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Solvent-induced syntheses of 2D/3D $[AgSCN]_n$-based supramolecular isomers with unusual topologies: structural, theoretical and nonlinear optical studies

Jianghua Li,[a] Suci Meng,[a] Yinglin Song,[b] Jinfang Zhang,[a] Zhipeng Huang,[a] Huajian Zhao,[c] Hongyang Wei,[c] Wenjiang Huang,[c] Marie P. Cifuentes,[d] Mark G. Humphrey[d] and Chi Zhang*[a,c,d]

[a] *Functional Molecular Materials Research Center, Scientific Research Academy, School of Chemistry and Chemical Engineering, Jiangsu University, Zhenjiang 212013, P. R. China*

[b] *School of Physical Science and Technology, Suzhou University, Suzhou 215006, P. R. China*

[c] *Functional Molecular Materials Research Center, School of Chemical Engineering, Nanjing University of Science and Technology, Nanjing 210094, P. R. China*

[d] *Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia*

Supporting Information

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Supplementary Index

1. The Ag···Ag bonds in 2

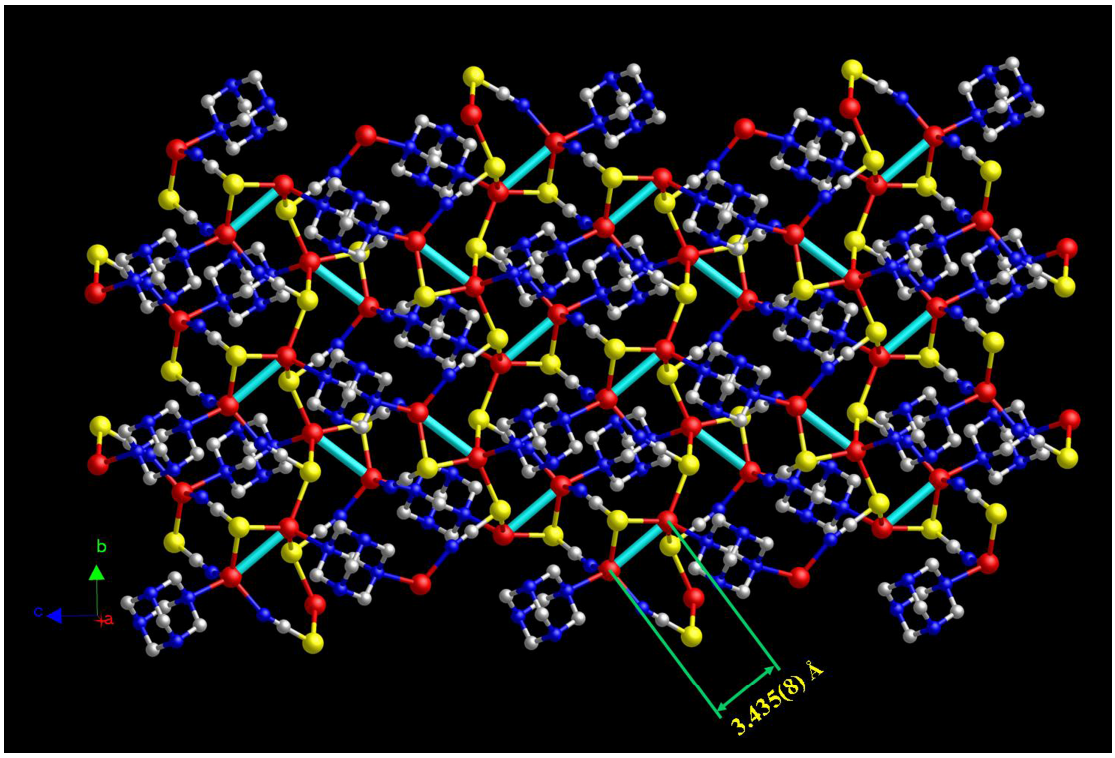

Figure S1. The Ag···Ag bonds (3.435(8) Å) were highlighted in turquoise for ball-and-stick diagram of CP **2**. Atom color codes: Ag red, S yellow, N blue and C gray.

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2. XRPD Patterns

X-ray powder diffraction (XRPD) has been used to check the phase purity of the bulk samples in the solid state. For CPs **1**-**3**, the measured XRD patterns closely match the simulated patterns generated from the results of single-crystal diffraction data, indicative of pure products.

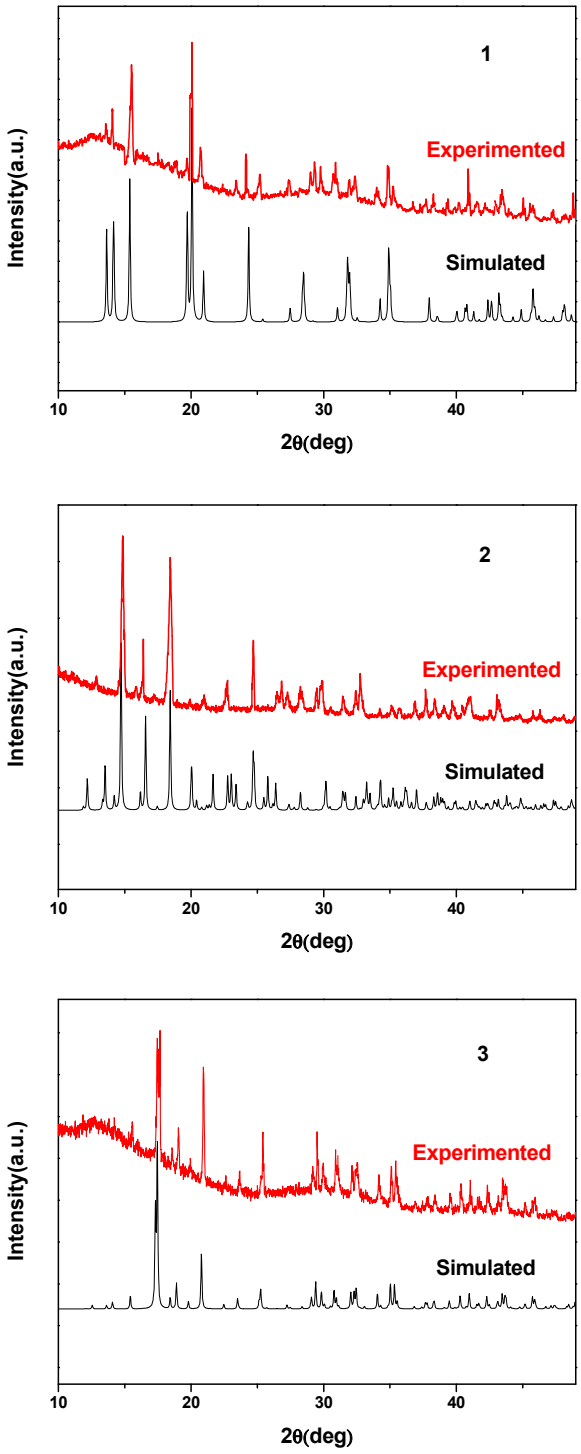

Figure S2. Experimental XRPD and simulated patterns for **1**-**3**

2. CP 1 B3LYP/LanL2DZ+6-31G* TD-PCM (150 states) in DMF (dielectric constant = 36.71)

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	4.8311 eV	256.64 nm	f=0.0056
213 ->216		0.15292			
213 ->217		-0.22557			
215 ->216		0.60803			
215 ->217		-0.16274			

Excited State	2:	Singlet-A	4.8394 eV	256.20 nm	f=0.0025
212 ->216		0.14770			
212 ->217		-0.19967			
214 ->216		0.63885			

Excited State	3:	Singlet-A	4.8942 eV	253.33 nm	f=0.0409
213 ->216		0.48851			
213 ->217		0.19748			
215 ->216		-0.15073			
215 ->217		-0.39352			

Excited State 4: Singlet-A 4.9265 eV 251.67 nm f=0.1437

212 ->216 -0.42613

214 ->217 0.52907

Excited State 5: Singlet-A 5.1189 eV 242.21 nm f=0.0036

207 ->216 -0.24633

211 ->216 -0.30131

211 ->217 0.12446

213 ->217 0.42539

215 ->216 0.19610

215 ->217 0.20948

Excited State 6: Singlet-A 5.1275 eV 241.80 nm f=0.0003

207 ->217 -0.14113

211 ->216 0.13255

211 ->217 -0.15256

213 ->216 0.38495

215 ->217 0.44127

215 ->219 -0.14191

Excited State 7: Singlet-A 5.1893 eV 238.92 nm f=0.0212

206 ->216 -0.22560

212 ->216 0.38893

212 ->217 0.37990

214 ->217 0.32175

214 ->220 0.10913

Excited State 8: Singlet-A 5.2279 eV 237.16 nm f=0.0224

206 ->216 0.34537

206 ->217 -0.25579

212 ->216 0.29312

212 ->217 -0.29993

214 ->216 -0.14343

214 ->217 0.22328

214 ->219 -0.20442

Excited State 9: Singlet-A 5.2499 eV 236.17 nm f=0.0069

205 ->216 -0.16269

207 ->217 -0.20410

211 ->216 0.34143

211 ->217 -0.26637

213 ->216 -0.21438

213 ->217 0.32411

213 ->219 -0.13159

215 ->216 0.15269

Excited State 10: Singlet-A 5.3115 eV 233.42 nm f=0.0128

203 ->216	-0.20166
203 ->217	-0.17184
205 ->216	0.22400
205 ->217	0.20991
207 ->216	0.26454
207 ->217	0.21487
211 ->216	0.12560
211 ->217	0.10235
213 ->217	0.23323
213 ->220	0.11322
215 ->219	0.20428

Excited State 11: Singlet-A 5.3353 eV 232.38 nm f=0.0150

206 ->216	0.35835
206 ->217	-0.30716
212 ->216	-0.11390
212 ->217	0.40000
212 ->219	-0.12053
214 ->216	0.19810
214 ->217	-0.12117

Excited State 12: Singlet-A 5.3979 eV 229.69 nm f=0.0001

203 ->216 0.13765

207 ->216 -0.22255

208 ->216 0.12744

211 ->216 0.18734

212 ->218 0.13565

213 ->217 -0.10179

213 ->219 0.10422

214 ->218 0.44706

214 ->224 -0.11214

215 ->219 0.18336

Excited State 13: Singlet-A 5.4003 eV 229.59 nm f=0.0008

210 ->216 0.64614

210 ->217 -0.22029

215 ->218 -0.12981

Excited State 14: Singlet-A 5.4062 eV 229.34 nm f=0.0002

207 ->216 0.24933

207 ->217 -0.12124

208 ->216 -0.14376

211 ->216 -0.26844

212 ->218 0.10406

213 ->219 -0.12801

214 ->218 0.42449

215 ->219 -0.19983

Excited State 15: Singlet-A 5.4302 eV 228.32 nm f=0.0043

205 ->216 -0.25383

207 ->216 0.14324

207 ->217 -0.14453

208 ->216 -0.33676

211 ->216 -0.12454

211 ->217 0.12131

213 ->217 -0.11795

213 ->219 0.14102

213 ->220 0.10494

215 ->219 0.34589

Excited State 16: Singlet-A 5.4514 eV 227.43 nm f=0.0075

206 ->216 0.11428

209 ->216 0.28986

209 ->217 0.12822

212 ->216 0.10349

212 ->219 0.13084

214 ->219 0.34131

215 ->218 0.39869

Excited State	17:	Singlet-A	5.4642 eV	226.90 nm	f=0.0044
200 ->216		-0.14313			
203 ->216		0.22271			
205 ->216		-0.12957			
207 ->216		0.29960			
208 ->216		0.38239			
208 ->217		0.22479			
211 ->216		-0.19076			
215 ->219		0.14807			

Excited State	18:	Singlet-A	5.4681 eV	226.74 nm	f=0.0114
209 ->216		0.55379			
209 ->217		0.23650			
214 ->219		-0.23209			
215 ->218		-0.13436			

Excited State	19:	Singlet-A	5.5015 eV	225.37 nm	f=0.0136
200 ->216		-0.13893			
203 ->216		0.17641			
213 ->216		-0.11488			
213 ->219		0.32510			
213 ->221		-0.17934			

