附　　錄　　B

附錄 B-1. 9F 正己烷溶液之理論計算:

A. S_0 state：

1. S_0 optimization Cartesian Coordinates：

command：b3lyp/6-31G(d,p) opt freq SCRF(pcm,read)

nosymmcav

eps=1.9

epsinf=1.8903

rsolv=4.60

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.468260	-0.065008	0.000063
2	6	0	-3.031498	-1.392777	-0.000023
3	6	0	-1.664340	-1.711325	-0.000063
4	6	0	-0.742158	-0.671558	-0.000037
5	6	0	-1.189390	0.665683	0.000017
6	6	0	-2.539249	0.984280	0.000078
7	6	0	-0.000001	1.576213	-0.000015
8	6	0	1.189389	0.665684	-0.000029
9	6	0	0.742159	-0.671557	-0.000036
10	6	0	1.664341	-1.711325	0.000004
11	6	0	3.031498	-1.392777	0.000050
12	6	0	3.468260	-0.065007	0.000036
13	6	0	2.539250	0.984281	-0.000003
14	8	0	-0.000002	2.796643	-0.000062
15	1	0	-4.532868	0.151942	0.000100
16	1	0	-3.764043	-2.195929	-0.000046
17	1	0	-1.346155	-2.750555	-0.000111
18	1	0	-2.857413	2.023549	0.000134
19	1	0	1.346157	-2.750555	0.000009
20	1	0	3.764043	-2.195929	0.000085
21	1	0	4.532869	0.151940	0.000072

22 1 0 2.857415 2.023550 0.000002

---

2. S_0 state frequency：

99	132	153	205	273	283	410	413	437	457
510	565	568	628	663	686	736	755	756	785
795	825	899	900	932	963	966	998	1000	1022
1043	1056	1101	1117	1175	1181	1186	1213	1230	1315
1321	1345	1415	1483	1492	1511	1515	1639	1645	1649
1662	1793	3169	3170	3178	3179	3185	3186	3194	3195

3. S_0 state TD：

command：PBE1PBE/6-31G(d,p) td(50-50,nstates=6) scrf (pcm,read)

nosymmcav

eps=1.9

epsinf=1.8903

rsolv=4.60

Excited State 1: Triplet-A 2.3936 eV 517.97 nm f=0.0000

43 -> 51 0.17198

44 -> 50 -0.18095

45 -> 48 0.19974

45 -> 49 0.16229

47 -> 48 0.69888

47 -> 49 -0.26178

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

Total Energy, E(RPA) = -574.701299835

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

Excited State 2: Triplet-A 2.6841 eV 461.92 nm f=0.0000

46 -> 48 0.72806

46 -> 52 -0.14050

Excited State 3: Triplet-A 3.1446 eV 394.28 nm f=0.0000

38 -> 48 0.16432

38 -> 52 -0.12320

43 -> 48 0.20406

43 -> 49	-0.12273				
44 -> 48	0.68116				
44 -> 49	0.16559				
45 -> 50	-0.26571				
47 -> 50	-0.11592				
47 -> 51	0.15360				
Excited State	4:	Singlet-A	3.2178 eV	385.31 nm	f=0.0000
46 -> 48	0.67518				
Excited State	5:	Singlet-A	3.2315 eV	383.68 nm	f=0.0061
47 -> 48	0.68033				
Excited State	6:	Triplet-A	3.4639 eV	357.93 nm	f=0.0000
44 -> 50	-0.23233				
45 -> 48	0.57221				
45 -> 49	0.20073				
47 -> 48	-0.27608				
47 -> 49	-0.27529				
Excited State	7:	Triplet-A	3.6742 eV	337.44 nm	f=0.0000
43 -> 51	-0.11951				
45 -> 48	0.38160				
45 -> 49	-0.16025				
47 -> 48	0.10441				
47 -> 49	0.59878				
Excited State	8:	Triplet-A	4.1111 eV	301.58 nm	f=0.0000
43 -> 48	0.49390				
43 -> 49	-0.21119				
44 -> 48	-0.30236				
44 -> 49	0.20997				
45 -> 50	-0.12224				
47 -> 50	-0.19437				
47 -> 51	0.31806				
Excited State	9:	Singlet-A	4.1745 eV	297.00 nm	f=0.0383
45 -> 48	0.61668				

47 -> 49 -0.32329

Excited State 10: Singlet-A 4.4029 eV 281.59 nm f=0.0411

43 -> 48 -0.15868

44 -> 48 0.60128

44 -> 49 -0.10811

47 -> 50 0.19684

Excited State 11: Singlet-A 4.5142 eV 274.65 nm f=0.0000

46 -> 49 0.65494

Excited State 12: Singlet-A 4.5976 eV 269.67 nm f=0.0626

43 -> 48 0.57622

44 -> 48 0.15404

44 -> 49 0.21554

4.

B. S_1(min) state：

1. S_1(min) state optimization Cartesian Coordinates：

command：CIS(root=1,nstates=6,direct)/6-31g* opt freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.402665	-0.043064	0.000016
2	6	0	-2.974321	-1.411786	0.000015
3	6	0	-1.656418	-1.738350	0.000000
4	6	0	-0.699374	-0.691629	-0.000008
5	6	0	-1.142232	0.689520	-0.000002
6	6	0	-2.508806	0.989708	0.000006
7	6	0	0.000000	1.590087	-0.000055
8	6	0	1.142232	0.689520	-0.000024
9	6	0	0.699374	-0.691629	-0.000027
10	6	0	1.656418	-1.738350	-0.000010
11	6	0	2.974321	-1.411786	0.000009
12	6	0	3.402665	-0.043064	0.000025

13	6	0	2.508806	0.989708	0.000004
14	8	0	0.000000	2.809764	0.000026
15	1	0	-4.458795	0.160263	0.000016
16	1	0	-3.721501	-2.184636	0.000014
17	1	0	-1.342774	-2.766650	-0.000008
18	1	0	-2.827634	2.015308	-0.000007
19	1	0	1.342774	-2.766650	-0.000003
20	1	0	3.721501	-2.184636	0.000027
21	1	0	4.458795	0.160263	0.000051
22	1	0	2.827634	2.015308	0.000007

---

2. S_1(min) state frequency：

91	142	172	223	270	291	411	445	448	497
543	552	598	639	654	699	766	794	810	841
845	857	959	962	973	1056	1064	1078	1092	1094
1120	1121	1194	1226	1264	1274	1282	1308	1347	1436
1453	1468	1502	1587	1589	1634	1660	1673	1687	1766
1779	1864	3350	3352	3360	3363	3376	3378	3389	3390

3. S_1(min) state TD：

command：PBE1PBE/6-31G(d,p) td(50-50,nstates=6) scrf (pcm,read)

nosymmcav

eps=1.9

epsinf=1.8903

rsolv=4.60

Excited State 1: Triplet-A 2.3936 eV 517.97 nm f=0.0000

43 -> 51 0.17198

44 -> 50 -0.18095

45 -> 48 0.19974

45 -> 49 0.16229

47 -> 48 0.69888

47 -> 49 -0.26178

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

Total Energy, E(RPA) = -574.701299835

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

Excited State	2:	Triplet-A	2.6841 eV	461.92 nm	f=0.0000
46 -> 48		0.72806			
46 -> 52		-0.14050			
Excited State	3:	Triplet-A	3.1446 eV	394.28 nm	f=0.0000
38 -> 48		0.16432			
38 -> 52		-0.12320			
43 -> 48		0.20406			
43 -> 49		-0.12273			
44 -> 48		0.68116			
44 -> 49		0.16559			
45 -> 50		-0.26571			
47 -> 50		-0.11592			
47 -> 51		0.15360			
Excited State	4:	Singlet-A	3.2178 eV	385.31 nm	f=0.0000
46 -> 48		0.67518			
Excited State	5:	Singlet-A	3.2315 eV	383.68 nm	f=0.0061
47 -> 48		0.68033			
Excited State	6:	Triplet-A	3.4639 eV	357.93 nm	f=0.0000
44 -> 50		-0.23233			
45 -> 48		0.57221			
45 -> 49		0.20073			
47 -> 48		-0.27608			
47 -> 49		-0.27529			
Excited State	7:	Triplet-A	3.6742 eV	337.44 nm	f=0.0000
43 -> 51		-0.11951			
45 -> 48		0.38160			
45 -> 49		-0.16025			
47 -> 48		0.10441			
47 -> 49		0.59878			
Excited State	8:	Triplet-A	4.1111 eV	301.58 nm	f=0.0000
43 -> 48		0.49390			
43 -> 49		-0.21119			

44 -> 48	-0.30236				
44 -> 49	0.20997				
45 -> 50	-0.12224				
47 -> 50	-0.19437				
47 -> 51	0.31806				
Excited State	9:	Singlet-A	4.1745 eV	297.00 nm	f=0.0383
45 -> 48	0.61668				
47 -> 49	-0.32329				
Excited State	10:	Singlet-A	4.4029 eV	281.59 nm	f=0.0411
43 -> 48	-0.15868				
44 -> 48	0.60128				
44 -> 49	-0.10811				
47 -> 50	0.19684				
Excited State	11:	Singlet-A	4.5142 eV	274.65 nm	f=0.0000
46 -> 49	0.65494				
Excited State	12:	Singlet-A	4.5976 eV	269.67 nm	f=0.0626
43 -> 48	0.57622				
44 -> 48	0.15404				
44 -> 49	0.21554				

附錄 B-2. 9F 二甲基亞碸溶液之理論計算:

A. S_0 state：

1. S_0 optimization Cartesian Coordinates：

command：b3lyp/6-31G(d,p) opt freq SCRF(pcm,read,solvent=DMSO)
nosymmcav

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.469155	-0.064854	0.000077
2	6	0	3.031676	-1.392923	0.000085
3	6	0	1.663255	-1.712376	0.000002
4	6	0	0.742272	-0.671838	-0.000082
5	6	0	1.189212	0.666809	-0.000069
6	6	0	2.540130	0.985591	0.000025
7	6	0	-0.000001	1.573101	-0.000206
8	6	0	-1.189211	0.666806	-0.000043
9	6	0	-0.742272	-0.671838	-0.000089
10	6	0	-1.663256	-1.712376	-0.000085
11	6	0	-3.031675	-1.392923	0.000016
12	6	0	-3.469154	-0.064854	0.000127
13	6	0	-2.540129	0.985589	0.000085
14	8	0	-0.000003	2.797924	0.000041
15	1	0	4.535543	0.152625	0.000142
16	1	0	3.765137	-2.197805	0.000171
17	1	0	1.344554	-2.753472	0.000026
18	1	0	2.864381	2.025214	0.000007
19	1	0	-1.344553	-2.753471	-0.000134
20	1	0	-3.765137	-2.197804	0.000034
21	1	0	-4.535542	0.152623	0.000222
22	1	0	-2.864377	2.025214	0.000142

2. S_0 state frequency：

99	132	154	205	273	286	409	411	436	456
508	564	567	623	660	687	737	754	756	780
794	826	901	904	929	967	969	1003	1005	1017
1040	1053	1096	1112	1172	1174	1179	1211	1225	1313
1320	1341	1413	1479	1488	1507	1511	1635	1041	1643
1656	1763	3135	3136	3142	3143	3148	3149	3157	3157

3. S_0 state TD：

command：PBE1PBE/6-31G(d,p) td(50-50,nstates=6)scrf(pcm,read,solvent=DMSO)
nosymmcav

Excited State 1: Triplet-A 2.3349 eV 531.00 nm f=0.0000

43 -> 51	0.16411
44 -> 50	-0.16980
46 -> 48	-0.19881
46 -> 49	-0.14787
47 -> 48	0.70455
47 -> 49	-0.24948

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

Total Energy, E(RPA) = -574.712669038

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

Excited State 2: Triplet-A 2.7855 eV 445.10 nm f=0.0000

45 -> 48	0.72649
45 -> 52	-0.13397

Excited State 3: Singlet-A 3.1149 eV 398.04 nm f=0.0051

47 -> 48	0.68118

Excited State 4: Triplet-A 3.1278 eV 396.40 nm f=0.0000

37 -> 48	0.15642
37 -> 52	-0.11128
43 -> 48	0.19370
43 -> 49	-0.11902
44 -> 48	0.69017
44 -> 49	0.14837

46 -> 50 0.26084

47 -> 50 -0.10635

47 -> 51 0.14760

Excited State 5: Singlet-A 3.3009 eV 375.61 nm f=0.0000

45 -> 48 0.67692

Excited State 6: Triplet-A 3.3661 eV 368.33 nm f=0.0000

44 -> 50 0.22342

46 -> 48 0.62297

46 -> 49 0.16532

47 -> 48 0.25135

47 -> 49 0.21612

Excited State 7: Triplet-A 3.6485 eV 339.82 nm f=0.0000

43 -> 51 -0.13408

46 -> 48 -0.31092

46 -> 49 0.19006

47 -> 48 0.12216

47 -> 49 0.62942

Excited State 8: Triplet-A 4.0626 eV 305.19 nm f=0.0000

43 -> 48 0.54531

43 -> 49 -0.18366

44 -> 48 -0.27863

44 -> 49 0.16277

47 -> 50 -0.20973

47 -> 51 0.29866

Excited State 9: Singlet-A 4.0935 eV 302.88 nm f=0.0704

46 -> 48 0.63069

47 -> 49 0.28994

Excited State 10: Singlet-A 4.4029 eV 281.59 nm f=0.0456

43 -> 48 -0.16281

44 -> 48 0.61083

47 -> 50 0.18035

Excited State 11: Singlet-A 4.5349 eV 273.40 nm f=0.8976

46 -> 48 -0.22983

47 -> 49 0.56217

Excited State 12: Singlet-A 4.5395 eV 273.12 nm f=0.0741

43 -> 48 0.59293

44 -> 48 0.14663

44 -> 49 0.17153

B. S_1(min) state：

1. S_1(min) state optimization Cartesian Coordinates：

command：CIS(root=1,nstates=6,direct)/6-31g* opt freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.402665	-0.043064	0.000016
2	6	0	-2.974321	-1.411786	0.000015
3	6	0	-1.656418	-1.738350	0.000000
4	6	0	-0.699374	-0.691629	-0.000008
5	6	0	-1.142232	0.689520	-0.000002
6	6	0	-2.508806	0.989708	0.000006
7	6	0	0.000000	1.590087	-0.000055
8	6	0	1.142232	0.689520	-0.000024
9	6	0	0.699374	-0.691629	-0.000027
10	6	0	1.656418	-1.738350	-0.000010
11	6	0	2.974321	-1.411786	0.000009
12	6	0	3.402665	-0.043064	0.000025
13	6	0	2.508806	0.989708	0.000004
14	8	0	0.000000	2.809764	0.000026
15	1	0	-4.458795	0.160263	0.000016
16	1	0	-3.721501	-2.184636	0.000014
17	1	0	-1.342774	-2.766650	-0.000008
18	1	0	-2.827634	2.015308	-0.000007
19	1	0	1.342774	-2.766650	-0.000003
20	1	0	3.721501	-2.184636	0.000027

21	1	0	4.458795	0.160263	0.000051
22	1	0	2.827634	2.015308	0.000007

---

2. S_1(min) state frequency：

91	142	172	223	270	291	411	445	448	497
543	552	598	639	654	699	766	794	810	841
845	857	959	962	973	1056	1064	1078	1092	1094
1120	1121	1194	1226	1264	1274	1282	1308	1347	1436
1453	1468	1502	1587	1589	1634	1660	1673	1687	1766
1779	1864	3350	3352	3360	3363	3376	3378	3389	3390

3. S_1(min) state TD：

command：PBE1PBE/6-31G(d,p) td(50-50,nstates=6) scrf (pcm,read,solvent=DMSO) nosymmcav

Excited State 1: Triplet-A 2.3936 eV 517.97 nm f=0.0000

43 -> 51	0.17198
44 -> 50	-0.18095
45 -> 48	0.19974
45 -> 49	0.16229
47 -> 48	0.69888
47 -> 49	-0.26178

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

Total Energy, E(RPA) = -574.701299835

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

Excited State 2: Triplet-A 2.6841 eV 461.92 nm f=0.0000

46 -> 48	0.72806
46 -> 52	-0.14050

Excited State 3: Triplet-A 3.1446 eV 394.28 nm f=0.0000

38 -> 48	0.16432
38 -> 52	-0.12320
43 -> 48	0.20406
43 -> 49	-0.12273
44 -> 48	0.68116

44 -> 49 0.16559
45 -> 50 -0.26571
47 -> 50 -0.11592
47 -> 51 0.15360

Excited State 4: Singlet-A 3.2178 eV 385.31 nm f=0.0000
46 -> 48 0.67518

Excited State 5: Singlet-A 3.2315 eV 383.68 nm f=0.0061
47 -> 48 0.68033

Excited State 6: Triplet-A 3.4639 eV 357.93 nm f=0.0000
44 -> 50 -0.23233
45 -> 48 0.57221
45 -> 49 0.20073
47 -> 48 -0.27608
47 -> 49 -0.27529

Excited State 7: Triplet-A 3.6742 eV 337.44 nm f=0.0000
43 -> 51 -0.11951
45 -> 48 0.38160
45 -> 49 -0.16025
47 -> 48 0.10441
47 -> 49 0.59878

Excited State 8: Triplet-A 4.1111 eV 301.58 nm f=0.0000
43 -> 48 0.49390
43 -> 49 -0.21119
44 -> 48 -0.30236
44 -> 49 0.20997
45 -> 50 -0.12224
47 -> 50 -0.19437
47 -> 51 0.31806

Excited State 9: Singlet-A 4.1745 eV 297.00 nm f=0.0383
45 -> 48 0.61668
47 -> 49 -0.32329

Excited State	10:	Singlet-A	4.4029 eV	281.59 nm	f=0.0411
43 -> 48		-0.15868			
44 -> 48		0.60128			
44 -> 49		-0.10811			
47 -> 50		0.19684			
Excited State	11:	Singlet-A	4.5142 eV	274.65 nm	f=0.0000
46 -> 49		0.65494			
Excited State	12:	Singlet-A	4.5976 eV	269.67 nm	f=0.0626
43 -> 48		0.57622			
44 -> 48		0.15404			
44 -> 49		0.21554			

附錄 B-3. 1-HOF 正己烷溶液之理論計算:

A. S_0 state：

1. S_0 optimization Cartesian Coordinates：

command：b3lyp/6-31G(d,p) opt freq SCRF(pcm,read)
nosymmcav
eps=1.9
epsinf=1.8903
rsolv=4.60

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.979451	-2.080835	0.000000
2	6	0	3.313704	-1.650606	0.000000
3	6	0	3.614448	-0.286204	0.000000
4	6	0	2.600464	0.685503	0.000000
5	6	0	0.980178	-1.119446	0.000000
6	6	0	1.277354	0.263578	0.000000
7	6	0	-0.505194	-1.282655	0.000000
8	6	0	-1.047463	0.081455	0.000000
9	6	0	0.000000	1.024452	0.000000
10	6	0	-2.389855	0.452274	0.000000
11	6	0	-2.691179	1.829357	0.000000
12	6	0	-1.653605	2.756626	0.000000
13	6	0	-0.292813	2.377905	0.000000
14	8	0	-1.169422	-2.321788	0.000000
15	8	0	-3.376376	-0.466899	0.000000
16	1	0	1.726157	-3.137664	0.000000
17	1	0	4.118780	-2.380007	0.000000
18	1	0	4.653987	0.031346	0.000000
19	1	0	2.856580	1.741623	0.000000
20	1	0	-3.729396	2.146590	0.000000
21	1	0	-1.902777	3.814824	0.000000

