857	-0.016548
H	5.779852	-0.411220	0.084992
S	-4.246806	1.709926	0.075621
S	5.209519	4.932831	-0.281214
C	-2.102313	-3.798915	0.224488
H	-3.190763	-3.816661	1.956758
H	-3.430212	-3.685181	-1.325700
H	-1.091646	-5.571954	0.076521
O	9.082634	-1.795211	-0.178326
H	10.100320	-0.301544	-0.234472
H	9.687517	-2.842702	-1.492904
O	-0.887909	8.029728	-0.166606
H	-2.429938	8.347595	0.703322
H	0.332654	9.137300	0.488424
O	11.260122	3.067403	-0.610759
H	9.829225	3.878011	-1.330719
H	11.451693	3.887269	0.974802
O	-5.687709	7.725420	2.241013
H	-7.038909	8.048920	1.117274
H	-5.460018	5.953531	2.196364

point05

C	-0.297139	-1.622988	0.186183
C	-1.195335	0.982758	0.124318
C	3.155368	2.423691	0.155838
C	2.229726	-1.980013	0.201263
N	0.600774	2.807368	0.098341
N	3.919570	-0.025443	0.179692
H	3.066024	-3.820646	0.240199
H	0.026946	4.629570	-0.001909
H	5.769498	-0.438057	0.117734
S	-4.252672	1.728733	0.059256
S	5.230155	4.912889	-0.316372
C	-2.127191	-3.789024	0.225618
H	-3.222559	-3.804497	1.953907
H	-3.448599	-3.670763	-1.329813
H	-1.123567	-5.566632	0.081241
O	9.099215	-1.773155	-0.172885
H	10.112198	-0.279226	-0.252157
H	9.707302	-2.840995	-1.468975
O	-0.884042	8.051870	-0.152851
H	-2.444342	8.342780	0.692728
H	0.297399	9.193519	0.511392
O	11.291869	3.095938	-0.647420
H	9.940472	3.914218	-1.500082
H	11.360021	3.944765	0.933001
O	-5.693885	7.733052	2.239055
H	-7.046360	8.027695	1.109233
H	-5.470294	5.961387	2.242513

point06

C	-0.313315	-1.620554	0.195880
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C	-1.200316	0.990814	0.128942
C	3.152415	2.413091	0.197159
C	2.211263	-1.987941	0.220399
N	0.596955	2.810482	0.113006
N	3.912553	-0.045034	0.209497
H	3.035065	-3.833780	0.259146
H	0.030375	4.633285	0.012733
H	5.759146	-0.464897	0.150473
S	-4.258538	1.747537	0.042889
S	5.250789	4.892947	-0.351529
C	-2.152069	-3.779133	0.226748
H	-3.254356	-3.792333	1.951053
H	-3.466986	-3.656348	-1.333926
H	-1.155486	-5.561309	0.085962
O	9.115795	-1.751098	-0.167447
H	10.124075	-0.256910	-0.269842
H	9.727087	-2.839289	-1.445045
O	-0.880174	8.074010	-0.139095
H	-2.458747	8.337965	0.682134
H	0.262145	9.249739	0.534360
O	11.323806	3.124284	-0.683892
H	10.062871	3.944063	-1.664144
H	11.267169	3.998260	0.883220
O	-5.700060	7.740683	2.237099
H	-7.053811	8.006469	1.101193
H	-5.480572	5.969242	2.288664
point07			
C	-0.329491	-1.618120	0.205576
C	-1.205298	0.998870	0.133564
C	3.149461	2.402490	0.238480