215 ->219 -0.19374

215 ->220 0.41535

215 ->221 0.10143

Excited State 20: Singlet-A 5.5117 eV 224.95 nm f=0.0561

206 ->216 -0.11306

210 ->216 0.10159

212 ->219 -0.12760

212 ->220 -0.11774

213 ->218 0.10789

213 ->222 -0.11292

214 ->219 -0.35647

215 ->218 0.48253

Excited State 21: Singlet-A 5.5141 eV 224.85 nm f=0.0010

200 ->216 -0.21073

203 ->216 0.31726

203 ->217 -0.20400

205 ->216 0.12459

205 ->217 0.17111

208 ->216 -0.29634

208 ->217 -0.17109

211 ->217 -0.13483

211 ->219 -0.13300

213 ->219 -0.15609

215 ->217 0.10182

215 ->220 -0.10742

Excited State 22: Singlet-A 5.5628 eV 222.88 nm f=0.0362

206 ->216 0.13959

206 ->217 0.14453

212 ->219 0.28652

212 ->221 -0.12031

213 ->218 0.20993

214 ->220 0.44160

214 ->221 0.22538

Excited State 23: Singlet-A 5.5667 eV 222.73 nm f=0.0078

200 ->217 -0.18681

200 ->219 0.10160

203 ->216 0.11796

203 ->217 0.13380

205 ->216 0.28137

207 ->217 -0.10458

207 ->219 0.10482

211 ->219 0.13314

212 ->218 -0.10981

213 ->220 0.26739

213 ->221 0.16407

215 ->217 -0.12264

215 ->219 0.13324

215 ->220 0.11884

215 ->221 -0.22959

Excited State 24: Singlet-A 5.5736 eV 222.45 nm f=0.0028

202 ->216 0.16501

202 ->217 -0.10406

204 ->216 0.61537

213 ->218 0.21081

Excited State 25: Singlet-A 5.5804 eV 222.18 nm f=0.0249

204 ->216 -0.22219

213 ->218 0.53501

214 ->219 0.12957

214 ->220 -0.18513

215 ->222 -0.16169

Excited State 26: Singlet-A 5.5807 eV 222.17 nm f=0.0003

203 ->216 0.28356

211 ->216 0.22661

211 ->217 0.48496

211 ->219 0.10115

211 ->220 0.12420

213 ->219 -0.12696

215 ->219 -0.17565

Excited State 27: Singlet-A 5.5969 eV 221.52 nm f=0.0144

200 ->216 0.13640

203 ->216 0.19250

203 ->217 0.10486

205 ->216 0.32127

207 ->216 0.11655

213 ->219 0.21372

213 ->220 -0.25991

215 ->219 0.17345

215 ->220 -0.25959

215 ->221 0.15924

Excited State 28: Singlet-A 5.6122 eV 220.92 nm f=0.0005

210 ->216 0.22057

210 ->217 0.64382

210 ->220 0.10783

Excited State 29: Singlet-A 5.6143 eV 220.84 nm f=0.0221

205 ->216 0.10839

212 ->218 0.52658

213 ->220 0.12570

214 ->218 -0.15441

214 ->222 -0.25713

215 ->220 0.16011

Excited State 30: Singlet-A 5.6377 eV 219.92 nm f=0.0002

200 ->216 -0.26365

201 ->217 0.10095

203 ->216 -0.15558

205 ->217 0.30446

207 ->216 -0.16312

207 ->217 -0.27466

208 ->217 0.21321

211 ->217 0.18280

212 ->218 0.15102

213 ->219 0.10515

215 ->219 0.10641

Excited State 31: Singlet-A 5.6604 eV 219.04 nm f=0.0035

206 ->216 0.30474

206 ->217 0.45792

206 ->219 0.17029

206 ->220 0.12678

212 ->216 0.10574

212 ->217 0.11382

214 ->219 -0.14489

214 ->220 -0.17068

214 ->221 -0.14860

Excited State 32: Singlet-A 5.6628 eV 218.95 nm f=0.0049

205 ->216 -0.17486

207 ->217 0.29272

208 ->216 -0.13818

211 ->219 0.13531

212 ->218 0.13134

213 ->217 0.11329

213 ->219 0.24637

213 ->221 0.23859

215 ->219 -0.10327

215 ->220 -0.18356

215 ->221 -0.15173

Excited State 33: Singlet-A 5.6763 eV 218.43 nm f=0.0287

212 ->219 0.13200

212 ->220 -0.35930

213 ->218 -0.16618

214 ->220 -0.24627

214 ->221 0.41166

Excited State 34: Singlet-A 5.6838 eV 218.14 nm f=0.0009

202 ->216 -0.14773

204 ->217 0.14624

209 ->216 -0.25903

209 ->217 0.59988

209 ->219 -0.11638

Excited State 35: Singlet-A 5.6977 eV 217.60 nm f=0.0015

202 ->216 -0.43551

204 ->216 0.13873

204 ->217 0.44649

208 ->217 0.10195

209 ->217 -0.20401

Excited State 36: Singlet-A 5.6986 eV 217.57 nm f=0.0010

200 ->216 0.15873

203 ->217 -0.12019

207 ->216 -0.12251

207 ->217 0.12257

207 ->219 -0.11454

208 ->216 -0.18763

208 ->217 0.52583

211 ->219 -0.11034

Excited State 37: Singlet-A 5.7093 eV 217.16 nm f=0.0000

200 ->216 -0.10686

201 ->216 -0.23355

203 ->217 0.28069

205 ->217 0.17860

207 ->217 0.24535

208 ->216 -0.10077

208 ->217 0.12969

211 ->219 0.11424

213 ->219 -0.19794

213 ->221 -0.18707

215 ->221 0.16197

Excited State 38: Singlet-A 5.7255 eV 216.55 nm f=0.0004

200 ->217 -0.13090

201 ->216 0.32655

203 ->217 -0.27663

205 ->217 -0.18609

206 ->218 -0.13563

211 ->219 0.15998

213 ->219 -0.12639

213 ->221 -0.11558

215 ->221 0.10679

Excited State 39: Singlet-A 5.7470 eV 215.74 nm f=0.0003

200 ->216 -0.12148

200 ->217 -0.14402

201 ->216 0.16578

205 ->216 -0.14290

206 ->218 0.27925

206 ->222 -0.15503

206 ->226 -0.18580

207 ->217 0.13878

212 ->222 -0.20511

212 ->224 0.12084

212 ->226 -0.15958

213 ->219 -0.10566

213 ->221 -0.11225

214 ->224 0.14842

214 ->226 -0.12467

215 ->219 0.10617

Excited State 40: Singlet-A 5.7780 eV 214.58 nm f=0.0004

206 ->217 -0.11685

212 ->219 0.47397

212 ->220 -0.16822

212 ->221 0.16565

214 ->219 -0.13306

214 ->220 -0.10400

214 ->221 -0.27069

214 ->223 -0.10309

Excited State 41: Singlet-A 5.7865 eV 214.26 nm f=0.0008

200 ->216 0.31725

201 ->216 0.31151

201 ->217 0.15003

203 ->216 0.17183

203 ->217 0.15758

205 ->216 -0.19379

205 ->217 0.31061

Excited State 42: Singlet-A 5.7989 eV 213.81 nm f=0.0016

202 ->216 0.42275

202 ->217 0.27900

204 ->217 0.44584

Excited State 43: Singlet-A 5.8090 eV 213.43 nm f=0.0023

200 ->216 -0.26451

201 ->216 0.19225

201 ->217 0.12346

203 ->217 0.28608

205 ->217 -0.24178

206 ->218 -0.11796

207 ->216 0.16130

211 ->216 0.11123

211 ->219 -0.16963

211 ->220 -0.12144

213 ->220 -0.11726

Excited State 44: Singlet-A 5.8225 eV 212.94 nm f=0.0810

199 ->216 0.11325

199 ->217 0.11229

206 ->216 0.11993

206 ->217 0.12402

206 ->219 -0.25976

206 ->220 -0.15024

206 ->227 0.11394

207 ->218 0.12768

211 ->218 0.29724

211 ->222 -0.14566

211 ->226 -0.12161

212 ->220 -0.11163

212 ->227 0.10683

213 ->222 -0.12558

214 ->219 0.10327

214 ->220 0.17489

214 ->223 -0.13535

215 ->222 -0.10813

Excited State 45: Singlet-A 5.8586 eV 211.63 nm f=0.0002

200 ->217 0.21874

200 ->219 -0.12143

201 ->216 0.22409

201 ->217 0.14443

203 ->217 0.24905

207 ->217 -0.12511

213 ->219 0.10762

213 ->220 0.27708

215 ->219 -0.18351

215 ->220 -0.16284

215 ->221 0.14530

215 ->223 0.15302

Excited State 46: Singlet-A 5.8722 eV 211.14 nm f=0.0222

203 ->221 -0.11627

205 ->221 0.13312

207 ->221 0.15577

211 ->219 -0.16826

211 ->220 -0.10118

213 ->219 0.22679

213 ->220 0.31855

213 ->221 -0.19991

215 ->220 -0.20551

215 ->221 -0.15555

Excited State 47: Singlet-A 5.8850 eV 210.68 nm f=0.0077

198 ->216 -0.13470

198 ->217 0.13746

199 ->216 0.51706

199 ->217 0.25398

202 ->216 0.10031

212 ->221 0.12712

Excited State 48: Singlet-A 5.9162 eV 209.57 nm f=0.0252

198 ->216 -0.10233

200 ->218 -0.12401

202 ->217 -0.13940

206 ->219 -0.24229

206 ->220 -0.14460

208 ->218 0.10075

212 ->217 0.14250

212 ->220 0.23961

214 ->219 -0.19327

214 ->220 -0.12549

214 ->223 0.32961

Excited State 49: Singlet-A 5.9207 eV 209.41 nm f=0.0085

200 ->217 -0.23137

207 ->221 -0.11516

211 ->220 -0.15872

213 ->220 0.22958

213 ->221 0.12147

215 ->221 0.46538

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Excited State 50: Singlet-A 5.9287 eV 209.12 nm f=0.0193

198 ->216	0.50384
198 ->217	-0.13866
199 ->217	0.27821
207 ->218	-0.14192
211 ->218	-0.11008

Excited State 51: Singlet-A 5.9363 eV 208.86 nm f=0.0673

198 ->216	-0.16567
202 ->216	-0.17860
202 ->217	0.53654
204 ->216	0.12782
204 ->217	-0.14596
206 ->219	-0.13354
211 ->218	-0.11851

Excited State 52: Singlet-A 5.9443 eV 208.58 nm f=0.1732

202 ->217	0.23530
206 ->219	0.16006
211 ->218	0.31166
212 ->219	0.17684
212 ->220	0.31737

214 ->220 -0.18881

214 ->221 0.18097

Excited State 53: Singlet-A 5.9672 eV 207.78 nm f=0.0017

200 ->217 -0.14717

201 ->216 -0.21432

201 ->217 0.42451

203 ->219 0.10374

205 ->217 -0.15067

208 ->219 0.10815

210 ->218 -0.10474

211 ->220 0.10159

213 ->221 -0.23259

214 ->222 0.11772

Excited State 54: Singlet-A 5.9701 eV 207.67 nm f=0.0004

210 ->219 0.58702

210 ->220 0.20073

211 ->218 -0.23511

Excited State 55: Singlet-A 5.9717 eV 207.62 nm f=0.0007

201 ->216 0.11215

201 ->217 -0.26698

207 ->220 0.11101

208 ->220 -0.13402

210 ->218 0.27061

211 ->219 -0.23693

211 ->220 0.11107

212 ->218 0.13695

213 ->221 -0.11762

213 ->223 0.15711

214 ->222 0.19498

214 ->224 0.15495

Excited State 56: Singlet-A 5.9783 eV 207.39 nm f=0.0003

200 ->217 0.15875

201 ->217 0.24638

207 ->219 0.10373

208 ->219 -0.20906

210 ->218 0.44316

211 ->220 -0.17251

214 ->224 0.12461

Excited State 57: Singlet-A 5.9866 eV 207.10 nm f=0.0065

200 ->217 -0.11365

208 ->219 0.33185

208 ->220 -0.22323

208 ->221 -0.11869

209 ->218 -0.25846

210 ->218 0.21964

213 ->223 -0.14205

214 ->222 -0.15964

215 ->223 0.21507

Excited State 58: Singlet-A 5.9887 eV 207.03 nm f=0.0068

206 ->219 -0.11482

208 ->218 -0.28902

209 ->216 -0.11139

209 ->219 0.44828

209 ->220 -0.29174

209 ->221 -0.17918

210 ->219 -0.12868

211 ->218 -0.12020

Excited State 59: Singlet-A 5.9910 eV 206.95 nm f=0.0001

207 ->219 -0.35973

208 ->219 0.20481

210 ->218 0.12883

211 ->219 0.40873

212 ->218 0.10321

214 ->222 0.19118

214 ->224 0.12637

Excited State 60: Singlet-A 5.9971 eV 206.74 nm f=0.0040

206 ->219 0.14047

207 ->218 -0.27289

209 ->219 0.16367

209 ->220 -0.10104

210 ->219 0.27524

210 ->220 -0.10805

211 ->218 0.32211

212 ->220 -0.21529

212 ->221 0.10353

214 ->220 0.12164

214 ->223 0.21722

Excited State 61: Singlet-A 6.0058 eV 206.44 nm f=0.0325

199 ->216 -0.12066

205 ->218 0.13009

206 ->221 -0.10362

207 ->218 0.11877

212 ->221 0.45260

213 ->222 -0.13381

214 ->221 0.26345

214 ->225 0.14162

Excited State 62: Singlet-A 6.0059 eV 206.44 nm f=0.0163

207 ->219 0.11942

210 ->218 -0.22362

212 ->218 0.13942

213 ->223 -0.30846

214 ->222 0.24944

214 ->224 0.15383

215 ->223 0.39316

Excited State 63: Singlet-A 6.0150 eV 206.12 nm f=0.0004

200 ->217 0.11089

201 ->217 0.14816

203 ->221 -0.12116

205 ->219 -0.10328

205 ->220 0.12685

205 ->221 0.19495

207 ->221 0.12206

209 ->218 -0.16159

210 ->218 -0.16918

213 ->221 0.29741

213 ->223 0.13766

214 ->222 0.14737

214 ->224 0.19571

215 ->223 -0.15351

Excited State 64: Singlet-A 6.0194 eV 205.97 nm f=0.0047

200 ->217 0.29853

203 ->219 -0.16298

205 ->221 -0.13069

207 ->219 0.27928

207 ->220 -0.12474

209 ->218 -0.16759

211 ->219 0.10803

211 ->220 -0.17200

213 ->221 -0.21824

215 ->223 -0.18658

Excited State 65: Singlet-A 6.0204 eV 205.94 nm f=0.0539

206 ->219 0.11661

207 ->218 0.28498

208 ->218 -0.17690

210 ->219 -0.11171

212 ->220 -0.19001

212 ->223 -0.20568

214 ->220 0.10906

214 ->223 0.44717

Excited State 66: Singlet-A 6.0366 eV 205.39 nm f=0.0081

206 ->218 -0.19691

206 ->222 0.14553

206 ->224 -0.11868

207 ->220 -0.17802

211 ->220 0.30436

212 ->224 0.16127

214 ->218 0.12367

214 ->222 -0.24398

214 ->224 0.29944

Excited State 67: Singlet-A 6.0423 eV 205.19 nm f=0.0056

198 ->216 0.13523

206 ->219 -0.10045

210 ->220 0.24593

211 ->218 0.13504

213 ->218 0.12223

213 ->224 -0.15193

215 ->222 0.54573

Excited State 68: Singlet-A 6.0531 eV 204.83 nm f=0.0054

208 ->218 0.10589

210 ->219 -0.15528

210 ->220 0.56834

211 ->218 0.10761

215 ->222 -0.19326

Excited State 69: Singlet-A 6.0540 eV 204.80 nm f=0.0019

203 ->219 -0.12021

206 ->218 0.11790

207 ->220 -0.24333

208 ->220 0.11692

209 ->218 -0.11358

210 ->218 0.19656

211 ->220 0.34650

212 ->224 -0.10808

213 ->223 -0.13119

214 ->222 0.18032

214 ->224 -0.21621

215 ->223 -0.10980

Excited State 70: Singlet-A 6.0714 eV 204.21 nm f=0.0012

205 ->219 -0.12746

208 ->219 0.24213

208 ->220 -0.14197

208 ->221 -0.14033

209 ->218 0.54080

209 ->222 0.10731

Excited State 71: Singlet-A 6.0759 eV 204.06 nm f=0.0121

207 ->218 0.34135

208 ->218 0.46176

208 ->222 0.10961

209 ->219 0.21185

209 ->220 -0.12551

209 ->221 -0.12028

212 ->221 -0.15163

Excited State 72: Singlet-A 6.0909 eV 203.56 nm f=0.0066

203 ->219 -0.26638

204 ->218 0.10329

205 ->220 0.13481

207 ->220 -0.22922

213 ->223 0.37865

215 ->220 -0.11924

215 ->223 0.21249

215 ->225 -0.22195

Excited State 73: Singlet-A 6.0928 eV 203.49 nm f=0.0160

198 ->216 -0.11011

203 ->218 0.25708

205 ->218 -0.29211

206 ->219 0.32137

206 ->220 -0.22678

207 ->222 -0.10436

215 ->222 0.13567

Excited State 74: Singlet-A 6.0936 eV 203.46 nm f=0.0006

203 ->219 0.31345

204 ->218 -0.21199

205 ->219 0.35226

205 ->220 -0.11045

207 ->219 0.18011

207 ->220 -0.20254

208 ->219 0.10189

209 ->218 0.13741

213 ->223 0.17004

Excited State 75: Singlet-A 6.1001 eV 203.25 nm f=0.0011

203 ->218	-0.21314
204 ->219	0.32282
204 ->220	-0.14312
205 ->218	-0.10875
207 ->218	-0.18262
208 ->218	0.24085
213 ->222	-0.30300
215 ->224	0.22508

Excited State 76: Singlet-A 6.1088 eV 202.96 nm f=0.1009

202 ->219	0.10682
203 ->218	-0.15504
204 ->219	0.37388
204 ->220	-0.13729
205 ->218	-0.18861
212 ->221	0.12295
213 ->222	0.33018
215 ->224	-0.20544