22	1	0	0.484571	3.135996	0.000000
23	1	0	-2.954469	-1.351628	0.000000

---

2. S_0 state frequency：

92	117	165	180	241	268	269	357
423	451	455	522	524	547	596	627
669	676	689	695	745	774	780	808
814	893	902	917	947	964	982	999
1044	1063	1096	1132	1173	1184	1190	1218
1263	1314	1333	1359	1386	1426	1487	1496
1510	1530	1640	1651	1655	1667	1749	3170
3174	3180	3187	3193	3196	3200	3573	

3. S_0 state TD：

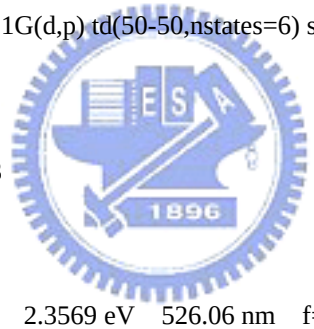
command：PBE1PBE/6-31G(d,p) td(50-50,nstates=6) scrf (pcm,read)

nosymmcav

eps=1.9

epsinf=1.8903

rsolv=4.60



Excited State 1: Triplet-A' 2.3569 eV 526.06 nm f=0.0000

47 -> 54 -0.12987

47 -> 55 0.13214

48 -> 52 -0.10781

48 -> 53 -0.11560

48 -> 54 -0.11082

50 -> 52 -0.39903

51 -> 52 0.60796

51 -> 53 -0.25908

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

Total Energy, E(RPA) = -649.862674611

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

Excited State 2: Triplet-A' 2.7456 eV 451.57 nm f=0.0000

48 -> 52 -0.13046

50 -> 52 0.61593

50 -> 54 -0.13641

51 -> 52 0.39282

Excited State 3: Triplet-A" 2.9691 eV 417.58 nm f=0.0000

49 -> 52 0.72119

49 -> 56 -0.12983

Excited State 4: Singlet-A' 3.1821 eV 389.62 nm f=0.0203

50 -> 52 -0.30213

51 -> 52 0.60858

Excited State 5: Triplet-A' 3.2614 eV 380.16 nm f=0.0000

43 -> 52 0.12090

47 -> 52 0.28034

48 -> 52 0.61419

48 -> 53 0.20553

48 -> 54 0.18874

50 -> 54 0.17686

51 -> 52 0.15206

51 -> 55 0.14650

Excited State 6: Singlet-A" 3.4502 eV 359.36 nm f=0.0000

49 -> 52 0.67883

Excited State 7: Singlet-A' 3.5654 eV 347.74 nm f=0.1425

50 -> 52 0.59120

51 -> 52 0.28354

51 -> 53 0.11039

Excited State 8: Triplet-A' 3.6943 eV 335.61 nm f=0.0000

47 -> 52 -0.15104

47 -> 55 -0.10338

48 -> 53 0.12845

50 -> 52 -0.15917

50 -> 54 -0.16454

51 -> 52 0.14717

51 -> 53 0.63882

51 -> 55 -0.14281

Excited State	9:	Triplet-A'	3.8917 eV	318.59 nm	f=0.0000
47 -> 52		0.47385			
47 -> 53		-0.14608			
48 -> 52		-0.35812			
48 -> 53		0.16409			
50 -> 53		-0.20550			
50 -> 54		0.16906			
51 -> 53		0.17250			
51 -> 54		-0.14053			
51 -> 55		0.21872			

Excited State	10:	Singlet-A'	4.2680 eV	290.50 nm	f=0.0203
47 -> 52		-0.13873			
48 -> 52		0.59541			
50 -> 53		-0.13417			
51 -> 53		0.19379			

Excited State	11:	Singlet-A'	4.4122 eV	281.00 nm	f=0.1923
47 -> 52		-0.22218			
48 -> 52		-0.17255			
50 -> 53		0.17907			
51 -> 53		0.52251			

Excited State	12:	Singlet-A'	4.5561 eV	272.13 nm	f=0.4175
47 -> 52		0.44671			
50 -> 53		-0.33251			
51 -> 53		0.25141			

B. S_1(min) state：

1. S_1(min) state optimization Cartesian Coordinates：

command：CIS(root=1,nstates=6,direct)/6-31g* opt freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	2.033376	-1.990484	0.000000
2	6	0	3.308117	-1.500240	0.000000
3	6	0	3.575881	-0.091171	0.000000
4	6	0	2.568800	0.819474	0.000000
5	6	0	0.969921	-1.080957	0.000000
6	6	0	1.230667	0.350704	0.000000
7	6	0	-0.458200	-1.320872	0.000000
8	6	0	-1.026976	0.003403	0.000000
9	6	0	0.000000	1.020579	0.000000
10	6	0	-2.389055	0.340523	0.000000
11	6	0	-2.715362	1.671048	0.000000
12	6	0	-1.700987	2.677597	0.000000
13	6	0	-0.370614	2.385483	0.000000
14	8	0	-1.079835	-2.383682	0.000000
15	8	0	-3.321350	-0.611247	0.000000
16	1	0	1.832809	-3.045544	0.000000
17	1	0	4.143641	-2.177260	0.000000
18	1	0	4.599404	0.237074	0.000000
19	1	0	2.777283	1.873873	0.000000
20	1	0	-3.750512	1.958417	0.000000
21	1	0	-2.018434	3.704916	0.000000
22	1	0	0.368949	3.164435	0.000000
23	1	0	-2.897067	-1.466991	0.000000

---

2. S_1(min) state frequency：

84	122	173	201	250	289	293	381
424	467	482	533	561	582	622	629
651	708	710	728	781	820	822	843
865	953	962	994	1012	1064	1093	1096
1121	1122	1163	1219	1272	1278	1285	1362
1382	1413	1453	1453	1507	1510	1589	1602
1642	1667	1672	1701	1768	1780	1840	3354
3356	3365	3376	3380	3385	3390	3964	

3. S_1(min) state TD：

command：PBE1PBE/6-31G(d,p) td(50-50,nstates=6) scrf (pcm,read)

nosymmcav

eps=1.9

epsinf=1.8903

rsolv=4.60

Excited State 1: Triplet-A' 1.5487 eV 800.54 nm f=0.0000

47 -> 54	-0.12221
47 -> 55	0.10956
50 -> 52	0.12419
51 -> 52	0.80219
51 -> 53	-0.16527

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

Total Energy, E(RPA) = -649.874177398

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

Excited State 2: Singlet-A' 2.4243 eV 511.43 nm f=0.0168

50 -> 52	0.13220
51 -> 52	0.65475

Excited State 3: Triplet-A' 2.4784 eV 500.26 nm f=0.0000

48 -> 52	0.15190
50 -> 52	0.73348
50 -> 54	-0.11596
51 -> 52	-0.10573

Excited State 4: Triplet-A" 2.6577 eV 466.52 nm f=0.0000

49 -> 52	0.72643
49 -> 56	-0.11597

Excited State 5: Triplet-A' 3.0314 eV 409.00 nm f=0.0000

43 -> 52	0.13462
47 -> 52	0.32179
48 -> 52	0.63535
48 -> 53	0.13576
48 -> 54	0.12788
50 -> 52	-0.13383
50 -> 54	-0.11112
51 -> 54	-0.18328
51 -> 55	0.11851

Excited State	6:	Singlet-A"	3.1331 eV	395.72 nm	f=0.0000
49 -> 52		0.67870			
Excited State	7:	Singlet-A'	3.2920 eV	376.63 nm	f=0.1374
50 -> 52		0.63817			
51 -> 52		-0.11868			
51 -> 53		-0.16226			
Excited State	8:	Triplet-A'	3.6121 eV	343.25 nm	f=0.0000
47 -> 52		0.57303			
48 -> 52		-0.35992			
51 -> 54		-0.23595			
51 -> 55		0.18222			
Excited State	9:	Triplet-A'	3.6707 eV	337.77 nm	f=0.0000
47 -> 55		-0.12101			
48 -> 53		0.14135			
50 -> 53		-0.13282			
51 -> 52		0.10440			
51 -> 53		0.69447			
Excited State	10:	Singlet-A'	4.1785 eV	296.72 nm	f=0.0268
47 -> 52		-0.16082			
48 -> 52		0.58646			
51 -> 53		0.26591			
51 -> 54		0.10648			
Excited State	11:	Singlet-A'	4.3512 eV	284.95 nm	f=0.1462
47 -> 52		0.53882			
48 -> 52		0.18751			
51 -> 53		-0.20707			
51 -> 54		0.22440			
Excited State	12:	Singlet-A'	4.6250 eV	268.07 nm	f=0.7382
47 -> 52		0.27021			
48 -> 52		-0.16412			
51 -> 53		0.52812			

附錄 B-4. 1-HOF-b 正己烷溶液之理論計算:

A. S_0 state：

1. S_0 optimization Cartesian Coordinates：

command：b3lyp/6-31G(d,p) opt freq SCRF(pcm,read)
nosymmcav
eps=1.9
epsinf=1.8903
rsolv=4.60

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.619081	1.226007	0.000164
2	6	0	-3.696686	0.330051	0.000258
3	6	0	-3.467946	-1.049338	0.000111
4	6	0	-2.165625	-1.571529	-0.000096
5	6	0	-1.333968	0.704643	-0.000059
6	6	0	-1.097072	-0.682045	-0.000152
7	6	0	-0.018699	1.428517	-0.000297
8	6	0	1.014511	0.348578	-0.000150
9	6	0	0.368251	-0.908622	-0.000186
10	6	0	2.409273	0.426591	0.000067
11	6	0	3.146169	-0.774807	0.000175
12	6	0	2.494182	-2.004094	0.000056
13	6	0	1.092906	-2.091642	-0.000109
14	8	0	0.142604	2.637945	-0.000226
15	8	0	3.002675	1.642903	0.000212
16	1	0	-2.773923	2.301732	0.000267
17	1	0	-4.716008	0.706341	0.000441
18	1	0	-4.314474	-1.731258	0.000184
19	1	0	-2.008088	-2.646903	-0.000165
20	1	0	4.233689	-0.733632	0.000330
21	1	0	3.088559	-2.914167	0.000122
22	1	0	0.602127	-3.060189	-0.000146