C	2.192802	-1.995866	0.239534
N	0.593136	2.813598	0.127670
N	3.905535	-0.064623	0.239304
H	3.004105	-3.846914	0.278094
H	0.033805	4.637001	0.027375
H	5.748793	-0.491735	0.183213
S	-4.264403	1.766342	0.026522
S	5.271423	4.873005	-0.386685
C	-2.176947	-3.769242	0.227878
H	-3.286152	-3.780168	1.948202
H	-3.485373	-3.641929	-1.338039
H	-1.187406	-5.555988	0.090682
O	9.132376	-1.729041	-0.162008
H	10.135954	-0.234592	-0.287527
H	9.746875	-2.837584	-1.421116
O	-0.876308	8.096150	-0.125340
H	-2.473151	8.333148	0.671541
H	0.226890	9.305958	0.557329
O	11.355553	3.152819	-0.720553
H	10.194026	3.967777	-1.820364
H	11.175411	4.047198	0.825578
O	-5.706236	7.748316	2.235142
H	-7.061262	7.985244	1.093154
H	-5.490849	5.977098	2.334815
point08			
C	-0.345665	-1.615686	0.215272
C	-1.210279	1.006925	0.138188
C	3.146507	2.391891	0.279802
C	2.174338	-2.003794	0.258669
N	0.589315	2.816714	0.142334

N	3.898518	-0.084212	0.269108
H	2.973148	-3.860045	0.297042
H	0.037235	4.640714	0.042014
H	5.738441	-0.518575	0.215954
S	-4.270269	1.785149	0.010155
S	5.292059	4.853062	-0.421842
C	-2.201826	-3.759349	0.229008
H	-3.317949	-3.768004	1.945350
H	-3.503758	-3.627514	-1.342153
H	-1.219327	-5.550664	0.095403
O	9.148956	-1.706986	-0.156569
H	10.147833	-0.212275	-0.305213
H	9.766660	-2.835878	-1.397186
O	-0.872441	8.118290	-0.111586
H	-2.487556	8.328333	0.660947
H	0.191635	9.362178	0.580297
O	11.387490	3.181354	-0.757213
H	10.331520	3.985771	-1.965818
H	11.086180	4.091348	0.760683
O	-5.712412	7.755946	2.233184
H	-7.068713	7.964018	1.085113
H	-5.501127	5.984955	2.380966

point09

C	-0.361841	-1.613252	0.224968
C	-1.215260	1.014981	0.142812
C	3.143554	2.381289	0.321123
C	2.155875	-2.011719	0.277805
N	0.585496	2.819829	0.157000
N	3.891500	-0.103801	0.298913
H	2.942188	-3.873179	0.315991

H	0.040665	4.644429	0.056656
H	5.728089	-0.545413	0.248694
S	-4.276135	1.803953	-0.006212
S	5.312693	4.833120	-0.456998
C	-2.226704	-3.749459	0.230138
H	-3.349746	-3.755840	1.942497
H	-3.522145	-3.613096	-1.346267
H	-1.251246	-5.545343	0.100121
O	9.165536	-1.684929	-0.151131
H	10.159710	-0.189957	-0.322899
H	9.786448	-2.834172	-1.373256
O	-0.868573	8.140430	-0.097831
H	-2.501960	8.323518	0.650353
H	0.156382	9.418399	0.603265
O	11.419237	3.209700	-0.793874
H	10.472811	3.998645	-2.099527
H	11.001464	4.130921	0.689264
O	-5.718587	7.763577	2.231226
H	-7.076165	7.942793	1.077072
H	-5.511405	5.992811	2.427117
point10			
C	-0.378017	-1.610818	0.234664
C	-1.220242	1.023037	0.147435
C	3.140600	2.370690	0.362446
C	2.137414	-2.019647	0.296940
N	0.581677	2.822945	0.171665
N	3.884483	-0.123390	0.328718
H	2.911229	-3.886312	0.334939
H	0.044095	4.648144	0.071296
H	5.717735	-0.572253	0.281433

S	-4.282000	1.822758	-0.022578
S	5.333329	4.813180	-0.492155
C	-2.251582	-3.739568	0.231268
H	-3.381542	-3.743676	1.939645
H	-3.540532	-3.598681	-1.350379
H	-1.283168	-5.540019	0.104842
O	9.182117	-1.662872	-0.145690
H	10.171589	-0.167639	-0.340585
H	9.806233	-2.832467	-1.349327
O	-0.864707	8.162570	-0.084076
H	-2.516365	8.318703	0.639759
H	0.121128	9.474618	0.626233
O	11.451128	3.238212	-0.830546
H	10.615416	4.006737	-2.219549
H	10.923518	4.164110	0.609333
O	-5.724765	7.771210	2.229268
H	-7.083616	7.921568	1.069031
H	-5.521681	6.000667	2.473266