Excited State 77: Singlet-A 6.1220 eV 202.52 nm f=0.0029

203 ->218	0.20966

205 ->218 -0.29200

206 ->219 -0.10252

206 ->220 0.47805

206 ->221 -0.16192

207 ->218 0.10647

Excited State 78: Singlet-A 6.1270 eV 202.36 nm f=0.0065

203 ->219 -0.21541

205 ->219 0.14576

205 ->220 -0.12010

206 ->218 0.37243

206 ->226 0.14032

207 ->219 -0.13585

207 ->220 0.14575

212 ->218 0.12322

212 ->222 0.19832

212 ->226 0.15488

214 ->218 0.11088

214 ->226 0.17206

Excited State 79: Singlet-A 6.1351 eV 202.09 nm f=0.0258

198 ->217 -0.13526

202 ->219 0.11230

203 ->218 0.22561

204 ->219 0.30215

205 ->218 0.24097

206 ->219 0.15517

207 ->218 0.10991

208 ->218 -0.14650

212 ->221 -0.14393

212 ->223 0.18716

213 ->222 -0.18267

214 ->225 -0.13783

Excited State 80: Singlet-A 6.1432 eV 201.82 nm f=0.0023

203 ->219 -0.25013

205 ->219 0.32021

205 ->220 -0.20030

206 ->218 -0.22055

207 ->220 0.17729

208 ->220 -0.11620

212 ->222 -0.16481

212 ->226 -0.11116

214 ->226 -0.12233

Excited State 81: Singlet-A 6.1543 eV 201.46 nm f=0.0000

202 ->218 0.15809

203 ->219 0.22797

203 ->220 0.14866

204 ->218 0.56401

205 ->219 0.13705

Excited State 82: Singlet-A 6.1621 eV 201.20 nm f=0.0341

198 ->216 0.10677

198 ->217 0.13201

199 ->217 -0.17113

203 ->218 0.33570

204 ->219 0.21555

205 ->218 0.22143

212 ->223 -0.22913

213 ->222 0.19230

214 ->225 0.15058

215 ->224 0.12647

Excited State 83: Singlet-A 6.1848 eV 200.46 nm f=0.0004

198 ->216 0.16904

198 ->217 0.23024

199 ->217 -0.20746

203 ->218 0.13350

205 ->218 -0.14032

206 ->220 -0.18429

212 ->221 0.10604

212 ->223 0.29941

212 ->227 -0.10955

214 ->225 -0.17303

215 ->224 0.17233

215 ->226 0.11012

Excited State 84: Singlet-A 6.1988 eV 200.01 nm f=0.0065

198 ->216 -0.18164

198 ->217 0.12179

198 ->219 -0.10629

199 ->216 -0.30529

199 ->217 0.41984

199 ->219 -0.13928

215 ->224 0.15590

Excited State 85: Singlet-A 6.2029 eV 199.88 nm f=0.0017

203 ->220 0.43608

204 ->218 -0.19983

205 ->220 0.12902

207 ->219 -0.12402

208 ->219 0.11649

208 ->220 0.15268

211 ->219 -0.10778

211 ->223 0.10609

211 ->227 -0.11209

212 ->222 -0.10844

215 ->225 0.10307

215 ->227 -0.10936

Excited State 86: Singlet-A 6.2200 eV 199.33 nm f=0.0006

202 ->219 0.27215

202 ->220 0.11861

203 ->218 -0.11963

204 ->220 0.56179

Excited State 87: Singlet-A 6.2215 eV 199.28 nm f=0.0012

200 ->219 -0.11645

203 ->220 0.33213

204 ->218 -0.11122

207 ->219 0.15798

207 ->220 0.12734

208 ->221 0.14000

211 ->227 0.10911

212 ->222 0.14485

214 ->224 0.12331

214 ->229 0.12033

215 ->225 -0.21593

215 ->227 0.13059

Excited State 88: Singlet-A 6.2341 eV 198.88 nm f=0.0007

200 ->219 -0.16687

201 ->219 -0.15163

203 ->220 -0.14745

205 ->219 -0.11759

205 ->220 -0.19485

208 ->219 0.26002

208 ->220 0.28297

208 ->221 0.23423

209 ->219 -0.15897

209 ->220 -0.17044

209 ->221 -0.12030

Excited State 89: Singlet-A 6.2349 eV 198.85 nm f=0.0008

208 ->219 0.11333

208 ->220 0.12305

208 ->221 0.10112

209 ->219 0.38625

209 ->220 0.41390

209 ->221 0.28956

Excited State 90: Singlet-A 6.2440 eV 198.56 nm f=0.0026

198 ->217 0.40752

202 ->219 0.13190

202 ->220 -0.11084

205 ->218 0.14722

206 ->219 0.13035

206 ->223 -0.10234

206 ->227 0.10531

212 ->228 0.11156

214 ->225 -0.21655

214 ->227 0.12019

215 ->226 -0.11145

Excited State 91: Singlet-A 6.2490 eV 198.41 nm f=0.0143

206 ->218 -0.17314

206 ->222 -0.18512

206 ->226 -0.18325

212 ->222 0.28985

212 ->226 -0.19155

213 ->225 0.10995

214 ->222 0.18660

214 ->224 0.10364

214 ->229 0.19922

215 ->225 0.26177

Excited State 92: Singlet-A 6.2594 eV 198.08 nm f=0.0012

198 ->217 -0.10661

200 ->218 -0.17163

201 ->218 -0.13724

202 ->219 0.34071

202 ->220 -0.31620

202 ->221 -0.11004

204 ->220 -0.11274

204 ->221 0.16010

213 ->222 0.13984

215 ->224 0.28795

Excited State 93: Singlet-A 6.2690 eV 197.77 nm f=0.0030

200 ->218 -0.20694

201 ->218 0.10006

202 ->219 -0.18688

202 ->220 0.19427

203 ->218 -0.11695

204 ->220 0.11184

212 ->227 0.11979

213 ->222 0.22840

214 ->228 0.13970

215 ->224 0.33085

Excited State 94: Singlet-A 6.2719 eV 197.68 nm f=0.0070

200 ->219 0.20329

201 ->219 0.25182

201 ->220 -0.13428

202 ->218 -0.19732

205 ->220 0.12098

207 ->219 0.12378

207 ->220 0.23549

208 ->219 0.19357

208 ->220 0.22287

208 ->221 0.12284

215 ->223 0.11051

215 ->225 0.13610

Excited State 95: Singlet-A 6.2811 eV 197.39 nm f=0.0051

201 ->219 -0.23755

201 ->220 0.20773

202 ->218 0.23186

211 ->223 -0.12276

213 ->223 0.17077

213 ->225 0.14994

213 ->227 0.10840

215 ->223 0.17907

215 ->225 0.29882

Excited State 96: Singlet-A 6.2902 eV 197.11 nm f=0.0860

198 ->217 0.23416

203 ->218 0.12004

205 ->218 -0.18291

212 ->221 -0.15390

212 ->228 -0.15102

213 ->229 0.12380

214 ->225 0.20922

214 ->227 -0.19845

214 ->228 0.20789

215 ->224 -0.19245

Excited State 97: Singlet-A 6.2986 eV 196.84 nm f=0.0081

200 ->217 0.11865

200 ->219 0.26906

201 ->219 -0.15592

201 ->220 0.12857

202 ->218 0.21094

203 ->221 -0.11834

205 ->221 -0.10388

207 ->220 0.15129

208 ->219 0.10517

208 ->220 0.16448

208 ->221 -0.10317

212 ->222 0.13344

213 ->223 -0.12619

213 ->225 -0.14626

215 ->221 0.12507

215 ->225 -0.19528

Excited State 98: Singlet-A 6.3109 eV 196.46 nm f=0.0156

201 ->218 -0.14892

213 ->222 -0.12916

213 ->224 0.60830

215 ->222 0.15942

Excited State 99: Singlet-A 6.3229 eV 196.09 nm f=0.0002

200 ->220 0.14564

201 ->219 0.12433

202 ->218 0.35266

203 ->220 -0.11437

203 ->221 0.14908

204 ->218 -0.10456

205 ->220 0.29641

208 ->220 -0.11111

208 ->221 0.21934

212 ->224 -0.13089

213 ->225 -0.10170

215 ->227 -0.10458

Excited State 100: Singlet-A 6.3301 eV 195.87 nm f=0.0022

209 ->220 -0.38659

209 ->221 0.57440

Excited State 101: Singlet-A 6.3345 eV 195.73 nm f=0.0001

201 ->219 0.21211

201 ->220 -0.19208

202 ->218 0.30789

205 ->219 -0.11546

205 ->220 -0.22656

205 ->221 0.15915

208 ->220 0.17213

208 ->221 -0.28071

212 ->224 -0.18013

Excited State 102: Singlet-A 6.3443 eV 195.43 nm f=0.0007

200 ->219 -0.22203

200 ->220 0.13724

202 ->218 -0.10835

203 ->219 -0.10747

205 ->219 0.17574

205 ->220 0.12976

207 ->220 0.10596

207 ->221 -0.14861

208 ->220 0.18634

208 ->221 -0.21114

211 ->221 0.43307

Excited State 103: Singlet-A 6.3535 eV 195.14 nm f=0.0026

200 ->219 0.10235

205 ->220 -0.14199

208 ->220 -0.15685

208 ->221 0.35418

211 ->220 0.12581

211 ->221 0.44196

Excited State 104: Singlet-A 6.3579 eV 195.01 nm f=0.0002

210 ->221 0.67468

210 ->225 0.12093

Excited State 105: Singlet-A 6.3654 eV 194.78 nm f=0.0087

201 ->218 0.41595

206 ->223 0.10548

212 ->223 -0.29843

212 ->225 -0.13343

214 ->225 -0.32438

Excited State 106: Singlet-A 6.3675 eV 194.71 nm f=0.0023

198 ->218 -0.10713

200 ->219 -0.12946

201 ->218 -0.11528

202 ->218 0.20662

205 ->221 0.11998

206 ->224 -0.10593

212 ->224 0.45821

212 ->229 0.10878

214 ->224 -0.22007

214 ->229 -0.16477

Excited State 107: Singlet-A 6.3682 eV 194.69 nm f=0.0177

200 ->218 0.13735

201 ->218 0.41321

206 ->223 -0.10520

212 ->223 0.27008

212 ->224 0.12525

212 ->225 0.12960

213 ->224 0.16640

214 ->225 0.16987

Excited State 108: Singlet-A 6.3780 eV 194.39 nm f=0.0001

199 ->218 -0.14041

200 ->219 -0.16982

205 ->220 -0.10466

205 ->221 0.12041

207 ->221 0.29013

212 ->222 0.27405

212 ->229 0.14745

213 ->225 -0.12496

213 ->227 0.12789

213 ->228 -0.11361

214 ->222 -0.15385

214 ->224 0.12098

214 ->229 -0.21171

215 ->228 0.10858

Excited State 109: Singlet-A 6.3961 eV 193.84 nm f=0.0018

199 ->218 -0.12517

203 ->221 0.10305

207 ->221 -0.19134

212 ->222 0.21812

212 ->229 0.14750

213 ->225 0.36731

213 ->227 -0.14976

214 ->222 -0.11976

214 ->229 -0.21565

215 ->225 -0.17178

215 ->228 -0.11966

Excited State 110: Singlet-A 6.4109 eV 193.40 nm f=0.0001

200 ->219 -0.10492

200 ->221 0.15782

201 ->219 0.12401

201 ->221 -0.11641

205 ->221 -0.23365

207 ->221 0.34340

213 ->225 0.32750

215 ->225 -0.12324

Excited State 111: Singlet-A 6.4246 eV 192.98 nm f=0.0977

198 ->217 -0.12960

198 ->219 -0.14667

199 ->219 0.17737

200 ->218 0.42213

201 ->218 -0.10589

213 ->222 0.11142

214 ->225 -0.16750

214 ->227 -0.13243

214 ->228 0.11297

215 ->226 -0.15008

Excited State 112: Singlet-A 6.4253 eV 192.96 nm f=0.0039

200 ->220 -0.20230

201 ->219 -0.17100

203 ->221 0.13699

203 ->223 0.14384

205 ->219 0.10931

205 ->221 0.36052

205 ->223 -0.20397

207 ->223 -0.17673

213 ->225 0.11807

213 ->227 0.10436

213 ->228 -0.15888

215 ->227 -0.12809

Excited State 113: Singlet-A 6.4459 eV 192.35 nm f=0.0002

202 ->219 -0.35210

202 ->220 -0.14230

204 ->219 0.18549

204 ->221 0.51660

Excited State 114: Singlet-A 6.4633 eV 191.83 nm f=0.0044

211 ->218 0.12256

211 ->222 0.49140

213 ->226 -0.20755

215 ->226 -0.37386

Excited State 115: Singlet-A 6.4717 eV 191.58 nm f=0.0020

206 ->219 -0.11673

206 ->220 0.15428

206 ->221 0.60692

206 ->225 0.11733

212 ->221 0.13776

Excited State 116: Singlet-A 6.4762 eV 191.44 nm f=0.0000

201 ->219 -0.24567

203 ->221 0.43946

205 ->223 0.14784

207 ->221 0.20733

207 ->223 0.19310

215 ->227 0.12623

Excited State 117: Singlet-A 6.4885 eV 191.08 nm f=0.0000

199 ->218 0.10668

210 ->222 0.64347

210 ->224 -0.11961

Excited State 118: Singlet-A 6.4951 eV 190.89 nm f=0.0044

200 ->220 0.18640

201 ->220 0.13263

205 ->221 0.12080

205 ->223 0.23396

207 ->223 0.21283

208 ->223 0.29896

209 ->222 -0.11223

213 ->225 0.21328

213 ->228 -0.15731

215 ->225 -0.10736

215 ->227 -0.21874

Excited State 119: Singlet-A 6.5010 eV 190.72 nm f=0.0016

208 ->222 -0.21215

209 ->223 0.61569

211 ->222 -0.11611

Excited State 120: Singlet-A 6.5055 eV 190.58 nm f=0.0003

200 ->220 -0.28129

201 ->219 -0.13309

201 ->220 -0.23838

203 ->221 -0.14983

205 ->220 0.18586

207 ->223 0.17796

208 ->223 0.34136

209 ->222 -0.14599

215 ->227 0.12124

Excited State 121:	Singlet-A	6.5076 eV	190.52 nm	f=0.0167
205 ->222	-0.10305			
207 ->222	0.37087			
207 ->226	0.10192			
208 ->222	-0.16102			
209 ->223	-0.24321			
211 ->222	-0.30548			
211 ->226	0.11542			
213 ->226	-0.10272			
215 ->226	-0.23016			

Excited State 122:	Singlet-A	6.5081 eV	190.51 nm	f=0.0025
199 ->218	0.29339			
200 ->220	0.12217			
201 ->219	0.10810			
201 ->220	0.13238			
203 ->221	0.11837			
203 ->223	0.12025			
205 ->220	-0.10844			
205 ->223	-0.12356			
206 ->222	0.20951			
207 ->221	0.11207			

208 ->223 0.20372

210 ->222 -0.15047

212 ->222 0.11717

212 ->224 -0.10491

212 ->226 -0.13266

214 ->226 -0.22962

Excited State 123: Singlet-A 6.5116 eV 190.40 nm f=0.0000

199 ->218 -0.20495

203 ->221 0.12771

203 ->223 0.13430

205 ->223 -0.17796

206 ->222 -0.19999

208 ->223 0.35056

209 ->222 -0.10849

211 ->223 -0.10481

212 ->226 0.12648

213 ->225 -0.13249

214 ->226 0.19820

Excited State 124: Singlet-A 6.5153 eV 190.30 nm f=0.0013

199 ->219 0.10264

202 ->219 0.20598

202 ->220	0.40663			
202 ->221	0.16651			
204 ->220	-0.17732			
204 ->221	0.34203			
204 ->223	0.11377			
212 ->225	0.13976			

Excited State 125:	Singlet-A	6.5222 eV	190.10 nm	f=0.0101
202 ->220	-0.10805			
204 ->221	-0.11554			
207 ->222	0.10818			
212 ->225	0.53880			
214 ->225	-0.26028			

Excited State 126:	Singlet-A	6.5277 eV	189.94 nm	f=0.0022
198 ->218	-0.16037			
199 ->218	0.43719			
206 ->222	-0.26182			
206 ->224	0.10292			
206 ->226	-0.11450			
212 ->224	-0.12155			
212 ->226	0.17143			
214 ->226	0.21362			

214 ->229 -0.16581

Excited State 127: Singlet-A 6.5345 eV 189.74 nm f=0.0014

200 ->220 0.10301

207 ->223 -0.11992

209 ->222 -0.11521

211 ->223 0.44138

211 ->225 -0.17870

211 ->227 -0.11044

213 ->227 0.17737

215 ->227 0.28473

215 ->228 0.17126

Excited State 128: Singlet-A 6.5419 eV 189.52 nm f=0.0001

208 ->223 0.24554

209 ->218 -0.13087

209 ->222 0.59194

209 ->224 0.19930

Excited State 129: Singlet-A 6.5429 eV 189.49 nm f=0.0023

199 ->216 -0.10685

199 ->219 0.33070

199 ->220 -0.24570

199 ->221	-0.17720
200 ->218	-0.15670
202 ->220	-0.13827
207 ->222	-0.13365
207 ->224	-0.10959
210 ->223	-0.28348

Excited State 130: Singlet-A 6.5516 eV 189.24 nm f=0.0084

199 ->219	0.10849
208 ->222	-0.42331
208 ->224	-0.13308
209 ->223	-0.11533
210 ->223	0.43003
210 ->225	-0.15421

Excited State 131: Singlet-A 6.5536 eV 189.18 nm f=0.0050

199 ->219	0.13474
200 ->218	-0.14820
208 ->222	0.39507
208 ->224	0.14497
209 ->223	0.10936
210 ->223	0.37563
210 ->225	-0.15760

215 ->226 -0.10918

Excited State 132: Singlet-A 6.5591 eV 189.03 nm f=0.0294

198 ->219 0.47724

198 ->220 0.10241

199 ->220 -0.19884

199 ->221 -0.12837

200 ->218 0.20673

200 ->224 0.11827

203 ->224 -0.11500

206 ->223 0.11133

207 ->224 0.13593

Excited State 133: Singlet-A 6.5640 eV 188.89 nm f=0.0029

200 ->220 0.36968

201 ->219 -0.20147

201 ->220 -0.14375

201 ->221 -0.33969

203 ->221 -0.21038

205 ->223 -0.16376

Excited State 134: Singlet-A 6.5758 eV 188.55 nm f=0.0034

200 ->220 0.10614

201 ->220	0.12900
205 ->223	-0.24317
207 ->223	0.36062
207 ->225	-0.13395
207 ->227	-0.14527
208 ->223	-0.10881
211 ->223	-0.23137
211 ->227	-0.13782
215 ->227	0.22268
215 ->228	0.10724

Excited State 135: Singlet-A 6.5772 eV 188.51 nm f=0.0322

199 ->219	0.20265
202 ->221	0.12149
203 ->222	-0.11825
205 ->222	0.17970
205 ->224	0.12431
207 ->222	0.39221
211 ->222	0.12619
211 ->226	-0.12290
212 ->225	-0.11390
214 ->227	0.22105
215 ->226	0.18044

Excited State 136:	Singlet-A	6.5902 eV	188.13 nm	f=0.0105
202 ->220	-0.24118			
202 ->221	0.58417			
204 ->220	0.14400			
204 ->223	0.14770			
204 ->225	0.11464			

Excited State 137:	Singlet-A	6.5958 eV	187.98 nm	f=0.0075
198 ->218	0.59833			
199 ->218	0.18989			
199 ->222	0.13369			
212 ->224	0.13329			

