

Supporting Information

Solvent-free Thermal Synthesis of Luminescent Dinuclear Cu(I) Complexes with Triarylphosphines

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Reference

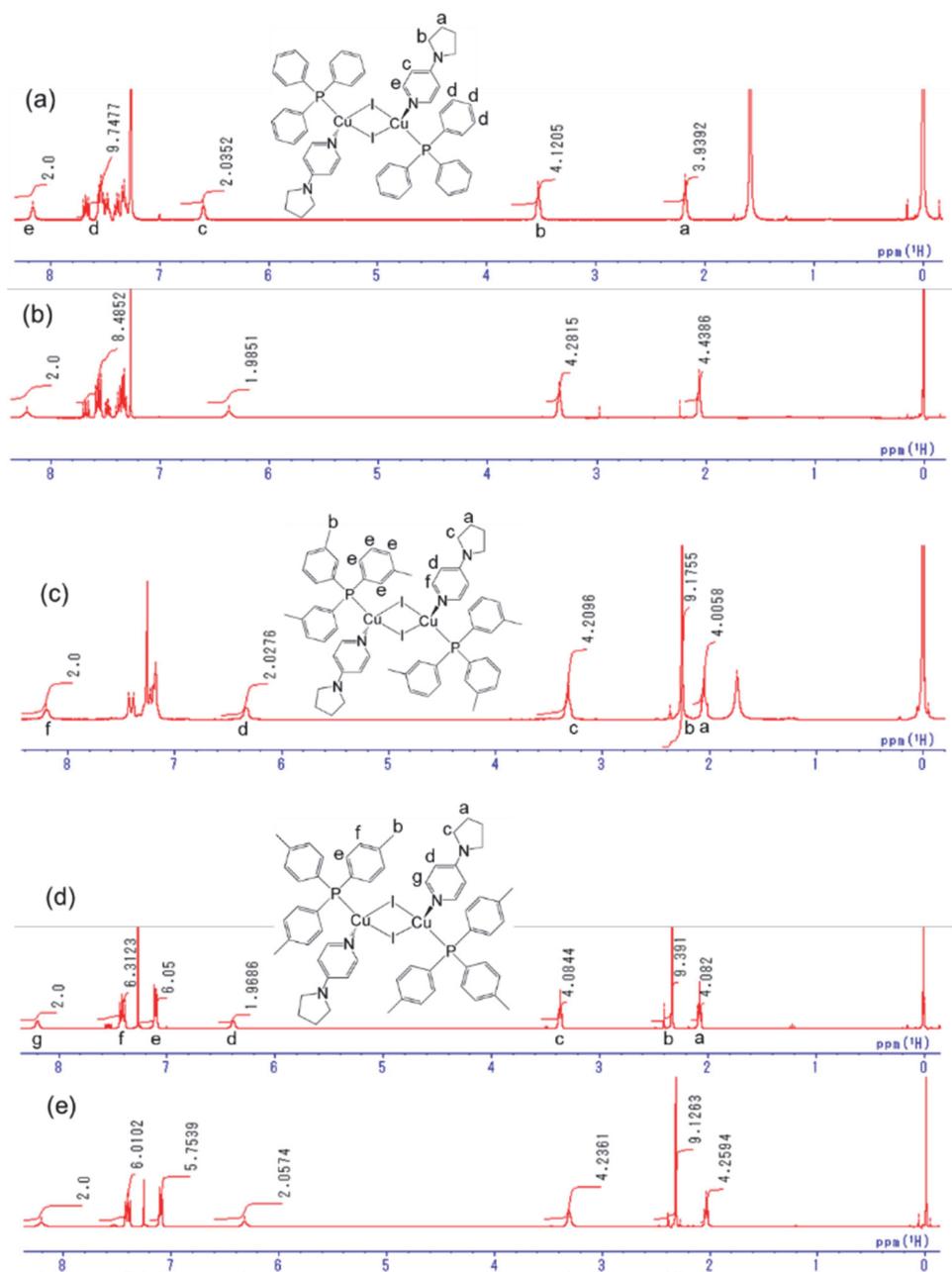


Figure S1. ¹H NMR spectra of **S1** (a) (CDCl₃), **T1** (b) (CDCl₃), **S2** (c) (CDCl₃), **S3** (d) (CDCl₃) and **T3** (e) (CDCl₃).

