Supporting Information

PCCP

Theoretical study on the mechanism of hot exciton combined with aggregation induced emission in efficient red fluorescent molecules

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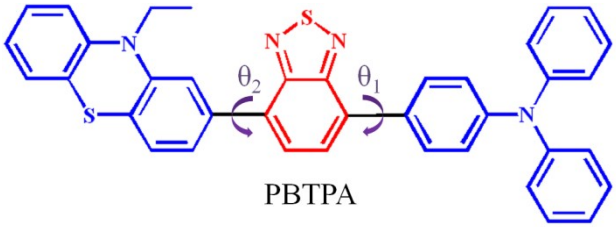
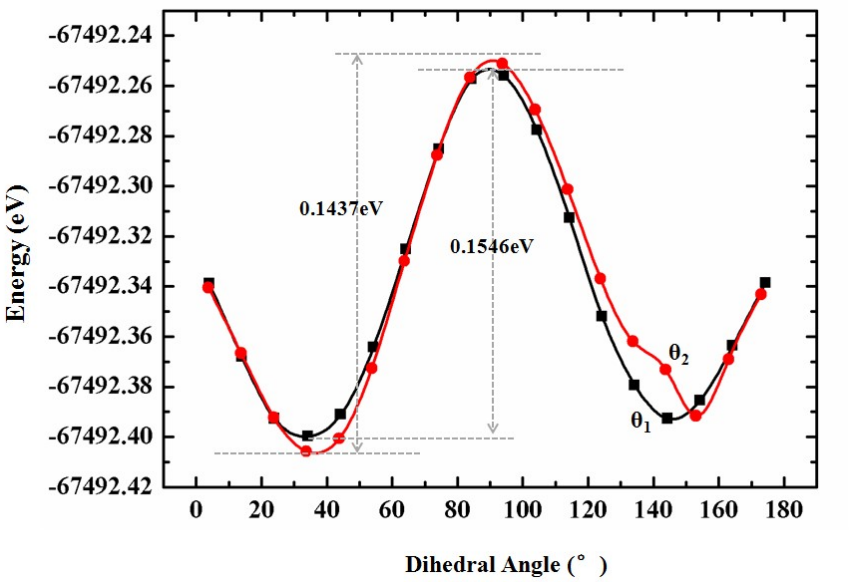
Contents

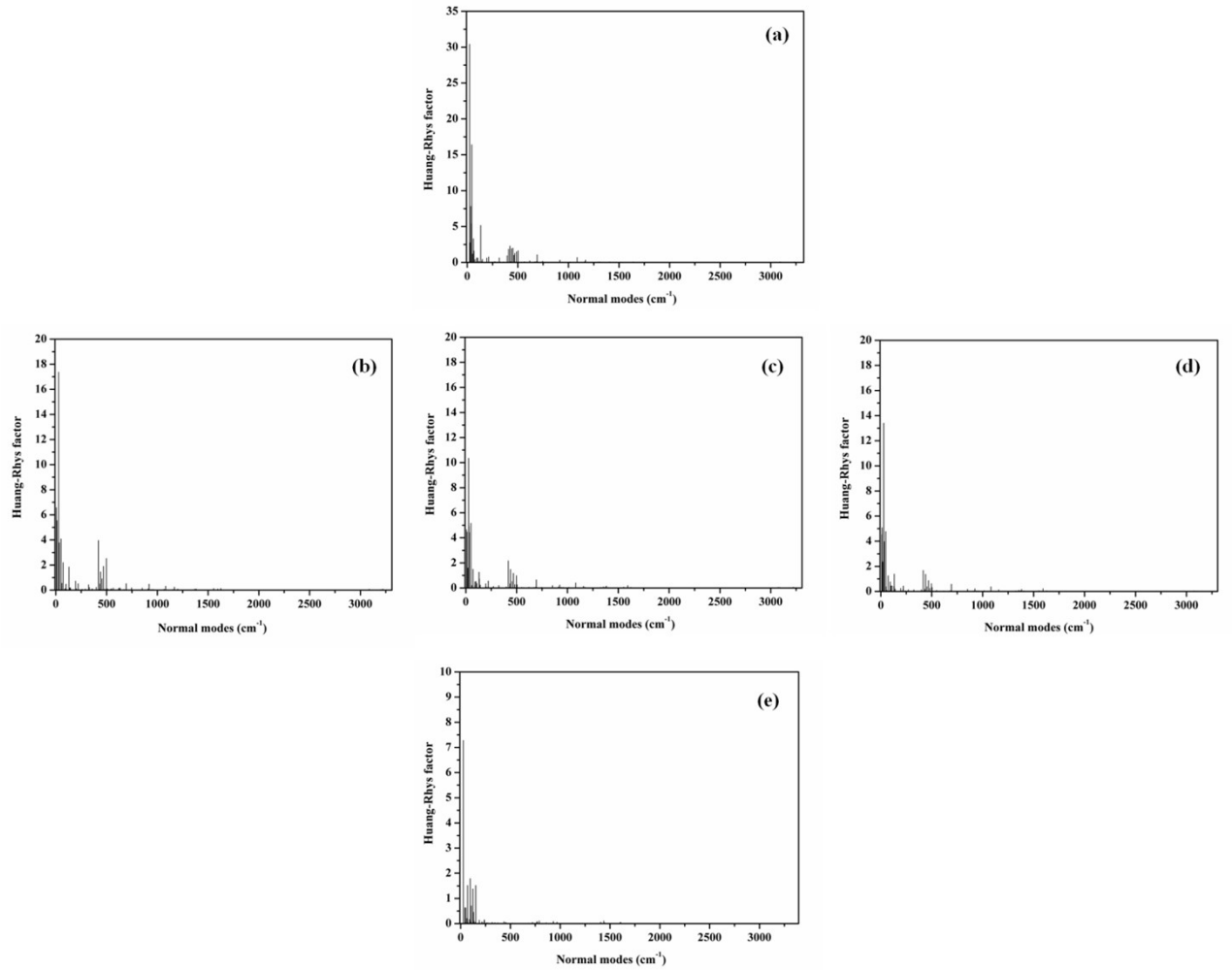
S1: Potential surface scanning of PBTPA in toluene.



PBTPA

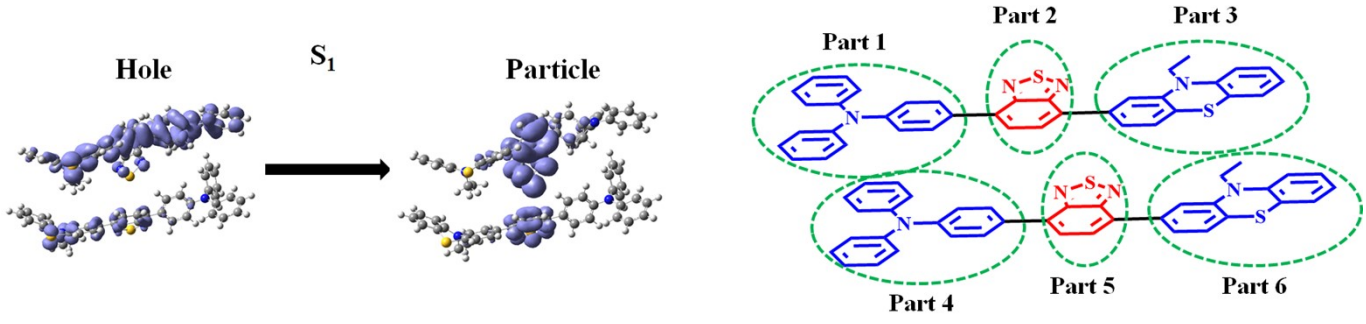


S2: The Huang-Rhys (HR) factor factors versus the normal mode frequencies in vacuum (a), solvents ((b): Toluene, (c): Tetrahydrofuran, (d): Acetonitrile) and (e):Aggregation state.



S3: The transition properties of dimer-4

The transition properties of dimer-4 (with the strongest interaction energy) are analyzed (see Figure S4). As shown in the figure we divide the molecule into 6 parts for calculating the charge transfer ratio, and the calculation results. It is found that the charge transfer during transition only occurs in one molecule, which indicates that dimers are not responsible for emission.



S4: Cartesian coordinates of optimized geometries.