Excited State 138:	Singlet-A	6.6142 eV	187.45 nm	f=0.0360
198 ->219	-0.18040			
203 ->222	0.15937			
206 ->223	0.25934			
206 ->227	-0.21048			
212 ->227	0.20815			
214 ->227	0.34594			
214 ->228	0.25684			

Excited State 139: Singlet-A 6.6152 eV 187.42 nm f=0.0000

200 ->219	-0.13870
200 ->220	-0.17466
200 ->221	0.18717
201 ->220	0.38757
201 ->221	-0.32527
203 ->220	-0.13338
203 ->225	-0.11214
205 ->221	0.14358
213 ->227	-0.10450
215 ->228	-0.10842

Excited State 140: Singlet-A 6.6295 eV 187.02 nm f=0.0012

200 ->219	0.13693
200 ->223	-0.11943
201 ->220	-0.13097
201 ->221	-0.11272
203 ->223	0.42538
203 ->225	-0.15987
205 ->223	0.33211
211 ->225	0.13128
215 ->227	0.10871

Excited State 141: Singlet-A 6.6361 eV 186.83 nm f=0.0477

203 ->222	0.12891
205 ->222	0.55722
205 ->224	0.11044
207 ->222	-0.11048
211 ->226	0.13643
215 ->226	-0.11797

Excited State 142: Singlet-A 6.6524 eV 186.37 nm f=0.0024

203 ->222	0.56281
204 ->223	0.19061
206 ->223	-0.11187
207 ->222	0.15995
211 ->224	-0.12072
211 ->226	-0.11353

Excited State 143: Singlet-A 6.6531 eV 186.36 nm f=0.0139

198 ->220	-0.16339
202 ->221	-0.15900
203 ->222	-0.16482
204 ->223	0.56474

Excited State 144: Singlet-A 6.6581 eV 186.21 nm f=0.0009

200 ->221	0.22683
201 ->221	0.14004
202 ->222	0.11507
203 ->223	0.10679
204 ->222	0.54898
206 ->222	0.10759
211 ->225	-0.10706

Excited State 145: Singlet-A 6.6643 eV 186.04 nm f=0.0001

200 ->219	-0.14182
200 ->220	0.13175
200 ->221	0.36439
200 ->223	0.10236
201 ->221	0.28229
204 ->222	-0.33669

Excited State 146: Singlet-A 6.6661 eV 185.99 nm f=0.0051

198 ->219	-0.11402
198 ->220	0.50663
199 ->220	-0.20681
199 ->221	0.11146
204 ->223	0.20649

Excited State 147: Singlet-A 6.6714 eV 185.84 nm f=0.0031

201 ->221	0.10449
203 ->223	-0.10638
207 ->225	-0.10467
210 ->224	-0.33053
211 ->221	-0.12908
211 ->223	0.16069
211 ->225	0.50815

Excited State 148: Singlet-A 6.6831 eV 185.52 nm f=0.0037

203 ->222	-0.11178
207 ->224	0.20484
208 ->224	-0.10064
210 ->223	0.10382
210 ->225	0.43827
211 ->224	-0.41332

Excited State 149: Singlet-A 6.6964 eV 185.15 nm f=0.0016

203 ->223	-0.12801
204 ->222	0.12204
206 ->222	-0.32087
206 ->224	0.11784
206 ->226	0.42700

207 ->225 0.10088

214 ->226 -0.29016

Excited State 150: Singlet-A 6.6999 eV 185.05 nm f=0.0005

200 ->223 -0.10095

201 ->221 0.12558

203 ->223 -0.17077

206 ->222 0.13421

206 ->226 -0.15712

207 ->225 0.21805

208 ->225 -0.11455

210 ->224 0.42945

211 ->225 0.20813

Orbital Coefficients of Atoms corresponding to Absorption Band of CP 1

Orbital transitions: 204→219; 213→222

204(HOMO-11)

17 N 1S -0.01967

2S 0.04127

2PX 0.25705

		2PY	-0.01542
		2PZ	-0.00070
		3S	0.05905
		3PX	0.22121
		3PY	-0.01560
		3PZ	0.00038
		4D 0	0.00186
		4D+1	0.00048
		4D-1	-0.00048
		4D+2	-0.00454
		4D-2	0.00000
18	N	1S	-0.01959
		2S	0.04110
		2PX	0.25605
		2PY	0.01536
		2PZ	-0.00067
		3S	0.05880
		3PX	0.22036
		3PY	0.01553
		3PZ	0.00041
		4D 0	0.00185
		4D+1	0.00048
		4D-1	0.00048

		4D+2	-0.00452
		4D-2	0.00000
		……	

219(LUMO+3)

7	N	1S	-0.00002
		2S	0.00005
		2PX	0.00013
		2PY	0.22116
		2PZ	0.00027
		3S	0.00004
		3PX	0.00024
		3PY	0.30589
		3PZ	0.00031
		4D 0	-0.00001
		4D+1	0.00001
		4D-1	-0.00421
		4D+2	0.00000
		4D-2	0.01324
26	C	1S	-0.00001
		2S	0.00001
		2PX	-0.00016
		2PY	-0.34579

2PZ	-0.00033
3S	0.00036
3PX	-0.00015
3PY	-0.43817
3PZ	-0.00050
4D 0	-0.00002
4D+1	0.00001
4D-1	-0.00722
4D+2	0.00002
4D-2	0.02022

.....

213→222

213(HOMO-2)

3	S	1S	-0.00236
		2S	0.01099
		2PX	-0.05179
		2PY	0.00000
		2PZ	-0.10873
		3S	-0.02417
		3PX	0.13548
		3PY	0.00000
		3PZ	0.28651
		4S	-0.03031
		4PX	0.08599
		4PY	0.00000
		4PZ	0.19991
		5D 0	-0.00011
		5D+1	0.01018
		5D-1	0.00000
		5D+2	0.00314
		5D-2	0.00000
5	S	1S	0.00114

	2S	-0.00542
	2PX	0.03715
	2PY	0.00000
	2PZ	0.07188
	3S	0.01135
	3PX	-0.09817
	3PY	0.00000
	3PZ	-0.19010
	4S	0.01378
	4PX	-0.06032
	4PY	0.00000
	4PZ	-0.13051
	5D 0	-0.00094
	5D+1	-0.00451
	5D-1	0.00000
	5D+2	-0.00141
	5D-2	0.00000
	……	

222(LUMO+6)

8	N	1S	0.00000

		2S	0.00000
		2PX	0.00000
		2PY	-0.20797
		2PZ	0.00000
		3S	0.00002
		3PX	0.00000
		3PY	-0.30470
		3PZ	0.00001
		4D 0	0.00000
		4D+1	0.00000
		4D-1	0.00486
		4D+2	0.00000
		4D-2	-0.01392
25	C	1S	0.00000
		2S	0.00000
		2PX	0.00000
		2PY	0.34681
		2PZ	-0.00001
		3S	-0.00001
		3PX	-0.00002
		3PY	0.43949
		3PZ	-0.00001
		4D 0	0.00000

4D+1	0.00000
4D-1	0.00617
4D+2	0.00000
4D-2	-0.01670

.....

3. CP 2 B3LYP/LanL2DZ+6-31G* TD-PCM (150 states) in DMF (dielectric constant = 36.71)

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	4.5921 eV	270.00 nm	f=0.0528
169 ->170		0.67431			

Excited State	2:	Singlet-A	4.7046 eV	263.54 nm	f=0.0328
168 ->170		0.68221			

Excited State	3:	Singlet-A	4.9122 eV	252.40 nm	f=0.0844
165 ->170		-0.31063			
166 ->170		0.54909			
169 ->171		-0.16995			

Excited State	4:	Singlet-A	4.9928 eV	248.33 nm	f=0.0219

162 ->170	0.12335
163 ->170	0.15392
164 ->170	-0.20849
165 ->170	0.26352
166 ->170	0.18787
167 ->170	0.48517
169 ->171	-0.17544

Excited State 5: Singlet-A 5.0647 eV 244.80 nm f=0.0087

161 ->170	0.18589
162 ->170	0.13553
163 ->170	-0.14697
164 ->170	0.10050
165 ->170	-0.25342
167 ->170	0.34857
169 ->171	0.41303
169 ->172	-0.12496

Excited State 6: Singlet-A 5.0892 eV 243.62 nm f=0.0356

162 ->170	0.39355
164 ->170	-0.12571
165 ->170	0.30058
166 ->170	0.16436

167 ->170 -0.28424

169 ->171 0.24656

169 ->172 -0.13366

Excited State 7: Singlet-A 5.1578 eV 240.38 nm f=0.0063

158 ->170 -0.10008

162 ->170 0.37872

163 ->170 0.27301

164 ->170 0.10388

165 ->170 -0.19022

166 ->170 -0.28942

169 ->171 -0.20347

169 ->172 -0.18363

Excited State 8: Singlet-A 5.1604 eV 240.26 nm f=0.0039

161 ->170 0.12304

162 ->170 0.24597

166 ->170 -0.10066

169 ->172 0.59744

Excited State 9: Singlet-A 5.2036 eV 238.27 nm f=0.0232

156 ->170 -0.11165

161 ->170 -0.15806

163 ->170 0.26860

164 ->170 0.31327

165 ->170 0.12549

168 ->171 -0.25289

168 ->172 0.22214

169 ->171 0.25636

169 ->172 0.17355

Excited State 10: Singlet-A 5.2074 eV 238.09 nm f=0.0107

161 ->170 0.13658

163 ->170 -0.11417

164 ->170 0.51671

165 ->170 0.25607

168 ->171 0.20163

168 ->172 -0.13798

169 ->171 -0.17566

Excited State 11: Singlet-A 5.2383 eV 236.69 nm f=0.0114

161 ->170 -0.11627

163 ->170 0.28329

168 ->171 0.54702

168 ->172 -0.11314

169 ->171 0.19326

169 ->172 0.10707

Excited State 12: Singlet-A 5.3373 eV 232.30 nm f=0.0011

161 ->170 0.31277

162 ->170 -0.14166

163 ->170 0.38226

168 ->171 -0.20621

168 ->172 -0.33034

Excited State 13: Singlet-A 5.3582 eV 231.39 nm f=0.0148

156 ->170 0.12561

157 ->170 0.10789

161 ->170 0.33799

163 ->170 0.10746

168 ->171 0.13275

168 ->172 0.49997

Excited State 14: Singlet-A 5.4050 eV 229.39 nm f=0.0017

166 ->171 -0.15096

167 ->170 -0.12919

167 ->171 0.32605

167 ->172 0.54808

Excited State 15: Singlet-A 5.4212 eV 228.70 nm f=0.0052

161 ->170	0.13501
165 ->171	-0.25715
165 ->172	0.11996
166 ->171	0.49612
166 ->172	-0.21682
167 ->172	0.20803
169 ->173	0.10524

Excited State 16: Singlet-A 5.4472 eV 227.61 nm f=0.0095

156 ->170	0.33104
157 ->170	0.25274
158 ->170	0.22537
159 ->170	-0.26144
161 ->170	-0.27860
165 ->172	-0.12701
167 ->172	0.12845

Excited State 17: Singlet-A 5.4650 eV 226.87 nm f=0.0082

161 ->170	-0.11914
164 ->171	-0.19171
165 ->171	0.20298
166 ->171	0.30203

166 ->172 0.29139

167 ->171 0.32873

167 ->172 -0.10846

169 ->173 0.12676

Excited State 18: Singlet-A 5.4769 eV 226.38 nm f=0.0173

164 ->171 0.11027

165 ->172 0.25315

166 ->172 0.44391

167 ->171 -0.28489

167 ->172 0.21333

169 ->173 -0.12264

169 ->174 0.18668

Excited State 19: Singlet-A 5.5097 eV 225.03 nm f=0.0059

164 ->171 -0.12284

164 ->172 -0.16688

165 ->172 -0.19892

167 ->171 -0.27680

167 ->172 0.12891

169 ->173 0.49828

Excited State 20: Singlet-A 5.5288 eV 224.25 nm f=0.0020

164 ->171 0.18888

164 ->172 0.27058

165 ->171 0.16166

165 ->172 0.37919

166 ->171 -0.10244

166 ->172 -0.10221

169 ->173 0.33546

Excited State 21: Singlet-A 5.5410 eV 223.76 nm f=0.0015

156 ->170 -0.29208

158 ->170 0.51137

160 ->170 0.11163

162 ->170 0.11562

164 ->171 0.11499

165 ->171 -0.19026

166 ->171 -0.10097

Excited State 22: Singlet-A 5.5480 eV 223.47 nm f=0.0041

157 ->170 -0.31813

158 ->170 0.19631

160 ->170 0.12329

164 ->172 0.32452

165 ->171 0.28105

165 ->172	-0.13747
166 ->171	0.12092
167 ->171	-0.15947
169 ->174	-0.13021

Excited State 23: Singlet-A 5.5528 eV 223.28 nm f=0.0106

156 ->170	-0.18190
157 ->170	0.12259
158 ->170	0.14416
164 ->171	-0.27573
164 ->172	-0.24141
165 ->171	0.29729
165 ->172	0.20231
166 ->172	-0.24869
167 ->171	-0.11138
169 ->174	0.11670

Excited State 24: Singlet-A 5.5697 eV 222.60 nm f=0.0006

156 ->170	-0.36393
157 ->170	0.42682
160 ->170	-0.18610
164 ->172	0.21029
165 ->172	-0.17523

167 ->171 -0.12422

Excited State 25: Singlet-A 5.5907 eV 221.77 nm f=0.0390

163 ->171 0.22476

163 ->172 0.24685

165 ->172 -0.20177

169 ->174 0.49713

Excited State 26: Singlet-A 5.6218 eV 220.54 nm f=0.0010

157 ->170 0.18844

158 ->170 -0.14430

160 ->170 0.61396

160 ->171 0.16992

Excited State 27: Singlet-A 5.6446 eV 219.65 nm f=0.0024

159 ->170 -0.23629

163 ->171 0.13187

164 ->171 0.37497

164 ->172 -0.34030

165 ->171 0.20814

168 ->173 -0.10660

169 ->174 -0.15639

Excited State 28: Singlet-A 5.6534 eV 219.31 nm f=0.0022

156 ->170 0.16705

157 ->170 0.12269

158 ->170 0.17629

159 ->170 0.45926

159 ->171 0.11760

162 ->171 -0.12029

163 ->171 0.25406

164 ->172 -0.12783

168 ->173 -0.13523

169 ->174 -0.12285

Excited State 29: Singlet-A 5.6565 eV 219.19 nm f=0.0060

159 ->170 0.28608

161 ->172 -0.12907

162 ->171 0.35004

163 ->171 -0.26155

164 ->171 0.19140

165 ->171 0.13306

169 ->173 0.10303

Excited State 30: Singlet-A 5.6639 eV 218.90 nm f=0.0066

161 ->171 0.14664

162 ->171 0.43774

162 ->172 -0.11171

163 ->171 0.12751

163 ->172 0.18042

164 ->171 -0.19253

165 ->171 -0.11433

165 ->172 0.14463

168 ->173 -0.13816

169 ->174 -0.14585

169 ->175 0.15158

Excited State 31: Singlet-A 5.6828 eV 218.17 nm f=0.0096

161 ->171 0.28280

162 ->171 -0.19114

162 ->172 -0.11194

163 ->171 -0.27186

163 ->172 0.38372

165 ->171 0.15865

166 ->171 0.11640

167 ->173 -0.14659

Excited State 32: Singlet-A 5.6949 eV 217.71 nm f=0.0123

161 ->171 0.11706

161 ->172 0.22431

163 ->171 0.16737

167 ->173 -0.13315

168 ->173 0.50821

168 ->175 0.15001

169 ->175 -0.11754

Excited State 33: Singlet-A 5.7164 eV 216.89 nm f=0.0038

155 ->170 -0.11610

161 ->171 0.10698

161 ->172 0.15340

163 ->171 0.12239

163 ->172 -0.17414

167 ->173 -0.13078

168 ->173 -0.12025

168 ->174 0.47522

168 ->175 -0.16208

169 ->175 -0.24223

Excited State 34: Singlet-A 5.7636 eV 215.12 nm f=0.0160

155 ->170 0.25741

162 ->172 0.31512

163 ->172 0.17369

166 ->173 0.14126

167 ->173 0.14652

168 ->173 0.13351

168 ->174 0.30873

169 ->175 0.21589

Excited State 35: Singlet-A 5.7719 eV 214.81 nm f=0.0091

155 ->170 -0.13021

162 ->172 0.45277

162 ->174 0.13694

168 ->173 -0.25364

168 ->174 -0.20594

169 ->175 -0.17824

169 ->176 0.11689

Excited State 36: Singlet-A 5.8004 eV 213.75 nm f=0.0058

161 ->171 -0.24590

161 ->172 0.14043

162 ->171 0.11276

162 ->172 -0.11395

163 ->172 0.28189

166 ->173 -0.19180

167 ->173 0.32766

169 ->174 -0.11913

169 ->175 -0.29285

Excited State 37: Singlet-A 5.8074 eV 213.49 nm f=0.0025

155 ->170 0.42376

161 ->172 0.28031

162 ->171 0.11403

163 ->171 -0.14526

164 ->173 0.15675

167 ->173 -0.13746

168 ->173 -0.12267

169 ->175 -0.12231

Excited State 38: Singlet-A 5.8198 eV 213.04 nm f=0.0019

155 ->170 0.22849

156 ->171 0.18552

159 ->171 -0.14415

161 ->171 0.35087

161 ->172 -0.15908

163 ->171 0.13560

167 ->173 0.25203

168 ->175 0.14441

169 ->175 -0.22362

Excited State	39:	Singlet-A	5.8441 eV	212.15 nm	f=0.0070

155 ->170	-0.14391
159 ->171	0.22436
159 ->172	0.12078
161 ->171	0.16715
161 ->172	0.28213
163 ->172	-0.10471
167 ->173	0.36402
169 ->174	0.11487
169 ->175	0.19231