23 1 0 3.968596 1.537432 0.000392

---

2. S_0 state frequency：

82	110	148	181	236	267	275	348
413	423	440	455	519	526	547	592
629	665	682	693	744	772	778	798
823	876	899	904	941	962	974	997
1043	1077	1097	1152	1166	1182	1191	1202
1239	1310	1316	1333	1358	1419	1480	1495
1511	1523	1642	1650	1654	1661	1789	3158
3169	3178	3186	3194	3195	3712		

附錄 B-5. 2,7-DMVECz 之理論計算:

A. FC state：

1. FC state optimization Cartesian Coordinates：

command：B3LYP/6-31G* opt freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.456004	-0.138446	-0.320834
2	6	0	3.045956	-1.494345	-0.340331
3	6	0	1.701815	-1.849851	-0.342098
4	6	0	0.722524	-0.850885	-0.330466
5	6	0	1.130062	0.510652	-0.338529
6	6	0	2.477069	0.869706	-0.338351
7	7	0	0.000034	1.323454	-0.358474
8	6	0	-1.130027	0.510690	-0.338432
9	6	0	-0.722531	-0.850864	-0.330433
10	6	0	-1.701864	-1.849785	-0.342050
11	6	0	-3.045993	-1.494227	-0.340185
12	6	0	-3.455998	-0.138314	-0.320617
13	6	0	-2.477011	0.869797	-0.338166
14	6	0	0.000158	3.324730	1.135642
15	6	0	0.000065	2.775628	-0.295577
16	6	0	-4.872800	0.270863	-0.335867
17	6	0	-5.939795	-0.294977	0.263151
18	6	0	-7.316067	0.296057	0.073393
19	6	0	-5.893304	-1.497494	1.173997
20	6	0	4.872847	0.270646	-0.336185
21	6	0	5.939729	-0.295015	0.263181
22	6	0	5.893036	-1.497037	1.174655
23	6	0	7.316095	0.295759	0.073233
24	1	0	3.799057	-2.272537	-0.394216
25	1	0	1.417159	-2.898816	-0.365129
26	1	0	2.783633	1.912230	-0.336654
27	1	0	-1.417266	-2.898765	-0.365113

28	1	0	-3.799109	-2.272402	-0.394042
29	1	0	-2.783536	1.912333	-0.336430
30	1	0	0.000174	4.420760	1.123932
31	1	0	0.886286	2.985916	1.682157
32	1	0	-0.885915	2.985941	1.682260
33	1	0	-0.876797	3.135321	-0.844531
34	1	0	0.876874	3.135289	-0.844636
35	1	0	-5.061659	1.186428	-0.898586
36	1	0	-7.303206	1.162502	-0.595186
37	1	0	-7.748845	0.608995	1.034301
38	1	0	-8.008303	-0.446549	-0.349056
39	1	0	-6.529615	-1.327540	2.052776
40	1	0	-4.883267	-1.723598	1.522411
41	1	0	-6.288887	-2.394918	0.676243
42	1	0	5.061823	1.185904	-0.899365
43	1	0	4.882859	-1.723342	1.522514
44	1	0	6.528672	-1.326347	2.053786
45	1	0	6.289335	-2.394565	0.677662
46	1	0	7.303376	1.161901	-0.595742
47	1	0	8.008255	-0.447131	-0.348836
48	1	0	7.748850	0.609083	1.034025

---

2. FC state optimization frequency：

26	40	46	50	59	69	79	102	133	156
173	193	194	198	217	225	239	242	285	288
315	333	355	370	400	406	417	444	451	460
479	491	531	575	606	609	630	646	670	737
754	760	772	788	815	816	838	839	850	859
860	888	891	921	950	953	964	979	979	991
1017	1026	1026	1077	1095	1096	1116	1116	1117	1157
1166	1178	1212	1214	1230	1236	1266	1272	1325	1339
1367	1369	1377	1390	1406	1411	1413	1437	1438	1438
1448	1449	1481	1502	1503	1504	1514	1515	1515	1520
1521	1524	1524	1526	1530	1535	1538	1610	1617	1657
1674	1724	1724	3021	3021	3028	3028	3057	3065	3065

3067	3071	3071	3103	3122	3122	3127	3134	3134	3138
3148	3148	3186	3188	3190	3191	3222	3222		

3. FC state TD:

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.5951 eV 477.76 nm f=0.0000

80 -> 84 0.19949

80 -> 86 0.11363

81 -> 86 0.13508

82 -> 83 0.72605

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 3.0632 eV 404.75 nm f=0.0000

79 -> 86 0.14883

80 -> 83 0.19347

81 -> 83 0.67100

82 -> 84 0.15830

Excited State 3: Triplet-A 3.2668 eV 379.53 nm f=0.0000

78 -> 84 0.14640

80 -> 83 0.46967

80 -> 87 -0.14966

81 -> 83 -0.26825

82 -> 84 0.43752

82 -> 86 0.15789

Excited State 4: Singlet-A 3.6314 eV 341.43 nm f=0.0331

81 -> 83 0.66172

82 -> 84 0.13745

82 -> 86 -0.13546

Excited State 5: Singlet-A 3.7175 eV 333.51 nm f=0.9296

81 -> 84 -0.13243

82 -> 83 0.64498

Excited State 6: Triplet-A 3.7976 eV 326.48 nm f=0.0000

77 -> 86 -0.11381
78 -> 83 -0.31568
79 -> 83 0.17333
79 -> 87 0.15162
80 -> 84 -0.22409
81 -> 84 -0.26251
81 -> 86 0.40589
82 -> 87 0.19680
82 -> 94 0.12473

Excited State 7: Singlet-A 3.8896 eV 318.76 nm f=0.0063
80 -> 83 0.55469
82 -> 84 -0.30091
82 -> 86 -0.12040

Excited State 8: Singlet-A 4.0780 eV 304.03 nm f=0.0758
79 -> 83 0.16167
81 -> 84 0.20937
82 -> 85 0.57751
82 -> 87 -0.10456

B. S_1 minima：

1. S_1（min） optimization Cartesian Coordinates：

command：CIS(root=1,nstates=2,direct)/6-31g* opt freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.432767	-0.122724	-0.241013
2	6	0	3.003576	-1.480717	-0.266277
3	6	0	1.684543	-1.828980	-0.288728
4	6	0	0.694779	-0.805888	-0.285240
5	6	0	1.125822	0.567364	-0.301138
6	6	0	2.446441	0.906928	-0.284786
7	7	0	0.000007	1.371069	-0.331337
8	6	0	-1.125811	0.567368	-0.301102

9	6	0	-0.694772	-0.805885	-0.285212
10	6	0	-1.684542	-1.828973	-0.288681
11	6	0	-3.003572	-1.480705	-0.266191
12	6	0	-3.432759	-0.122709	-0.240925
13	6	0	-2.446427	0.906938	-0.284710
14	6	0	0.000022	3.391194	1.111791
15	6	0	0.000009	2.816080	-0.302710
16	6	0	-4.825957	0.278606	-0.241265
17	6	0	-5.928425	-0.348872	0.209415
18	6	0	-7.284399	0.273943	-0.001543
19	6	0	-5.952280	-1.650606	0.968978
20	6	0	4.825969	0.278581	-0.241340
21	6	0	5.928409	-0.348882	0.209425
22	6	0	5.952213	-1.650561	0.969083
23	6	0	7.284401	0.273904	-0.001503
24	1	0	3.743158	-2.255123	-0.310954
25	1	0	1.391968	-2.862578	-0.324303
26	1	0	2.762936	1.933538	-0.279438
27	1	0	-1.391972	-2.862572	-0.324266
28	1	0	-3.743156	-2.255110	-0.310855
29	1	0	-2.762916	1.933550	-0.279352
30	1	0	0.000023	4.476631	1.078928
31	1	0	0.877855	3.066446	1.659431
32	1	0	-0.877802	3.066448	1.659447
33	1	0	-0.867200	3.161094	-0.851956
34	1	0	0.867208	3.161092	-0.851972
35	1	0	-4.986893	1.260651	-0.660112
36	1	0	-7.224255	1.205826	-0.551070
37	1	0	-7.777739	0.469028	0.949354
38	1	0	-7.936750	-0.399629	-0.556176
39	1	0	-6.742275	-1.628718	1.714900
40	1	0	-5.018903	-1.849610	1.477765
41	1	0	-6.167324	-2.494205	0.313469
42	1	0	4.986927	1.260602	-0.660235
43	1	0	5.018790	-1.849548	1.477793
44	1	0	6.742133	-1.628601	1.715082
45	1	0	6.167341	-2.494202	0.313656
46	1	0	7.224297	1.205754	-0.551090

47	1	0	7.936772	-0.399711	-0.556060
48	1	0	7.777694	0.469042	0.949408

---

2. S_1（min）optimization frequency：

26	45	49	62	63	70	85	117	136	161
185	195	197	211	225	238	242	249	295	305
309	353	372	383	398	427	438	462	469	498
510	513	565	592	636	646	656	671	680	765
788	804	805	837	860	863	877	883	892	922
924	960	971	989	1018	1040	1057	1058	1059	1064
1066	1096	1102	1132	1155	1176	1182	1202	1205	1205
1246	1256	1287	1292	1318	1319	1336	1348	1385	1413
1430	1473	1480	1519	1525	1525	1536	1553	1563	1563
1567	1568	1570	1610	1611	1612	1616	1618	1623	1630
1631	1634	1638	1640	1642	1648	1648	1661	1672	1676
1796	1797	1816	3170	3170	3175	3176	3209	3209	3209
3227	3228	3243	3271	3275	3276	3276	3296	3300	3301
3302	3302	3371	3375	3377	3378	3416	3416		

3. S_1（min）TD:

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.1373 eV 580.10 nm f=0.0000

80 -> 84 -0.19608

81 -> 86 -0.10409

82 -> 83 0.76899

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 2.9169 eV 425.06 nm f=0.0000