${}^1\Pi_{7\Pi_8}^*$ to ${}^1n_{8\Pi_8}^*$

point01

C	-0.413850	-1.625164	0.221098
C	-1.349264	0.865495	0.158737
C	3.006554	2.299797	0.130391
C	2.165626	-2.099486	0.249444
N	0.583925	2.787346	0.122832
N	3.851264	-0.062361	0.207870
H	3.014113	-3.930632	0.326923
H	0.028346	4.616603	0.032125
H	5.723982	-0.410071	0.126612
S	-4.416292	1.848152	0.015118

S	5.230764	4.796127	-0.009449
C	-2.237436	-3.800241	0.258892
H	-3.276787	-3.830477	2.020117
H	-3.607489	-3.609377	-1.243440
H	-1.252888	-5.584143	0.045353
O	9.063128	-1.475876	-0.274010
H	10.070354	-0.001890	-0.548021
H	9.562016	-2.666404	-1.513671
O	-0.784236	8.088030	-0.090707
H	-2.501997	8.112596	0.489439
H	0.041574	9.410838	0.786126
O	11.563238	3.240880	-1.082813
H	10.650500	4.533455	-0.245664
H	13.292337	3.518670	-0.716206
O	-5.587922	7.568355	2.158067
H	-7.014665	7.823468	1.105490
H	-5.295014	5.782564	2.082478

point02

C	-0.398487	-1.622800	0.214153
C	-1.327039	0.864550	0.154345
C	3.024044	2.315823	0.115568
C	2.182647	-2.088873	0.236427
N	0.590307	2.788191	0.114710
N	3.864414	-0.049112	0.191754
H	3.033759	-3.919439	0.309475
H	0.031471	4.614961	0.023399
H	5.737112	-0.399658	0.110927
S	-4.414808	1.821991	0.028136
S	5.225934	4.816027	-0.027779
C	-2.218002	-3.800714	0.256094

H	-3.260309	-3.829868	2.015629
H	-3.585513	-3.620037	-1.250029
H	-1.228515	-5.581943	0.049044
O	9.061055	-1.516250	-0.262814
H	10.071515	-0.040434	-0.503824
H	9.571236	-2.685373	-1.515715
O	-0.796873	8.073218	-0.102115
H	-2.491944	8.137123	0.513509
H	0.081275	9.365286	0.749972
O	11.524117	3.214235	-1.014405
H	10.502489	4.491316	-0.283192
H	13.202846	3.555382	-0.490174
O	-5.595768	7.576876	2.165717
H	-7.016810	7.847624	1.110613
H	-5.308632	5.792963	2.079602
point03			
C	-0.383123	-1.620436	0.207208
C	-1.304814	0.863607	0.149954
C	3.041533	2.331848	0.100745
C	2.199668	-2.078260	0.223411
N	0.596687	2.789034	0.106590
N	3.877565	-0.035863	0.175639
H	3.053402	-3.908248	0.292027
H	0.034599	4.613320	0.014672
H	5.750242	-0.389248	0.095242
S	-4.413327	1.795828	0.041154
S	5.221104	4.835928	-0.046109
C	-2.198566	-3.801188	0.253295
H	-3.243830	-3.829258	2.011139
H	-3.563540	-3.630693	-1.256619

H	-1.204141	-5.579743	0.052733
O	9.058980	-1.556624	-0.251619
H	10.072677	-0.078977	-0.459629
H	9.580454	-2.704342	-1.517758
O	-0.809508	8.058406	-0.113523
H	-2.481889	8.161648	0.537576
H	0.120976	9.319732	0.713816
O	11.484999	3.187590	-0.945997
H	10.356973	4.437190	-0.333312
H	13.087688	3.593477	-0.256090
O	-5.603616	7.585395	2.173366
H	-7.018955	7.871779	1.115736
H	-5.322247	5.803360	2.076724

point04

C	-0.367760	-1.618072	0.200264
C	-1.282589	0.862662	0.145562
C	3.059023	2.347875	0.085922
C	2.216688	-2.067648	0.210396
N	0.603066	2.789876	0.098468
N	3.890716	-0.022616	0.159523
H	3.073046	-3.897056	0.274579
H	0.037725	4.611680	0.005945
H	5.763372	-0.378835	0.079559
S	-4.411845	1.769666	0.054173
S	5.216275	4.855829	-0.064442
C	-2.179132	-3.801660	0.250496
H	-3.227354	-3.828649	2.006651
H	-3.541564	-3.641353	-1.263208
H	-1.179767	-5.577544	0.056423
O	9.056906	-1.596998	-0.240422