The cartesian coordinates of optimized ground state (S_0) geometry in vacuum

No.	Symbols	X	Y	Z
1	N	-6.69084000	-0.14758800	-0.19250500
2	C	-5.28286100	-0.20813000	-0.06518300
3	C	-4.66086100	-1.31622500	0.53597500
4	C	-4.46938900	0.84040100	-0.52761700
5	C	-3.27873700	-1.37101700	0.65371700
6	C	-3.08827900	0.78491700	-0.39048200
7	C	-2.45350100	-0.32730100	0.19336100
8	C	-7.43421500	-1.32509300	-0.48722600
9	C	-8.62976600	-1.60043000	0.19486400
10	C	-9.36161200	-2.74717000	-0.10675400
11	C	-8.90852300	-3.64456100	-1.07566800
12	C	-7.71545100	-3.37691800	-1.74988500
13	C	-6.98594100	-2.22373700	-1.46831400
14	C	-7.37511100	1.08910700	-0.02104400
15	C	-7.02931500	1.95619900	1.02746400
16	C	-7.69958700	3.16727500	1.18638400
17	C	-8.73456400	3.52520900	0.32019400
18	C	-9.08753800	2.65928100	-0.71661900
19	C	-8.41066000	1.45448600	-0.89524700
20	H	-5.26904400	-2.12586800	0.92419100
21	H	-2.83209600	-2.22416500	1.15517100
22	H	-4.92747600	1.70128000	-1.00204000
23	H	-2.49000800	1.60921700	-0.75781500
24	H	-8.97850800	-0.91199500	0.95728600
25	H	10.28475400	-2.94565500	0.43020700
26	H	-9.47809800	-4.54036000	-1.30287300
27	H	-7.35511000	-4.06170300	-2.51223600
28	H	-6.06752500	-2.01143600	-2.00529500
29	H	-6.23538600	1.67596400	1.71151300
30	H	-7.41913100	3.82714600	2.00232500
31	H	-9.25937500	4.46636800	0.45163800
32	H	-9.88647500	2.92725100	-1.40204700
33	H	-8.67889700	0.79020900	-1.70985400
34	C	-0.98496700	-0.43596000	0.30304100
35	C	-0.33412800	-1.65231500	0.20701200
36	C	-0.12410000	0.69794200	0.52522000
37	C	1.07239700	-1.80503100	0.32342300
38	C	1.32357300	0.54135100	0.64006800
39	C	1.94366600	-0.75463000	0.54152200
40	N	-0.53008400	1.96432700	0.67265800
41	N	1.96119100	1.69690300	0.86592800
42	S	0.81406300	2.87139800	0.92680300
43	H	1.48129500	-2.80262400	0.19883700

44	H	-0.91942100	-2.54182900	-0.00270600
45	C	3.40184800	-0.96974700	0.67412000
46	C	4.32312200	-0.03357400	0.17489200
47	C	3.89045700	-2.14092000	1.27000900
48	C	5.70964100	-0.21686200	0.27844800
49	H	3.93061800	0.85554000	-0.29056600
50	C	5.26232400	-2.34714600	1.36972000
51	H	3.20610900	-2.87148400	1.68731300
52	C	6.16867600	-1.39361000	0.90741000
53	H	5.64350800	-3.24501700	1.84688900
54	C	7.91885200	0.40880800	-0.63335600
55	C	8.59129400	-0.71015800	-0.09587600
56	C	8.61058300	1.17337900	-1.59048700
57	C	9.86455000	-1.06659300	-0.53912000
58	H	8.14730200	2.04611700	-2.02932400
59	C	9.90237700	0.83633400	-1.99683000
60	C	10.53519500	-0.29178200	-1.48530800
61	H	10.33798100	-1.94717100	-0.11499600
62	H	10.40198200	1.46109800	-2.73110900
63	H	11.53337300	-0.56747800	-1.80942000
64	N	6.61601200	0.75442400	-0.20705400
65	S	7.89240200	-1.61431100	1.26740300
66	C	6.10339900	2.09332400	-0.52564700
67	H	5.36463700	2.34536400	0.24029700
68	H	6.93338700	2.79353300	-0.39307400
69	C	5.48359200	2.28004000	-1.92137000
70	H	5.15777400	3.31921000	-2.03746400
71	H	6.19308400	2.05673300	-2.72108200
72	H	4.61424700	1.63704600	-2.07310600

The cartesian coordinates of optimized the first singlet excited state (S_1) geometry in vacuum

No.	Symbols	X	Y	Z
1	N	6.678683	-0.078423	0.067804
2	C	5.27562	-0.179709	0.045335
3	C	4.646882	-1.324823	-0.470938
4	C	4.470772	0.865198	0.524873
5	C	3.269257	-1.414776	-0.49291
6	C	3.091656	0.776485	0.483188
7	C	2.441268	-0.37273	-0.017925
8	C	7.474847	-1.228426	0.289424
9	C	8.649052	-1.426782	-0.44616
10	C	9.432545	-2.551321	-0.217056
11	C	9.05274	-3.498045	0.731693
12	C	7.880443	-3.303825	1.458818
13	C	7.097655	-2.174937	1.24942
14	C	7.308484	1.171794	-0.152356

15	C	6.818338	2.048481	-1.12722
16	C	7.438636	3.274347	-1.334909
17	C	8.560288	3.635825	-0.592038
18	C	9.053416	2.758764	0.371287
19	C	8.430942	1.537468	0.599365
20	H	5.252711	-2.130079	-0.873199
21	H	2.818066	-2.292426	-0.943018
22	H	4.942306	1.750842	0.938081
23	H	2.494375	1.596715	0.857181
24	H	8.937577	-0.694005	-1.192657
25	H	10.340244	-2.693506	-0.794785
26	H	9.664164	-4.377396	0.903111
27	H	7.577149	-4.029534	2.206671
28	H	6.190671	-2.014817	1.823196
29	H	5.950506	1.761247	-1.71176
30	H	7.047625	3.945614	-2.092668
31	H	9.044706	4.591362	-0.761679
32	H	9.922603	3.030949	0.96149
33	H	8.806169	0.857892	1.357617
34	C	0.990465	-0.511445	-0.045393
35	C	0.392392	-1.788817	-0.056649
36	C	0.095187	0.608272	-0.062498
37	C	-0.974161	-1.979574	-0.120609
38	C	-1.348538	0.41266	-0.132007
39	C	-1.900963	-0.911485	-0.184638
40	N	0.459404	1.889806	-0.051349
41	N	-2.030156	1.560996	-0.164529
42	S	-0.922058	2.79758	-0.111857
43	H	-1.338416	-2.998233	-0.069245
44	H	1.026171	-2.663038	0.040181
45	C	-3.325397	-1.177578	-0.298382
46	C	-4.27777	-0.16416	-0.11532
47	C	-3.815636	-2.480207	-0.597849
48	C	-5.649643	-0.381743	-0.228552
49	H	-3.901822	0.815847	0.119153
50	C	-5.166709	-2.721369	-0.688909
51	H	-3.132326	-3.297971	-0.785253
52	C	-6.102158	-1.693483	-0.506631
53	H	-5.526415	-3.720204	-0.917004
54	C	-7.898502	0.533304	0.17587
55	C	-8.570627	-0.688763	-0.048245
56	C	-8.668231	1.605351	0.670427
57	C	-9.936793	-0.817016	0.214611
58	H	-8.199922	2.556506	0.881067
59	C	-10.025068	1.468652	0.914723
60	C	-10.672724	0.254575	0.690416
61	H	-10.413736	-1.775728	0.034338

62	H	-10.578096	2.320303	1.295602
63	H	-11.73235	0.144573	0.889066
64	N	-6.53987	0.691103	-0.094048
65	S	-7.777735	-2.079619	-0.755837
66	C	-5.981247	2.050602	-0.102568
67	H	-5.140251	2.052056	-0.798203
68	H	-6.741428	2.706594	-0.531348
69	C	-5.531878	2.551226	1.27031
70	H	-5.193272	3.586658	1.186571
71	H	-6.344265	2.508706	1.999649
72	H	-4.701516	1.957381	1.6558

The cartesian coordinates of optimized the first triplet excited state (T_1) geometry in vacuum

No.	Symbols	X	Y	Z
1	N	6.67653500	-0.10414400	0.04000100
2	C	5.28268800	-0.18013800	0.07827000
3	C	4.61218200	-1.37998600	-0.23361500
4	C	4.50508400	0.94338800	0.42186300
5	C	3.23824500	-1.44528400	-0.19714700
6	C	3.12978100	0.87928900	0.44389000
7	C	2.43018400	-0.32181800	0.13733300
8	C	7.47617700	-1.25222500	0.28821900
9	C	8.57621000	-1.52728800	-0.52934000
10	C	9.36970200	-2.63965800	-0.27431300
11	C	9.06940200	-3.49385400	0.78412500
12	C	7.97045400	-3.22066900	1.59535000
13	C	7.18044400	-2.10142100	1.35898100
14	C	7.32722200	1.11850000	-0.28227500
15	C	6.86479000	1.90710500	-1.34002200
16	C	7.51049200	3.09828800	-1.65063400
17	C	8.62991400	3.50392100	-0.92784700
18	C	9.09674400	2.71010400	0.11726200
19	C	8.44771500	1.52586200	0.44697100
20	H	5.18710800	-2.25120500	-0.52754000
21	H	2.77272200	-2.37670000	-0.49552600
22	H	5.00210900	1.87045300	0.68604000
23	H	2.56515600	1.75731900	0.72284900
24	H	8.80096400	-0.86295400	-1.35750400
25	H	10.22146800	-2.84470700	-0.91462900
26	H	9.68774700	-4.36390000	0.97676600
27	H	7.73272900	-3.87404100	2.42852300
28	H	6.33171000	-1.87578900	1.99679100
29	H	5.99959700	1.58077800	-1.90817800
30	H	7.14261700	3.70495100	-2.47164600
31	H	9.13506900	4.43064400	-1.17771500
32	H	9.96579100	3.01862400	0.68916900