78 -> 84 -0.10390

79 -> 86 -0.11373

80 -> 83 0.33708

81 -> 83 0.56400

82 -> 84 -0.32497

Excited State	3:	Triplet-A	3.1008 eV	399.85 nm	f=0.0000
78 -> 84		0.10049			
80 -> 83		-0.40847			
81 -> 83		0.46163			
82 -> 84		0.38726			
Excited State	4:	Singlet-A	3.3703 eV	367.87 nm	f=1.2000
82 -> 83		0.63454			
Excited State	5:	Singlet-A	3.5435 eV	349.89 nm	f=0.0360
81 -> 83		0.65505			
82 -> 84		-0.13196			
82 -> 86		0.16013			
Excited State	6:	Triplet-A	3.7584 eV	329.88 nm	f=0.0000
78 -> 83		0.36861			
80 -> 84		-0.34385			
82 -> 85		-0.18597			
82 -> 87		0.39139			
82 -> 89		-0.18302			
82 -> 92		0.10667			
82 ->108		-0.10247			
Excited State	7:	Singlet-A	3.9485 eV	314.00 nm	f=0.0073
80 -> 83		0.53543			
82 -> 84		0.39337			
Excited State	8:	Singlet-A	4.0612 eV	305.29 nm	f=0.0144
79 -> 83		-0.10110			
82 -> 85		0.66089			

C. P_1：

1. P1 optimization Cartesian Coordinates：

command：CIS(root=1,nstates=2)/6-31g* opt=modred

D 2 1 20 21 -90.0 F

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.404038	-0.051416	-0.181024
2	6	0	3.064778	-1.443438	-0.130511
3	6	0	1.778162	-1.882988	-0.185084
4	6	0	0.718220	-0.931773	-0.291689
5	6	0	1.053476	0.466463	-0.388116
6	6	0	2.337925	0.904741	-0.340813
7	7	0	-0.131064	1.179235	-0.517873
8	6	0	-1.189201	0.298782	-0.472783
9	6	0	-0.669632	-1.034551	-0.342144
10	6	0	-1.580841	-2.119670	-0.292591
11	6	0	-2.926999	-1.858728	-0.363412
12	6	0	-3.428237	-0.546859	-0.476957
13	6	0	-2.541174	0.542959	-0.535255
14	6	0	-0.329959	3.294496	0.766312
15	6	0	-0.235493	2.618808	-0.599672
16	6	0	-4.894747	-0.312470	-0.601599
17	6	0	-5.755737	-0.126769	0.389445
18	6	0	-7.220969	0.110585	0.117174
19	6	0	-5.374595	-0.136561	1.848796
20	6	0	4.748773	0.449120	-0.146571
21	6	0	5.901731	-0.094188	0.317520
22	6	0	6.018741	-1.380481	1.091514
23	6	0	7.204283	0.629068	0.102511
24	1	0	3.855542	-2.165047	-0.092442
25	1	0	1.557138	-2.934516	-0.165678
26	1	0	2.582176	1.949499	-0.391723
27	1	0	-1.219380	-3.127623	-0.198924
28	1	0	-3.629660	-2.671862	-0.328506
29	1	0	-2.931688	1.539800	-0.620856
30	1	0	-0.402289	4.371842	0.651077
31	1	0	0.545561	3.073365	1.366625
32	1	0	-1.204849	2.949946	1.306669
33	1	0	-1.103310	2.857926	-1.201541

34	1	0	0.625970	2.984404	-1.144580
35	1	0	-5.271572	-0.278235	-1.614684
36	1	0	-7.440214	0.108221	-0.943960
37	1	0	-7.539716	1.065860	0.528042
38	1	0	-7.830350	-0.655270	0.591472
39	1	0	-5.639116	0.809461	2.316101
40	1	0	-4.316929	-0.306141	1.995735
41	1	0	-5.922239	-0.912641	2.378671
42	1	0	4.843644	1.444878	-0.553768
43	1	0	5.115244	-1.616487	1.638317
44	1	0	6.833565	-1.309944	1.807081
45	1	0	6.249428	-2.226146	0.442308
46	1	0	7.072205	1.553349	-0.447574
47	1	0	7.906242	0.007876	-0.454325
48	1	0	7.686786	0.862059	1.051267

---

2. P1 optimization frequency：

-60	26	48	59	60	68	76	111	126	151
159	184	192	205	220	227	242	250	286	291
310	352	369	382	416	424	436	456	463	495
506	512	552	592	618	640	647	662	686	762
782	793	811	837	854	861	872	890	892	908
926	952	963	983	1014	1044	1049	1052	1056	1058
1061	1091	1108	1125	1156	1172	1184	1199	1203	1218
1239	1255	1281	1309	1310	1320	1333	1350	1355	1394
1427	1467	1476	1488	1514	1524	1531	1551	1560	1564
1566	1567	1573	1595	1603	1613	1617	1619	1621	1629
1630	1634	1638	1639	1640	1642	1647	1657	1661	1718
1761	1811	1892	3159	3164	3186	3193	3196	3209	3224
3230	3236	3244	3272	3273	3275	3277	3287	3292	3296
3297	3309	3362	3374	3379	3382	3383	3424		

3. P1 TD：

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.2324 eV 555.39 nm f=0.0000

80 -> 85 0.10354

82 -> 83 0.77267

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 3.0567 eV 405.62 nm f=0.0000

78 -> 86 -0.10327

81 -> 83 0.71444

Excited State 3: Triplet-A 3.4103 eV 363.56 nm f=0.0000

79 -> 83 -0.31097

80 -> 83 0.36357

81 -> 83 -0.12650

81 -> 86 -0.10356

82 -> 84 0.19130

82 -> 85 0.44502

Excited State 4: Singlet-A 3.5812 eV 346.21 nm f=0.8213

81 -> 83 -0.24915

82 -> 83 0.58418

Excited State 5: Singlet-A 3.6446 eV 340.18 nm f=0.1639

81 -> 83 0.60808

82 -> 83 0.23130

82 -> 85 0.13863

82 -> 86 0.13255

Excited State 6: Triplet-A 4.0166 eV 308.68 nm f=0.0000

78 -> 83 -0.31307

80 -> 83 0.10356

81 -> 86 0.42450

81 -> 89 -0.14355

82 -> 86 -0.38495

82 -> 89 0.11617

Excited State	7:	Singlet-A	4.0505 eV	306.10 nm	f=0.0160
78 -> 83		-0.10162			
82 -> 84		0.64557			

Excited State	8:	Singlet-A	4.1726 eV	297.14 nm	f=0.0468
78 -> 83		-0.11610			
79 -> 83		0.14854			
80 -> 83		-0.26339			
82 -> 85		0.52184			
82 -> 86		-0.18831			
82 -> 87		-0.11948			

D. P_2：

1. P2 optimization Cartesian Coordinates：

command：CIS(root=1,nstates=2)/6-31g* opt=modred

D 11 12 16 17 90.0 F

D 2 1 20 21 -90.0 F

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.416986	-0.519761	-0.377739
2	6	0	3.005880	-1.843698	-0.113310
3	6	0	1.682500	-2.201977	-0.052783
4	6	0	0.693043	-1.194654	-0.271847
5	6	0	1.124742	0.154391	-0.560083
6	6	0	2.449529	0.493302	-0.609046
7	7	0	-0.000004	0.933501	-0.750055
8	6	0	-1.124748	0.154388	-0.560095
9	6	0	-0.693048	-1.194658	-0.271862
10	6	0	-1.682504	-2.201982	-0.052795
11	6	0	-3.005884	-1.843704	-0.113323
12	6	0	-3.416992	-0.519768	-0.377757
13	6	0	-2.449537	0.493296	-0.609063
14	6	0	-0.000006	3.207273	0.245013
15	6	0	-0.000004	2.354392	-1.021175

16	6	0	-4.862765	-0.191086	-0.503264
17	6	0	-5.682538	0.178465	0.471779
18	6	0	-7.130429	0.501599	0.195400
19	6	0	-5.267706	0.304709	1.916347
20	6	0	4.862758	-0.191079	-0.503262
21	6	0	5.682546	0.178465	0.471772
22	6	0	5.267737	0.304693	1.916348
23	6	0	7.130433	0.501600	0.195373
24	1	0	3.766272	-2.587144	0.045441
25	1	0	1.388702	-3.214509	0.153757
26	1	0	2.774029	1.497095	-0.809129
27	1	0	-1.388704	-3.214511	0.153755
28	1	0	-3.766275	-2.587149	0.045434
29	1	0	-2.774037	1.497089	-0.809143
30	1	0	-0.000006	4.262547	-0.010565
31	1	0	0.878050	3.002021	0.847375
32	1	0	-0.878063	3.002021	0.847373
33	1	0	-0.867852	2.576940	-1.629131
34	1	0	0.867845	2.576941	-1.629129
35	1	0	-5.260229	-0.233817	-1.509189
36	1	0	-7.374261	0.396436	-0.855124
37	1	0	-7.362753	1.520134	0.498168
38	1	0	-7.787220	-0.153248	0.763491
39	1	0	-5.448652	1.315329	2.276020
40	1	0	-4.222294	0.071080	2.063942
41	1	0	-5.858570	-0.361426	2.541025
42	1	0	5.260205	-0.233798	-1.509193
43	1	0	4.222327	0.071064	2.063957
44	1	0	5.448691	1.315309	2.276029
45	1	0	5.858609	-0.361450	2.541010
46	1	0	7.374247	0.396446	-0.855156
47	1	0	7.787233	-0.153253	0.763447
48	1	0	7.362762	1.520132	0.498146

---

2. P_2 optimization frequency：

-75	-72	25	57	58	66	72	98	116	142
159	160	184	205	216	220	230	253	263	295
307	345	362	409	409	418	428	454	454	479
507	510	538	539	601	622	635	654	680	749
775	783	794	831	836	850	873	877	886	902
916	929	934	967	979	1020	1036	1040	1047	1048
1051	1081	1107	1107	1132	1177	1177	1201	1217	1217
1230	1244	1283	1299	1307	1309	1321	1334	1341	1389
1418	1459	1473	1485	1490	1516	1526	1527	1565	1566
1567	1572	1572	1596	1598	1601	1608	1619	1619	1629
1629	1634	1638	1638	1639	1639	1642	1661	1674	1703
1778	1887	1888	3186	3186	3192	3193	3209	3229	3229
3235	3235	3245	3267	3268	3273	3276	3282	3282	3298
3307	3307	3364	3366	3385	3385	3386	3389		