H	10.073837	-0.117522	-0.415432
H	9.589674	-2.723311	-1.519801
O	-0.822144	8.043597	-0.124932
H	-2.471835	8.186173	0.561646
H	0.160678	9.274181	0.677661
O	11.445693	3.160945	-0.877589
H	10.216424	4.371054	-0.393993
H	12.946293	3.631050	-0.019373
O	-5.611462	7.593915	2.181014
H	-7.021100	7.895935	1.120859
H	-5.335865	5.813759	2.073848

point05

C	-0.352396	-1.615708	0.193321
C	-1.260364	0.861719	0.141170
C	3.076512	2.363900	0.071099
C	2.233709	-2.057035	0.197380
N	0.609448	2.790719	0.090346
N	3.903866	-0.009367	0.143408
H	3.092690	-3.885865	0.257129
H	0.040852	4.610038	-0.002780
H	5.776502	-0.368425	0.063875
S	-4.410364	1.743503	0.067191
S	5.211445	4.875730	-0.082772
C	-2.159696	-3.802135	0.247698
H	-3.210875	-3.828041	2.002161
H	-3.519590	-3.652009	-1.269798
H	-1.155394	-5.575346	0.060114
O	9.054832	-1.637372	-0.229226
H	10.074999	-0.156067	-0.371237
H	9.598892	-2.742278	-1.521844

O	-0.834779	8.028785	-0.136342
H	-2.461780	8.210697	0.585713
H	0.200379	9.228627	0.641505
O	11.406576	3.134300	-0.809181
H	10.084801	4.292726	-0.462350
H	12.779237	3.664566	0.212555
O	-5.619310	7.602434	2.188664
H	-7.023245	7.920090	1.125982
H	-5.349482	5.824159	2.070972

point06

C	-0.337033	-1.613344	0.186376
C	-1.238137	0.860774	0.136780
C	3.094001	2.379927	0.056276
C	2.250728	-2.046420	0.184364
N	0.615828	2.791562	0.082224
N	3.917019	0.003881	0.127292
H	3.112334	-3.874672	0.239682
H	0.043978	4.608398	-0.011507
H	5.789633	-0.358012	0.048190
S	-4.408882	1.717342	0.080209
S	5.206615	4.895632	-0.101102
C	-2.140262	-3.802607	0.244897
H	-3.194397	-3.827432	1.997673
H	-3.497615	-3.662667	-1.276387
H	-1.131020	-5.573146	0.063805
O	9.052758	-1.677744	-0.218031
H	10.076160	-0.194612	-0.327040
H	9.608112	-2.761247	-1.523888
O	-0.847416	8.013973	-0.147750
H	-2.451725	8.235224	0.609783

H	0.240080	9.183073	0.605351
O	11.367459	3.107655	-0.740773
H	9.964790	4.202904	-0.535142
H	12.589962	3.691215	0.431519
O	-5.627157	7.610955	2.196313
H	-7.025389	7.944246	1.131107
H	-5.363099	5.834556	2.068094

point07

C	-0.321669	-1.610980	0.179431
C	-1.215912	0.859829	0.132389
C	3.111491	2.395952	0.041453
C	2.267749	-2.035808	0.171347
N	0.622209	2.792405	0.074102
N	3.930169	0.017128	0.111176
H	3.131979	-3.863481	0.222234
H	0.047105	4.606755	-0.020233
H	5.802763	-0.347600	0.032505
S	-4.407399	1.691178	0.093228
S	5.201787	4.915533	-0.119434
C	-2.120826	-3.803081	0.242098
H	-3.177918	-3.826824	1.993183
H	-3.475641	-3.673327	-1.282977
H	-1.106646	-5.570947	0.067493
O	9.050683	-1.718118	-0.206834
H	10.077322	-0.233156	-0.282845
H	9.617330	-2.780216	-1.525931
O	-0.860052	7.999162	-0.159158
H	-2.441672	8.259749	0.633850
H	0.279782	9.137521	0.569195
O	11.328152	3.081009	-0.672365

