Supporting Information for Investigating the influence of substituent groups in TTM based radicals to the excitation process: A theoretical study.

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1.Table S1a The calculated emissive bands of TTM and TTM PCz radicals with different kinds of functional in cyclohexane solvent.

Radicals	b3lyp	cam-b3lyp	wb97xd	m062x	Exp.
TTM	557	500	498	542	570
TTM-PCz	738	583	569	634	703

Table S1b The calculated emissive bands of radicals in different solvents.

Radicals	cyclohexane	toluene	chloroform
TTM	557	558	559
TTM-IMz	751	759	787
TTM-PCz	784	783	785
TTM-3PCz	738	745	768
TTM-3NCz	748	755	778
2Br-TTM-3PCz	739	746	769
2F-TTM-3PCz	690	696	717

Table S1c The calculated adsorption bands of radicals in different solvents.

| Radicals	cyclohexane	toluene	chloroform
TTM	468	468	506
TTM-IMz	602	609	629
TTM-PCz	675	676	677
TTM-3PCz	651	657	671
TTM-3NCz	658	662	676
2Br-TTM-3PCz	653	657	672
2F-TTM-3PCz	617	621	633

2. Figure S1 and table S2: The characteristic bonds and dihedrals for TTM based radicals in cyclohexane solvent.
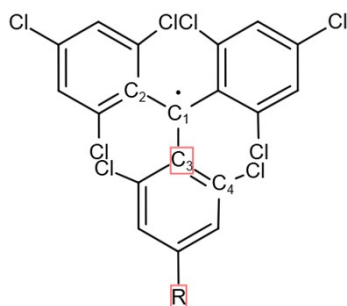
radicals	C1-C2 (Å)	C1-C3 (Å)	C1-C2-C3-C4
TTM	1.475(1.456)	1.475(1.449)	131.1(133.7)
TTM-IMz	1.476(1.449)	1.461(1.489)	134.4(121.4)
TTM-PCz	1.475(1.459)	1.470(1.450)	132.2(136.5)
TTM-3PCz	1.475(1.455)	1.469(1.463)	132.7(132.4)
TTM-3NCz	1.475(1.455)	1.463(1.461)	132.7(132.9)
2Br-TTM-3PCz	1.475(1.453)	1.469(1.466)	132.7(131.3)
2F-TTM-PCz	1.476(1.459)	1.470(1.458)	127.7(133.5)

()The characteristic bonds and dihedrals of D_1 state.