Excited State	40:	Singlet-A	5.8486 eV	211.99 nm	f=0.0117

156 ->171	0.15025
157 ->171	0.10932
158 ->171	0.13824
161 ->171	-0.10369
161 ->172	0.16212
162 ->172	-0.12478
163 ->171	-0.12727
164 ->173	-0.16246
166 ->173	0.36499
166 ->174	-0.18316

168 ->175 0.18307

169 ->175 -0.14855

169 ->176 -0.17055

Excited State 41: Singlet-A 5.8616 eV 211.52 nm f=0.0015

158 ->171 0.13330

158 ->172 0.10576

159 ->171 0.45714

159 ->172 0.32726

161 ->172 -0.21095

Excited State 42: Singlet-A 5.8758 eV 211.01 nm f=0.0055

156 ->171 0.15138

156 ->172 0.16606

157 ->171 0.16012

157 ->172 0.10913

158 ->171 0.15623

161 ->172 0.12621

163 ->172 -0.11699

164 ->173 -0.13268

164 ->174 -0.10946

165 ->174 0.16740

166 ->173 -0.11839

167 ->174 0.35853

168 ->174 -0.10903

168 ->175 -0.10187

168 ->176 0.11513

Excited State 43: Singlet-A 5.8791 eV 210.89 nm f=0.0056

156 ->171 -0.13031

157 ->171 -0.11379

158 ->171 -0.10996

161 ->171 0.10278

164 ->173 0.18096

164 ->174 -0.10929

165 ->173 -0.16318

165 ->174 0.13859

166 ->173 0.28609

166 ->174 -0.23991

167 ->173 0.16766

168 ->175 -0.19404

169 ->175 -0.12278

169 ->177 -0.10543

Excited State 44: Singlet-A 5.8871 eV 210.60 nm f=0.0024

157 ->171 0.13926

159 ->172 0.11074

160 ->170 -0.14028

160 ->171 0.53690

160 ->172 0.28340

160 ->176 0.11498

Excited State 45: Singlet-A 5.8953 eV 210.31 nm f=0.0030

155 ->170 0.14619

161 ->171 -0.16217

163 ->174 0.16602

164 ->173 -0.12481

164 ->174 0.15258

166 ->173 0.12152

167 ->174 0.11858

169 ->176 0.42108

169 ->177 -0.10751

Excited State 46: Singlet-A 5.9135 eV 209.66 nm f=0.0093

155 ->170 0.11333

156 ->172 0.13328

160 ->171 0.10542

164 ->173 -0.11256

165 ->173 0.50207

166 ->173 0.14066

166 ->175 -0.10589

168 ->175 -0.17890

169 ->175 -0.10016

Excited State 47: Singlet-A 5.9242 eV 209.29 nm f=0.0020

156 ->172 -0.13325

157 ->171 0.16384

157 ->172 -0.12134

160 ->171 -0.15163

164 ->173 0.22818

164 ->174 -0.20417

166 ->173 0.25724

166 ->174 0.32325

Excited State 48: Singlet-A 5.9277 eV 209.16 nm f=0.0070

156 ->171 -0.14187

156 ->172 0.12743

158 ->171 0.50389

158 ->172 -0.12136

167 ->174 -0.22700

169 ->176 0.18075

Excited State 49: Singlet-A 5.9331 eV 208.97 nm f=0.0102

156 ->171	-0.14361
158 ->171	0.19532
164 ->173	0.27011
164 ->175	-0.10043
165 ->173	0.22862
166 ->174	-0.11704
167 ->174	0.31419
168 ->175	0.19742
168 ->176	-0.11074
169 ->176	-0.12397

Excited State 50: Singlet-A 5.9361 eV 208.86 nm f=0.0245

156 ->172	0.14743
157 ->172	0.11814
158 ->171	-0.14174
158 ->172	0.13423
159 ->172	-0.12425
162 ->172	-0.10209
163 ->174	-0.16309
164 ->174	-0.18415
165 ->174	0.18021
168 ->174	0.12609

168 ->175 0.39306

169 ->176 0.10717

Excited State 51: Singlet-A 5.9486 eV 208.43 nm f=0.0087

157 ->171 -0.27807

157 ->172 0.11569

158 ->171 0.10096

160 ->171 0.14921

161 ->171 0.10108

164 ->173 -0.11682

165 ->173 -0.24092

165 ->174 -0.11913

166 ->173 0.10244

166 ->174 0.32363

167 ->174 0.15172

169 ->176 -0.20228

Excited State 52: Singlet-A 5.9756 eV 207.48 nm f=0.0045

156 ->171 -0.37762

156 ->172 0.20024

157 ->171 0.46145

159 ->172 -0.10263

165 ->173 -0.11320

166 ->174 0.10743

Excited State 53: Singlet-A 5.9980 eV 206.71 nm f=0.0202

156 ->171 0.25117

156 ->172 0.12755

157 ->172 0.12413

158 ->172 0.21235

159 ->172 -0.11324

160 ->171 0.11381

160 ->172 -0.18852

164 ->173 0.27076

164 ->174 0.18830

164 ->175 -0.15733

165 ->174 -0.12710

Excited State 54: Singlet-A 6.0120 eV 206.23 nm f=0.0003

156 ->171 0.12480

157 ->172 0.11032

159 ->172 -0.20531

160 ->171 -0.21329

160 ->172 0.52967

164 ->173 0.11532

Excited State 55: Singlet-A 6.0302 eV 205.60 nm f=0.0109

160 ->172	-0.13763
161 ->173	0.10173
163 ->174	0.25188
163 ->175	-0.18014
164 ->174	-0.10824
164 ->175	0.11043
165 ->174	0.17529
166 ->175	-0.11407
167 ->174	-0.18302
167 ->175	-0.14838
169 ->177	0.22157

Excited State 56: Singlet-A 6.0341 eV 205.47 nm f=0.0029

156 ->172	0.10641
157 ->171	-0.13610
157 ->172	0.16526
158 ->172	0.17391
159 ->171	-0.30014
159 ->172	0.41475
160 ->171	-0.10850
160 ->172	0.13090
163 ->173	-0.12614

165 ->174 0.12096

Excited State 57: Singlet-A 6.0413 eV 205.23 nm f=0.0048

158 ->172 0.31270

159 ->171 -0.10618

162 ->172 0.13339

162 ->173 -0.12025

163 ->173 0.22463

163 ->174 -0.11847

164 ->174 -0.10415

165 ->174 -0.22062

165 ->175 0.14582

166 ->174 -0.22104

166 ->175 -0.17299

Excited State 58: Singlet-A 6.0577 eV 204.67 nm f=0.0042

156 ->172 0.32144

158 ->171 -0.11059

158 ->172 -0.30181

159 ->172 0.13952

163 ->173 0.32523

Excited State 59: Singlet-A 6.0619 eV 204.53 nm f=0.0033

158 ->172 -0.13559

163 ->173 -0.15408

165 ->174 -0.10844

168 ->175 0.16948

168 ->176 0.55684

Excited State 60: Singlet-A 6.0634 eV 204.48 nm f=0.0090

157 ->172 -0.21101

162 ->173 -0.10110

163 ->173 0.24539

164 ->174 0.18659

164 ->175 -0.11647

165 ->174 0.31354

166 ->175 -0.19424

167 ->175 0.17088

168 ->176 0.12879

Excited State 61: Singlet-A 6.0758 eV 204.06 nm f=0.0015

157 ->172 -0.22189

158 ->171 0.11185

158 ->172 0.29985

160 ->172 0.11048

162 ->174 -0.12290

163 ->173 0.14934

163 ->174 0.18409

166 ->175 0.27939

166 ->176 -0.11560

Excited State 62: Singlet-A 6.0831 eV 203.82 nm f=0.0083

156 ->171 -0.11370

156 ->172 -0.31600

157 ->172 0.46017

160 ->172 -0.10277

163 ->173 0.18725

164 ->174 0.11862

168 ->176 0.11112

Excited State 63: Singlet-A 6.0984 eV 203.31 nm f=0.0100

154 ->170 -0.10416

161 ->173 0.25217

163 ->174 -0.24947

164 ->173 0.11636

164 ->174 0.26692

164 ->175 0.13094

165 ->175 -0.19807

167 ->175 -0.11862

167 ->176 -0.11376

169 ->177 0.16398

Excited State 64: Singlet-A 6.1200 eV 202.59 nm f=0.0065

155 ->172 -0.13630

165 ->175 -0.13545

165 ->176 0.13619

165 ->177 -0.12030

165 ->178 -0.14656

166 ->176 0.10624

166 ->177 -0.10266

166 ->178 -0.10183

167 ->174 0.15160

167 ->175 0.13071

167 ->176 0.17688

167 ->180 -0.10233

167 ->181 -0.12924

169 ->178 0.18690

169 ->179 -0.13007

169 ->181 0.12464

Excited State 65: Singlet-A 6.1291 eV 202.29 nm f=0.0082

161 ->173 0.10847

162 ->174 -0.15676

162 ->175 0.12441

164 ->173 -0.10348

164 ->174 -0.10962

164 ->175 -0.10980

167 ->175 0.29825

169 ->176 0.11955

169 ->177 0.37205

Excited State 66: Singlet-A 6.1419 eV 201.87 nm f=0.0107

155 ->171 -0.12988

163 ->173 0.19841

165 ->174 -0.11266

165 ->175 -0.15604

166 ->175 0.12909

167 ->176 0.21934

169 ->176 0.13954

169 ->177 0.10535

169 ->178 -0.20134

169 ->179 0.29554

Excited State 67: Singlet-A 6.1614 eV 201.23 nm f=0.0258

154 ->170 -0.19346

161 ->173 -0.13536

161 ->174 0.16440

162 ->173 0.26973

164 ->173 -0.11986

164 ->175 -0.10482

166 ->176 0.19485

167 ->175 -0.21787

169 ->178 0.20385

169 ->179 0.11399

Excited State 68: Singlet-A 6.1649 eV 201.11 nm f=0.0154

162 ->173 0.33198

162 ->175 0.14911

166 ->175 -0.18479

166 ->177 -0.13066

167 ->175 0.11383

168 ->177 0.24575

168 ->178 -0.10956

169 ->177 -0.17895

169 ->179 0.16833

Excited State 69: Singlet-A 6.1751 eV 200.78 nm f=0.0022

154 ->170 -0.16079

161 ->173 0.24477

162 ->173 -0.13744

162 ->174 0.20642

162 ->175 -0.18020

162 ->176 0.11889

163 ->174 0.10091

163 ->175 -0.12519

165 ->174 -0.12392

165 ->175 -0.11466

166 ->175 0.15273

169 ->179 0.14737

Excited State 70: Singlet-A 6.1829 eV 200.53 nm f=0.0115

154 ->170 0.29675

161 ->174 0.25111

162 ->174 0.10385

165 ->175 -0.13629

167 ->175 0.20765

167 ->176 -0.13597

168 ->178 0.10038

169 ->177 -0.15115

169 ->178 0.10823

Excited State 71: Singlet-A 6.1868 eV 200.40 nm f=0.0310

154 ->170	-0.22472
161 ->173	0.30116
162 ->173	0.22922
162 ->174	0.14058
165 ->175	0.15719
165 ->178	0.10644
167 ->176	0.16371
168 ->177	-0.16081
168 ->178	0.10536
168 ->179	-0.12071
168 ->183	-0.10067

Excited State 72: Singlet-A 6.2013 eV 199.93 nm f=0.0120

154 ->170	0.33348
161 ->173	0.27003
161 ->174	-0.22920
162 ->173	0.11512
164 ->175	-0.11055
166 ->176	0.16623
167 ->175	-0.15784
168 ->177	-0.10409

Excited State 73: Singlet-A 6.2094 eV 199.67 nm f=0.0049

153 ->170	0.11409
154 ->170	0.17443
162 ->172	-0.11905
162 ->174	0.38020
165 ->175	0.18034
168 ->177	0.22504
169 ->177	0.20613
169 ->179	-0.10095

Excited State 74: Singlet-A 6.2139 eV 199.53 nm f=0.0019

162 ->174	-0.19748
164 ->175	0.18175
164 ->178	0.10104
165 ->175	0.15640
165 ->176	-0.17671
166 ->175	0.25731
166 ->176	0.19056
167 ->175	0.12236
167 ->178	-0.11674
169 ->178	0.11706
169 ->179	0.16976

Excited State 75: Singlet-A 6.2209 eV 199.30 nm f=0.0092

156 ->172	-0.11537
161 ->173	0.18999
161 ->174	0.21096
162 ->173	-0.19913
163 ->173	-0.11410
163 ->174	-0.16618
164 ->174	0.11501
164 ->175	-0.15763
164 ->178	-0.10481
165 ->174	0.10046
165 ->175	0.19473
167 ->175	-0.10685
167 ->176	0.14781
168 ->177	0.13739
169 ->177	-0.10086

Excited State 76: Singlet-A 6.2480 eV 198.44 nm f=0.0123

156 ->173	0.13362
159 ->173	-0.14967
161 ->174	0.13922
162 ->173	0.10979
162 ->175	-0.15407

162 ->176	0.10422
163 ->175	-0.16398
164 ->174	0.17378
164 ->175	0.11418
166 ->176	-0.12411
167 ->176	0.18360
168 ->177	-0.13741
168 ->179	0.16071
169 ->177	0.10989
169 ->178	0.11908
169 ->179	-0.13395

Excited State 77: Singlet-A 6.2734 eV 197.63 nm f=0.0086

155 ->171	0.26207
155 ->172	-0.12061
161 ->174	0.10752
162 ->174	-0.23362
162 ->175	-0.10321
162 ->177	-0.10149
163 ->174	-0.11824
164 ->176	-0.16986
166 ->176	0.14165
167 ->177	0.11129

168 ->177 0.22921

169 ->178 -0.14402

Excited State 78: Singlet-A 6.2864 eV 197.23 nm f=0.0067

155 ->171 0.20091

155 ->172 0.13086

162 ->174 0.12594

162 ->175 0.12007

162 ->176 -0.10127

163 ->174 -0.12913

166 ->176 0.26096

168 ->177 -0.15860

168 ->179 0.24275

169 ->178 -0.24619

Excited State 79: Singlet-A 6.2922 eV 197.04 nm f=0.0073

155 ->171 0.20098

155 ->172 -0.19215

156 ->173 -0.13080

157 ->173 -0.10566

159 ->173 0.19972

160 ->173 -0.12908

162 ->175 0.14564

165 ->175 -0.13449

165 ->176 -0.16531

166 ->175 -0.16288

167 ->176 0.17328

167 ->177 0.10163

169 ->179 0.12022

Excited State 80: Singlet-A 6.2996 eV 196.81 nm f=0.0005

160 ->173 0.61641

160 ->174 -0.10955

166 ->176 -0.11379

Excited State 81: Singlet-A 6.3057 eV 196.62 nm f=0.0117

156 ->173 -0.15477

158 ->173 0.10485

159 ->173 0.38416

160 ->173 -0.10628

162 ->173 0.13370

164 ->175 0.11463

164 ->176 0.11527

167 ->176 -0.15366

169 ->178 -0.17300

Excited State 82: Singlet-A 6.3084 eV 196.54 nm f=0.0128

155 ->171	-0.15909
156 ->174	0.13919
159 ->173	0.28468
159 ->174	-0.13574
163 ->175	0.10845
164 ->174	-0.10881
164 ->175	-0.13090
164 ->176	-0.12047
168 ->177	-0.15874
168 ->179	0.23727
169 ->178	0.21647