33	H	8.80169600	0.90716700	1.26538800
34	C	1.00321500	-0.42294300	0.14721900
35	C	0.35554500	-1.74606700	0.15052000
36	C	0.09772300	0.69666100	0.16501500
37	C	-0.97132500	-1.92214600	0.06608600
38	C	-1.35501800	0.50410100	0.06861400
39	C	-1.92904900	-0.80923400	-0.05124000
40	N	0.45554800	1.96694900	0.21595500
41	N	-2.03028000	1.64386800	0.05717900
42	S	-0.93485300	2.90405700	0.16924000
43	H	-1.36283900	-2.92727500	0.15194100
44	H	0.97956400	-2.61808900	0.30079600
45	C	-3.32635200	-1.08286100	-0.26570000
46	C	-4.31407700	-0.08156800	-0.11012900
47	C	-3.76311700	-2.37578700	-0.64265500
48	C	-5.66426500	-0.31504700	-0.33935600
49	H	-3.98016800	0.89570500	0.18791300
50	C	-5.10413100	-2.62198000	-0.86448100
51	H	-3.05715100	-3.17921300	-0.80632000
52	C	-6.05769300	-1.61133100	-0.73559700
53	H	-5.43183700	-3.61109300	-1.16889300
54	C	-7.94815300	0.46596300	0.11382300
55	C	-8.55818000	-0.75649600	-0.22277600
56	C	-8.74163700	1.41935600	0.76936000
57	C	-9.87727100	-1.02316800	0.12618700
58	H	-8.32653100	2.38001200	1.04227100
59	C	-10.07340300	1.16064400	1.08035700
60	C	-10.64937400	-0.06431500	0.77402900
61	H	-10.30130300	-1.98772500	-0.13616600
62	H	-10.65366900	1.92936800	1.57984900
63	H	-11.68200700	-0.27457600	1.02806900
64	N	-6.60708700	0.72352600	-0.22133100
65	S	-7.71101500	-1.94380400	-1.22520700
66	C	-6.10886700	2.09174400	-0.08250200
67	H	-5.26315700	2.20082500	-0.76697500
68	H	-6.89470600	2.75446600	-0.45442200
69	C	-5.69111200	2.50283200	1.33350800
70	H	-5.45733000	3.57077200	1.34998600
71	H	-6.48536700	2.31304000	2.05834000
72	H	-4.80445400	1.96285600	1.66954000

The cartesian coordinates of optimized the second triplet excited state (T_2) geometry in vacuum

No.	Symbols	X	Y	Z
1	N	6.73960100	-0.09788400	0.07517200
2	C	5.32823700	-0.17850900	0.00696500
3	C	4.69652000	-1.32472900	-0.51882500
4	C	4.51792100	0.88479300	0.45305100

5	C	3.31086200	-1.40108000	-0.57953700
6	C	3.13095600	0.80830600	0.37910700
7	C	2.47548700	-0.34394800	-0.12817600
8	C	7.49041000	-1.23289700	0.46275900
9	C	8.71633000	-1.53272900	-0.16356700
10	C	9.45034200	-2.65451800	0.22880100
11	C	8.97416300	-3.50391200	1.23531900
12	C	7.75177400	-3.21168300	1.85308700
13	C	7.01627600	-2.08471200	1.47977300
14	C	7.39409000	1.11634800	-0.24191700
15	C	6.92428200	1.92258400	-1.29727000
16	C	7.56458600	3.12589100	-1.60119900
17	C	8.68763100	3.54109900	-0.87483300
18	C	9.15959800	2.73774000	0.17060900
19	C	8.51823600	1.53981400	0.49414500
20	H	5.30464100	-2.14537800	-0.89173000
21	H	2.86404000	-2.28274300	-1.03082500
22	H	4.98779700	1.77462700	0.86523900
23	H	2.53217600	1.64236600	0.72558700
24	H	9.08383000	-0.88300900	-0.95366500
25	H	10.39431900	-2.87114100	-0.26732300
26	H	9.54625800	-4.37949800	1.53280900
27	H	7.37027000	-3.85729900	2.64155200
28	H	6.07270600	-1.85511800	1.96779000
29	H	6.05720700	1.60006600	-1.86766700
30	H	7.18702000	3.73568700	-2.41940500
31	H	9.18599700	4.47641400	-1.11824200
32	H	10.02554200	3.04974600	0.75108900
33	H	8.88026100	0.92603600	1.31488900
34	C	1.01171200	-0.47058600	-0.18250400
35	C	0.39470900	-1.74420600	-0.24566000
36	C	0.11017500	0.65271900	-0.16840600
37	C	-0.98546500	-1.93473900	-0.32952800
38	C	-1.34851300	0.45639400	-0.25843200
39	C	-1.91077600	-0.86662400	-0.35972200
40	N	0.45398900	1.93996900	-0.10036600
41	N	-2.02677000	1.60815700	-0.25429400
42	S	-0.92697800	2.83554500	-0.14304000
43	H	-1.35543800	-2.95618100	-0.32828100
44	H	1.02159600	-2.62934000	-0.18203100
45	C	-3.35744900	-1.11911500	-0.50179100
46	C	-4.29648600	-0.14787700	-0.12969300
47	C	-3.86365600	-2.36449000	-0.99310200
48	C	-5.69354700	-0.34808700	-0.23668300
49	H	-3.90519400	0.77785300	0.26119000
50	C	-5.22522200	-2.59307900	-1.08416700
51	H	-3.17838500	-3.13975500	-1.32049000

52	C	-6.16070000	-1.60836600	-0.71583600
53	H	-5.59003000	-3.54413500	-1.46760400
54	C	-7.92824200	0.49140000	0.36564800
55	C	-8.63217900	-0.66238200	-0.09066700
56	C	-8.68482100	1.47685200	1.05923300
57	C	-10.01356600	-0.79584800	0.13821800
58	H	-8.19673200	2.35823700	1.45380500
59	C	-10.04780900	1.32770600	1.27435500
60	C	-10.72700500	0.18695700	0.81238600
61	H	-10.51507800	-1.69050800	-0.22483100
62	H	-10.58395000	2.10280100	1.81594000
63	H	-11.79319900	0.06770200	0.98483200
64	N	-6.56408200	0.67293500	0.14263900
65	S	-7.86877300	-1.92085600	-1.06013000
66	C	-5.99565300	2.01463800	0.38289400
67	H	-5.15422800	2.14250200	-0.30096600
68	H	-6.75177800	2.74577800	0.08594100
69	C	-5.53985600	2.24334000	1.83668000
70	H	-5.16211700	3.26708000	1.93756100
71	H	-6.36078200	2.10136500	2.54796600
72	H	-4.73400100	1.55378400	2.10641900

The cartesian coordinates of optimized ground state (S_0) geometry in toluene

No.	Symbols	X	Y	Z
1	N	6.69336000	-0.14896400	0.19277600
2	C	5.29049300	-0.20484300	0.05581000
3	C	4.66846000	-1.32443400	-0.53322800
4	C	4.47651500	0.85718400	0.49813600
5	C	3.28238500	-1.37904600	-0.65553800
6	C	3.09109900	0.80158400	0.35596000
7	C	2.45913500	-0.32307900	-0.21253700
8	C	7.43094800	-1.32694100	0.48119900
9	C	8.65498000	-1.57521900	-0.16733900
10	C	9.38611200	-2.72896000	0.12895300
11	C	8.90468000	-3.65892300	1.05889400
12	C	7.68318600	-3.41619100	1.69962800
13	C	6.95320500	-2.25669700	1.42368800
14	C	7.38055200	1.08486600	0.04783800
15	C	7.02915000	1.98345600	-0.97659000
16	C	7.71032700	3.19650700	-1.11073600
17	C	8.75966000	3.52482500	-0.24313800
18	C	9.11596800	2.62673000	0.77062900
19	C	8.42928300	1.41926800	0.92442700
20	H	5.27844200	-2.14440200	-0.90257100
21	H	2.83333900	-2.24236100	-1.14199400

22	H	4.93642700	1.72744500	0.95861400
23	H	2.49004900	1.63432300	0.70715400
24	H	9.02644000	-0.85878900	-0.89588800
25	H	10.33096700	-2.90536300	-0.38107900
26	H	9.47322200	-4.55871100	1.28171400
27	H	7.29943700	-4.12491600	2.43073200
28	H	6.01119900	-2.06503600	1.93154200
29	H	6.22184400	1.72643700	-1.65800600
30	H	7.42573700	3.88055100	-1.90764800
31	H	9.29191100	4.46636000	-0.35585200
32	H	9.92515300	2.86966400	1.45633300
33	H	8.70182600	0.72745900	1.71757900
34	C	0.98374900	-0.43455600	-0.32089500
35	C	0.33197600	-1.64727200	-0.20262100
36	C	0.12391400	0.70264700	-0.56664700
37	C	-1.08547600	-1.79877000	-0.31774100
38	C	-1.32547200	0.54895100	-0.67802200
39	C	-1.95053700	-0.74863000	-0.55372800
40	N	0.51899800	1.96410400	-0.74228600
41	N	-1.94409100	1.70411600	-0.92767500
42	S	-0.80590500	2.85273500	-1.01217600
43	H	-1.49906000	-2.79526900	-0.17964200
44	H	0.91708200	-2.53666500	0.01999200
45	C	-3.41672100	-0.95832500	-0.68651900
46	C	-4.33013900	-0.00972700	-0.18877700
47	C	-3.90443300	-2.13492300	-1.27816600
48	C	-5.72299100	-0.19152000	-0.28766800
49	H	-3.92960200	0.88253600	0.26994100
50	C	-5.28165400	-2.33385300	-1.38224400
51	H	-3.21794200	-2.87113800	-1.68763900
52	C	-6.18225900	-1.36999100	-0.92183100
53	H	-5.67052400	-3.23088500	-1.85953800
54	C	-7.91761900	0.41953000	0.64908100
55	C	-8.60062400	-0.69657600	0.10956700
56	C	-8.59899300	1.17097700	1.63093700
57	C	-9.86547500	-1.07083100	0.57164600
58	H	-8.13750200	2.04551100	2.07152900
59	C	-9.88397600	0.81675000	2.05879100
60	C	-10.52294900	-0.31261100	1.54622600
61	H	-10.34103200	-1.94921500	0.14004300
62	H	-10.37294700	1.43158300	2.81118300
63	H	-11.51423400	-0.59892500	1.88781600
64	N	-6.62626600	0.77209200	0.20592200
65	S	-7.91976500	-1.57402500	-1.29815800
66	C	-6.09993400	2.08650200	0.57996000
67	H	-5.35741100	2.36755700	-0.17471100
68	H	-6.92302500	2.80342400	0.48429800