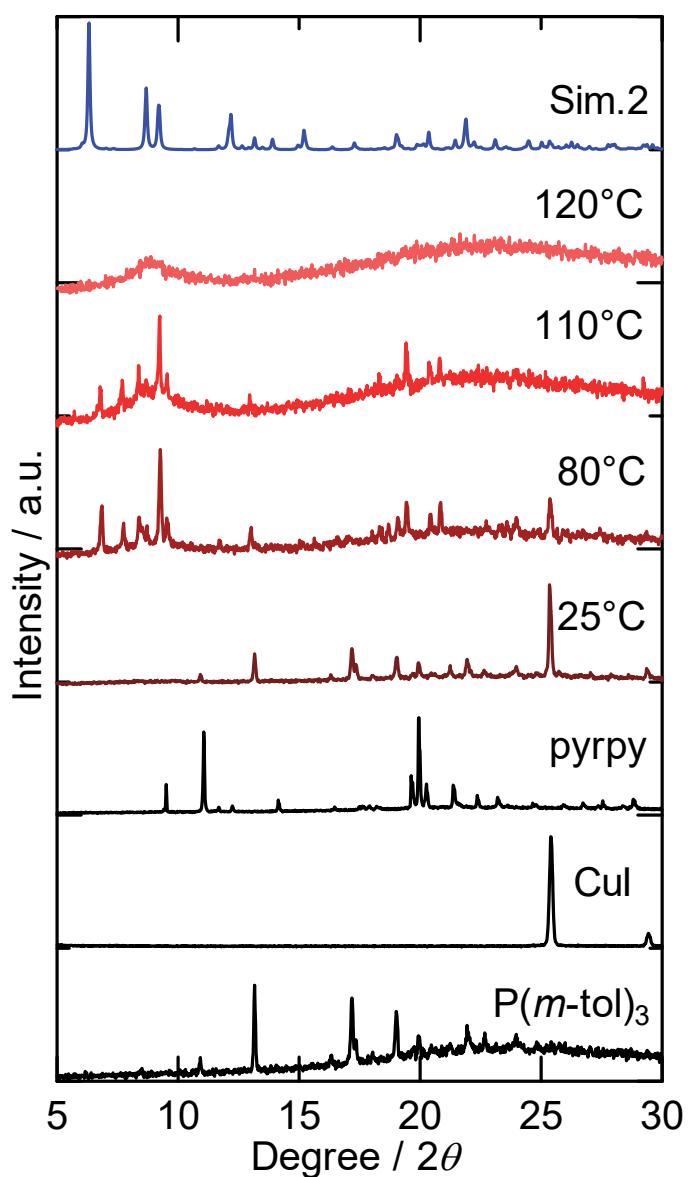


Figure S2. Temperature dependences of PXRD patterns of the ground mixtures of 1 eq. CuI, 1 eq. pyrpy, and 2 eq. P(*m*-tol)₃ to thermally synthesize complex **2**. The top blue line shows the simulation pattern calculated from the X-ray structure of **2**.

