Supplementary materials: Optimized structures (Cartesian coordinates, Å) and energies (a.u.) for ground and excited states of 9-Mesityl-10-methylacridinium.

Electronic Structure of 9-Mesityl-10-methylacridinium in ground and excited states: Charge-Shift Mechanism introduced by counter anion shift.

S. Zilberg **07.05.10**

B3LYP/cc-pVDZ and TD/B3LYP/cc-pVDZ

Ground State 1^1A'\HF=-944.3203206

Charge = 1 Multiplicity = 1

C	0.00978	-1.39831	0.
C	0.00903	-2.0961	1.22981
C	0.00903	-2.0961	-1.22981
C	0.00903	-3.49588	1.20085
C	0.00903	-3.49588	-1.20085
C	0.01175	-4.21727	0.
H	0.00471	-4.03836	2.14992
H	0.00471	-4.03836	-2.14992
C	0.0033	0.09789	0.
N	-0.00975	2.9304	0.
C	1.21664	0.82564	0.
C	-1.21837	0.81081	0.
C	1.20255	2.26669	0.
C	-1.2094	2.24697	0.
C	2.47454	0.14469	0.
C	-2.47507	0.1295	0.
C	2.44654	2.95255	0.

C	-2.44768	2.94108	0.
C	3.65997	0.83558	0.
C	-3.66008	0.82382	0.
C	3.63514	2.25091	0.
C	-3.63737	2.23943	0.
H	2.46217	-0.94472	0.
H	-2.4649	-0.96005	0.
H	2.49875	4.0371	0.
H	-2.48371	4.02666	0.
H	4.61275	0.30488	0.
H	-4.61304	0.29333	0.
H	4.57392	2.80815	0.
H	-4.5775	2.79451	0.
C	0.00502	-1.36657	-2.55419
H	0.88969	-0.71828	-2.66899
H	0.00573	-2.0769	-3.39211
H	-0.88319	-0.7227	-2.66668
C	0.00502	-1.36657	2.55419
H	0.88969	-0.71828	2.66899
H	-0.88319	-0.7227	2.66668
H	0.00573	-2.0769	3.39211
C	0.04245	-5.72522	0.
H	1.08309	-6.0935	0.
H	-0.45041	-6.13957	0.8919
H	-0.45041	-6.13957	-0.8919

C -0.07744 4.40437 0.

H 0.91924 4.84026 0.

H -0.60793 4.74998 -0.89754

H -0.60793 4.74998 0.89754

Excitation energies and oscillator strengths:

Excited State 1: Triplet-A' 1.9495 eV 635.99 nm f=0.0000

79 -> 86 0.13175

81 -> 84 0.78893

This state for optimization and/or second-order correction.

Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: Triplet-A" 2.1068 eV 588.51 nm f=0.0000

83 -> 84 0.70660

Excited State 3: Singlet-A" 2.1266 eV 583.02 nm f=0.0000

83 -> 84 0.70392

Excited State 4: Triplet-A' 2.2344 eV 554.90 nm f=0.0000

82 -> 84 0.70799

Excited State 5: Singlet-A' 2.2501 eV 551.02 nm f=0.0000

82 -> 84 0.70573

Excited State 6: Singlet-A' 2.9687 eV 417.64 nm f=0.0777

81 -> 84 0.64880

B3LYP/cc-pVDZ

T_1 $1^3A'$ -944.3203206

Charge = 1 Multiplicity = 3

C	-0.006645	-1.417625	0.000000
C	-0.005608	-2.122006	1.227309
C	-0.005608	-2.122006	-1.227309
C	-0.005608	-3.521952	1.200824
C	-0.005608	-3.521952	-1.200824
C	-0.008353	-4.243442	0.000000
H	-0.001153	-4.064940	2.149815
H	-0.001153	-4.064940	-2.149815
C	-0.001292	0.075165	0.000000
N	0.004355	2.936311	0.000000
C	-1.229653	0.821145	0.000000
C	1.231798	0.810523	0.000000
C	-1.222930	2.260036	0.000000
C	1.224343	2.245094	0.000000
C	-2.474994	0.173590	0.000000
C	2.479217	0.165796	0.000000
C	-2.450706	2.954914	0.000000
C	2.443127	2.951464	0.000000
C	-3.693979	0.888469	0.000000
C	3.692909	0.888048	0.000000
C	-3.680691	2.273973	0.000000