69	C	-5.47791300	2.18800400	1.99169400
70	H	-5.13337300	3.21536800	2.16314000
71	H	-6.19973800	1.93277700	2.77379700
72	H	-4.62164700	1.51670200	2.10874400

The cartesian coordinates of optimized the first singlet excited state (S_1) geometry in toluene

No.	Symbols	X	Y	Z
1	N	6.72670400	-0.08685600	0.07669300
2	C	5.32258600	-0.18468600	0.05887000
3	C	4.68132300	-1.34615300	-0.42782100
4	C	4.51486900	0.88132500	0.51046600
5	C	3.29620600	-1.42912700	-0.45274300
6	C	3.12836300	0.79810200	0.46779500
7	C	2.46540300	-0.36459200	-0.00753100
8	C	7.52310700	-1.23174800	0.33036000
9	C	8.69624700	-1.46069200	-0.41413700
10	C	9.48407800	-2.58469300	-0.15449000
11	C	9.11194300	-3.50277100	0.83586600
12	C	7.94171700	-3.27902200	1.57270600
13	C	7.15384800	-2.15067200	1.33159900
14	C	7.35897300	1.15420800	-0.19396800
15	C	6.87732400	1.99040600	-1.21921500
16	C	7.50297500	3.21205000	-1.47912600
17	C	8.62210600	3.61173100	-0.73744500
18	C	9.10693600	2.77603700	0.27688300
19	C	8.47981600	1.55895800	0.55555600
20	H	5.28020300	-2.17036300	-0.80631800
21	H	2.84515600	-2.32117500	-0.87854400
22	H	4.98666400	1.77946100	0.90070600
23	H	2.53365800	1.63469600	0.81511600
24	H	8.98152300	-0.75531500	-1.19042000
25	H	10.38678100	-2.74812100	-0.73955700
26	H	9.72512800	-4.37932700	1.03118500
27	H	7.64388600	-3.97870900	2.35091400
28	H	6.25263600	-1.97193200	1.91266700
29	H	6.01463300	1.67753100	-1.80187800
30	H	7.11871800	3.84735000	-2.27435600
31	H	9.10928300	4.56120200	-0.94650100
32	H	9.97112500	3.07629500	0.86587500
33	H	8.85063300	0.91601400	1.34992800
34	C	1.00423900	-0.49242100	-0.04087900
35	C	0.39261200	-1.77240400	-0.07485200
36	C	0.10633500	0.63578600	-0.04556800
37	C	-0.98126800	-1.95777500	-0.14931500
38	C	-1.34812900	0.44364700	-0.12323500
39	C	-1.91109400	-0.88168100	-0.19916900
40	N	0.46827400	1.92166600	-0.01258700
41	N	-2.02707100	1.59777500	-0.14013300

42	S	-0.91462100	2.82828600	-0.06640600
43	H	-1.34773700	-2.97865400	-0.12095100
44	H	1.02026500	-2.65502100	0.00593800
45	C	-3.34686500	-1.14541900	-0.32572400
46	C	-4.31056100	-0.14155400	-0.10043800
47	C	-3.82746200	-2.44420400	-0.68303200
48	C	-5.69266200	-0.36495300	-0.22693500
49	H	-3.94020100	0.83205100	0.17681200
50	C	-5.18263800	-2.69258800	-0.79435800
51	H	-3.13527100	-3.25026500	-0.89991100
52	C	-6.13013800	-1.67536300	-0.57144300
53	H	-5.53306200	-3.68517000	-1.07022300
54	C	-7.96059600	0.51230200	0.20210200
55	C	-8.63539600	-0.70250000	-0.09490100
56	C	-8.74682600	1.56136100	0.74491600
57	C	-10.01329000	-0.84675500	0.13694600
58	H	-8.28656800	2.50189600	1.01822100
59	C	-10.11361100	1.40985900	0.96084600
60	C	-10.76130400	0.20361700	0.65884100
61	H	-10.48739000	-1.79646000	-0.10257100
62	H	-10.67346300	2.24224200	1.38010300
63	H	-11.82689300	0.08342300	0.83360900
64	N	-6.59560500	0.68901600	-0.03626200
65	S	-7.81981700	-2.07749200	-0.85871000
66	C	-6.05506700	2.05719900	0.02197700
67	H	-5.20899500	2.10766500	-0.66818700
68	H	-6.82279400	2.72556200	-0.37784900
69	C	-5.61977800	2.50582200	1.43103600
70	H	-5.28057100	3.54720700	1.38864100
71	H	-6.44517900	2.43656300	2.14808900
72	H	-4.79321800	1.89360500	1.80470400

The cartesian coordinates of optimized the first triplet excited state (T_1) geometry in toluene

No.	Symbols	X	Y	Z
1	N	6.56693300	-0.04912100	-0.27295000
2	C	5.19932600	-0.13974800	0.01975300
3	C	4.52227200	-1.38305900	-0.03957400
4	C	4.44932700	1.00610300	0.38418900
5	C	3.17624800	-1.47438000	0.26685000
6	C	3.10022200	0.91850900	0.68159400
7	C	2.39864800	-0.33085400	0.64624600
8	C	7.44040900	-1.13698700	0.00321500
9	C	8.41196400	-1.51858500	-0.93905000
10	C	9.28146200	-2.57658400	-0.65966900
11	C	9.18599400	-3.27525700	0.55040600
12	C	8.21527600	-2.89799200	1.48679800
13	C	7.35224900	-1.83041100	1.22381200

14	C	7.11040500	1.13632100	-0.84075700
15	C	6.45131100	1.78725400	-1.89903700
16	C	6.99360700	2.95130400	-2.45117200
17	C	8.20329300	3.46927100	-1.97187800
18	C	8.86479100	2.81423100	-0.92548500
19	C	8.32211500	1.65933100	-0.35547900
20	H	5.06681700	-2.27403300	-0.33962700
21	H	2.70323500	-2.44642800	0.17143000
22	H	4.94684700	1.97037100	0.44275300
23	H	2.56370100	1.81349200	0.97359900
24	H	8.48048900	-0.98060800	-1.88139300
25	H	10.02856000	-2.86119900	-1.39758400
26	H	9.86050300	-4.10163600	0.76172700
27	H	8.13582900	-3.42604300	2.43473800
28	H	6.60717500	-1.52893200	1.95605700
29	H	5.51797500	1.37853400	-2.27865900
30	H	6.47253000	3.44574900	-3.26829700
31	H	8.62531600	4.37122500	-2.40879800
32	H	9.80285900	3.20841400	-0.54032800
33	H	8.83090000	1.15517300	0.46248000
34	C	1.00396000	-0.45997400	0.94268400
35	C	0.37094500	-1.83075000	1.04516000
36	C	0.08006200	0.64635100	1.20401200
37	C	-0.94527900	-2.02859300	0.97639800
38	C	-1.37707500	0.43240400	1.12647800
39	C	-1.91701100	-0.88540000	0.76517100
40	N	0.40662500	1.89118600	1.46245300
41	N	-2.07882700	1.51989200	1.33810300
42	S	-1.01159000	2.78615800	1.63880700
43	H	-1.35349300	-3.01674100	1.16687200
44	H	1.02093400	-2.66841800	1.28338600
45	C	-3.23285800	-1.13673000	0.24671200
46	C	-4.21723900	-0.10729500	0.14629600
47	C	-3.59282100	-2.44555200	-0.19224200
48	C	-5.49448600	-0.33538600	-0.37330900
49	H	-3.93877300	0.87340000	0.49760800
50	C	-4.85650900	-2.68103200	-0.71478000
51	H	-2.88392600	-3.26450400	-0.15145900
52	C	-5.80074100	-1.64933400	-0.82707600
53	H	-5.12467600	-3.67599200	-1.06360300
54	C	-7.82342000	0.46085000	-0.44480800
55	C	-8.36835100	-0.76266300	-0.89933100
56	C	-8.73553900	1.43170000	0.02348500
57	C	-9.74195800	-1.01603000	-0.84404000
58	H	-8.37666800	2.38976700	0.37871200
59	C	-10.11321100	1.18820000	0.04052400
60	C	-10.62846100	-0.03869300	-0.38050600

61	H	-10.11182400	-1.97975100	-1.18827500
62	H	-10.77862800	1.96899500	0.40197000
63	H	-11.69688500	-0.23608400	-0.35482300
64	N	-6.43657600	0.70543900	-0.47881000
65	S	-7.32083200	-1.98453400	-1.69106800
66	C	-5.97474900	2.08332900	-0.28999900
67	H	-5.00819500	2.17696500	-0.79753100
68	H	-6.67334700	2.72955800	-0.83230600
69	C	-5.84403900	2.55838500	1.17511800
70	H	-5.63066000	3.63441500	1.18666100
71	H	-6.76601000	2.38391500	1.73936900
72	H	-5.02973500	2.04913600	1.69965700

The cartesian coordinates of optimized the second triplet excited state (T_2) geometry in toluene