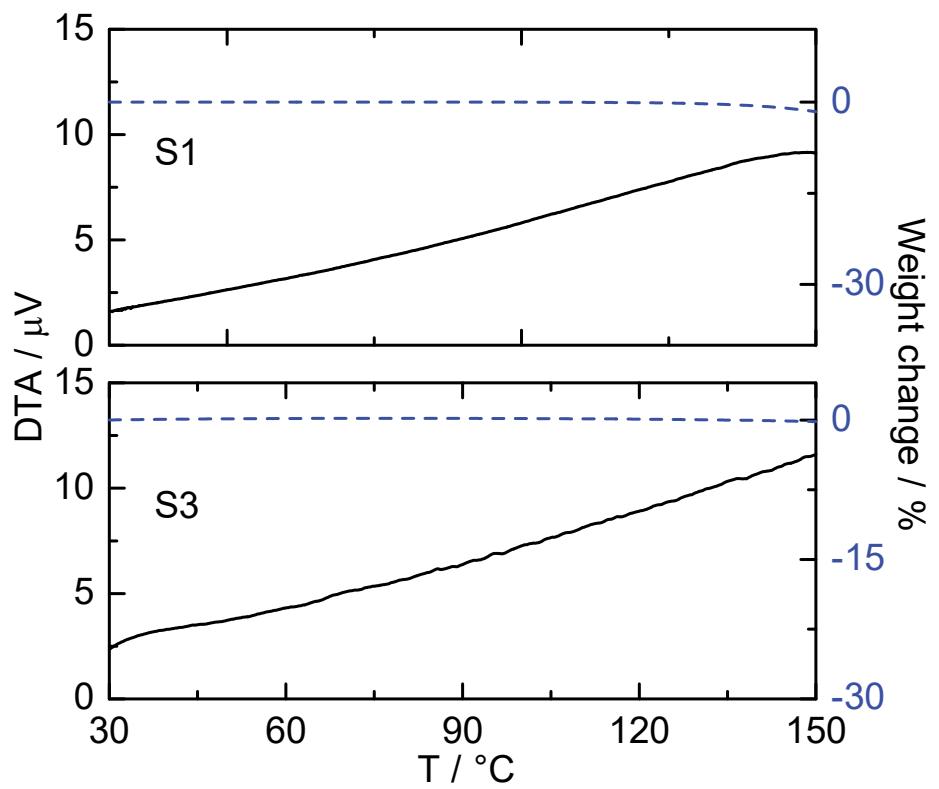


Figure S3. TG (dotted lines) and DTA (solid lines) curves of the solution synthesized complexes **S1** and **S3**, under Ar flow (flow rate: 250 mL/min).

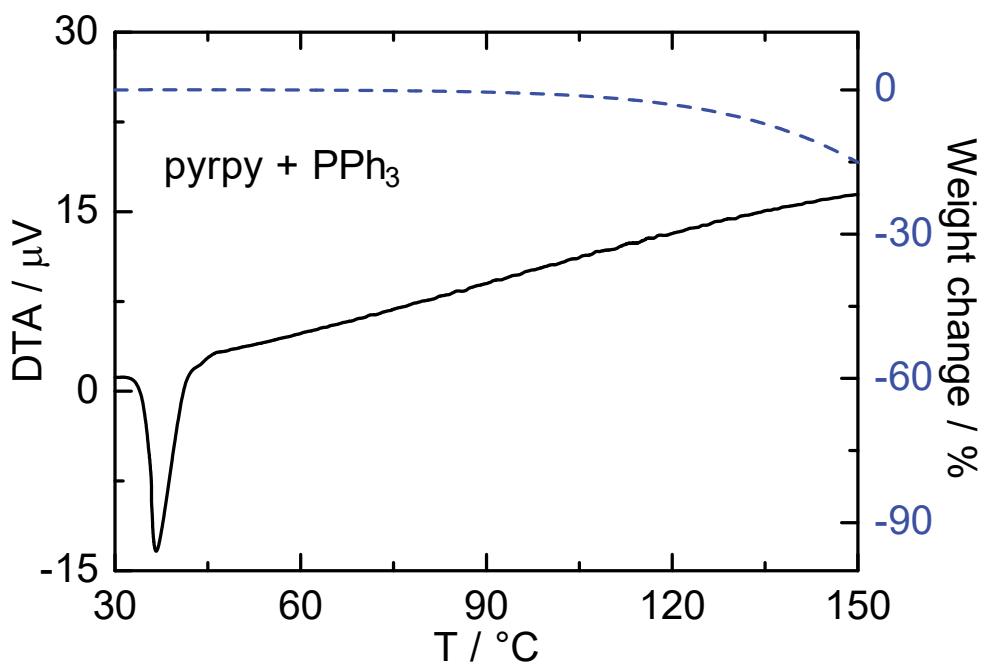


Figure S4. TG (blue dotted lines) and DTA (black solid lines) curves of the mixture of pyrpy and PPh_3 under Ar flow (flow rate: 250 mL/min).