H	9.858858	4.103928	-0.607987
H	12.384842	3.708272	0.631197
O	-5.635005	7.619476	2.203963
H	-7.027536	7.968401	1.136230
H	-5.376717	5.844955	2.065217

point08

C	-0.306306	-1.608616	0.172487
C	-1.193687	0.858884	0.127997
C	3.128978	2.411978	0.026630
C	2.284770	-2.025195	0.158331
N	0.628589	2.793248	0.065982
N	3.943320	0.030377	0.095061
H	3.151623	-3.852288	0.204786
H	0.050231	4.605115	-0.028960
H	5.815893	-0.337189	0.016820
S	-4.405917	1.665015	0.106246
S	5.196957	4.935434	-0.137765
C	-2.101392	-3.803554	0.239300
H	-3.161442	-3.826215	1.988695
H	-3.453665	-3.683983	-1.289564
H	-1.082273	-5.568747	0.071184
O	9.048610	-1.758492	-0.195638
H	10.078482	-0.271699	-0.238648
H	9.626550	-2.799185	-1.527974
O	-0.872687	7.984350	-0.170567
H	-2.431616	8.284274	0.657919
H	0.319481	9.091967	0.533041
O	11.289035	3.054364	-0.603956
H	9.767900	3.997803	-0.677463
H	12.172491	3.715202	0.807469

O	-5.642851	7.627995	2.211611
H	-7.029681	7.992557	1.141353
H	-5.390334	5.855354	2.062339
point09			
C	-0.290942	-1.606252	0.165542
C	-1.171462	0.857941	0.123605
C	3.146468	2.428003	0.011807
C	2.301790	-2.014582	0.145314
N	0.634971	2.794092	0.057860
N	3.956470	0.043626	0.078945
H	3.171267	-3.841097	0.187338
H	0.053358	4.603473	-0.037687
H	5.829023	-0.326777	0.001138
S	-4.404436	1.638854	0.119264
S	5.192128	4.955334	-0.156095
C	-2.081957	-3.804028	0.236501
H	-3.144963	-3.825607	1.984205
H	-3.431692	-3.694643	-1.296154
H	-1.057899	-5.566549	0.074875
O	9.046535	-1.798866	-0.184443
H	10.079644	-0.310244	-0.194453
H	9.635768	-2.818152	-1.530017
O	-0.885323	7.969540	-0.181975
H	-2.421563	8.308799	0.681989
H	0.359182	9.046416	0.496885
O	11.249918	3.027719	-0.535548
H	9.691738	3.887751	-0.739892
H	11.961127	3.711766	0.959639
O	-5.650699	7.636516	2.219260
H	-7.031826	8.016711	1.146476

H -5.403950 5.865753 2.059463

point10

C -0.275579 -1.603888 0.158597

C -1.149237 0.856996 0.119213

C 3.163957 2.444028 -0.003016

C 2.318811 -2.003968 0.132300

N 0.641350 2.794935 0.049738

N 3.969621 0.056875 0.062830

H 3.190910 -3.829904 0.169890

H 0.056484 4.601833 -0.046414

H 5.842153 -0.316365 -0.014547

S -4.402954 1.612690 0.132283

S 5.187298 4.975235 -0.174426

C -2.062523 -3.804501 0.233702

H -3.128485 -3.824998 1.979717

H -3.409718 -3.705299 -1.302743

H -1.033525 -5.564350 0.078563

O 9.044460 -1.839240 -0.173246

H 10.080804 -0.348789 -0.150256

H 9.644988 -2.837121 -1.532061

O -0.897958 7.954728 -0.193383

H -2.411508 8.333326 0.706056

H 0.398883 9.000862 0.460730

O 11.210744 3.001157 -0.467127

H 9.616249 3.782495 -0.795955

H 11.757109 3.699834 1.090160

O -5.658545 7.645034 2.226910

H -7.033971 8.040868 1.151599

H -5.417567 5.876151 2.056585