No.	Symbols	X	Y	Z
1	N	6.71021300	-0.12656300	0.12321100
2	C	5.29650700	-0.19461800	0.02636700
3	C	4.66507300	-1.33269500	-0.50724800
4	C	4.48926600	0.87530700	0.45098800
5	C	3.28378800	-1.39432200	-0.59782800
6	C	3.10757700	0.81250400	0.34575900
7	C	2.45049100	-0.32990700	-0.17212900
8	C	7.44862700	-1.26916200	0.52890300
9	C	8.66109600	-1.59747600	-0.10173600
10	C	9.38197200	-2.71765100	0.30493800
11	C	8.90498800	-3.53591100	1.33181900
12	C	7.69646800	-3.21596000	1.95515200
13	C	6.97414300	-2.09054300	1.56600200
14	C	7.38674300	1.08267800	-0.18779600
15	C	6.97909900	1.86415800	-1.28243000
16	C	7.64015100	3.05362200	-1.57870200
17	C	8.72208800	3.47810500	-0.80372300
18	C	9.13293100	2.70002600	0.28129100
19	C	8.47021300	1.51603800	0.59556200
20	H	5.26799900	-2.15874500	-0.86965000
21	H	2.84053300	-2.27195100	-1.05528700
22	H	4.95509000	1.75860300	0.87555800
23	H	2.51051100	1.65283000	0.67306900
24	H	9.02784900	-0.97448700	-0.91023200
25	H	10.31557800	-2.95915100	-0.19485900
26	H	9.46736000	-4.41113100	1.64182800
27	H	7.31732000	-3.83834900	2.76047300
28	H	6.04356100	-1.83741700	2.06198900
29	H	6.14739000	1.53252100	-1.89415200
30	H	7.31330800	3.64512300	-2.42885400
31	H	9.23724600	4.40361900	-1.04121000
32	H	9.96638600	3.02270000	0.89852000

33	H	8.78244500	0.92416800	1.44911200
34	C	0.98955900	-0.43531500	-0.26115800
35	C	0.36772600	-1.70809300	-0.29895400
36	C	0.11293300	0.69892800	-0.30470000
37	C	-1.00582600	-1.87866400	-0.40427800
38	C	-1.33356500	0.51733500	-0.42280100
39	C	-1.89941300	-0.79143100	-0.48780100
40	N	0.49768700	1.98783400	-0.27295100
41	N	-2.03096500	1.67117200	-0.48067400
42	S	-0.90173700	2.91711200	-0.38072100
43	H	-1.40376400	-2.88807000	-0.38114800
44	H	0.98288900	-2.59460800	-0.19199900
45	C	-3.35396100	-1.02959400	-0.64414000
46	C	-4.28421800	-0.11973500	-0.13518500
47	C	-3.85372900	-2.19138000	-1.27192300
48	C	-5.67890700	-0.31205100	-0.24274700
49	H	-3.89107200	0.75725200	0.35009500
50	C	-5.21844800	-2.41746400	-1.36108500
51	H	-3.16957700	-2.91286700	-1.70308600
52	C	-6.14088400	-1.49231900	-0.86355000
53	H	-5.58513900	-3.31602400	-1.84867100
54	C	-7.91017100	0.42997700	0.51334600
55	C	-8.60134100	-0.68297100	-0.04199100
56	C	-8.66056900	1.31759000	1.32274200
57	C	-9.96376100	-0.87823400	0.22184200
58	H	-8.18132800	2.16722500	1.78567900
59	C	-10.00959000	1.11381400	1.56467800
60	C	-10.67341100	0.01056900	1.01565400
61	H	-10.46020600	-1.74019400	-0.21275700
62	H	-10.54430600	1.81581800	2.19557100
63	H	-11.72763900	-0.15416800	1.20942500
64	N	-6.55316800	0.66277100	0.27385300
65	S	-7.85349000	-1.79605300	-1.17410100
66	C	-5.99227300	1.98980500	0.62920300
67	H	-5.18259000	2.19618800	-0.06982100
68	H	-6.76827000	2.72863700	0.42396400
69	C	-5.49256900	2.10642300	2.07376500
70	H	-5.11178700	3.11871500	2.23639800
71	H	-6.28496300	1.91698700	2.80194000
72	H	-4.68038600	1.40503000	2.27456200

The cartesian coordinates of optimized ground state (S_0) geometry in Tetrahydrofuran

No.	Symbols	X	Y	Z
1	N	6.68691900	-0.14458900	0.20298500
2	C	5.28514700	-0.20836000	0.06323800
3	C	4.66879000	-1.33228600	-0.52444100

4	C	4.46492900	0.85093800	0.50226200
5	C	3.28293100	-1.39333300	-0.65110100
6	C	3.08003400	0.78902500	0.35573700
7	C	2.45442700	-0.33870700	-0.21434000
8	C	7.43393000	-1.31916500	0.48360000
9	C	8.65761400	-1.55458100	-0.17065400
10	C	9.39961600	-2.70388800	0.11773500
11	C	8.92885600	-3.64188600	1.04570300
12	C	7.70740400	-3.41194900	1.69218700
13	C	6.96688100	-2.25681300	1.42384300
14	C	7.36697800	1.09474800	0.06577100
15	C	7.02045000	1.99117200	-0.96236000
16	C	7.69490600	3.20922700	-1.08927000
17	C	8.73293300	3.54426200	-0.20997600
18	C	9.08478500	2.64805200	0.80764700
19	C	8.40425400	1.43561300	0.95361200
20	H	5.28164900	-2.15180800	-0.88988200
21	H	2.83904900	-2.26135800	-1.13398500
22	H	4.91832700	1.72358700	0.96463700
23	H	2.47459100	1.61847100	0.70775900
24	H	9.02116700	-0.83288300	-0.89805900
25	H	10.34398000	-2.87032900	-0.39651000
26	H	9.50545100	-4.53801600	1.26261600
27	H	7.33191100	-4.12694900	2.42143400
28	H	6.02540600	-2.07595200	1.93675000
29	H	6.22311400	1.72922000	-1.65363900
30	H	7.41451800	3.89142900	-1.88924600
31	H	9.26011600	4.48935500	-0.31686100
32	H	9.88512600	2.89607700	1.50184200
33	H	8.67339100	0.74585800	1.74982800
34	C	0.97943600	-0.45289600	-0.32929300
35	C	0.32725400	-1.66427900	-0.19861300
36	C	0.12305800	0.68166200	-0.59717200
37	C	-1.09056000	-1.81514800	-0.31466700
38	C	-1.32508400	0.52865500	-0.71018000
39	C	-1.95223700	-0.76522700	-0.56407700
40	N	0.52076900	1.93922000	-0.79780500
41	N	-1.94046800	1.67999600	-0.98668100
42	S	-0.80095900	2.82544800	-1.08996400
43	H	-1.50488100	-2.80977400	-0.16570100
44	H	0.90982300	-2.55244200	0.03524500
45	C	-3.42015500	-0.97022200	-0.69038500
46	C	-4.32623900	-0.01549700	-0.19010700
47	C	-3.91551700	-2.14641100	-1.27709600
48	C	-5.72108200	-0.18961400	-0.28291000
49	H	-3.91881600	0.87381300	0.26866500
50	C	-5.29462000	-2.33751400	-1.37665200

51	H	-3.23517600	-2.88920500	-1.68494000
52	C	-6.18758700	-1.36676000	-0.91504200
53	H	-5.68910300	-3.23334300	-1.85165800
54	C	-7.90804700	0.43119600	0.66369700
55	C	-8.60019400	-0.68071900	0.12672300
56	C	-8.58052900	1.18444900	1.65095600
57	C	-9.86493700	-1.05057500	0.59408400
58	H	-8.11385900	2.05644300	2.09104500
59	C	-9.86480400	0.83484900	2.08535400
60	C	-10.51284700	-0.29084700	1.57423000
61	H	-10.34843000	-1.92495800	0.16304400
62	H	-10.34627800	1.45069600	2.84169100
63	H	-11.50366900	-0.57280300	1.92077400
64	N	-6.61755100	0.77880400	0.21312900
65	S	-7.92879900	-1.55932700	-1.28639500
66	C	-6.08098500	2.08939100	0.59296700
67	H	-5.34034700	2.36968300	-0.16357400
68	H	-6.89943200	2.81198300	0.50410600
69	C	-5.45304600	2.17952600	2.00229000
70	H	-5.09950500	3.20353000	2.17391500
71	H	-6.17464300	1.93031100	2.78650200
72	H	-4.60188900	1.50086000	2.11473400

The cartesian coordinates of optimized the first singlet excited state (S_1) geometry in Tetrahydrofuran

No.	Symbols	X	Y	Z
1	N	6.70911700	-0.10240800	0.08181000
2	C	5.31933600	-0.18034700	0.02713400
3	C	4.67044700	-1.37228200	-0.39014900
4	C	4.50740400	0.92814300	0.37856400
5	C	3.29048200	-1.44541000	-0.43811800
6	C	3.12592300	0.85098300	0.31613900
7	C	2.45397000	-0.34224300	-0.08481300
8	C	7.49600200	-1.26303800	0.31991900
9	C	8.65092300	-1.49566400	-0.44909700
10	C	9.43482300	-2.62613100	-0.20514000
11	C	9.07487100	-3.53754200	0.79678000
12	C	7.92362100	-3.30508700	1.56112600
13	C	7.13812400	-2.17191800	1.33292100
14	C	7.37850200	1.13976300	-0.09662000
15	C	7.00115600	2.01044300	-1.13578800
16	C	7.67162000	3.22494500	-1.30426000
17	C	8.72770500	3.57801100	-0.45348200
18	C	9.10800900	2.70523000	0.57490400
19	C	8.43765200	1.49342300	0.75935900
20	H	5.26602600	-2.22565900	-0.70140200
21	H	2.84628900	-2.36318600	-0.81157600
22	H	4.97768200	1.84640800	0.71905300