3. Figure S2: The calculated molecular orbitals of the radicals in the ground state.
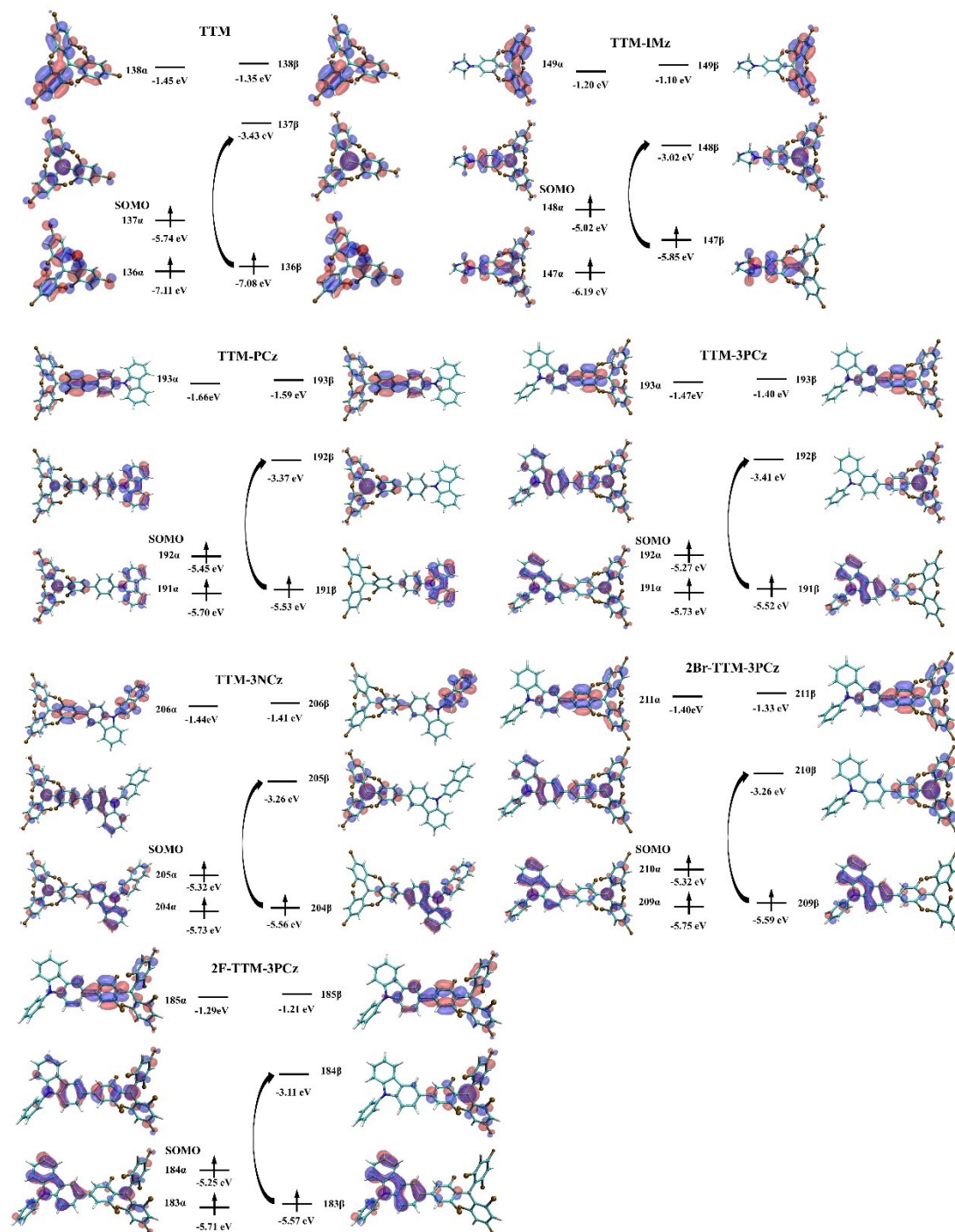
4. Figure S3 the hole-electron overlap for the selected radicals. The overlap is directly related to the value of transition dipole moment.

TTM   **TTM-IMz**

TTM-PCz   **TTM-3PCz**
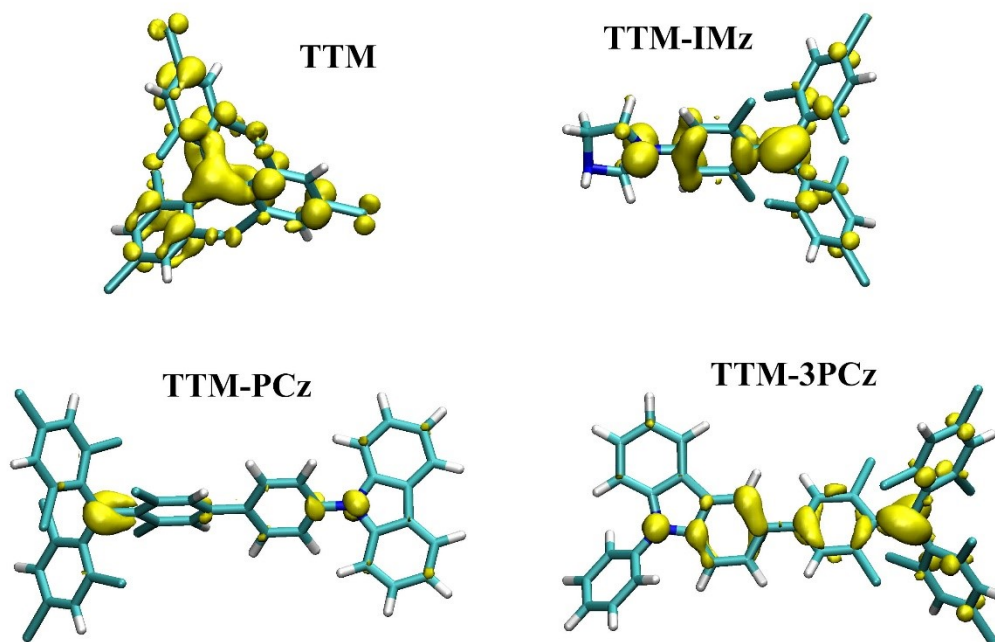
Generalized Mulliken–Hush for obtaining H_{ab}