Excited State 83: Singlet-A 6.3132 eV 196.39 nm f=0.0033

155 ->171	0.20674
155 ->172	-0.12704
159 ->173	-0.16212
160 ->173	-0.12589
164 ->176	-0.10500
165 ->175	0.18279
165 ->176	0.31076
166 ->176	-0.19570
168 ->177	-0.16466

169 ->179 0.17133

Excited State 84: Singlet-A 6.3224 eV 196.10 nm f=0.0117

153 ->170 -0.12591

155 ->171 0.15154

156 ->173 0.34629

157 ->173 0.27810

158 ->173 0.21630

159 ->173 0.28151

162 ->173 -0.10822

165 ->176 0.11062

168 ->179 -0.10420

Excited State 85: Singlet-A 6.3393 eV 195.58 nm f=0.0041

153 ->170 0.10946

155 ->171 -0.19131

155 ->172 0.11147

158 ->173 -0.17647

162 ->175 0.11826

163 ->175 -0.12568

164 ->176 -0.15875

165 ->176 0.17607

166 ->176 0.26625

167 ->178	0.11498
168 ->179	-0.16505
169 ->178	0.12418
169 ->179	-0.16773

Excited State 86: Singlet-A 6.3563 eV 195.06 nm f=0.0082

155 ->172	0.19551
156 ->174	-0.11466
158 ->173	0.12932
161 ->174	-0.14536
164 ->175	-0.11021
165 ->175	0.11970
165 ->177	-0.11778
165 ->180	0.13784
166 ->175	0.12843
166 ->176	-0.10959
167 ->175	-0.17359
167 ->176	0.12162
167 ->177	0.21083
167 ->178	0.13298
167 ->180	-0.15639
168 ->178	0.10098

Excited State 87: Singlet-A 6.3613 eV 194.90 nm f=0.0016

156 ->173 -0.17079

157 ->173 -0.19594

158 ->173 0.53987

158 ->174 -0.11214

159 ->173 -0.14593

160 ->173 0.11344

168 ->179 -0.10013

Excited State 88: Singlet-A 6.3638 eV 194.83 nm f=0.0010

155 ->171 0.24123

155 ->172 0.48695

163 ->174 0.12264

Excited State 89: Singlet-A 6.3729 eV 194.55 nm f=0.0073

161 ->174 0.11479

161 ->175 -0.10570

162 ->175 -0.11692

163 ->174 0.22352

163 ->175 0.32415

164 ->175 0.20979

165 ->175 0.16591

165 ->176 0.10503

167 ->177 0.10160

Excited State 90: Singlet-A 6.3858 eV 194.16 nm f=0.0098

153 ->170 0.54852

154 ->170 -0.15460

156 ->173 0.18535

Excited State 91: Singlet-A 6.3993 eV 193.75 nm f=0.0071

156 ->174 0.19332

157 ->173 0.23584

157 ->174 0.14632

158 ->174 0.12056

159 ->174 -0.15927

161 ->174 -0.23379

165 ->177 0.10835

167 ->176 -0.21100

167 ->177 0.11407

167 ->180 -0.20649

167 ->181 -0.13177

167 ->184 0.10844

Excited State 92: Singlet-A 6.4033 eV 193.63 nm f=0.0312

156 ->173 -0.26467

157 ->173 0.27917

161 ->175 -0.18560

166 ->177 -0.10519

167 ->176 0.18639

167 ->180 0.15637

167 ->181 0.11110

169 ->181 -0.15139

Excited State 93: Singlet-A 6.4095 eV 193.44 nm f=0.0104

155 ->171 -0.10082

156 ->173 -0.23770

157 ->173 0.38242

157 ->175 0.10640

161 ->174 0.19926

163 ->176 0.11118

166 ->177 0.12687

169 ->181 0.14881

Excited State 94: Singlet-A 6.4194 eV 193.14 nm f=0.0105

156 ->174 0.16731

157 ->174 0.12278

158 ->174 0.10481

159 ->174 -0.14495

161 ->175 0.15873

162 ->175 0.15563

164 ->175 0.18353

164 ->176 0.24587

166 ->177 -0.20753

167 ->176 0.12917

167 ->180 0.11843

167 ->181 0.11952

169 ->178 -0.13833

Excited State 95: Singlet-A 6.4381 eV 192.58 nm f=0.0040

156 ->173 0.17977

157 ->174 0.10118

161 ->174 -0.14583

161 ->175 -0.21274

164 ->176 0.23725

166 ->177 0.28228

167 ->176 0.11741

168 ->179 0.13069

169 ->180 -0.11678

Excited State 96: Singlet-A 6.4522 eV 192.16 nm f=0.0238

158 ->174 -0.11783

161 ->175 0.27531

162 ->175 -0.18740

163 ->175 -0.17501

164 ->176 0.18210

165 ->176 0.13483

166 ->177 0.14414

167 ->177 0.21134

168 ->177 0.11577

Excited State 97: Singlet-A 6.4580 eV 191.98 nm f=0.0145

162 ->175 0.10267

163 ->175 0.15988

164 ->175 -0.15623

164 ->176 0.26618

164 ->178 0.14194

165 ->176 0.29371

165 ->177 0.21349

166 ->178 0.11519

167 ->177 0.12372

168 ->177 -0.10837

Excited State 98: Singlet-A 6.4650 eV 191.78 nm f=0.0038

156 ->174 -0.15815

157 ->174 -0.13084

158 ->174 0.53288

159 ->174 -0.11366

160 ->174 0.13749

169 ->180 0.17404

169 ->181 -0.10616

Excited State 99: Singlet-A 6.4739 eV 191.51 nm f=0.0444

157 ->174 0.17471

158 ->174 -0.17092

163 ->176 0.10850

164 ->175 -0.12964

168 ->177 0.11887

168 ->178 0.21861

168 ->179 0.10787

169 ->180 0.41879

Excited State 100: Singlet-A 6.4854 eV 191.17 nm f=0.0017

156 ->174 -0.11122

157 ->174 -0.18174

159 ->174 0.11275

163 ->176 -0.14083

165 ->177 0.20896

165 ->178 0.16557

166 ->179 0.11631

168 ->177 0.13170

168 ->178 0.30800

168 ->179 0.17778

169 ->180 -0.10119

169 ->181 0.21925

Excited State 101: Singlet-A 6.4936 eV 190.93 nm f=0.0106

156 ->174 0.24570

157 ->174 -0.23501

160 ->174 0.25276

163 ->176 0.30080

166 ->179 -0.10772

167 ->177 -0.11096

168 ->178 0.17771

169 ->180 -0.10306

169 ->181 -0.11182

Excited State 102: Singlet-A 6.4964 eV 190.85 nm f=0.0192

156 ->174 -0.27861

157 ->174 0.29599

158 ->174 0.10663

160 ->174 -0.17329

161 ->175 0.13004

162 ->175 0.10428

162 ->176 0.12037

166 ->179 -0.10649

168 ->178 0.17888

169 ->180 -0.18904

169 ->181 -0.10125

169 ->183 -0.11980

Excited State 103: Singlet-A 6.5068 eV 190.55 nm f=0.0098

160 ->174 -0.12268

161 ->175 -0.12645

161 ->176 -0.10996

162 ->175 -0.12384

163 ->176 0.33805

164 ->176 0.10765

165 ->178 0.10821

166 ->177 -0.13127

166 ->178 -0.11894

167 ->177 -0.14031

167 ->179 -0.10466

168 ->178 -0.11208

168 ->185	-0.11352
169 ->180	-0.10370
169 ->181	0.15266
169 ->185	0.14697

Excited State 104: Singlet-A 6.5115 eV 190.41 nm f=0.0005

156 ->174	-0.18311
157 ->174	0.24555
158 ->174	-0.14065
160 ->174	0.50174
168 ->178	-0.10211

Excited State 105: Singlet-A 6.5157 eV 190.29 nm f=0.0092

157 ->174	-0.18417
160 ->174	-0.10543
162 ->175	0.21177
162 ->176	0.22274
163 ->176	-0.15694
165 ->179	-0.12267
166 ->179	0.13094
168 ->178	-0.20493
168 ->179	0.11534
168 ->185	-0.10299

169 ->185 0.11018

169 ->186 0.10471

Excited State 106: Singlet-A 6.5240 eV 190.04 nm f=0.0041

156 ->174 0.22829

157 ->174 0.16107

158 ->174 0.16184

159 ->172 0.11026

159 ->174 0.54003

160 ->174 0.11970

169 ->181 -0.10904

Excited State 107: Singlet-A 6.5266 eV 189.97 nm f=0.0178

160 ->174 0.14924

162 ->175 -0.12439

162 ->176 0.14578

162 ->179 -0.10572

163 ->176 -0.13293

164 ->176 0.20079

165 ->177 -0.11697

166 ->177 0.11277

166 ->179 -0.17950

167 ->177 -0.10117

167 ->178	0.14150
167 ->179	-0.14023
169 ->181	0.24475
169 ->182	0.11817
169 ->183	-0.13859

Excited State 108: Singlet-A 6.5422 eV 189.51 nm f=0.0018

156 ->175	-0.22167
157 ->175	-0.14498
158 ->175	-0.10470
159 ->175	0.14665
161 ->175	-0.11541
162 ->176	0.28535
162 ->177	-0.10301
163 ->176	0.12831
163 ->178	0.10263
164 ->176	0.10739
165 ->179	0.11469
167 ->179	0.15369

Excited State 109: Singlet-A 6.5516 eV 189.24 nm f=0.0054

156 ->174	0.13683
156 ->175	0.12607

161 ->175 -0.12068

162 ->176 0.11033

164 ->176 -0.10633

165 ->178 -0.14704

166 ->177 0.15737

166 ->178 0.13924

167 ->177 0.17336

167 ->178 -0.20502

169 ->179 0.10612

169 ->181 0.22828

169 ->185 0.14165

Excited State 110: Singlet-A 6.5756 eV 188.55 nm f=0.0244

156 ->175 0.12898

162 ->176 0.33823

162 ->178 0.10141

162 ->179 -0.11004

164 ->178 -0.13407

165 ->178 0.12164

166 ->178 -0.19020

166 ->179 -0.11375

168 ->179 -0.11411

168 ->180 0.10028

168 ->185 0.12907

169 ->182 -0.12645

Excited State 111: Singlet-A 6.5852 eV 188.28 nm f=0.0024

155 ->173 0.10567

163 ->176 0.13740

164 ->177 -0.15715

165 ->179 -0.12812

166 ->181 -0.10074

167 ->177 0.18890

168 ->179 0.11980

168 ->181 -0.15621

168 ->187 0.10977

169 ->180 0.11830

169 ->182 0.11092

169 ->183 -0.15212

169 ->185 -0.16963

169 ->186 0.15430

Excited State 112: Singlet-A 6.5974 eV 187.93 nm f=0.0154

155 ->173 -0.12088

161 ->176 0.22471

163 ->175 -0.13401

163 ->179	-0.10644
164 ->177	0.20465
165 ->177	-0.11635
165 ->178	0.10383
166 ->177	-0.16507
167 ->178	-0.17483
167 ->179	0.13112
168 ->178	-0.14693
168 ->179	0.11294
168 ->183	-0.12632
169 ->181	0.12632
169 ->182	-0.14670

Excited State 113: Singlet-A 6.6020 eV 187.80 nm f=0.0393

155 ->173	0.10603
161 ->176	0.39098
161 ->177	-0.13457
163 ->178	-0.10013
165 ->177	0.12497
167 ->177	-0.10590
168 ->178	0.10698
168 ->183	0.15660
169 ->180	-0.11465

169 ->182 0.10877

169 ->186 0.10289

Excited State 114: Singlet-A 6.6115 eV 187.53 nm f=0.0069

161 ->176 -0.13124

162 ->175 -0.12147

163 ->175 0.10009

163 ->176 -0.15740

164 ->177 0.11602

164 ->178 -0.12513

165 ->177 -0.11728

165 ->178 0.19322

166 ->177 -0.15974

167 ->177 0.10281

167 ->178 -0.10784

167 ->179 0.14315

168 ->185 -0.17412

169 ->182 0.25574

Excited State 115: Singlet-A 6.6333 eV 186.91 nm f=0.0110

161 ->176 0.27388

162 ->176 -0.13661

162 ->179 0.12453

163 ->176 0.12974

166 ->177 0.18041

166 ->178 -0.13983

166 ->186 -0.11992

167 ->177 0.14382

169 ->182 0.19253

169 ->183 -0.17527

169 ->186 -0.16257

Excited State 116: Singlet-A 6.6371 eV 186.80 nm f=0.0251

155 ->173 -0.17568

157 ->175 -0.12450

158 ->175 -0.10054

159 ->175 0.11328

161 ->175 0.12698

162 ->179 -0.11152

165 ->179 -0.14491

166 ->179 0.13948

167 ->178 -0.14446

168 ->185 0.11531

169 ->180 -0.11498

169 ->181 -0.21717

169 ->182 0.26047

169 ->187 -0.16080

Excited State 117: Singlet-A 6.6527 eV 186.37 nm f=0.0134

155 ->173 0.36988

155 ->174 -0.15494

161 ->176 -0.12362

163 ->177 0.12024

164 ->177 0.11358

165 ->177 -0.15665

165 ->179 -0.10903

166 ->178 0.13869

168 ->179 -0.10910

168 ->183 0.11961

169 ->182 -0.10586

Excited State 118: Singlet-A 6.6638 eV 186.06 nm f=0.0064

155 ->173 0.33154

158 ->175 -0.27031

159 ->175 0.18071

160 ->175 -0.12088

165 ->179 0.10779

166 ->178 -0.12830

167 ->179 -0.11701

168 ->180 -0.15563

168 ->181 0.10449

168 ->182 0.12003

Excited State 119: Singlet-A 6.6714 eV 185.84 nm f=0.0038

155 ->173 -0.10109

156 ->175 -0.15888

157 ->175 -0.26529

158 ->175 0.34454

160 ->175 0.10194

161 ->176 -0.12627

163 ->178 -0.10170

164 ->177 0.14889

165 ->179 0.10435

166 ->178 -0.18126

168 ->180 -0.12564

168 ->181 0.10717

Excited State 120: Singlet-A 6.6765 eV 185.70 nm f=0.0119

155 ->173 0.24868

158 ->175 0.26515

159 ->175 -0.17522

160 ->175 0.21860

162 ->177	0.13562
163 ->175	0.10819
168 ->183	-0.11850
169 ->182	0.17316
169 ->183	0.10687
169 ->184	-0.13275

Excited State 121: Singlet-A 6.6773 eV 185.68 nm f=0.0083

158 ->175	-0.23544
159 ->175	-0.10286
160 ->175	0.11632
160 ->176	0.13255
164 ->177	0.20771
168 ->181	0.34840
169 ->182	0.11640
169 ->186	0.13714

Excited State 122: Singlet-A 6.6870 eV 185.41 nm f=0.0019

158 ->175	-0.20496
159 ->175	-0.16459
159 ->176	-0.21906
160 ->175	0.28042
160 ->176	0.20995

165 ->177	0.10199
166 ->178	-0.16994
168 ->181	-0.19691

Excited State 123: Singlet-A 6.6941 eV 185.21 nm f=0.0042

156 ->175	-0.29375
157 ->175	0.40942
157 ->176	-0.10496
164 ->177	0.21804
166 ->178	-0.14805

Excited State 124: Singlet-A 6.7020 eV 185.00 nm f=0.0421

154 ->170	-0.11488
154 ->171	0.17603
154 ->172	0.23427
156 ->175	0.13183
157 ->175	-0.16471
160 ->175	-0.17338
160 ->176	-0.17189
164 ->177	0.26416
164 ->178	-0.11741
164 ->179	0.11008
165 ->178	-0.12432