23	H	2.53543000	1.71355800	0.60076300
24	H	8.92343900	-0.79150900	-1.23129700
25	H	10.32399500	-2.79881200	-0.80748200
26	H	9.68594000	-4.41786800	0.98146300
27	H	7.64031800	-3.99997100	2.34863000
28	H	6.25301600	-1.98167900	1.93502600
29	H	6.19064200	1.72864900	-1.80342100
30	H	7.37410700	3.88992100	-2.11205700
31	H	9.24963800	4.52191500	-0.59170300
32	H	9.92323000	2.97114900	1.24421300
33	H	8.72506100	0.81871700	1.56193300
34	C	1.00358800	-0.46215000	-0.12744100
35	C	0.38000200	-1.74713000	-0.11771200
36	C	0.10433100	0.66726100	-0.17493400
37	C	-0.98914700	-1.93029800	-0.17593000
38	C	-1.35275800	0.47401600	-0.24213600
39	C	-1.92591200	-0.85361100	-0.26228700
40	N	0.46579400	1.95154900	-0.19923300
41	N	-2.02673600	1.62545200	-0.30951700
42	S	-0.91805000	2.85959600	-0.28863500
43	H	-1.35702200	-2.94817300	-0.10581100
44	H	1.00149900	-2.63024200	-0.00544800
45	C	-3.35749400	-1.12105200	-0.36212700
46	C	-4.32897300	-0.10903800	-0.15803800
47	C	-3.83205800	-2.43363500	-0.66223700
48	C	-5.70895200	-0.34437800	-0.25548300
49	H	-3.96341100	0.87695600	0.07750700
50	C	-5.18972500	-2.68832000	-0.75094000
51	H	-3.14103300	-3.24618900	-0.85781100
52	C	-6.13702500	-1.66673800	-0.55855300
53	H	-5.53967400	-3.69051300	-0.99001100
54	C	-7.97264100	0.50264000	0.25525700
55	C	-8.63575600	-0.72654700	0.01383500
56	C	-8.74097600	1.53370100	0.84677700
57	C	-9.97965000	-0.91499900	0.36328900
58	H	-8.29132800	2.49363300	1.06635900
59	C	-10.08637400	1.34661800	1.17077200
60	C	-10.71758700	0.12026100	0.93864000
61	H	-10.44267100	-1.88019100	0.16769600
62	H	-10.63562600	2.17069900	1.61998700
63	H	-11.76137300	-0.03074700	1.20039200
64	N	-6.62742000	0.70472800	-0.08903200
65	S	-7.83422300	-2.06617300	-0.85097000
66	C	-6.11100100	2.07948200	-0.08383600
67	H	-5.29686500	2.12539400	-0.81368700
68	H	-6.90705600	2.72705600	-0.46423100
69	C	-5.61820800	2.58457800	1.28841100

70	H	-5.29708900	3.62864000	1.19399500
71	H	-6.40853500	2.53317900	2.04467400
72	H	-4.76908100	1.99718600	1.65149900

The cartesian coordinates of optimized the first triplet excited state (T_1) geometry in Tetrahydrofuran

No.	Symbols	X	Y	Z
1	N	6.55058300	-0.04296800	-0.29581000
2	C	5.18633100	-0.13770700	0.00499400
3	C	4.51582800	-1.38624600	-0.03273700
4	C	4.42980600	1.00812900	0.35833400
5	C	3.17280100	-1.48335600	0.28445600
6	C	3.08396200	0.91416300	0.66864200
7	C	2.38980300	-0.34041600	0.65748500
8	C	7.43136500	-1.12582000	-0.01849900
9	C	8.39260000	-1.51324400	-0.96891100
10	C	9.27000200	-2.56517800	-0.68908800
11	C	9.19202400	-3.25095800	0.53010300
12	C	8.23131800	-2.86743700	1.47486000
13	C	7.36065200	-1.80583400	1.21075300
14	C	7.08928700	1.14399200	-0.86645600
15	C	6.43271200	1.78445600	-1.93276100
16	C	6.97128800	2.94927200	-2.48803700
17	C	8.17458400	3.47785600	-2.00293500
18	C	8.83354600	2.83306500	-0.94801900
19	C	8.29431000	1.67727500	-0.37553000
20	H	5.06290300	-2.27845700	-0.32423700
21	H	2.70793500	-2.46088000	0.20711200
22	H	4.91902200	1.97749000	0.39940900
23	H	2.54494200	1.81040100	0.95208800
24	H	8.44738500	-0.98597500	-1.91828800
25	H	10.00910200	-2.85492900	-1.43300200
26	H	9.87239200	-4.07242200	0.74196500
27	H	8.16568900	-3.38551100	2.42931800
28	H	6.62398400	-1.49962500	1.94958300
29	H	5.50547100	1.36710400	-2.31811900
30	H	6.45308100	3.43540400	-3.31194000
31	H	8.59390600	4.37990000	-2.44233500
32	H	9.76646000	3.23542600	-0.55885200
33	H	8.80115500	1.18143400	0.44878300
34	C	0.99945100	-0.47454600	0.96943000
35	C	0.36937300	-1.84626300	1.07652000
36	C	0.07695800	0.62792200	1.25429900
37	C	-0.94739200	-2.04814700	1.01897900
38	C	-1.38049700	0.41001500	1.18993000
39	C	-1.91910000	-0.90521900	0.80998900
40	N	0.40019100	1.86926900	1.53326300
41	N	-2.08495900	1.48743200	1.43428500

42	S	-1.02203900	2.75396000	1.74556800
43	H	-1.35197500	-3.03732600	1.21117100
44	H	1.02200200	-2.68428100	1.30610000
45	C	-3.23013600	-1.14860200	0.27499400
46	C	-4.20543200	-0.11218900	0.15613800
47	C	-3.59109500	-2.45751700	-0.16208000
48	C	-5.47864700	-0.33482800	-0.37769900
49	H	-3.92548800	0.86958400	0.50362500
50	C	-4.84968200	-2.68781000	-0.69975800
51	H	-2.88941200	-3.28165600	-0.10493600
52	C	-5.78518100	-1.64995900	-0.82858800
53	H	-5.11833100	-3.68296200	-1.04750500
54	C	-7.80242500	0.47209500	-0.47954200
55	C	-8.34870300	-0.75062300	-0.93476000
56	C	-8.71511000	1.44879000	-0.02370300
57	C	-9.72405500	-0.99938900	-0.89235700
58	H	-8.35723900	2.40779400	0.33002200
59	C	-10.09404900	1.21028000	-0.01866300
60	C	-10.61074000	-0.01651500	-0.44017000
61	H	-10.09538700	-1.96216400	-1.23775900
62	H	-10.75948300	1.99529100	0.33338500
63	H	-11.68017200	-0.20942200	-0.42398400
64	N	-6.41350600	0.71043000	-0.50175700
65	S	-7.29682200	-1.97996300	-1.71132300
66	C	-5.94716000	2.08734600	-0.30797600
67	H	-4.97519500	2.17635700	-0.80565200
68	H	-6.63513900	2.73790000	-0.85789000
69	C	-5.83092500	2.56160300	1.15820100
70	H	-5.59947900	3.63367400	1.17022800
71	H	-6.76432400	2.40550000	1.70863500
72	H	-5.03424600	2.03851400	1.69625500

The cartesian coordinates of optimized the second triplet excited state (T_2) geometry in Tetrahydrofuran

No.	Symbols	X	Y	Z
1	N	6.70690500	-0.13064600	0.13843300
2	C	5.29611400	-0.19423400	0.02996700
3	C	4.66354100	-1.33129800	-0.50633300
4	C	4.48757000	0.87861100	0.44728400
5	C	3.28232200	-1.38931100	-0.60704600
6	C	3.10618000	0.81865200	0.33116900
7	C	2.44916800	-0.32166200	-0.19030800
8	C	7.44444100	-1.28379000	0.52079600
9	C	8.65054800	-1.60410700	-0.12527600
10	C	9.37272000	-2.73220700	0.25804800
11	C	8.90201700	-3.56495900	1.27661500
12	C	7.69956900	-3.25205600	1.91583400
13	C	6.97667800	-2.11863300	1.54985900

14	C	7.39025700	1.08508500	-0.13589400
15	C	7.01134100	1.88368600	-1.22830200
16	C	7.68052700	3.07759100	-1.48862600
17	C	8.74248200	3.48821100	-0.67866900
18	C	9.12549700	2.69207600	0.40389900
19	C	8.45386200	1.50347300	0.68165400
20	H	5.26502200	-2.16071300	-0.86294300
21	H	2.83963700	-2.26814400	-1.06324300
22	H	4.95130100	1.76052100	0.87672600
23	H	2.51037300	1.66017500	0.65859500
24	H	9.01218100	-0.96967500	-0.92722500
25	H	10.30161600	-2.96791400	-0.25288100
26	H	9.46497200	-4.44594800	1.56845300
27	H	7.32637000	-3.88558100	2.71507600
28	H	6.05191700	-1.87081500	2.05944900
29	H	6.19723800	1.56181600	-1.86847200
30	H	7.37726000	3.68255600	-2.33796100
31	H	9.26452200	4.41655800	-0.88811600
32	H	9.94361700	3.00338200	1.04672100
33	H	8.74462700	0.89712000	1.53267300
34	C	0.98726600	-0.42481900	-0.28710700
35	C	0.36089900	-1.69566200	-0.29122600
36	C	0.11629400	0.71046000	-0.37430700
37	C	-1.01379900	-1.86580400	-0.39412400
38	C	-1.33203400	0.52970500	-0.49237200
39	C	-1.90428600	-0.77847700	-0.50972800
40	N	0.50597200	1.99934500	-0.39102600
41	N	-2.02487800	1.68174100	-0.60358100
42	S	-0.89303900	2.92930300	-0.54483900
43	H	-1.41564400	-2.87262500	-0.34332400
44	H	0.97387800	-2.58061200	-0.15921600
45	C	-3.35865600	-1.01372400	-0.65277400
46	C	-4.28549400	-0.10810200	-0.12957800
47	C	-3.85921300	-2.17745300	-1.27898500
48	C	-5.68195200	-0.30595600	-0.21796400
49	H	-3.89243100	0.76538300	0.36198400
50	C	-5.22322500	-2.40813800	-1.35474000
51	H	-3.17615800	-2.89537600	-1.71806800
52	C	-6.14479400	-1.48931900	-0.84152000
53	H	-5.59124600	-3.30591000	-1.84230300
54	C	-7.91489700	0.42497700	0.54458500
55	C	-8.60587100	-0.68253200	-0.01791800
56	C	-8.66457600	1.30980900	1.35679000
57	C	-9.97175400	-0.87385300	0.23291500
58	H	-8.18663800	2.15499600	1.82872300
59	C	-10.01552100	1.10932500	1.58993400
60	C	-10.68142400	0.01344800	1.02766000