$$|H_{ab}| = |\mu_{12}| \Delta E_{12} / |\Delta \mu_{ab}| \qquad (1)$$

$$|\Delta \mu_{ab}| = [(\mu_{11} - \mu_{22})^2 + 4(\mu_{12})^2]^{1/2} \qquad (2)$$

where μ_{12} is the transition dipole moment connecting the two adiabatic states in the charge transition, μ_{11}-μ_{22} is the difference of two adiabatic state dipole moments (in this case, D_0 and D_1), ΔE_{12} is the zero-point energy difference between the initial and final adiabatic states. These values can be extract from the computing results of geometry optimization results of D_0 and D_1.(J. Chem. Phys. 106, 9213 (1997); J. AM. CHEM. SOC. 2005, 127, 11303-11310)

5. Table S3 parameters in eq.s(1) and eq.s(2) for obtaining H_{ab}. Dipole moments (in Debye) and ΔE_{12} (in a.u.)

Solvents	cyclohexane				Toluene				chloroform			
Radicals	μ_{11}	μ_{22}	μ_{12}	ΔE_{12}	μ_{11}	μ_{22}	μ_{12}	ΔE_{12}	μ_{11}	μ_{22}	μ_{12}	ΔE_{12}
TTM	0.001	3.57	2.19	0.087	0.00	3.70	2.26	0.087	0.00	4.11	2.50	0.087
IMz	6.64	18.92	3.82	0.067	6.80	19.42	3.98	0.067	7.32	20.99	4.52	0.064
PCz	1.34	43.74	3.70	0.061	1.33	43.89	3.94	0.061	1.31	44.32	4.69	0.061
3PCz	6.16	34.55	5.27	0.065	6.23	35.18	5.44	0.064	6.43	37.13	6.00	0.062
3NCz	6.33	37.24	5.19	0.064	6.40	37.83	5.35	0.063	6.57	39.70	5.89	0.062
2Br3PCz	5.93	34.38	5.31	0.065	6.00	35.01	5.48	0.064	6.18	36.96	6.04	0.062
2F3PCz	5.94	31.32	5.29	0.068	5.43	32.01	5.45	0.068	5.60	34.12	5.98	0.066

Solvents	cyclohexane	Toluene	chloroform
Radicals	H_{ab}	H_{ab}	H_{ab}
TTM	7402	7387	7366
IMz	3911	3901	3901
PCz	1155	1223	1426
3PCz	2467	2475	2499
3NCz	2229	2240	2274
2Br3PCz	1294	1389	1638
2F3PCz	1388	1486	1752

6. Table S4 The calculated k_r and k_{nr} ($10^7\,S^{-1}$) of TTM based radicals in toluene.

Toluene	
k_r	k_{nr}
1.11	93.4
1.54	598.7
1.17	14.82
2.57	1.52
2.40	4.04
2.60	2.50
3.09	0.16

7.Table S5: Considering Huang-Rhys factors (S) of each radical in cyclohexane contributed from different vibrational modes. Where B represents bond length; A represents bond angle; D represents the dihedral.

Item	S^S_{TTM}	S^S_{Sub}	S^B_{TTM}	S^B_{Sub}	S^T_{TTM}	S^T_{Sub}	S_{total}
TTM	0.448	0.000	1.134	0.000	8.976	0.000	10.558
IMz	0.504	0.009	1.180	0.014	14.951	1.721	18.379
PCz	0.045	0.021	0.122	0.068	2.548	1.855	4.659
3PCz	0.022	0.008	0.090	0.033	2.544	2.254	4.951
3NCz	0.024	0.005	0.088	0.049	2.772	2.125	5.063
2Br3PCz	0.015	0.004	0.066	0.032	1.383	2.122	3.622
2F3PCz	0.033	0.004	0.130	0.022	2.782	2.300	5.271

8.Atomic coordinates of all the radicals at their ground-state geometry.