C	3.675528	2.274789	0.000000
H	-2.487243	-0.916520	0.000000
H	2.496881	-0.924265	0.000000
H	-2.487101	4.040806	0.000000
H	2.459554	4.038419	0.000000
H	-4.638031	0.340929	0.000000
H	4.639819	0.345395	0.000000
H	-4.607624	2.847559	0.000000
H	4.601827	2.849566	0.000000
C	-0.000571	-1.391580	2.551247
C	-0.000571	-1.391580	-2.551247
H	-0.884691	-0.742227	2.665003
H	-0.884691	-0.742227	-2.665003
H	0.886631	-0.745731	2.660425
H	0.886631	-0.745731	-2.660425
H	0.000061	-2.099825	3.391285
H	0.000061	-2.099825	-3.391285
C	-0.038992	-5.751687	0.000000
H	-1.079306	-6.121076	0.000000
H	0.454132	-6.166181	0.891802
H	0.454132	-6.166181	-0.891802
C	0.067087	4.406229	0.000000
H	-0.928500	4.844064	0.000000
H	0.598038	4.753169	0.897329
H	0.598038	4.753169	-0.897329

CAS(12/9)/cc-pVDZ PC-GAMESS results

THE ELECTRONIC STATE IS 1-A'

TOTAL ENERGY = -938.2057533100

C	6.0	0.0076759613	-1.4002372081	0.0000000000
C	6.0	0.0078703201	-2.0918237456	-1.2179256620
C	6.0	0.0078703201	-2.0918237456	1.2179256620
C	6.0	0.0091055577	-3.4814716640	-1.1933299546
C	6.0	0.0091055577	-3.4814716640	1.1933299546
C	6.0	0.0120532014	-4.1950141018	0.0000000000
H	1.0	0.0064379244	-4.0199199898	-2.1316313452
H	1.0	0.0064379244	-4.0199199898	2.1316313452
C	6.0	0.0033411376	0.1030903015	0.0000000000
N	7.0	-0.0116735198	2.9085598940	0.0000000000
C	6.0	1.2099916447	0.8279676952	0.0000000000
C	6.0	-1.2126317892	0.8163044021	0.0000000000
C	6.0	1.1864101448	2.2537836402	0.0000000000
C	6.0	-1.2005386693	2.2292022954	0.0000000000
C	6.0	2.4781807189	0.1484557749	0.0000000000
C	6.0	-2.4734443539	0.1375647848	0.0000000000
C	6.0	2.4396852559	2.9496529304	0.0000000000
C	6.0	-2.4406459638	2.9310717581	0.0000000000
C	6.0	3.6416868415	0.8301823490	0.0000000000
C	6.0	-3.6393059994	0.8252876511	0.0000000000
C	6.0	3.6180300761	2.2528913568	0.0000000000

C	6.0	-3.6133073861	2.2434663152	0.0000000000
H	1.0	2.4741315208	-0.9292107539	0.0000000000
H	1.0	-2.4722216239	-0.9401086758	0.0000000000
H	1.0	2.4950541654	4.0213896672	0.0000000000
H	1.0	-2.4745414360	4.0049027041	0.0000000000
H	1.0	4.5870279027	0.3081235832	0.0000000000
H	1.0	-4.5854714638	0.3047772590	0.0000000000
H	1.0	4.5485234565	2.8023100613	0.0000000000
H	1.0	-4.5440508824	2.7931051451	0.0000000000
C	6.0	0.0049843665	-1.3677768456	-2.5472574338
C	6.0	0.0049843665	-1.3677768456	2.5472574338
H	1.0	0.8844722179	-0.7310724583	-2.6606467018
H	1.0	0.8844722179	-0.7310724583	2.6606467018
H	1.0	-0.8773519547	-0.7348149140	-2.6598474826
H	1.0	-0.8773519547	-0.7348149140	2.6598474826
H	1.0	0.0060296792	-2.0800360438	-3.3695685938
H	1.0	0.0060296792	-2.0800360438	3.3695685938
C	6.0	0.0435817712	-5.7041203416	0.0000000000
H	1.0	1.0751071567	-6.0642254285	0.0000000000
H	1.0	-0.4490739296	-6.1094745478	-0.8832361317
H	1.0	-0.4490739296	-6.1094745478	0.8832361317
C	6.0	-0.0832217512	4.3832200621	0.0000000000
H	1.0	0.9006697708	4.8155514565	0.0000000000
H	1.0	-0.6067116252	4.7161244203	-0.8910780863
H	1.0	-0.6067116252	4.7161244203	0.8910780863