61	H	-10.46958000	-1.73085800	-0.20940400
62	H	-10.55047100	1.80873800	2.22309400
63	H	-11.73761500	-0.14716600	1.21311000
64	N	-6.55370100	0.65742500	0.31113700
65	S	-7.85284300	-1.81005100	-1.13115700
66	C	-5.99554100	1.98147700	0.68437800
67	H	-5.19240500	2.20289000	-0.01730900
68	H	-6.77386600	2.72073300	0.49504200
69	C	-5.49121400	2.07302100	2.12873200
70	H	-5.11139400	3.08298600	2.30663000
71	H	-6.28325900	1.87270700	2.85396600
72	H	-4.68006000	1.36663500	2.31750700

The cartesian coordinates of optimized ground state (S_0) geometry in Acetonitrile

No.	Symbols	X	Y	Z
1	N	6.68361000	-0.14074900	0.21035100
2	C	5.28230700	-0.21079600	0.07211900
3	C	4.66914800	-1.33794200	-0.51317600
4	C	4.45835600	0.84633500	0.51034700
5	C	3.28330300	-1.40358500	-0.64031900
6	C	3.07370000	0.77989000	0.36316400
7	C	2.45179100	-0.35001100	-0.20681100
8	C	7.43875000	-1.31260300	0.48167500
9	C	8.66006300	-1.53757700	-0.18067000
10	C	9.41105700	-2.68352900	0.09843600
11	C	8.95136700	-3.62835800	1.02523900
12	C	7.73205900	-3.40887600	1.67973100
13	C	6.98273200	-2.25711900	1.42051600
14	C	7.35769100	1.10259400	0.07626100
15	C	7.01045700	1.99786900	-0.95264600
16	C	7.67940700	3.21947300	-1.07654000
17	C	8.71271200	3.55894200	-0.19311900
18	C	9.06549800	2.66373100	0.82530400
19	C	8.39023400	1.44774900	0.96796600
20	H	5.28376300	-2.15688100	-0.87687600
21	H	2.84214500	-2.27460200	-1.12037900
22	H	4.90821900	1.72075600	0.97278100
23	H	2.46550800	1.60740200	0.71542600
24	H	9.01517300	-0.81100400	-0.90740800
25	H	10.35344800	-2.84191900	-0.42190400
26	H	9.53474000	-4.52177000	1.23512900
27	H	7.36507400	-4.12929800	2.40793600
28	H	6.04303900	-2.08471000	1.93964000
29	H	6.21728800	1.73247100	-1.64743100
30	H	7.39874900	3.90074000	-1.87720600
31	H	9.23565900	4.50666000	-0.29756000

32	H	9.86223600	2.91521200	1.52237000
33	H	8.66000800	0.75891700	1.76482600
34	C	0.97702400	-0.46579400	-0.32478000
35	C	0.32400100	-1.67530900	-0.18191000
36	C	0.12317900	0.66635400	-0.61012300
37	C	-1.09402300	-1.82575600	-0.29859500
38	C	-1.32443600	0.51375900	-0.72417300
39	C	-1.95332000	-0.77710900	-0.56105700
40	N	0.52302600	1.92038300	-0.82941000
41	N	-1.93751800	1.66163000	-1.02030500
42	S	-0.79657700	2.80425200	-1.13784700
43	H	-1.50946400	-2.81825300	-0.13898300
44	H	0.90457400	-2.56177300	0.06300400
45	C	-3.42192900	-0.98002400	-0.68471100
46	C	-4.32478100	-0.01936100	-0.18956500
47	C	-3.92058500	-2.15896100	-1.26325700
48	C	-5.72047300	-0.18996000	-0.28011100
49	H	-3.91410800	0.87074500	0.26488400
50	C	-5.30047200	-2.34639300	-1.36138200
51	H	-3.24272600	-2.90713100	-1.66538800
52	C	-6.19009400	-1.36962900	-0.90566400
53	H	-5.69741500	-3.24408800	-1.83078100
54	C	-7.90482100	0.44014200	0.66586800
55	C	-8.60065600	-0.67232900	0.13467000
56	C	-8.57392600	1.19863300	1.65168700
57	C	-9.86566200	-1.03800200	0.60521800
58	H	-8.10546500	2.07131100	2.08839800
59	C	-9.85820300	0.85316200	2.08963900
60	C	-10.50998300	-0.27309600	1.58381300
61	H	-10.35229100	-1.91261200	0.17815700
62	H	-10.33676900	1.47287600	2.84462400
63	H	-11.50084000	-0.55151600	1.93309200
64	N	-6.61434600	0.78342300	0.21089700
65	S	-7.93246800	-1.55817200	-1.27609200
66	C	-6.07397200	2.09455000	0.58638000
67	H	-5.33411900	2.37112500	-0.17222300
68	H	-6.89085600	2.81861300	0.49655100
69	C	-5.44376600	2.18796300	1.99426400
70	H	-5.08724900	3.21172800	2.16034300
71	H	-6.16518800	1.94515200	2.78063000
72	H	-4.59421400	1.50758300	2.10852100

The cartesian coordinates of optimized the first singlet excited state (S_1) geometry in Acetonitrile

No.	Symbols	X	Y	Z
1	N	6.70462600	-0.10493400	0.08514900
2	C	5.31950500	-0.18046500	0.02725700
3	C	4.66761700	-1.38095800	-0.36799100

4	C	4.50692300	0.93751800	0.35519900
5	C	3.28939100	-1.45268200	-0.41837700
6	C	3.12713900	0.86058400	0.29226400
7	C	2.45161800	-0.34000800	-0.08833800
8	C	7.49219200	-1.26725300	0.32041300
9	C	8.63907000	-1.50273800	-0.45911000
10	C	9.42357100	-2.63352600	-0.21812400
11	C	9.07184900	-3.53952500	0.79190700
12	C	7.92882500	-3.30262800	1.56738300
13	C	7.14210200	-2.16973400	1.34142600
14	C	7.37959500	1.13667600	-0.08506100
15	C	7.02209200	2.00356300	-1.13402000
16	C	7.69921600	3.21554800	-1.29497900
17	C	8.74066100	3.56821900	-0.42595900
18	C	9.10078400	2.69828900	0.61238300
19	C	8.42451600	1.48846200	0.78852700
20	H	5.26182000	-2.24121000	-0.66189100
21	H	2.84679800	-2.37722100	-0.77600900
22	H	4.97647700	1.86049100	0.68293800
23	H	2.53879400	1.72847000	0.56407300
24	H	8.90429800	-0.80228700	-1.24714100
25	H	10.30656500	-2.81042100	-0.82814000
26	H	9.68375600	-4.41967500	0.97461100
27	H	7.65314100	-3.99333300	2.36112300
28	H	6.26401700	-1.97477400	1.95226700
29	H	6.22454500	1.72030400	-1.81652100
30	H	7.41901800	3.87825400	-2.11070900
31	H	9.26784600	4.51003600	-0.55828400
32	H	9.90488100	2.96457300	1.29474100
33	H	8.69570700	0.81533300	1.59804600
34	C	1.00488100	-0.45735200	-0.13299600
35	C	0.37690800	-1.74341500	-0.11705600
36	C	0.10474100	0.67284300	-0.18826200
37	C	-0.99104700	-1.92455000	-0.17376700
38	C	-1.35348000	0.47979300	-0.25517100
39	C	-1.92912200	-0.84748300	-0.26736000
40	N	0.46561400	1.95610600	-0.22265200
41	N	-2.02546400	1.63110700	-0.33171500
42	S	-0.91747100	2.86551400	-0.31909100
43	H	-1.35963700	-2.94174700	-0.09849400
44	H	0.99562000	-2.62761100	0.00025100
45	C	-3.36022400	-1.11533500	-0.36737300
46	C	-4.33347600	-0.10128600	-0.16870400
47	C	-3.83323500	-2.42892200	-0.66074200
48	C	-5.71308100	-0.33749300	-0.26816200
49	H	-3.96956100	0.88622000	0.06285700
50	C	-5.19187400	-2.68276600	-0.75317500