TTM
0 2
```
 C                    -3.19433386    -2.74390259     0.34410931
 C                    -2.51718384    -1.74293908     1.29864580
 C                    -1.70998450    -0.71971923     0.78350280
 C                    -2.70817669    -1.85528213     2.68241700
 C                    -1.09377538     0.19115561     1.65213120
 C                    -2.09196858    -0.94440653     3.55104532
 C                    -1.28476585     0.07881079     3.03590258
 H                    -0.47745859     0.97240505     1.25880826
 H                    -2.23779620    -1.03018268     4.60758531
 C                    -2.46801661    -4.04310729    -0.05102409
 C                    -2.63663834    -5.20202686     0.71864732
 C                    -1.63844615    -4.06646397    -1.18026688
 C                    -1.97568745    -6.38430240     0.35907752
 C                    -0.97749328    -5.24873884    -1.53983525
 C                    -1.14611318    -6.40765780    -0.77016250
 H                    -2.10443509    -7.26916362     0.94673784
 H                    -0.34409634    -5.26657168    -2.40203609
 C                    -4.59780114    -2.44566141    -0.21529376
 C                    -4.73728266    -1.74218023    -1.41927927
 C                    -5.73547484    -2.87774312     0.47963494
 C                    -6.01443786    -1.47078148    -1.92833649
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H	-7.88126906	-2.93625323	0.50116834
Cl	-0.31603178	-7.89246163	-1.22174023
Cl	-1.42668123	-2.61099363	-2.14689076
Cl	-3.67848718	-5.17269422	2.13684709
Cl	-8.75607397	-1.56202529	-1.87273097
Cl	-3.30849319	-1.19952923	-2.29202811
Cl	-5.56030184	-3.76123536	1.99170501
Cl	-0.51087270	1.22276352	4.12680199
Cl	-1.47012054	-0.57862796	-0.95435754
Cl	-3.72193020	-3.14032883	3.32937819

TTM-IMz

0 2

C	0.07054079	0.46818084	-0.08665929
C	0.15633989	1.22917982	-1.42274276
C	-1.01478170	1.66307782	-2.05845396
C	1.40553864	1.48779091	-2.00286752
C	-0.93670439	2.35558924	-3.27428858
C	1.48361583	2.18030019	-3.21870337
C	0.31249439	2.61420061	-3.85441318
H	-1.83088168	2.68688035	-3.75966798
H	2.43740664	2.37775288	-3.66164301
C	0.09610738	1.24313992	1.24389878
C	1.31790036	1.50810281	1.87709586
C	-1.10241998	1.68338982	1.82150952
C	1.34116614	2.21331736	3.08790266
C	-1.07915411	2.38860535	3.03231575
C	0.14263904	2.65357014	3.66551172
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C	1.01732160	-3.25200338	-0.04580215
C	-0.24350984	-3.86322095	-0.07108244

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Cl	2.87633478	0.94286081	-1.20448798
Cl	-0.37078453	-5.61860165	-0.06477391
Cl	2.70212579	-1.08666129	-0.01907275
Cl	2.82311482	0.95519375	1.15168494
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C	0.98292520	4.58193027	4.45868641
C	0.75883334	5.71975653	5.44444704
H	0.11140008	5.27414175	7.47879818
H	-1.84209160	3.88856267	5.76141443
H	-0.65447168	3.17387776	6.91000736
H	2.05771518	4.27117132	4.45536621
H	0.73267513	4.91254206	3.41923277
H	1.71106383	5.97022626	5.97615669
H	0.43011089	6.64393789	4.90606393
N	0.09298498	3.41917307	4.87391811
N	-0.30413451	5.27646513	6.43970455
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Cl	-2.75784318	-0.69123432	-0.14447619

TTM-PCz
0 2

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C	-6.37125279	-0.52239825	0.02352775
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H	-6.61559117	1.59555171	-0.26210700