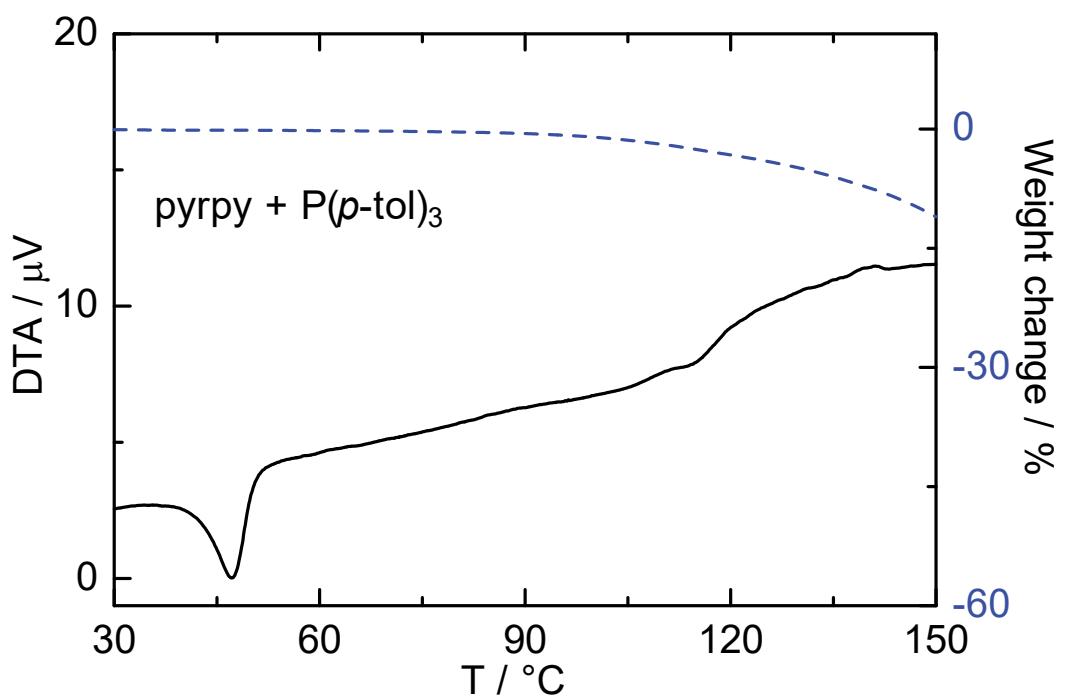


Figure S5. TG (dotted lines) and DTA (solid lines) curves of the mixture of pyrpy and $P(p\text{-tol})_3$ under Ar flow (flow rate: 250 mL/min).