51	H	-3.14279000	-3.24349900	-0.84985100
52	C	-6.13850600	-1.65967100	-0.57135900
53	H	-5.54113600	-3.68570700	-0.99011500
54	C	-7.97493400	0.50013000	0.26306500
55	C	-8.63494700	-0.73020600	0.02268400
56	C	-8.73777900	1.52142300	0.87642800
57	C	-9.96857400	-0.93277400	0.39971900
58	H	-8.29149300	2.48415200	1.09080600
59	C	-10.07627000	1.32241300	1.22567900
60	C	-10.70258600	0.09324400	0.99899300
61	H	-10.42896600	-1.89933200	0.20464300
62	H	-10.62240700	2.14013700	1.69015100
63	H	-11.73974000	-0.06758600	1.28068700
64	N	-6.63559700	0.71047800	-0.10565400
65	S	-7.83821000	-2.04946100	-0.88363200
66	C	-6.12244300	2.08582700	-0.09456100
67	H	-5.31279100	2.13674900	-0.82956400
68	H	-6.92147100	2.73486200	-0.46640700
69	C	-5.62031200	2.58801100	1.27589000
70	H	-5.30127600	3.63278400	1.18172900
71	H	-6.40469500	2.53496900	2.03799000
72	H	-4.76849600	2.00028400	1.63244900

The cartesian coordinates of optimized the first triplet excited state (T_1) geometry in Acetonitrile

No.	Symbols	X	Y	Z
1	N	6.53965900	-0.03955800	-0.30752600
2	C	5.17746300	-0.13612100	-0.00021200
3	C	4.50972100	-1.38669100	-0.02836500
4	C	4.41907800	1.00923400	0.35160700
5	C	3.16872500	-1.48644100	0.29661600
6	C	3.07522900	0.91245500	0.67022100
7	C	2.38439700	-0.34412800	0.66945700
8	C	7.42348800	-1.12171400	-0.03513500
9	C	8.37531300	-1.51174900	-0.99389000
10	C	9.25610100	-2.56248600	-0.71927800
11	C	9.19048700	-3.24398600	0.50323900
12	C	8.23894100	-2.85775200	1.45637300
13	C	7.36505300	-1.79740100	1.19711600
14	C	7.07602300	1.14903900	-0.87747500
15	C	6.41883900	1.78870000	-1.94394400
16	C	6.95581800	2.95479600	-2.49855300
17	C	8.15798600	3.48535000	-2.01227500
18	C	8.81754700	2.84132900	-0.95704000
19	C	8.27984300	1.68416900	-0.38547900
20	H	5.05717200	-2.27917700	-0.31821900
21	H	2.70706800	-2.46609000	0.22737500
22	H	4.90485100	1.98057600	0.38535400

23	H	2.53574100	1.80897000	0.95206500
24	H	8.42026100	-0.98805200	-1.94581200
25	H	9.98785500	-2.85460500	-1.46948300
26	H	9.87328300	-4.06445200	0.71114900
27	H	8.18301000	-3.37269600	2.41312200
28	H	6.63566100	-1.48923100	1.94234400
29	H	5.49289200	1.36974600	-2.33075900
30	H	6.43755900	3.44021100	-3.32284000
31	H	8.57610500	4.38821600	-2.45114500
32	H	9.74955200	3.24508900	-0.56716400
33	H	8.78716500	1.18914600	0.43907300
34	C	0.99629500	-0.48073300	0.99042300
35	C	0.36851600	-1.85276100	1.10254900
36	C	0.07435200	0.62008200	1.28409800
37	C	-0.94849400	-2.05717600	1.05147600
38	C	-1.38290700	0.39975000	1.22681000
39	C	-1.92024400	-0.91508400	0.84045000
40	N	0.39594000	1.86035600	1.57016300
41	N	-2.08871200	1.47254900	1.48466900
42	S	-1.02783100	2.73979000	1.79790100
43	H	-1.35099300	-3.04645800	1.24717900
44	H	1.02309100	-2.69002300	1.32946500
45	C	-3.22778400	-1.15559700	0.29559800
46	C	-4.19725100	-0.11533600	0.16223200
47	C	-3.59000200	-2.46575500	-0.13642600
48	C	-5.46767500	-0.33601700	-0.37974000
49	H	-3.91597500	0.86807000	0.50403800
50	C	-4.84522800	-2.69411800	-0.68298100
51	H	-2.89294400	-3.29287100	-0.06702200
52	C	-5.77510600	-1.65289300	-0.82530800
53	H	-5.11473800	-3.69030500	-1.02696800
54	C	-7.78794500	0.47763400	-0.50208700
55	C	-8.33507600	-0.74565900	-0.95486100
56	C	-8.70065400	1.45903200	-0.05605300
57	C	-9.71144900	-0.99096700	-0.91976300
58	H	-8.34305700	2.41914300	0.29498200
59	C	-10.08031700	1.22393200	-0.05797400
60	C	-10.59801900	-0.00352300	-0.47708300
61	H	-10.08363600	-1.95404600	-1.26342000
62	H	-10.74559200	2.01236600	0.28656900
63	H	-11.66805400	-0.19342100	-0.46638400
64	N	-6.39780900	0.71176600	-0.51770700
65	S	-7.28110600	-1.98174000	-1.71879100
66	C	-5.92841400	2.08839700	-0.32579800
67	H	-4.95348900	2.17292000	-0.81833700
68	H	-6.61049100	2.73959100	-0.88192200
69	C	-5.81973700	2.56740600	1.13926900

70	H	-5.58278400	3.63821300	1.14816300
71	H	-6.75784500	2.41923700	1.68375300
72	H	-5.02973100	2.04204900	1.68502500

The cartesian coordinates of optimized the second triplet excited state (T_2) geometry in Acetonitrile

No.	Symbols	X	Y	Z
1	N	6.70502400	-0.13116800	0.14480300
2	C	5.29569200	-0.19521900	0.03309400
3	C	4.66335000	-1.33347300	-0.50198500
4	C	4.48562400	0.87859400	0.44639100
5	C	3.28223400	-1.39132200	-0.60640400
6	C	3.10445500	0.81830900	0.32661400
7	C	2.44825100	-0.32225600	-0.19509500
8	C	7.44543100	-1.28692600	0.51607800
9	C	8.64874600	-1.60050100	-0.13813800
10	C	9.37494000	-2.72989100	0.23421900
11	C	8.91051500	-3.56997300	1.24981700
12	C	7.71071500	-3.26341800	1.89732000
13	C	6.98407400	-2.12868400	1.54224300
14	C	7.38855100	1.08831400	-0.11537400
15	C	7.02166700	1.89072400	-1.20897100
16	C	7.69166900	3.08728400	-1.45574900
17	C	8.74259000	3.49612800	-0.63040000
18	C	9.11393800	2.69577400	0.45330500
19	C	8.44116100	1.50443000	0.71715300
20	H	5.26470700	-2.16440700	-0.85499200
21	H	2.84049700	-2.27193700	-1.06026500
22	H	4.94775200	1.76082100	0.87677300
23	H	2.50864600	1.66039200	0.65301800
24	H	9.00538200	-0.96027000	-0.93773900
25	H	10.30173700	-2.96058100	-0.28263900
26	H	9.47645100	-4.45177100	1.53316700
27	H	7.34287200	-3.90266600	2.69440900
28	H	6.06188800	-1.88565500	2.05885400
29	H	6.21717600	1.56944700	-1.86158000
30	H	7.39860600	3.69525700	-2.30649000
31	H	9.26561000	4.42619900	-0.82928400
32	H	9.92366500	3.00554800	1.10728100
33	H	8.72286700	0.89446700	1.56866300
34	C	0.98617900	-0.42509700	-0.29549000
35	C	0.35799900	-1.69495100	-0.28600800
36	C	0.11740700	0.71008900	-0.40044800
37	C	-1.01719200	-1.86483300	-0.38734500
38	C	-1.33179300	0.52973000	-0.51671500
39	C	-1.90672300	-0.77781900	-0.51501100
40	N	0.50908700	1.99839000	-0.43831800
41	N	-2.02244500	1.68070500	-0.64810700

42	S	-0.88948800	2.92831400	-0.60797400
43	H	-1.42021900	-2.87051600	-0.32536000
44	H	0.96990800	-2.57924000	-0.14426500
45	C	-3.36105800	-1.01206600	-0.65220000
46	C	-4.28649400	-0.10512800	-0.12833200
47	C	-3.86242500	-2.17933400	-1.27229800
48	C	-5.68350200	-0.30500800	-0.20883600
49	H	-3.89319300	0.76930200	0.36140600
50	C	-5.22620900	-2.41149900	-1.34215000
51	H	-3.18017000	-2.89860700	-1.71053300
52	C	-6.14716600	-1.49221300	-0.82764700
53	H	-5.59497300	-3.31122200	-1.82531700
54	C	-7.91640100	0.42633900	0.55337200
55	C	-8.60774500	-0.68170900	-0.00625700
56	C	-8.66509600	1.31408900	1.36294000
57	C	-9.97481600	-0.86997200	0.24127600
58	H	-8.18718000	2.15962000	1.83412100
59	C	-10.01670400	1.11624000	1.59442800
60	C	-10.68388400	0.02074100	1.03253300
61	H	-10.47361500	-1.72690800	-0.19990000
62	H	-10.55123500	1.81772200	2.22551500
63	H	-11.74078200	-0.13711000	1.21602000
64	N	-6.55383500	0.65736300	0.31978400
65	S	-7.85363500	-1.82012000	-1.10720200
66	C	-5.99604300	1.98210000	0.69152000
67	H	-5.19534400	2.20434900	-0.01270200
68	H	-6.77489100	2.72080100	0.50393800
69	C	-5.48903900	2.07332000	2.13488700
70	H	-5.11028600	3.08378800	2.31210800
71	H	-6.28035500	1.87286600	2.86066200
72	H	-4.67775300	1.36668700	2.32277900