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C	-1.15774816	-0.39046076	1.84677940
C	-0.61947875	2.29613463	2.44327269
C	-0.69049807	-0.03982666	3.11931766
C	-0.43883148	1.31100132	3.42111973
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Cl	-2.93003725	-2.65245836	0.03415635
Cl	-3.96957459	2.66957028	-0.66387710
Cl	0.55175751	-0.41277427	-5.83834354
Cl	-1.82630364	2.76717537	-2.07125739
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H	0.53324496	3.73615145	4.21691747
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C	1.69064552	1.76593121	9.58235667
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C	3.03086082	4.63148329	7.78924664
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C	3.52672397	3.18952229	9.62221816
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H	4.61830044	6.01759710	7.32248949

H	6.06562586	5.30536674	9.22325970
H	5.32172038	3.42980161	10.70422925
N	1.37488666	2.91102379	8.69274274

TTM-3PCz

0 2

C	5.37782309	-1.46427514	-6.03441271
C	5.92889513	-0.33581239	-6.92314492
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C	5.85644599	-0.45354317	-8.31755758
C	7.02359403	1.81718559	-7.16325527
C	6.37446074	0.55935233	-9.13530867
C	6.96166417	1.69321109	-8.55827257
H	7.46754315	2.68552133	-6.72340572
H	6.32279190	0.46655299	-10.20014305
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C	2.90820531	-1.98597684	-6.37505408
C	3.58176214	-0.88970891	-4.31688449
C	1.57569369	-1.98328723	-5.94031874
C	2.25085405	-0.90710032	-3.87141781
C	1.24916240	-1.46039358	-4.68080700
H	0.80781934	-2.38466836	-6.56865411
H	1.99971302	-0.49870736	-2.91469331
C	6.30096013	-2.62418393	-5.61672428
C	7.05042319	-2.52652233	-4.43733847
C	6.39209273	-3.77356408	-6.41184201
C	7.88767409	-3.58048240	-4.04935005
C	7.22937874	-4.82829263	-6.02357910
C	7.97570342	-4.73207159	-4.84152766
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H	7.29871875	-5.70724203	-6.62954895
Cl	7.62245030	2.96109297	-9.58602577
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Cl	6.93897485	-1.07778314	-3.44359154
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C	-5.19820847	-3.64370315	-6.68290112
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C	-5.97171207	-2.94599348	-4.46523153
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H	-7.17541517	-4.02038515	-5.89433655
H	-6.72988229	-2.89015762	-3.71310178
H	-3.13368302	-3.15463111	-7.12210238
C	-2.81655279	-1.54098308	-3.30639209
C	-1.87833695	-1.11148753	-2.43725596
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C	-0.20988044	-1.50032337	-4.18981265
C	-1.22398944	-1.97311724	-5.04345580
C	-2.47766356	-2.00438758	-4.55995401
H	-2.14360205	-0.80151499	-1.44754025
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H	-3.59366724	-2.43043782	1.40277747
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TTM-3NCz
0 2

C	3.06082642	-0.02786672	-0.31490466
C	3.80593875	0.42396098	0.95440651
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C	5.19969655	0.28547711	1.00162224
C	3.83241493	1.35716975	3.19676274
C	5.91025551	0.68037284	2.13877172
C	5.22793214	1.21697414	3.23712022
H	3.31276257	1.76674937	4.03813591
H	6.97473435	0.57380331	2.16775078
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C	3.85870621	1.22552546	-2.39550815
C	1.55563032	1.50712989	-1.67151241
C	3.61287640	2.05458651	-3.50358513

C	1.30493283	2.29262820	-2.79207776
C	2.31891077	2.54229759	-3.72067439