CAS(12/9)/cc-pVDZ PC-GAMESS results

THE ELECTRONIC STATE IS $1^1A''$

TOTAL ENERGY = -938.0940281223

C	6.0	0.0121419348	-1.3858556251	0.0000000000
C	6.0	0.0090316673	-2.1182844652	-1.2607913122
C	6.0	0.0090316673	-2.1182844652	1.2607913122
C	6.0	0.0046426063	-3.4799792920	-1.2277462973
C	6.0	0.0046426063	-3.4799792920	1.2277462973
C	6.0	0.0024273939	-4.1843822832	0.0000000000
H	1.0	0.0002329123	-4.0433119948	-2.1492768849
H	1.0	0.0002329123	-4.0433119948	2.1492768849
C	6.0	0.0108827126	0.1009651145	0.0000000000
N	7.0	-0.0161279136	2.9130702434	0.0000000000
C	6.0	1.2369023330	0.8191826725	0.0000000000
C	6.0	-1.2486567903	0.8130449102	0.0000000000
C	6.0	1.2163679936	2.2440275068	0.0000000000
C	6.0	-1.2229624919	2.2227886917	0.0000000000
C	6.0	2.4925834388	0.1514619681	0.0000000000
C	6.0	-2.4832756224	0.1475316078	0.0000000000
C	6.0	2.4500226038	2.9213911370	0.0000000000
C	6.0	-2.4489249242	2.9049358384	0.0000000000
C	6.0	3.6748841467	0.8326260305	0.0000000000
C	6.0	-3.6789257630	0.8315485738	0.0000000000
C	6.0	3.6570367222	2.2330501802	0.0000000000

C	6.0	-3.6493277435	2.2210751313	0.0000000000
H	1.0	2.5130899756	-0.9306869308	0.0000000000
H	1.0	-2.5031498150	-0.9349156368	0.0000000000
H	1.0	2.5003877542	3.9946585800	0.0000000000
H	1.0	-2.4810700562	3.9797037292	0.0000000000
H	1.0	4.6139542855	0.2975062474	0.0000000000
H	1.0	-4.6178305138	0.2976131492	0.0000000000
H	1.0	4.5823344641	2.7902628874	0.0000000000
H	1.0	-4.5720454742	2.7840833201	0.0000000000
C	6.0	0.0089562035	-1.3624180318	-2.5575980594
C	6.0	0.0089562035	-1.3624180318	2.5575980594
H	1.0	0.8885149049	-0.7216403968	-2.6230207473
H	1.0	0.8885149049	-0.7216403968	2.6230207473
H	1.0	-0.8678338835	-0.7174296787	-2.6201175082
H	1.0	-0.8678338835	-0.7174296787	2.6201175082
H	1.0	0.0059522200	-2.0475535559	-3.4016948611
H	1.0	0.0059522200	-2.0475535559	3.4016948611
C	6.0	0.0310047418	-5.6789819148	0.0000000000
H	1.0	1.0781398681	-5.9995992391	0.0000000000
H	1.0	-0.4421102987	-6.0875258998	-0.8905280926
H	1.0	-0.4421102987	-6.0875258998	0.8905280926
C	6.0	-0.0907022174	4.3683568831	0.0000000000
H	1.0	0.8923923218	4.8085477830	0.0000000000
H	1.0	-0.6123525146	4.7253445371	-0.8876784420
H	1.0	-0.6123525146	4.7253445371	0.8876784420