3. P_2 TD：

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.6488 eV 468.07 nm f=0.0000

77 -> 92 0.11330

78 -> 83 0.10783

81 -> 85 -0.14463

82 -> 83 0.75887

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 3.1765 eV 390.31 nm f=0.0000

78 -> 85 -0.11631

81 -> 83 0.72571

Excited State 3: Singlet-A 3.8034 eV 325.99 nm f=0.0381

81 -> 83 0.65806

82 -> 85 0.18469

Excited State 4: Singlet-A 3.9750 eV 311.91 nm f=0.5118

81 -> 85 -0.17562

82 -> 83 0.62521

Excited State 5: Triplet-A 4.0361 eV 307.19 nm f=0.0000

78 -> 83 -0.36735

78 -> 93 -0.13171

81 -> 85 0.55653

81 -> 89 0.19657

82 -> 83 0.15626

Excited State 6: Triplet-A 4.1023 eV 302.23 nm f=0.0000

77 -> 83 0.39297

78 -> 85 0.15725

79 -> 83 -0.12204

79 -> 87 -0.16967

79 -> 88 0.14671

79 -> 93 0.10359

80 -> 85 0.14746

80 -> 89 -0.17208

80 -> 96 -0.12724

81 -> 88 0.12770

81 -> 93 -0.15926

82 -> 85 0.23120

82 -> 92 0.28433

82 -> 98 -0.15036

82 ->100 -0.10239

Excited State 7: Singlet-A 4.1596 eV 298.07 nm f=0.0016

82 -> 84 0.64911

Excited State 8: Singlet-A 4.1729 eV 297.12 nm f=0.0058

81 -> 84 0.64208

82 -> 85 -0.10052

附錄 B-6. 3,6-DMVECz 之理論計算:

A. FC state：

1. FC state optimization Cartesian Coordinates：

command：B3LYP/6-31G* opt freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.418398	1.188415	-0.276320
2	6	0	3.053002	-0.179192	-0.344211
3	6	0	1.688275	-0.502217	-0.370834
4	6	0	0.724765	0.507238	-0.294420
5	6	0	1.128379	1.864922	-0.205614
6	6	0	2.482845	2.213267	-0.198378
7	7	0	0.000040	2.677149	-0.164952
8	6	0	-1.128311	1.864941	-0.205632
9	6	0	-0.724718	0.507253	-0.294431
10	6	0	-1.688240	-0.502194	-0.370845
11	6	0	-3.052957	-0.179158	-0.344248
12	6	0	-3.418338	1.188461	-0.276374
13	6	0	-2.482775	2.213301	-0.198421
14	6	0	0.000012	4.583058	1.449535
15	6	0	0.000045	4.122814	-0.012693
16	6	0	-4.127545	-1.185860	-0.433342
17	6	0	-4.191983	-2.421751	0.100623
18	6	0	-3.144447	-3.034697	0.997532
19	6	0	-5.393865	-3.298567	-0.156048
20	6	0	4.127556	-1.185928	-0.433307
21	6	0	4.191934	-2.421828	0.100658
22	6	0	3.144225	-3.034806	0.997356
23	6	0	5.393817	-3.298652	-0.155984
24	1	0	4.475762	1.442132	-0.273141
25	1	0	1.378104	-1.536073	-0.484238
26	1	0	2.806325	3.248295	-0.136894
27	1	0	-1.378071	-1.536054	-0.484244

28	1	0	-4.475698	1.442191	-0.273215
29	1	0	-2.806247	3.248333	-0.136954
30	1	0	0.000013	5.677759	1.504610
31	1	0	0.886051	4.211838	1.974725
32	1	0	-0.886054	4.211840	1.974682
33	1	0	-0.876980	4.515618	-0.538271
34	1	0	0.877095	4.515609	-0.538232
35	1	0	-5.001065	-0.853421	-0.996594
36	1	0	-2.556193	-3.799535	0.469480
37	1	0	-3.624161	-3.545608	1.843196
38	1	0	-2.449239	-2.292775	1.397223
39	1	0	-6.126117	-2.811419	-0.807643
40	1	0	-5.895990	-3.568585	0.784001
41	1	0	-5.097839	-4.245556	-0.630307
42	1	0	5.001133	-0.853488	-0.996466
43	1	0	2.449366	-2.292770	1.397455
44	1	0	3.623756	-3.546380	1.842712
45	1	0	2.555552	-3.799084	0.468957
46	1	0	6.126311	-2.811314	-0.807166
47	1	0	5.097853	-4.245423	-0.630727
48	1	0	5.895621	-3.569102	0.784107

---

2. FC state optimization frequency：

34	42	45	50	56	68	89	94	126	149
171	190	193	203	220	235	244	280	283	293
317	337	346	375	387	413	436	440	442	465
484	484	529	556	585	607	617	654	660	723
746	759	779	791	804	813	834	842	867	876
881	903	912	914	940	940	946	972	979	980
1028	1028	1049	1077	1091	1093	1116	1116	1119	1162
1180	1188	1197	1213	1213	1242	1272	1275	1314	1319
1344	1368	1390	1405	1408	1411	1425	1438	1438	1439
1448	1449	1471	1503	1504	1506	1515	1515	1517	1521
1523	1524	1524	1527	1529	1536	1538	1616	1619	1655
1676	1725	1726	3020	3020	3026	3027	3057	3063	3063

3067	3069	3070	3103	3121	3121	3127	3133	3133	3139
3143	3143	3181	3181	3202	3202	3207	3210		

3. FC state TD:

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.9073 eV 426.46 nm f=0.0000

80 -> 83	-0.32963
80 -> 85	0.13761
81 -> 83	-0.29097
81 -> 85	-0.26516
81 -> 86	0.13406
82 -> 84	0.55598

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 2.9921 eV 414.38 nm f=0.0000

80 -> 84	-0.17972
81 -> 84	0.20955
82 -> 83	0.64691
82 -> 85	-0.20149

Excited State 3: Triplet-A 3.2544 eV 380.98 nm f=0.0000

79 -> 85	-0.12953
80 -> 84	0.18755
81 -> 84	-0.39814
82 -> 83	0.32378
82 -> 85	0.42634
82 -> 86	-0.20017

Excited State 4: Triplet-A 3.3540 eV 369.66 nm f=0.0000

79 -> 84	-0.11563
80 -> 83	0.18535
80 -> 85	0.11551
81 -> 83	0.60084
82 -> 84	0.31072

Excited State 5: Singlet-A 3.6051 eV 343.91 nm f=0.0117

80 -> 84	0.12455				
81 -> 84	0.13669				
82 -> 83	0.66410				
Excited State	6:	Singlet-A	3.9199 eV	316.29 nm	f=0.0276
81 -> 83	-0.44264				
82 -> 84	0.52324				
Excited State	7:	Singlet-A	3.9750 eV	311.91 nm	f=0.6138
80 -> 83	-0.16066				
81 -> 83	0.44929				
81 -> 85	-0.13051				
82 -> 84	0.39599				
Excited State	8:	Singlet-A	4.1550 eV	298.40 nm	f=0.0516
81 -> 84	0.26001				
82 -> 85	0.60512				
82 -> 86	0.15777				

B. S_1（sym）:

1. S_1（sym） optimization Cartesian Coordinates：

command：CIS(root=1,nstates=2,direct)/6-31g* opt freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.418348	1.192526	-0.261623
2	6	0	3.052366	-0.161589	-0.327190
3	6	0	1.687370	-0.520423	-0.361103
4	6	0	0.712238	0.475178	-0.288787
5	6	0	1.123591	1.841166	-0.197236
6	6	0	2.459915	2.210127	-0.182194
7	7	0	0.000047	2.622223	-0.154832
8	6	0	-1.123591	1.841134	-0.197312
9	6	0	-0.712262	0.475199	-0.288848
10	6	0	-1.687395	-0.520390	-0.361167

11	6	0	-3.052403	-0.161575	-0.327314
12	6	0	-3.418350	1.192487	-0.261800
13	6	0	-2.459861	2.210084	-0.182370
14	6	0	-0.000045	4.538326	1.414225
15	6	0	0.000047	4.068822	-0.038640
16	6	0	-4.135180	-1.156086	-0.419757
17	6	0	-4.211746	-2.384480	0.092474
18	6	0	-3.183679	-3.034613	0.985178
19	6	0	-5.425342	-3.241426	-0.173738
20	6	0	4.135176	-1.156026	-0.419606
21	6	0	4.211726	-2.384531	0.092398
22	6	0	3.183592	-3.034910	0.984840
23	6	0	5.425417	-3.241338	-0.173807
24	1	0	4.460825	1.452141	-0.249817
25	1	0	1.405627	-1.547038	-0.489334
26	1	0	2.765835	3.237020	-0.109978
27	1	0	-1.405647	-1.547021	-0.489298
28	1	0	-4.460818	1.452146	-0.250065
29	1	0	-2.765782	3.236983	-0.110205
30	1	0	-0.000059	5.623001	1.454382
31	1	0	0.878425	4.175514	1.935271
32	1	0	-0.878565	4.175496	1.935172
33	1	0	-0.868595	4.443334	-0.562443
34	1	0	0.868754	4.443334	-0.562336
35	1	0	-4.994167	-0.807644	-0.971168
36	1	0	-2.633610	-3.805446	0.448423
37	1	0	-3.680402	-3.527430	1.816911
38	1	0	-2.473605	-2.327515	1.387967
39	1	0	-6.132534	-2.752312	-0.832630
40	1	0	-5.936760	-3.487876	0.754107
41	1	0	-5.134749	-4.184736	-0.631707
42	1	0	4.994253	-0.807429	-0.970779
43	1	0	2.473443	-2.327941	1.387716
44	1	0	3.680250	-3.527898	1.816508
45	1	0	2.633624	-3.805645	0.447841
46	1	0	6.132664	-2.752057	-0.832514
47	1	0	5.134945	-4.184583	-0.631986
48	1	0	5.936723	-3.487924	0.754063