H	4.40494941	2.30195923	-4.18188764
H	0.33122586	2.70793831	-2.94295257
C	2.54157368	-1.46825067	-0.43666084
C	1.26381803	-1.78746763	0.04716637
C	3.33298866	-2.45609909	-1.03143378
C	0.77277893	-3.09236457	-0.08022799
C	2.84047717	-3.76088152	-1.16205891
C	1.55819232	-4.07787441	-0.69159708
H	-0.20272866	-3.33625454	0.28824196
H	3.44175538	-4.51527815	-1.62282605
Cl	6.12526599	1.71442011	4.66687614
Cl	6.05897731	-0.38836043	-0.37692741
Cl	1.36907229	1.14692063	2.00803544
Cl	0.93433372	-5.71357716	-0.86782450
Cl	0.27482624	-0.54999436	0.81621518
Cl	4.94391643	-2.05817578	-1.61612310
Cl	5.46382718	0.55142859	-2.13894508
Cl	0.27372928	1.22554615	-0.50257260
C	5.10597058	6.63760538	-8.80562586
C	4.18091356	7.27602565	-9.66897292
C	2.81188755	6.91400706	-9.63784620
C	2.42849812	5.96438938	-8.75478334
C	3.33267385	5.42653017	-7.85578030
C	4.64981320	5.68313800	-7.88237251
H	6.14778721	6.88044848	-8.85358823
H	4.52193864	8.03144336	-10.34688375
H	2.10736712	7.37372768	-10.29858715
H	5.32533331	5.18581921	-7.21669223
C	1.22258957	4.68463977	-7.24846793
C	0.23929650	4.23797863	-6.45418939
C	0.60511222	3.58056821	-5.26816436
C	1.96849428	3.35329846	-4.97369016
C	2.96635876	3.86390624	-5.82379218
C	2.54649037	4.57945042	-6.88393887
H	-0.78906028	4.37452968	-6.71847174
H	-0.14801283	3.24335126	-4.59133319
H	4.00871457	3.70414003	-5.63197894
N	1.08103780	5.33950181	-8.57307759
C	-0.07184138	6.25803643	-8.61539103
C	-1.30676061	5.76234857	-9.06388066
C	-2.43655628	6.58591981	-9.08552584
C	-2.34088205	7.91424458	-8.65507647

C	-1.10296347	8.42340927	-8.22663990
C	0.03547025	7.59498315	-8.20901687
H	-3.73483751	5.05987966	-9.86202789
H	-1.38414219	4.74677935	-9.39056161
C	-3.66296171	6.07825222	-9.53563674
C	-3.48227692	8.73183715	-8.65266271
H	-1.02739082	9.44283278	-7.91425412
H	0.97632010	7.98050969	-7.88440812
C	-4.70638958	8.22848604	-9.11743229
C	-4.79578335	6.90325961	-9.55794363
H	-3.41819136	9.73906730	-8.29739936
H	-5.57406676	8.85697774	-9.13435432
H	-5.72787374	6.51855072	-9.91195981

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C	2.47431300	-0.05192200	0.00590700
C	3.18130900	1.24125800	0.06992500
C	2.86392000	2.24003000	1.02726300
C	4.23409600	1.58632200	-0.81678300
C	3.52050100	3.46444700	1.10004300
C	4.91186600	2.80012700	-0.76374500
C	4.54451700	3.73286300	0.19914400
H	3.24585200	4.18327000	1.86149100
H	5.69751200	3.01514900	-1.47681800
C	1.00542000	-0.08994000	0.00749100
C	0.20761100	0.74139200	-0.82370100
C	0.25330400	-0.96046600	0.84074400
C	-1.17906400	0.71202300	-0.82739200
C	-1.13329500	-0.99980000	0.85023600
C	-1.88581100	-0.16096400	0.01397300
H	-1.71186000	1.34361700	-1.52832100
H	-1.63075400	-1.65795500	1.55266600
C	3.24801400	-1.30620300	-0.05938600
C	4.31903800	-1.59545900	0.82542600
C	2.98207700	-2.32009100	-1.01650600
C	5.05992500	-2.77171000	0.77066700
C	3.70231300	-3.50808900	-1.09097000
C	4.74076000	-3.72219400	-0.19203900
H	5.85715100	-2.94518000	1.48220000
H	3.46468700	-4.24020600	-1.85221600
Cl	1.65791900	1.95470500	2.27045000
Cl	4.69851000	0.51843100	-2.13061200

Cl	4.72862200	-0.50492300	2.13893400
Cl	1.76034500	-2.09835000	-2.25728700
Cl	1.05185700	-1.98525000	2.02899800
Cl	0.94983100	1.80276100	-2.01632000
C	-7.72115400	3.98875100	-0.73955900
C	-8.94496800	3.31002000	-0.60039400
C	-8.99292300	1.93997600	-0.35010800
C	-7.77796300	1.25724800	-0.24508100
C	-6.53465000	1.92764200	-0.37150100
C	-6.51423400	3.30483000	-0.62370900