CAS(12/9)/cc-pVDZ PC-GAMESS results

THE ELECTRONIC STATE IS $1^3A'$

TOTAL ENERGY = -938.1191297272

C	6.0	0.0069952808	-1.4238322536	0.0000000000
C	6.0	0.0065833965	-2.1215827470	-1.2153607992
C	6.0	0.0065833965	-2.1215827470	1.2153607992
C	6.0	0.0084276687	-3.5114671708	-1.1932510517
C	6.0	0.0084276687	-3.5114671708	1.1932510517
C	6.0	0.0119042629	-4.2252853831	0.0000000000
H	1.0	0.0044488031	-4.0498901072	-2.1317009800
H	1.0	0.0044488031	-4.0498901072	2.1317009800
C	6.0	0.0040874155	0.0743771423	0.0000000000
N	7.0	0.0107947074	2.9216711872	0.0000000000
C	6.0	1.2168191674	0.8129494095	0.0000000000
C	6.0	-1.2488744671	0.8199413822	0.0000000000
C	6.0	1.1926957453	2.2676735747	0.0000000000
C	6.0	-1.2398091795	2.2233611323	0.0000000000
C	6.0	2.4662039577	0.1838824887	0.0000000000
C	6.0	-2.4836090484	0.1689640760	0.0000000000
C	6.0	2.4340499500	2.9579427836	0.0000000000
C	6.0	-2.4383816062	2.9374122991	0.0000000000
C	6.0	3.7035784674	0.9225752547	0.0000000000
C	6.0	-3.6702016064	0.8797066408	0.0000000000
C	6.0	3.6839886113	2.2688781722	0.0000000000

C	6.0	-3.6477635591	2.2669449710	0.0000000000
H	1.0	2.5005829349	-0.8933442825	0.0000000000
H	1.0	-2.5017012631	-0.9093082088	0.0000000000
H	1.0	2.4786564995	4.0303818018	0.0000000000
H	1.0	-2.4602130202	4.0124186701	0.0000000000
H	1.0	4.6364324731	0.3775114696	0.0000000000
H	1.0	-4.6126119540	0.3511052416	0.0000000000
H	1.0	4.5932344779	2.8504157185	0.0000000000
H	1.0	-4.5677303631	2.8327151818	0.0000000000
C	6.0	0.0001457676	-1.3951685338	-2.5430559755
C	6.0	0.0001457676	-1.3951685338	2.5430559755
H	1.0	0.8813155418	-0.7608136735	-2.6583729446
H	1.0	0.8813155418	-0.7608136735	2.6583729446
H	1.0	-0.8792827457	-0.7566844779	-2.6470128338
H	1.0	-0.8792827457	-0.7566844779	2.6470128338
H	1.0	-0.0062012604	-2.1037565086	-3.3690012237
H	1.0	-0.0062012604	-2.1037565086	3.3690012237
C	6.0	0.0436031402	-5.7347236850	0.0000000000
H	1.0	1.0748858896	-6.0959904369	0.0000000000
H	1.0	-0.4491945987	-6.1404738678	-0.8831565412
H	1.0	-0.4491945987	-6.1404738678	0.8831565412
C	6.0	-0.0725022491	4.3928800278	0.0000000000
H	1.0	0.9035900868	4.8429565447	0.0000000000
H	1.0	-0.6047844484	4.7114531266	-0.8908020728
H	1.0	-0.6047844484	4.7114531266	0.8908020728