---

2. S_1（sym）optimization frequency：

-921	34	45	48	60	60	76	100	103	135
150	173	182	192	212	230	242	255	281	298
314	335	353	362	389	398	411	444	469	480
485	515	516	566	614	624	646	653	678	743
746	752	777	783	822	826	851	875	884	900
907	935	939	940	950	980	984	1003	1028	1053
1053	1110	1113	1122	1147	1176	1177	1206	1215	215
1235	1248	1271	1276	1302	1308	1330	1351	1383	1396
1424	1462	1483	1509	1517	1520	1552	1559	1564	1566
1566	1574	1577	1582	1592	1609	1621	1621	1630	1631
1631	1633	1639	1641	1642	1647	1648	1665	1709	1712
1795	1850	1857	3184	3184	3190	3191	3213	3227	3227
3234	3234	3262	3282	3282	3284	3285	3313	3319	3319
3320	3320	3370	3371	3387	3391	3401	3406		

3. S_1（sym）TD：

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.8885 eV 429.24 nm f=0.0000

77 -> 90 -0.10060

79 -> 90 -0.10242

80 -> 83 0.36535

80 -> 85 -0.10377

81 -> 83 -0.39869

81 -> 85 -0.18603

81 -> 86 0.15692

82 -> 84 0.49701

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 2.8893 eV 429.12 nm f=0.0000

80 -> 84 0.12915

81 -> 84 0.10758

82 -> 83 0.70454

Excited State	3:	Triplet-A	3.3199 eV	373.45 nm	f=0.0000
80 -> 84		-0.13908			
81 -> 83		0.44302			
81 -> 84		-0.25869			
82 -> 83		0.10274			
82 -> 84		0.32827			
82 -> 85		0.24080			
82 -> 86		-0.18669			
Excited State	4:	Triplet-A	3.3201 eV	373.43 nm	f=0.0000
80 -> 84		0.18365			
81 -> 83		0.33546			
81 -> 84		0.34171			
82 -> 83		-0.13543			
82 -> 84		0.24872			
82 -> 85		-0.31778			
82 -> 86		0.24632			
Excited State	5:	Singlet-A	3.4934 eV	354.91 nm	f=0.0155
80 -> 84		-0.11706			
81 -> 84		0.13362			
82 -> 83		0.66455			
Excited State	6:	Singlet-A	3.8825 eV	319.34 nm	f=0.0013
81 -> 83		0.50472			
82 -> 84		-0.46052			
Excited State	7:	Singlet-A	3.9378 eV	314.86 nm	f=0.6281
80 -> 83		0.18925			
81 -> 83		0.37560			
81 -> 85		-0.10009			
82 -> 84		0.45767			
Excited State	8:	Singlet-A	4.1766 eV	296.86 nm	f=0.0488
81 -> 84		0.17860			
82 -> 85		0.63374			
82 -> 86		0.17581			

C. S_1（min） optimization Cartesian Coordinates：

1. S_1（min）optimization Cartesian Coordinates：

command：CIS(root=1,nstates=2,direct)/6-31g* opt freq

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.401772	1.162675	-0.309895
2	6	0	3.036292	-0.175395	-0.398304
3	6	0	1.676996	-0.523541	-0.417860
4	6	0	0.700195	0.478707	-0.320556
5	6	0	1.116618	1.834656	-0.218108
6	6	0	2.432387	2.191501	-0.210781
7	7	0	-0.035057	2.633914	-0.152142
8	6	0	-1.133388	1.856088	-0.186854
9	6	0	-0.710977	0.467834	-0.302941
10	6	0	-1.687248	-0.540555	-0.374610
11	6	0	-3.038048	-0.185988	-0.314939
12	6	0	-3.416192	1.184200	-0.225574
13	6	0	-2.480189	2.212138	-0.141979
14	6	0	0.027429	4.537995	1.431425
15	6	0	-0.028292	4.077744	-0.023147
16	6	0	-4.135386	-1.159591	-0.387331
17	6	0	-4.208132	-2.406024	0.085028
18	6	0	-3.151129	-3.105701	0.902372
19	6	0	-5.448801	-3.231165	-0.153004
20	6	0	4.103554	-1.200378	-0.533643
21	6	0	4.237705	-2.350104	0.117302
22	6	0	3.320770	-2.844705	1.209271
23	6	0	5.392124	-3.274167	-0.188100
24	1	0	4.443076	1.429267	-0.305263
25	1	0	1.388263	-1.550993	-0.537005
26	1	0	2.748316	3.215578	-0.130924
27	1	0	-1.396496	-1.560877	-0.524524
28	1	0	-4.462819	1.424873	-0.193780

29	1	0	-2.794040	3.234036	-0.047548
30	1	0	0.039822	5.622310	1.480007
31	1	0	0.918773	4.162959	1.921094
32	1	0	-0.836818	4.179992	1.979503
33	1	0	-0.913880	4.460691	-0.512114
34	1	0	0.822209	4.453438	-0.576524
35	1	0	-5.015025	-0.779645	-0.882580
36	1	0	-2.620468	-3.841733	0.301158
37	1	0	-3.619252	-3.648124	1.719305
38	1	0	-2.426978	-2.422284	1.319954
39	1	0	-6.174766	-2.709322	-0.764457
40	1	0	-5.922764	-3.497333	0.789103
41	1	0	-5.195943	-4.164649	-0.651475
42	1	0	4.869017	-0.946743	-1.250350
43	1	0	2.618681	-2.091385	1.536363
44	1	0	3.907322	-3.159983	2.068954
45	1	0	2.758053	-3.715480	0.878348
46	1	0	6.021792	-2.888076	-0.980861
47	1	0	5.030953	-4.254466	-0.492026
48	1	0	6.010001	-3.426791	0.693994

---

2. S_1（min） optimization frequency：

31	41	46	59	62	74	96	98	131	148
169	181	189	212	228	230	247	273	295	299
335	350	360	387	401	414	439	470	473	490
510	514	556	583	606	639	644	674	693	745
766	770	778	807	847	849	858	884	889	915
922	930	944	970	976	982	986	1028	1051	1054
1105	1112	1116	1132	1170	1175	1187	1204	1214	1218
1226	1249	1275	1294	1295	1320	1324	1347	1373	1398
1424	1461	1483	1509	1516	1519	1529	1550	1565	1566
1567	1574	1575	1586	1589	1620	1621	1630	1632	1632
1635	1638	1640	1642	1644	1647	1652	1663	1702	1732
1742	1842	1889	3184	3185	3191	3192	3212	3226	3229
3232	3237	3255	3279	3281	3282	3284	3307	3315	3318

3319	3323	3364	3373	3383	3386	3396	3411		

3. S_1（min）TD：

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.7773 eV 446.41 nm f=0.0000

80 -> 83 0.24860

81 -> 83 -0.33702

82 -> 83 0.57659

82 -> 84 0.24356

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 2.9336 eV 422.64 nm f=0.0000

80 -> 83 -0.18488

80 -> 84 0.13576

81 -> 83 0.36173

82 -> 83 0.42589

82 -> 84 -0.40047

82 -> 85 -0.11344

82 -> 86 0.13197

Excited State 3: Triplet-A 3.3001 eV 375.69 nm f=0.0000

80 -> 84 -0.13894

81 -> 83 0.47150

81 -> 84 -0.12829

82 -> 83 0.11520

82 -> 84 0.40673

82 -> 85 0.17994

82 -> 86 -0.19818

Excited State 4: Singlet-A 3.4731 eV 356.99 nm f=0.0449

81 -> 84 0.14823

82 -> 83 0.66046

Excited State 5: Triplet-A 3.5366 eV 350.58 nm f=0.0000

79 -> 85 -0.10058

79 -> 86 0.11125

80 -> 83	0.13065				
80 -> 84	0.22501				
80 -> 85	-0.12983				
80 -> 86	0.11884				
81 -> 83	0.21141				
81 -> 84	0.34143				
81 -> 85	-0.17782				
81 -> 86	0.15465				
82 -> 84	0.19944				
82 -> 85	-0.26023				
82 -> 86	0.23042				
Excited State	6:	Singlet-A	3.8946 eV	318.35 nm	f=0.0052
81 -> 83	0.51585				
82 -> 84	-0.41751				
Excited State	7:	Singlet-A	3.9843 eV	311.18 nm	f=0.6073
80 -> 83	0.21547				
81 -> 83	0.31491				
81 -> 85	-0.10137				
81 -> 86	0.10253				
82 -> 84	0.47819				
Excited State	8:	Singlet-A	4.1685 eV	297.43 nm	f=0.0472
82 -> 85	0.64326				
82 -> 86	0.18129				

D. P_1：

1. P1 optimization Cartesian Coordinates：

command：CIS(root=1,nstates=2)/6-31g* opt=modred

D 3 2 20 21 -90.0 F

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.334005	0.968314	-0.473387

2	6	0	2.918343	-0.349654	-0.586601
3	6	0	1.552969	-0.658191	-0.556900
4	6	0	0.610202	0.374178	-0.412919
5	6	0	1.075174	1.714747	-0.303977
6	6	0	2.398877	2.028832	-0.326464
7	7	0	-0.048959	2.551127	-0.182569
8	6	0	-1.170806	1.807495	-0.185988
9	6	0	-0.795763	0.406919	-0.340064
10	6	0	-1.806206	-0.572143	-0.389314
11	6	0	-3.139112	-0.178189	-0.270103
12	6	0	-3.471087	1.202585	-0.143971
13	6	0	-2.502728	2.201584	-0.081906
14	6	0	0.131417	4.423556	1.430143
15	6	0	0.009076	3.990961	-0.028848
16	6	0	-4.270037	-1.115497	-0.311874
17	6	0	-4.365105	-2.363754	0.150795
18	6	0	-3.300736	-3.105298	0.920267
19	6	0	-5.639659	-3.146645	-0.047934
20	6	0	-3.921126	-1.439338	-0.787870
21	6	0	4.505808	-2.158132	0.159200
22	6	0	4.245371	-1.980680	1.634479
23	6	0	5.505062	-3.236365	-0.182594
24	1	0	4.383079	1.198868	-0.496440
25	1	0	1.233384	-1.680700	-0.643939
26	1	0	2.750521	3.040277	-0.235350
27	1	0	-1.551588	-1.597786	-0.566308
28	1	0	-4.508046	1.473333	-0.066769
29	1	0	-2.782128	3.230584	0.039713
30	1	0	0.180484	5.505908	1.496537
31	1	0	1.027059	4.011917	1.881125
32	1	0	-0.723817	4.083328	2.003187
33	1	0	-0.880509	4.410919	-0.478924
34	1	0	0.851023	4.349582	-0.606330
35	1	0	-5.154344	-0.702221	-0.770885
36	1	0	-2.818770	-3.852630	0.292609
37	1	0	-3.754187	-3.639688	1.750678
38	1	0	-2.538305	-2.449968	1.314026
39	1	0	-6.371204	-2.595313	-0.625977