168 ->180 0.11324

168 ->181 -0.10613

169 ->184 -0.10718

Excited State 125: Singlet-A 6.7076 eV 184.84 nm f=0.0034

154 ->172 0.11004

156 ->176 -0.26035

157 ->176 -0.14236

158 ->176 -0.17533

159 ->175 0.13805

159 ->176 0.27567

160 ->175 0.25835

160 ->176 0.17745

161 ->176 0.10686

167 ->179 -0.12106

168 ->180 0.11825

168 ->181 -0.11833

Excited State 126: Singlet-A 6.7155 eV 184.62 nm f=0.0027

153 ->171 -0.12531

154 ->172 -0.14858

155 ->173 0.12259

156 ->175 0.19007

157 ->176 0.10692

158 ->175 0.10535

159 ->175 0.24188

159 ->176 0.17317

160 ->175 0.10014

164 ->177 0.11734

165 ->177 0.10392

166 ->181 -0.10565

167 ->179 0.12926

168 ->180 -0.10921

169 ->184 0.13439

Excited State 127: Singlet-A 6.7173 eV 184.57 nm f=0.0066

153 ->172 0.10518

154 ->171 0.16289

154 ->172 0.29642

156 ->175 -0.14968

159 ->176 -0.13197

161 ->177 0.10152

163 ->177 -0.10962

167 ->179 -0.16853

168 ->181 0.15186

169 ->183 0.11033

169 ->184 0.20117

Excited State 128: Singlet-A 6.7214 eV 184.46 nm f=0.0006

154 ->171 0.14578

154 ->172 0.28476

155 ->173 -0.11626

156 ->176 0.18048

157 ->175 0.22522

157 ->176 0.16469

158 ->176 0.16408

159 ->175 0.26850

160 ->175 0.14885

160 ->176 0.14763

Excited State 129: Singlet-A 6.7276 eV 184.29 nm f=0.0033

154 ->172 -0.13166

156 ->176 0.11892

161 ->177 0.10991

163 ->177 -0.10389

166 ->179 -0.10044

167 ->177 0.10791

167 ->179 -0.27314

168 ->180 0.38840

168 ->182 0.13472

Excited State 130: Singlet-A 6.7344 eV 184.11 nm f=0.0107

153 ->171 -0.10431

153 ->172 0.10748

156 ->175 -0.12745

163 ->177 -0.13017

165 ->181 0.12366

166 ->178 -0.11183

167 ->177 -0.13051

167 ->179 0.27839

168 ->180 0.26891

168 ->181 0.10631

168 ->182 0.15877

169 ->183 -0.26752

Excited State 131: Singlet-A 6.7472 eV 183.76 nm f=0.0018

153 ->171 0.11095

156 ->175 0.20907

156 ->178 -0.11449

157 ->175 -0.12410

161 ->175 -0.14538

163 ->177 0.18799

164 ->178 0.12441

164 ->179 -0.10055

164 ->180 -0.12213

166 ->178 -0.19953

166 ->179 -0.11355

167 ->182 0.10126

169 ->184 0.15959

Excited State 132: Singlet-A 6.7608 eV 183.39 nm f=0.0107

153 ->171 0.11968

154 ->170 -0.10406

154 ->171 0.48755

154 ->172 -0.37023

163 ->177 -0.10933

Excited State 133: Singlet-A 6.7680 eV 183.19 nm f=0.0092

155 ->174 0.16233

162 ->177 0.16241

163 ->177 0.34606

166 ->178 0.13273

166 ->179 0.11232

167 ->178 0.12117

168 ->180 0.16106

168 ->182 0.15192

168 ->183 -0.12168

Excited State 134: Singlet-A 6.7691 eV 183.16 nm f=0.0007

153 ->171 -0.18047

158 ->176 0.30691

163 ->177 0.11900

165 ->177 -0.12630

165 ->181 0.11703

166 ->179 0.16551

166 ->181 -0.11815

167 ->179 -0.13805

167 ->181 0.12381

168 ->182 -0.10270

168 ->183 0.10013

169 ->183 -0.10534

169 ->184 -0.21254

Excited State 135: Singlet-A 6.7813 eV 182.83 nm f=0.0013

153 ->171 0.17286

154 ->171 -0.11012

156 ->176 -0.19513

157 ->176 -0.13382

158 ->176 0.44048

160 ->176 0.17177

163 ->177 -0.20692

167 ->181 -0.10102

169 ->184 0.12753

Excited State 136: Singlet-A 6.7854 eV 182.72 nm f=0.0144

155 ->174 0.14950

157 ->176 0.11918

158 ->176 -0.11893

160 ->176 -0.20055

161 ->177 0.12434

162 ->177 0.18139

163 ->177 -0.13272

164 ->178 0.12032

165 ->177 -0.11957

166 ->179 0.27284

167 ->179 -0.12230

167 ->181 -0.11786

168 ->182 -0.13040

169 ->183 -0.17889

Excited State 137: Singlet-A 6.7901 eV 182.59 nm f=0.0007

157 ->175 -0.11600

158 ->176 -0.19614

160 ->175 -0.36018

160 ->176 0.46159

Excited State 138: Singlet-A 6.8031 eV 182.25 nm f=0.0027

156 ->176 0.11406

157 ->176 -0.25570

162 ->177 0.37666

162 ->178 -0.15877

162 ->179 0.11839

164 ->177 0.10197

165 ->179 -0.18526

166 ->179 -0.10246

166 ->182 0.10230

168 ->183 0.10648

169 ->187 0.10743

Excited State 139: Singlet-A 6.8092 eV 182.08 nm f=0.0015

153 ->171 -0.16892

155 ->174 0.17771

157 ->176 0.28053

158 ->175 -0.11189

158 ->176 0.12338

159 ->175 -0.25925

159 ->176 0.33681

166 ->179 -0.10936

168 ->183 0.13453

Excited State 140: Singlet-A 6.8113 eV 182.03 nm f=0.0038

153 ->171 -0.13959

155 ->174 0.33759

156 ->175 0.10739

157 ->176 -0.11762

159 ->175 0.18361

159 ->176 -0.28299

166 ->179 -0.11211

168 ->183 0.15041

169 ->184 0.17699

Excited State 141: Singlet-A 6.8162 eV 181.90 nm f=0.0019

155 ->174 0.11053

156 ->176 0.40210

157 ->176 -0.37234

159 ->175 -0.13558

159 ->176 0.19168

165 ->179 0.11342

Excited State 142: Singlet-A 6.8238 eV 181.69 nm f=0.0559

153 ->171 -0.11725

155 ->174 -0.12206

161 ->178 0.10253

163 ->178 -0.14834

166 ->180 -0.10510

166 ->181 -0.10146

167 ->178 0.17622

167 ->181 -0.18897

168 ->181 -0.20911

168 ->182 0.30735

169 ->184 -0.12335

Excited State 143: Singlet-A 6.8337 eV 181.43 nm f=0.0304

161 ->177 -0.14615

162 ->177 0.10707

163 ->177 -0.13133

163 ->178 0.14894

165 ->179 0.25213

167 ->178 -0.15263

168 ->181 -0.10213

168 ->182 0.23618

168 ->183 0.13010

168 ->184 0.11563

169 ->184 0.20775

Excited State 144: Singlet-A 6.8383 eV 181.31 nm f=0.0148

152 ->170 0.11598

153 ->171 0.15755

155 ->174 0.18682

155 ->175 -0.10769

161 ->175 0.10062

161 ->177 -0.15009

162 ->177 -0.14103

163 ->182 -0.16122

164 ->179 -0.12054

166 ->180 -0.13435

166 ->181 -0.17803

167 ->184 0.10945

Excited State 145: Singlet-A 6.8550 eV 180.87 nm f=0.0012

153 ->171 0.32846

156 ->176 0.18871

161 ->177 0.26448

164 ->179 0.14162

165 ->181 0.15977

166 ->181 -0.12225

167 ->180 -0.10492

168 ->183 0.13571

169 ->184 -0.12200

Excited State 146: Singlet-A 6.8699 eV 180.47 nm f=0.0026

161 ->178 0.13661

162 ->177 -0.13406

163 ->178 -0.10414

163 ->179 0.18719

164 ->178 0.11993

164 ->181 0.12077

165 ->179 -0.14354

166 ->180 0.31745

166 ->181 -0.17443

167 ->178 -0.10223

167 ->182 -0.12732

168 ->182 0.13062

168 ->183 -0.16495

Excited State 147: Singlet-A 6.8732 eV 180.39 nm f=0.0066

161 ->177	-0.20286
163 ->177	-0.14070
163 ->179	-0.20499
164 ->178	0.12817
165 ->180	-0.15082
166 ->180	0.25627
166 ->181	-0.17851
167 ->181	-0.15475
168 ->181	0.15606
168 ->182	-0.18217

Excited State 148: Singlet-A 6.8885 eV 179.99 nm f=0.0312

155 ->174	-0.16707
156 ->177	0.10809
162 ->177	0.10418
163 ->179	0.11758
165 ->179	0.26128
166 ->178	0.11326
167 ->182	-0.11390
168 ->182	-0.10388
168 ->183	-0.11930
169 ->184	0.11185
169 ->186	0.17399

169 ->187 -0.12169

Excited State 149: Singlet-A 6.8988 eV 179.72 nm f=0.0462

153 ->171 -0.14138

153 ->172 0.12578

156 ->177 -0.10208

161 ->178 0.15533

163 ->178 -0.26428

164 ->177 -0.10879

164 ->179 0.38235

168 ->183 -0.10233

Excited State 150: Singlet-A 6.9051 eV 179.55 nm f=0.0070

161 ->177 -0.19750

161 ->178 0.20703

162 ->177 0.12768

162 ->178 0.15487

163 ->178 -0.13199

164 ->178 -0.14533

164 ->179 -0.12925

164 ->180 0.13109

165 ->178 -0.16625

165 ->181 0.20108

166 ->181	0.14543
167 ->182	0.12604
168 ->183	-0.13825
169 ->186	0.13215
169 ->187	-0.12494

Orbital Coefficients of Atoms corresponding to Absorption Band of CP 2

Orbital transitions: 156→174; 157→174

156(HOMO-13)

3	S	1S	-0.00040
		2S	0.00155
		2PX	0.06300
		2PY	-0.03893
		2PZ	0.03215
		3S	-0.00513
		3PX	-0.16277
		3PY	0.10073
		3PZ	-0.08340
		4S	0.00218
		4PX	-0.11089
		4PY	0.06940

		4PZ	-0.05753
		5D 0	0.00297
		5D+1	0.00260
		5D-1	-0.00250
		5D+2	-0.00375
		5D-2	0.00029
4	S	1S	0.00162
		2S	-0.00759
		2PX	0.01829
		2PY	0.06499
		2PZ	-0.02988
		3S	0.01615
		3PX	-0.04709
		3PY	-0.17002
		3PZ	0.07829
		4S	0.02012
		4PX	-0.04715
		4PY	-0.10041
		4PZ	0.04788
		5D 0	0.00156
		5D+1	0.00357
		5D-1	0.00136
		5D+2	-0.00080

		5D-2	0.00649
6	S	1S	-0.00139
		2S	0.00640
		2PX	-0.04542
		2PY	0.00679
		2PZ	0.05738
		3S	-0.01465
		3PX	0.11923
		3PY	-0.01869
		3PZ	-0.15224
		4S	-0.01300
		4PX	0.07006
		4PY	-0.02529
		4PZ	-0.08657
		5D 0	-0.00395
		5D+1	0.00006
		5D-1	-0.00346
		5D+2	0.00375
		5D-2	0.00383
18	N	1S	0.01723
		2S	-0.03662
		2PX	-0.10839
		2PY	0.18906

		2PZ	-0.06326
		3S	-0.06161
		3PX	-0.09778
		3PY	0.15501
		3PZ	-0.05769
		4D 0	-0.00304
		4D+1	0.00204
		4D-1	-0.00043
		4D+2	-0.00170
		4D-2	-0.00400
20	N	1S	-0.01250
		2S	0.02939
		2PX	-0.07823
		2PY	0.08877
		2PZ	-0.15245
		3S	0.02371
		3PX	-0.07121
		3PY	0.07057
		3PZ	-0.12875
		4D 0	-0.00241
		4D+1	-0.00271
		4D-1	0.00065
		4D+2	-0.00121

		4D-2	0.00231

……

157(HOMO-12)

9	N	1S	-0.00641
		2S	0.01409
		2PX	0.02607
		2PY	0.07795
		2PZ	0.15719
		3S	0.02328
		3PX	0.01670
		3PY	0.06458
		3PZ	0.14514
		4D 0	0.00115
		4D+1	-0.00428
		4D-1	-0.00068
		4D+2	0.00046
		4D-2	-0.00142
10	N	1S	-0.02500
		2S	0.05723
		2PX	-0.12820
		2PY	0.02877
		2PZ	0.32297

		3S	0.06058
		3PX	-0.11041
		3PY	0.02026
		3PZ	0.27755
		4D 0	-0.00588
		4D+1	0.00507
		4D-1	0.00039
		4D+2	-0.00286
		4D-2	0.00050
18	N	1S	0.00696
		2S	-0.01468
		2PX	-0.03744
		2PY	0.07446
		2PZ	0.15602
		3S	-0.02546
		3PX	-0.03557
		3PY	0.06086
		3PZ	0.14075
		4D 0	-0.00130
		4D+1	-0.00490
		4D-1	0.00127
		4D+2	-0.00086
		4D-2	-0.00125

20	N	1S	0.02500
		2S	-0.05538
		2PX	0.11175
		2PY	0.03715
		2PZ	0.32630
		3S	-0.06755
		3PX	0.09137
		3PY	0.03024
		3PZ	0.28385
		4D 0	0.00637
		4D+1	0.00462
		4D-1	0.00053
		4D+2	0.00267
		4D-2	0.00137

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174(LUMO+4)

13	N	1S	-0.00762
		2S	0.02671
		2PX	0.05784
		2PY	-0.03099
		2PZ	0.10020
		3S	-0.03945

		3PX	0.09015
		3PY	-0.01342
		3PZ	0.14368
		4D 0	0.00081
		4D+1	-0.00066
		4D-1	0.00158
		4D+2	0.00049
		4D-2	0.00025
15	N	1S	0.01571
		2S	-0.04227
		2PX	-0.05746
		2PY	0.02618
		2PZ	-0.01519
		3S	-0.00634
		3PX	-0.10584
		3PY	0.03950
		3PZ	-0.00728
		4D 0	0.00668
		4D+1	-0.00065
		4D-1	-0.00474
		4D+2	-0.00532
		4D-2	-0.00088
23	C	1S	-0.01142

		2S	0.02149
		2PX	0.12652
		2PY	-0.04667
		2PZ	0.08857
		3S	0.05297
		3PX	0.10115
		3PY	-0.13342
		3PZ	0.22684
		4D 0	0.00061
		4D+1	0.00748
		4D-1	-0.00084
		4D+2	-0.00619
		4D-2	-0.00360
30	C	1S	0.00450
		2S	0.00077
		2PX	-0.04922
		2PY	0.03929
		2PZ	-0.10274
		3S	-0.02903
		3PX	-0.05316
		3PY	0.16077
		3PZ	-0.14039
		4D 0	0.00157

4D+1	0.00421
4D-1	0.01296
4D+2	0.00355
4D-2	0.00808

……

4. CP 3 B3LYP/LanL2DZ+6-31G* TD-PCM (50 states) in DMF (dielectric constant = 36.71)

Excitation energies and oscillator strengths:

Excited State	1:	Singlet-A	4.4642 eV	277.73 nm	f=0.0599
243 ->246		0.16600			
245 ->246		0.64662			
245 ->247		-0.12350			

This state for optimization and/or second-order correction.
Total Energy, E(RPA) = -4565.86827983
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State	2:	Singlet-A	4.5930 eV	269.94 nm	f=0.0025
244 ->246		0.68067			
244 ->247		-0.12717			
245 ->246		0.10500			

Excited State	3:	Singlet-A	4.7480 eV	261.13 nm	f=0.0014
243 ->246		-0.12248			
245 ->246		0.13083			
245 ->247		0.54395			
245 ->248		0.33936			
245 ->249		-0.12399			

Excited State	4:	Singlet-A	4.8488 eV	255.70 nm	f=0.0053
244 ->247		0.54621			
244 ->248		0.28853			
245 ->248		0.25499			

Excited State	5:	Singlet-A	4.8553 eV	255.36 nm	f=0.0068
243 ->247		-0.10779			
244 ->247		-0.18846			
244 ->248		-0.19330			
245 ->247		-0.35825			
245 ->248		0.49275			

Excited State	6:	Singlet-A	4.9340 eV	251.28 nm	f=0.0325
238 ->246		-0.22447			
243 ->246		0.56192			
245 ->246		-0.18806			

245 ->248 0.18020

Excited State 7: Singlet-A 4.9492 eV 250.51 nm f=0.0007
244 ->247 -0.33512
244 ->248 0.58641

Excited State 8: Singlet-A 5.0036 eV 247.79 nm f=0.1003
237 ->246 0.38485
237 ->247 -0.10630
238 ->246 -0.25261
239 ->246 0.32860
240 ->246 0.15922
241 ->246 -0.24703

Excited State 9: Singlet-A 5.1505 eV 240.72 nm f=0.0028
243 ->247 0.16106
245 ->249 0.60598
245 ->250 -0.17899
245 ->252 0.12895

Excited State 10: Singlet-A 5.2047 eV 238.21 nm f=0.0127
237 ->246 0.18973
238 ->246 0.12451
240 ->246 -0.10135
241 ->247 0.10141
241 ->248 0.10136
242 ->246 0.58300
243 ->246 0.18654