CAS(12/9)/cc-pVDZ PC-GAMESS results

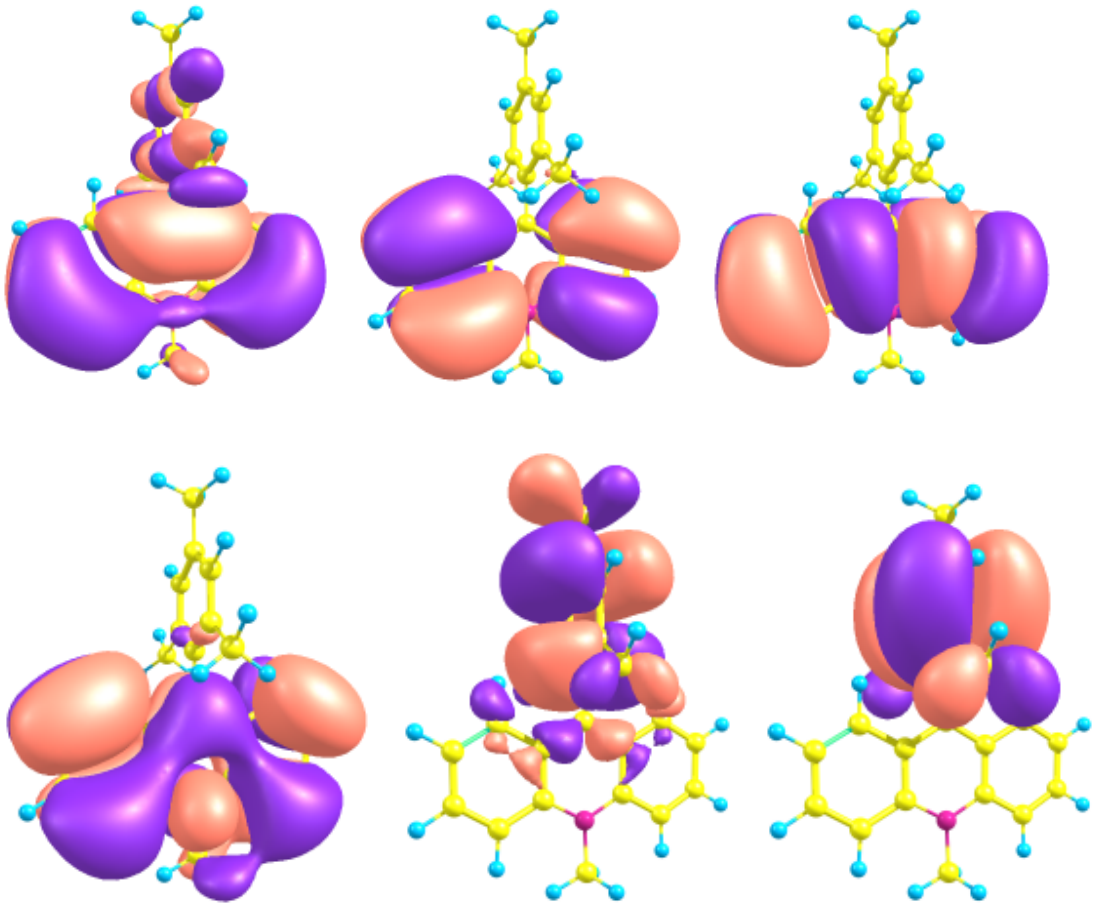
THE ELECTRONIC STATE IS $1^3A''$

TOTAL ENERGY = -938.0949732191

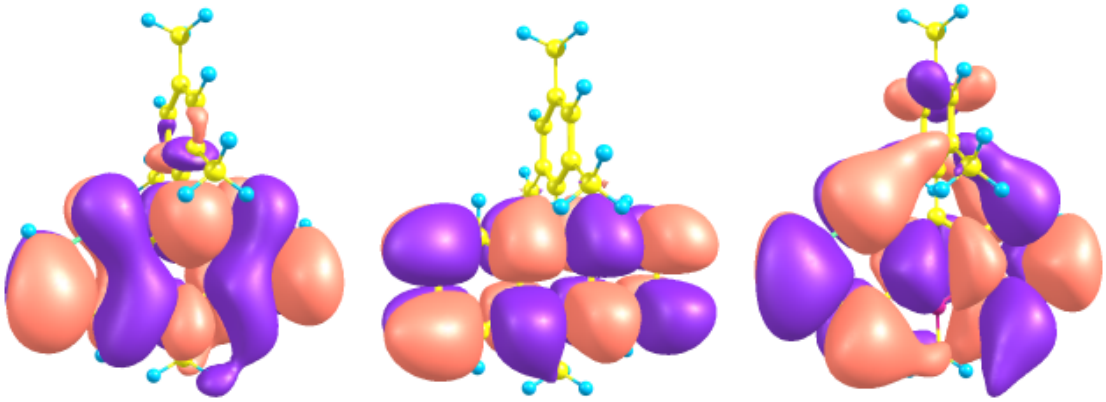
C	6.0	0.0121359419	-1.3846616561	0.0000000000
C	6.0	0.0089821836	-2.1182096467	-1.2608195232
C	6.0	0.0089821836	-2.1182096467	1.2608195232
C	6.0	0.0046643463	-3.4800577210	-1.2276552805
C	6.0	0.0046643463	-3.4800577210	1.2276552805
C	6.0	0.0025097646	-4.1842656054	0.0000000000
H	1.0	0.0003230723	-4.0432842597	-2.1492563147
H	1.0	0.0003230723	-4.0432842597	2.1492563147
C	6.0	0.0107597590	0.0999193863	0.0000000000
N	7.0	-0.0160558855	2.9130416969	0.0000000000
C	6.0	1.2376329085	0.8194722771	0.0000000000
C	6.0	-1.2487317326	0.8128718080	0.0000000000
C	6.0	1.2163737012	2.2436270968	0.0000000000
C	6.0	-1.2228227531	2.2226139141	0.0000000000
C	6.0	2.4924174907	0.1517923546	0.0000000000
C	6.0	-2.4834592400	0.1475047119	0.0000000000
C	6.0	2.4500900887	2.9211933668	0.0000000000
C	6.0	-2.4488705617	2.9048615791	0.0000000000
C	6.0	3.6753560248	0.8329090377	0.0000000000
C	6.0	-3.6791098768	0.8315172071	0.0000000000
C	6.0	3.6571120043	2.2328335599	0.0000000000