40	1	0	-6.085891	-3.408193	0.908891
41	1	0	-5.435833	-4.082008	-0.564967
42	1	0	4.177174	-1.645720	-1.816158
43	1	0	3.522187	-1.202432	1.833404
44	1	0	5.167863	-1.732667	2.154959
45	1	0	3.879230	-2.908199	2.069160
46	1	0	5.656463	-3.322284	-1.252156
47	1	0	5.174188	-4.202478	0.191896
48	1	0	6.467581	-3.032005	0.280976

---

2. P1 optimization frequency：

-30	37	45	57	63	72	92	99	125	145
155	172	187	209	216	229	237	264	295	301
336	351	362	388	403	416	436	465	470	493
504	515	549	591	613	635	639	671	695	745
768	770	784	809	843	848	857	885	888	913
922	935	941	945	975	978	987	1028	1049	1054
1105	1111	1112	1131	1169	1175	1193	1203	1215	1218
1225	1254	1277	1296	1304	1314	1322	1343	1372	1401
1424	1464	1480	1489	1515	1520	1533	1552	1565	1566
1567	1574	1575	1582	1589	1619	1620	1630	1630	1631
1633	1638	1639	1640	1642	1648	1661	1668	1703	1721
1746	1844	1900	3185	3185	3192	3193	3212	3228	3229
3234	3237	3254	3278	3280	3282	3283	3306	3310	3313
3318	3323	3368	3373	3374	3386	3396	3411		

3. P1 TD：

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.7542 eV 450.17 nm f=0.0000

80 -> 83 -0.19226

81 -> 83 -0.34333

82 -> 83 0.61523

82 -> 84 -0.20750

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	2.9633 eV	418.40 nm	f=0.0000
80 -> 84		0.17789			
81 -> 83		0.42919			
82 -> 83		0.37516			
82 -> 84		0.45302			
Excited State	3:	Triplet-A	3.3365 eV	371.60 nm	f=0.0000
80 -> 84		-0.17826			
81 -> 83		0.48402			
82 -> 83		0.10477			
82 -> 84		-0.47486			
82 -> 88		0.12444			
Excited State	4:	Singlet-A	3.4801 eV	356.27 nm	f=0.0628
81 -> 84		-0.15456			
82 -> 83		0.65936			
Excited State	5:	Triplet-A	3.8221 eV	324.38 nm	f=0.0000
77 -> 83		-0.17477			
78 -> 83		0.14188			
80 -> 83		0.44033			
80 -> 84		-0.16057			
80 -> 88		-0.10431			
81 -> 83		-0.16749			
81 -> 84		0.16573			
82 -> 85		-0.13193			
82 -> 86		-0.17730			
82 -> 88		0.28355			
82 -> 91		0.13635			
Excited State	6:	Singlet-A	4.1227 eV	300.74 nm	f=0.0294
80 -> 83		-0.10841			
81 -> 83		0.51852			
82 -> 84		0.38789			
82 -> 88		0.11159			

Excited State	7:	Singlet-A	4.1790 eV	296.69 nm	f=0.1885
81 -> 83		-0.13004			
82 -> 84		0.32332			
82 -> 85		0.56663			

Excited State	8:	Singlet-A	4.2365 eV	292.66 nm	f=0.6510
80 -> 83		0.13413			
81 -> 83		-0.28332			
82 -> 84		0.39109			
82 -> 85		-0.35724			

E. P_2：

1. P_2 optimization Cartesian Coordinates：

command：CIS(root=1,nstates=2)/6-31g* opt=modred

D 10 11 16 17 90.0 F

D 3 2 20 21 -90.0 F

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.396920	0.980312	-0.354054
2	6	0	3.006638	-0.374072	-0.543455
3	6	0	1.672880	-0.713699	-0.600478
4	6	0	0.693482	0.311053	-0.469666
5	6	0	1.128693	1.690764	-0.286961
6	6	0	2.470290	2.018617	-0.222785
7	7	0	0.025555	2.479459	-0.205486
8	6	0	-1.120486	1.679630	-0.293501
9	6	0	-0.700002	0.322195	-0.471344
10	6	0	-1.683415	-0.693998	-0.603522
11	6	0	-3.030098	-0.351946	-0.551169
12	6	0	-3.399818	0.980021	-0.370433
13	6	0	-2.436495	2.019947	-0.235867
14	6	0	-0.006266	4.293455	1.485577
15	6	0	0.024130	3.910957	0.007880
16	6	0	-4.079999	-1.398978	-0.736923

17	6	0	-4.638942	-2.132280	0.214842
18	6	0	-4.294484	-2.019350	1.679128
19	6	0	-5.692520	-3.162775	-0.110361
20	6	0	4.065192	-1.408245	-0.734634
21	6	0	4.627920	-2.144557	0.212336
22	6	0	4.273942	-2.049267	1.675626
23	6	0	5.694061	-3.160224	-0.117918
24	1	0	4.446326	1.207303	-0.309337
25	1	0	1.371720	-1.734226	-0.745125
26	1	0	2.802069	3.028838	-0.074296
27	1	0	-1.387799	-1.717595	-0.743492
28	1	0	-4.443055	1.234969	-0.330538
29	1	0	-2.763519	3.033211	-0.092852
30	1	0	-0.011918	5.373601	1.594548
31	1	0	0.863745	3.902211	2.001198
32	1	0	-0.892052	3.896684	1.968772
33	1	0	-0.833512	4.321504	-0.509885
34	1	0	0.902718	4.320553	-0.473708
35	1	0	-4.398134	-1.557550	-1.756209
36	1	0	-3.935170	-2.973331	2.058606
37	1	0	-5.179650	-1.764594	2.257838
38	1	0	-3.537262	-1.271356	1.867152
39	1	0	-5.902870	-3.204051	-1.172545
40	1	0	-6.621339	-2.943347	0.411359
41	1	0	-5.376814	-4.152514	0.211708
42	1	0	4.390948	-1.548296	-1.754631
43	1	0	3.513175	-1.305619	1.867510
44	1	0	5.154842	-1.798970	2.262496
45	1	0	3.914288	-3.008196	2.041755
46	1	0	5.909404	-3.189271	-1.179463
47	1	0	5.387338	-4.156066	0.193478
48	1	0	6.617898	-2.935466	0.410146

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2. P_2 optimization frequency：

-40	-28	41	48	67	71	83	97	112	140
152	155	167	206	207	219	224	237	286	301

343	351	363	391	395	408	431	448	457	486
504	508	542	556	607	616	631	670	679	743
762	778	790	818	846	852	855	882	894	904
917	931	939	943	957	961	976	1021	1047	1049
1052	1110	1112	1121	1149	1170	1176	1202	1206	1218
1218	1249	1278	1281	1311	1314	1319	1331	1350	1398
1428	1457	1466	1487	1491	1505	1516	1527	1558	1566
1567	1567	1574	1574	1588	1618	1619	1625	1631	1631
1633	1637	1638	1639	1641	1642	1658	1679	1686	1690
1743	1899	1899	3186	3187	3193	3194	3211	3228	3230
3235	3236	3247	3276	3278	3279	3280	3300	3307	3311
3311	3313	3370	3372	3377	3385	3387	3392		

3. P_2 TD：

command：B3LYP/6-31+G* td(50-50,nstates=4)

Excited State 1: Triplet-A 2.7386 eV 452.73 nm f=0.0000

77 -> 94 -0.11128

78 -> 83 -0.12844

81 -> 83 -0.48338

82 -> 83 0.56904

82 -> 85 0.14505

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 3.1018 eV 399.72 nm f=0.0000

78 -> 85 -0.10486

81 -> 83 0.55187

82 -> 83 0.47447

Excited State 3: Singlet-A 3.6980 eV 335.27 nm f=0.0647

81 -> 83 0.20285

81 -> 85 0.15784

82 -> 83 0.62774

Excited State 4: Triplet-A 3.9148 eV 316.71 nm f=0.0000

78 -> 83 -0.36571

81 -> 83 0.17961

81 -> 85 0.16737

82 -> 85 0.54013

Excited State 5: Triplet-A 4.0874 eV 303.33 nm f=0.0000

77 -> 83 -0.31311

78 -> 83 -0.16660

78 -> 85 -0.26411

80 -> 90 0.10021

81 -> 94 -0.14965

82 -> 84 0.17595

82 -> 86 0.17947

82 -> 88 0.19359

82 -> 89 0.22513

82 -> 90 -0.11011

82 -> 92 -0.16093

82 -> 94 0.16058

82 -> 98 0.10707

Excited State 6: Singlet-A 4.1136 eV 301.40 nm f=0.2810

81 -> 83 0.58701

82 -> 83 -0.17841

82 -> 85 -0.23931

Excited State 7: Singlet-A 4.1692 eV 297.38 nm f=0.0139

82 -> 84 0.66101

Excited State 8: Singlet-A 4.1732 eV 297.10 nm f=0.0025

80 -> 83 0.64949