Excited State 11: Singlet-A 5.2194 eV 237.54 nm f=0.0018
237 ->246 0.11661
238 ->246 0.39302
240 ->246 -0.17900
241 ->246 -0.33447
241 ->248 -0.14618
242 ->246 -0.20919
243 ->246 0.19631

Excited State 12: Singlet-A 5.2370 eV 236.75 nm f=0.0017
244 ->247 0.10685
244 ->249 0.58901
244 ->250 -0.27869
244 ->252 0.15893
245 ->250 -0.11233

Excited State 13:	Singlet-A	5.2541 eV	235.98 nm	f=0.0162
237 ->246	0.19386			
238 ->246	0.22691			
239 ->246	0.17332			
241 ->246	0.41698			
241 ->247	0.13041			
241 ->248	0.19297			
242 ->246	-0.24079			
242 ->247	0.13745			
Excited State 14:	Singlet-A	5.2842 eV	234.63 nm	f=0.0061
243 ->246	0.11243			
243 ->247	0.52996			
245 ->248	0.10604			
245 ->250	0.32360			
Excited State 15:	Singlet-A	5.3059 eV	233.67 nm	f=0.0030
238 ->246	0.12056			
240 ->246	0.21286			
243 ->247	-0.25429			
243 ->248	0.29937			
245 ->249	0.14145			
245 ->250	0.43608			
Excited State 16:	Singlet-A	5.3274 eV	232.73 nm	f=0.0053
238 ->246	0.20813			
239 ->246	-0.15650			
240 ->246	0.56962			
243 ->247	0.14399			
245 ->249	-0.10110			
245 ->250	-0.17113			
Excited State 17:	Singlet-A	5.3576 eV	231.42 nm	f=0.0108
225 ->246	-0.12850			
230 ->246	0.12364			
232 ->246	0.29935			
233 ->246	-0.15220			
236 ->246	-0.13798			
237 ->246	-0.28195			
238 ->246	0.12050			
239 ->246	0.38338			
239 ->247	-0.17039			

Excited State 18:	Singlet-A	5.3595 eV	231.34 nm	f=0.0095
230 ->246	-0.11237			
232 ->246	-0.34230			
233 ->246	0.16182			
236 ->246	0.19059			
237 ->246	-0.19197			
237 ->247	0.12242			
238 ->246	0.11020			
238 ->247	-0.11156			
239 ->246	0.35860			
241 ->247	-0.16108			
Excited State 19:	Singlet-A	5.3811 eV	230.41 nm	f=0.0036
237 ->247	0.11296			
238 ->247	0.10660			
243 ->248	0.48401			
244 ->249	-0.12697			
244 ->250	-0.19454			
245 ->249	-0.19037			
245 ->250	-0.19646			
245 ->251	0.14837			
Excited State 20:	Singlet-A	5.3967 eV	229.74 nm	f=0.0075
232 ->246	0.10139			
236 ->246	-0.27279			
237 ->246	0.21733			
241 ->246	0.30026			
241 ->247	-0.28624			
241 ->248	-0.21670			
242 ->247	-0.20122			
242 ->248	-0.16521			
Excited State 21:	Singlet-A	5.4142 eV	229.00 nm	f=0.0055
243 ->248	0.18765			
244 ->248	0.10451			
244 ->249	0.29334			
244 ->250	0.54617			
244 ->252	-0.11067			
Excited State 22:	Singlet-A	5.4323 eV	228.24 nm	f=0.0193
232 ->246	0.22812			
236 ->246	0.11194			
237 ->247	0.24591			
237 ->248	-0.11633			

238 ->247	-0.14150			
239 ->247	0.25283			
241 ->248	0.18541			
243 ->248	-0.11966			
245 ->251	0.27522			
245 ->252	-0.13337			

Excited State 23:	Singlet-A	5.4457 eV	227.67 nm	f=0.0344
232 ->246	-0.18950			
238 ->247	0.18019			
239 ->247	-0.14127			
243 ->248	-0.10758			
245 ->251	0.41503			
245 ->252	-0.25758			
245 ->253	-0.10879			
245 ->254	0.11451			

Excited State 24:	Singlet-A	5.4799 eV	226.25 nm	f=0.0017
232 ->246	0.16433			
236 ->246	0.50946			
237 ->247	-0.10559			
238 ->247	0.14631			
241 ->246	0.12604			
242 ->247	-0.23489			
242 ->248	-0.13679			

Excited State 25:	Singlet-A	5.4856 eV	226.02 nm	f=0.0054
232 ->246	0.10223			
236 ->246	0.23318			
239 ->247	-0.22423			
239 ->248	-0.16702			
240 ->247	-0.17119			
240 ->248	-0.11546			
241 ->247	-0.25908			
241 ->248	-0.16978			
242 ->247	0.32657			
242 ->248	0.12797			

Excited State 26:	Singlet-A	5.5039 eV	225.26 nm	f=0.0106
243 ->248	-0.15034			
243 ->249	-0.13586			
244 ->251	-0.14863			
244 ->252	0.16181			
245 ->250	0.14287			

245 ->251	0.29538			
245 ->252	0.40181			
245 ->253	0.14640			
Excited State 27:	Singlet-A	5.5249 eV	224.41 nm	f=0.0014
235 ->246	0.22166			
243 ->249	-0.11550			
244 ->251	0.41732			
244 ->252	-0.28930			
244 ->253	-0.15456			
244 ->254	0.16434			
245 ->252	0.19876			
Excited State 28:	Singlet-A	5.5393 eV	223.83 nm	f=0.0015
237 ->247	0.22179			
238 ->247	0.11668			
239 ->247	-0.27642			
239 ->248	-0.22652			
240 ->247	0.33633			
240 ->248	0.20087			
243 ->248	-0.12302			
244 ->251	0.12973			
245 ->251	-0.15015			
Excited State 29:	Singlet-A	5.5443 eV	223.62 nm	f=0.0026
225 ->246	0.14460			
235 ->246	0.49775			
242 ->247	0.22369			
242 ->248	-0.18245			
244 ->251	-0.21349			
245 ->252	-0.11965			
Excited State 30:	Singlet-A	5.5514 eV	223.34 nm	f=0.0024
235 ->246	0.26307			
238 ->247	-0.10322			
239 ->247	-0.17988			
241 ->247	0.14592			
241 ->248	-0.10610			
242 ->247	-0.34828			
242 ->248	0.39714			
Excited State 31:	Singlet-A	5.5824 eV	222.10 nm	f=0.0023
240 ->247	-0.19814			
240 ->248	-0.11082			

241 ->248	0.10568
242 ->248	-0.20604
244 ->250	0.13348
244 ->251	0.36559
244 ->252	0.32694
244 ->253	0.26461

Excited State 32: Singlet-A 5.5939 eV 221.64 nm f=0.0085

238 ->247	0.33938
239 ->247	0.17251
240 ->248	0.10260
241 ->247	-0.12140
242 ->248	0.27373
243 ->247	0.10846
243 ->249	0.16037
243 ->250	-0.13297
244 ->252	0.10259
245 ->253	0.31796

Excited State 33: Singlet-A 5.5988 eV 221.45 nm f=0.0184

238 ->247	-0.22173
239 ->247	-0.14840
240 ->247	0.13077
242 ->248	-0.14529
243 ->249	0.27929
244 ->252	-0.11093
244 ->253	-0.10759
245 ->251	0.14307
245 ->253	0.41444

Excited State 34: Singlet-A 5.6108 eV 220.98 nm f=0.0013

237 ->247	-0.20654
238 ->247	-0.20101
239 ->247	0.13143
239 ->248	0.18361
240 ->247	0.32538
241 ->248	-0.26073
242 ->247	0.21129
242 ->248	0.12042
244 ->251	0.21851
244 ->252	0.11351
244 ->253	0.10959
245 ->251	0.10577

Excited State	35:	Singlet-A	5.6307 eV	220.19 nm	f=0.0043
225 ->246		0.38098			
226 ->246		-0.11444			
228 ->246		0.19086			
230 ->246		-0.25929			
231 ->246		-0.12590			
232 ->246		0.14247			
235 ->246		-0.28020			
241 ->247		0.13048			
245 ->252		-0.10300			
245 ->253		0.11369			
Excited State	36:	Singlet-A	5.6568 eV	219.18 nm	f=0.0047
227 ->246		0.11239			
230 ->246		0.18288			
237 ->247		0.26012			
237 ->248		0.26488			
238 ->247		-0.15741			
238 ->248		-0.24328			
239 ->248		0.13229			
240 ->248		0.26987			
241 ->248		-0.12249			
241 ->249		-0.11033			
Excited State	37:	Singlet-A	5.6706 eV	218.64 nm	f=0.0035
225 ->246		0.12970			
243 ->249		0.44286			
243 ->250		-0.18354			
245 ->252		0.22870			
245 ->253		-0.29642			
Excited State	38:	Singlet-A	5.6756 eV	218.45 nm	f=0.0032
237 ->247		0.23424			
239 ->247		0.11072			
239 ->248		-0.14834			
240 ->248		-0.30564			
241 ->247		0.34825			
241 ->248		-0.32414			
Excited State	39:	Singlet-A	5.6839 eV	218.13 nm	f=0.0119
227 ->246		-0.14240			
228 ->246		-0.16833			
230 ->246		-0.23267			
231 ->246		0.18098			

233 ->246	-0.16426			
237 ->247	0.13684			
238 ->248	-0.23483			
239 ->248	0.18107			
240 ->247	0.13771			
240 ->248	-0.20504			
244 ->252	-0.17243			
244 ->253	0.25466			

Excited State 40:	Singlet-A	5.6866 eV	218.03 nm	f=0.0069
227 ->246	-0.15680			
228 ->246	-0.14912			
230 ->246	-0.10426			
231 ->246	0.14304			
233 ->246	-0.10779			
237 ->248	-0.22808			
239 ->247	0.13918			
239 ->248	-0.25141			
240 ->247	-0.14211			
240 ->248	0.33401			
241 ->247	0.17867			
241 ->248	-0.11171			

Excited State 41:	Singlet-A	5.6947 eV	217.72 nm	f=0.0009
228 ->246	0.13758			
230 ->246	0.17566			
233 ->246	0.11801			
237 ->247	-0.12084			
238 ->248	0.13661			
244 ->252	-0.31447			
244 ->253	0.46021			

Excited State 42:	Singlet-A	5.7164 eV	216.89 nm	f=0.0010
225 ->246	-0.10880			
228 ->246	-0.14754			
230 ->246	-0.31107			
231 ->246	-0.14080			
237 ->248	0.18160			
238 ->248	0.32694			
240 ->247	-0.17151			
243 ->250	-0.27700			

Excited State 43:	Singlet-A	5.7281 eV	216.45 nm	f=0.0038
225 ->246	0.15174			

227 ->246	-0.19176
230 ->246	0.19629
231 ->246	0.36736
233 ->246	-0.11593
237 ->247	0.10130
238 ->248	0.25539
239 ->247	-0.12201
239 ->248	0.21870
243 ->250	-0.11500

Excited State 44: Singlet-A 5.7444 eV 215.84 nm f=0.0017

227 ->246	-0.17842
233 ->246	-0.14904
234 ->246	0.18777
237 ->247	-0.17074
237 ->248	0.36736
239 ->247	0.22224
239 ->248	-0.28192
243 ->250	-0.13244

Excited State 45: Singlet-A 5.7469 eV 215.74 nm f=0.0012

227 ->246	0.11981
232 ->246	-0.10177
233 ->246	-0.22057
234 ->246	0.60649
237 ->248	-0.12901

Excited State 46: Singlet-A 5.7623 eV 215.16 nm f=0.0018

228 ->246	-0.28764
230 ->246	0.10362
232 ->246	0.13711
233 ->246	0.28472
234 ->246	0.17128
242 ->249	0.32983
242 ->250	-0.24685
242 ->252	0.10950
243 ->249	-0.11181

Excited State 47: Singlet-A 5.7637 eV 215.11 nm f=0.0106

228 ->246	0.24451
232 ->246	-0.15832
233 ->246	-0.32281
234 ->246	-0.12696
242 ->249	0.34984

242 ->250	-0.25936			
242 ->252	0.10734			
Excited State 48:	Singlet-A	5.7693 eV	214.90 nm	f=0.0047
225 ->246	0.16867			
227 ->246	0.52446			
228 ->246	-0.11936			
231 ->246	0.34866			
Excited State 49:	Singlet-A	5.7837 eV	214.37 nm	f=0.0054
225 ->246	-0.26688			
228 ->246	0.29308			
230 ->246	-0.26656			
231 ->246	0.32216			
232 ->246	0.13393			
233 ->246	0.24484			
234 ->246	0.14506			
Excited State 50:	Singlet-A	5.7946 eV	213.96 nm	f=0.0016
230 ->247	0.10130			
232 ->247	0.38327			
232 ->248	-0.14954			
233 ->247	-0.18747			
236 ->247	-0.31993			
238 ->248	-0.15184			
243 ->250	-0.21558			

Orbital Coefficients of Atoms corresponding to Absorption Band of CP 3

Orbital transitions: 245→251

			245(HOMO)
5	S	1S	0.00483
		2S	-0.02166
		2PX	0.09551
		2PY	-0.02354
		2PZ	0.02418
		3S	0.05181
		3PX	-0.25560
		3PY	0.06234
		3PZ	-0.06460
		4S	0.04114
		4PX	-0.14728
		4PY	0.05073

		4PZ	-0.02822
		5D 0	0.00612
		5D+1	0.00777
		5D-1	-0.00223
		5D+2	-0.00718
		5D-2	0.00569
6	S	1S	0.00043
		2S	-0.00116
		2PX	0.07747
		2PY	-0.01778
		2PZ	0.01841
		3S	0.00761
		3PX	-0.20344
		3PY	0.04670
		3PZ	-0.04772
		4S	-0.01888
		4PX	-0.13961
		4PY	0.03603
		4PZ	-0.02311
		5D 0	0.00091
		5D+1	0.00097
		5D-1	-0.00006
		5D+2	-0.00139
		5D-2	0.00110
7	S	1S	0.00509
		2S	-0.02184
		2PX	-0.13411
		2PY	0.02048
		2PZ	-0.03239
		3S	0.05828
		3PX	0.35055
		3PY	-0.05316
		3PZ	0.08562
		4S	0.03001
		4PX	0.25201
		4PY	-0.04150
		4PZ	0.05182
		5D 0	0.00596
		5D+1	0.00788
		5D-1	-0.00138
		5D+2	-0.00791
		5D-2	0.00607
22	N	1S	0.00273
		2S	-0.00749

		2PX	-0.15492
		2PY	0.01419
		2PZ	-0.07016
		3S	-0.00942
		3PX	-0.12608
		3PY	0.01379
		3PZ	-0.04893
		4D 0	0.00386
		4D+1	0.00587
		4D-1	0.00028
		4D+2	-0.00075
		4D-2	0.00213
24	N	1S	0.00113
		2S	-0.00391
		2PX	0.10900
		2PY	-0.01752
		2PZ	0.05370
		3S	0.01383
		3PX	0.08682
		3PY	-0.01476
		3PZ	0.04680
		4D 0	0.00306
		4D+1	0.00357
		4D-1	0.00011
		4D+2	-0.00049
		4D-2	0.00136

……

251(LUMO+5)

21	N	1S	0.00250
		2S	-0.00679
		2PX	-0.06585
		2PY	-0.17062
		2PZ	-0.01729
		3S	0.02121
		3PX	-0.09981
		3PY	-0.24099
		3PZ	-0.01920
		4D 0	0.00135
		4D+1	0.00026
		4D-1	0.00390
		4D+2	-0.00062
		4D-2	-0.00221
24	N	1S	-0.00659

		2S	0.01961
		2PX	0.10326
		2PY	0.05888
		2PZ	0.02102
		3S	0.04914
		3PX	0.13943
		3PY	0.08862
		3PZ	0.02000
		4D 0	-0.00019
		4D+1	-0.00368
		4D-1	-0.00140
		4D+2	0.00134
		4D-2	-0.00164
31	C	1S	-0.00415
		2S	0.01708
		2PX	-0.14229
		2PY	-0.07005
		2PZ	-0.01066
		3S	0.00501
		3PX	-0.25941
		3PY	-0.09552
		3PZ	-0.00139
		4D 0	0.00426
		4D+1	-0.01441
		4D-1	-0.00303
		4D+2	0.00339
		4D-2	-0.00412
32	C	1S	-0.00038
		2S	0.00730
		2PX	0.06845
		2PY	0.19364
		2PZ	0.02876
		3S	-0.04809
		3PX	0.08185
		3PY	0.29219
		3PZ	0.08458
		4D 0	0.00500
		4D+1	0.00402
		4D-1	0.01569
		4D+2	-0.00332
		4D-2	-0.00849