C	6.0	-3.6492759459	2.2210804206	0.0000000000
H	1.0	2.5125792861	-0.9304701975	0.0000000000
H	1.0	-2.5031038481	-0.9349651959	0.0000000000
H	1.0	2.5002965596	3.9945034910	0.0000000000
H	1.0	-2.4809299633	3.9796197775	0.0000000000
H	1.0	4.6142963782	0.2976807181	0.0000000000
H	1.0	-4.6179935195	0.2976835809	0.0000000000
H	1.0	4.5822797225	2.7902356112	0.0000000000
H	1.0	-4.5719761092	2.7841189231	0.0000000000
C	6.0	0.0088462785	-1.3624731086	-2.5576200830
C	6.0	0.0088462785	-1.3624731086	2.5576200830
H	1.0	0.8883073336	-0.7215151054	-2.6228246316
H	1.0	0.8883073336	-0.7215151054	2.6228246316
H	1.0	-0.8679642968	-0.7175569523	-2.6200008440
H	1.0	-0.8679642968	-0.7175569523	2.6200008440
H	1.0	0.0060176042	-2.0475609831	-3.4017095322
H	1.0	0.0060176042	-2.0475609831	3.4017095322
C	6.0	0.0310560312	-5.6789560075	0.0000000000
H	1.0	1.0780751592	-5.9997359660	0.0000000000
H	1.0	-0.4421425579	-6.0874959517	-0.8905137849
H	1.0	-0.4421425579	-6.0874959517	0.8905137849
C	6.0	-0.0906565688	4.3682573719	0.0000000000
H	1.0	0.8923333139	4.8086552945	0.0000000000
H	1.0	-0.6123825289	4.7253909502	-0.8876466225
H	1.0	-0.6123825289	4.7253909502	0.8876466225

Scheme 1. Active space MOs: 9 orbitals, 12 electrons; cc-pVDZ basis set.

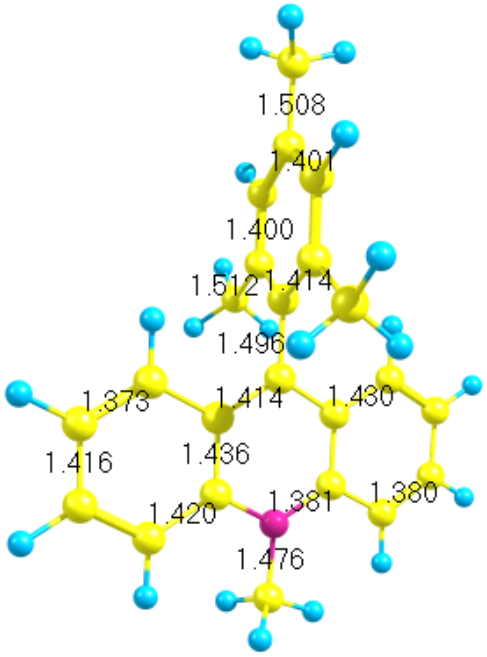


HOMO-1 HOMO

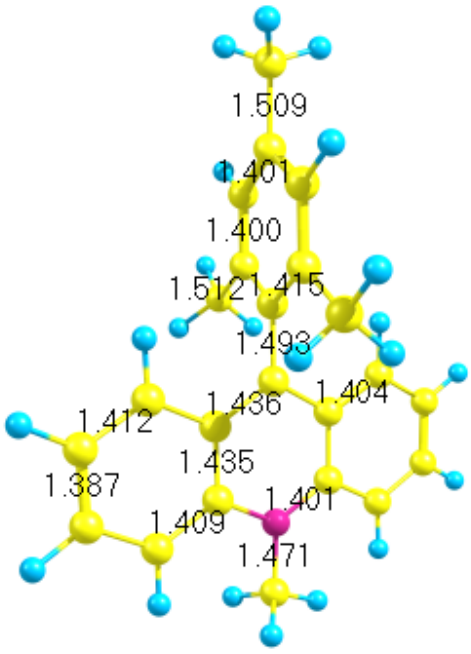


LUMO LUMO+1 LUMO+2

B3LYP/cc-pVDZ optimized structures



GS $1^1A'$ - 944.32032



T_1 $1^3A'$ - 944.248 86