H	-7.71974700	5.05699600	-0.93569300
H	-9.87581400	3.86362200	-0.68723000
H	-9.94094700	1.42474400	-0.23745600
H	-5.56934500	3.83242000	-0.72315700
C	-6.16331000	-0.30320100	0.06014500
C	-5.44136500	-1.48309600	0.26612200
C	-4.05404700	-1.40999600	0.24765800
C	-3.36488600	-0.19371500	0.02064100
C	-4.10728500	0.97562900	-0.19871900
C	-5.50198300	0.92952800	-0.18159700
H	-5.94319200	-2.43163700	0.42450500
H	-3.48381100	-2.32439200	0.38019200
H	-3.59917300	1.92288300	-0.35492700
C	-9.49004200	-1.33792900	-0.78654200
C	-10.47085600	-2.31016800	-0.58900400
C	-10.49596300	-3.05627300	0.59145600
C	-9.53981400	-2.81983000	1.58163400
C	-8.56711400	-1.83619700	1.40037100
C	-8.53833300	-1.09661600	0.21178200
H	-9.45072000	-0.77154800	-1.71178600
H	-11.20822700	-2.49220400	-1.36568200
H	-11.25648800	-3.81761300	0.73892700
H	-9.55653100	-3.39252100	2.50457500
H	-7.83675600	-1.63077000	2.17682900
N	-7.54075100	-0.09839600	0.01757600
Br	5.74069100	-5.34066400	-0.28059500
Br	5.45712300	5.40224600	0.28530300

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C	3.28264800	-0.05950800	0.00224700
C	3.99585100	1.22370100	0.15309400
C	3.68748100	2.15344600	1.18132900

C	5.04677000	1.62561500	-0.71274100
C	4.34860500	3.36671800	1.33884200
C	5.73277800	2.82768700	-0.57737600
C	5.36666100	3.68187700	0.45171000
H	4.09513200	4.04315700	2.14561700
H	6.51851000	3.10638200	-1.26851100
C	1.81336000	-0.09108000	0.00250300
C	1.01786500	0.79757900	-0.76954200
C	1.05692200	-1.01258100	0.77491700
C	-0.36907500	0.77399300	-0.77510600
C	-0.32996500	-1.04724000	0.78223500
C	-1.07944700	-0.15122800	0.00489300
H	-0.89910800	1.45411500	-1.43134000
H	-0.82969300	-1.74968400	1.43869100
C	4.05077400	-1.31061300	-0.14855200
C	5.11778300	-1.66683600	0.71762500
C	3.78336700	-2.25255800	-1.17713000
C	5.85536900	-2.83795200	0.58218000
C	4.49663600	-3.43591800	-1.33477900
C	5.52709600	-3.70685900	-0.44735500
H	6.65216800	-3.08251300	1.27356200
H	4.27304200	-4.12244800	-2.14187300
Cl	2.48385400	1.78471800	2.40472800
Cl	5.49871200	0.65039800	-2.10094100
Cl	5.52626500	-0.67338100	2.10637500
Cl	2.56509900	-1.93608600	-2.40064700
Cl	1.85011200	-2.11992800	1.89145600
Cl	1.76283800	1.93631000	-1.88767000
C	-6.90026000	4.05811100	-0.48686100
C	-8.12661600	3.37655000	-0.39052900
C	-8.17969700	1.99373300	-0.22626100
C	-6.96734400	1.30111900	-0.16415400
C	-5.72149600	1.97359100	-0.24813700
C	-5.69593000	3.36375500	-0.41372500
H	-6.89481900	5.13650300	-0.61601700
H	-9.05540400	3.93791800	-0.44275900
H	-9.12968300	1.47605100	-0.14605000
H	-4.74900500	3.89292800	-0.47989300
C	-5.35813000	-0.28119600	0.04195300
C	-4.64025300	-1.47421600	0.17208800
C	-3.25261400	-1.40486100	0.15762800
C	-2.55895700	-0.17907100	0.00926700
C	-3.29748500	1.00423500	-0.13484700
C	-4.69244600	0.96184800	-0.12128400

H	-5.14530900	-2.42922400	0.26973000
H	-2.68563900	-2.32789400	0.23100400
H	-2.78628500	1.95785800	-0.23024900
C	-8.69153100	-1.24827400	-0.86245000
C	-9.67549200	-2.22747800	-0.72360100
C	-9.70010300	-3.04662900	0.40739500
C	-8.74027500	-2.87658700	1.40760500
C	-7.76442000	-1.88698000	1.28579000
C	-7.73604700	-1.07383100	0.14619000
H	-8.65271100	-0.62495500	-1.75035400
H	-10.41573200	-2.35750800	-1.50797100
H	-10.46306300	-3.81305000	0.50881200
H	-8.75650700	-3.50630500	2.29263800
H	-7.03109100	-1.73364800	2.07142500
N	-6.73513500	-0.06916200	0.01268300
F	6.22803400	-4.84466700	-0.58915300
F	6.01750900	4.84906000	0.59340600