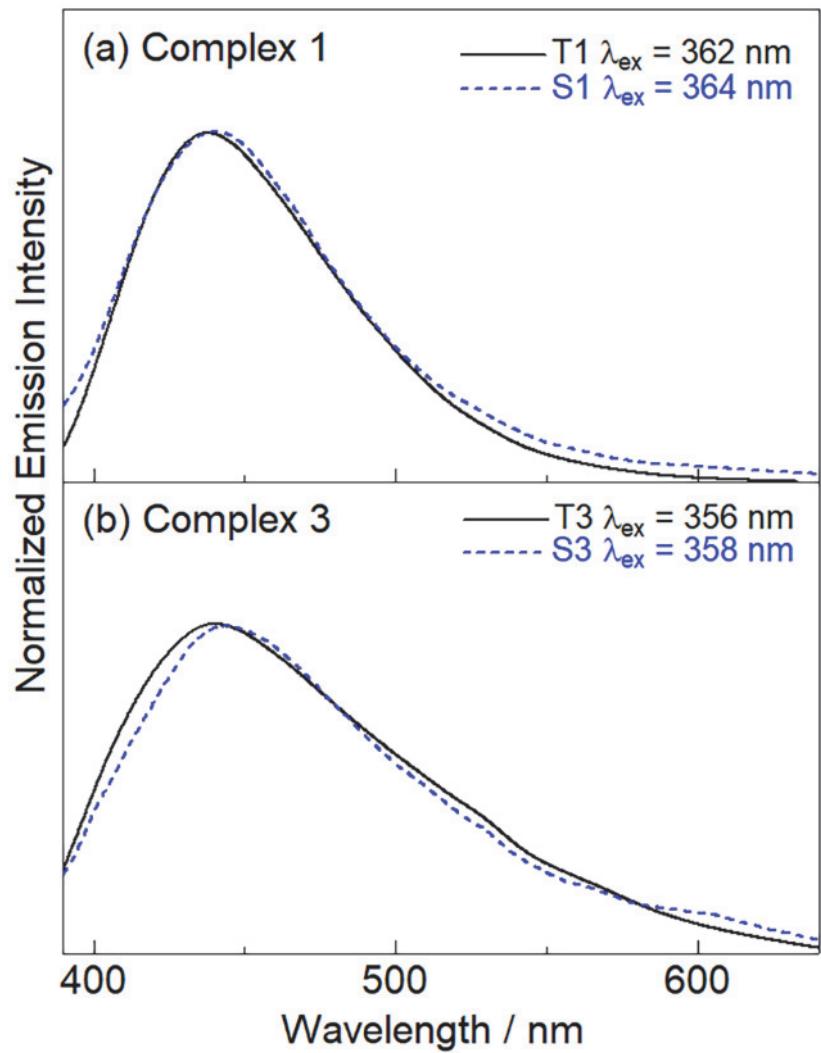


Figure S6. Emission spectra of complexes (a) S1 and T1, (b) S3 and T3 in the solid state at 298 K.

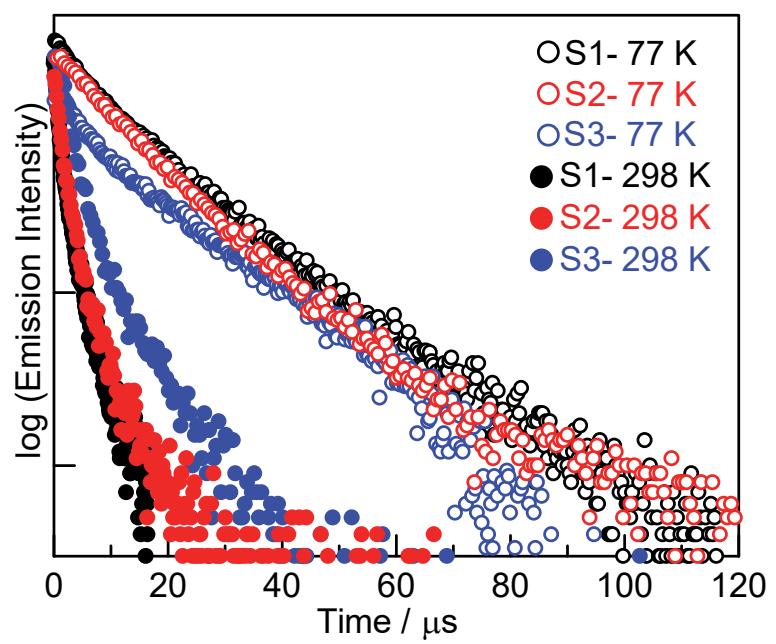


Figure S7. Emission decay curve of complexes **S1**, **S2** and **S3** in the solid state at 77 K and 298 K.

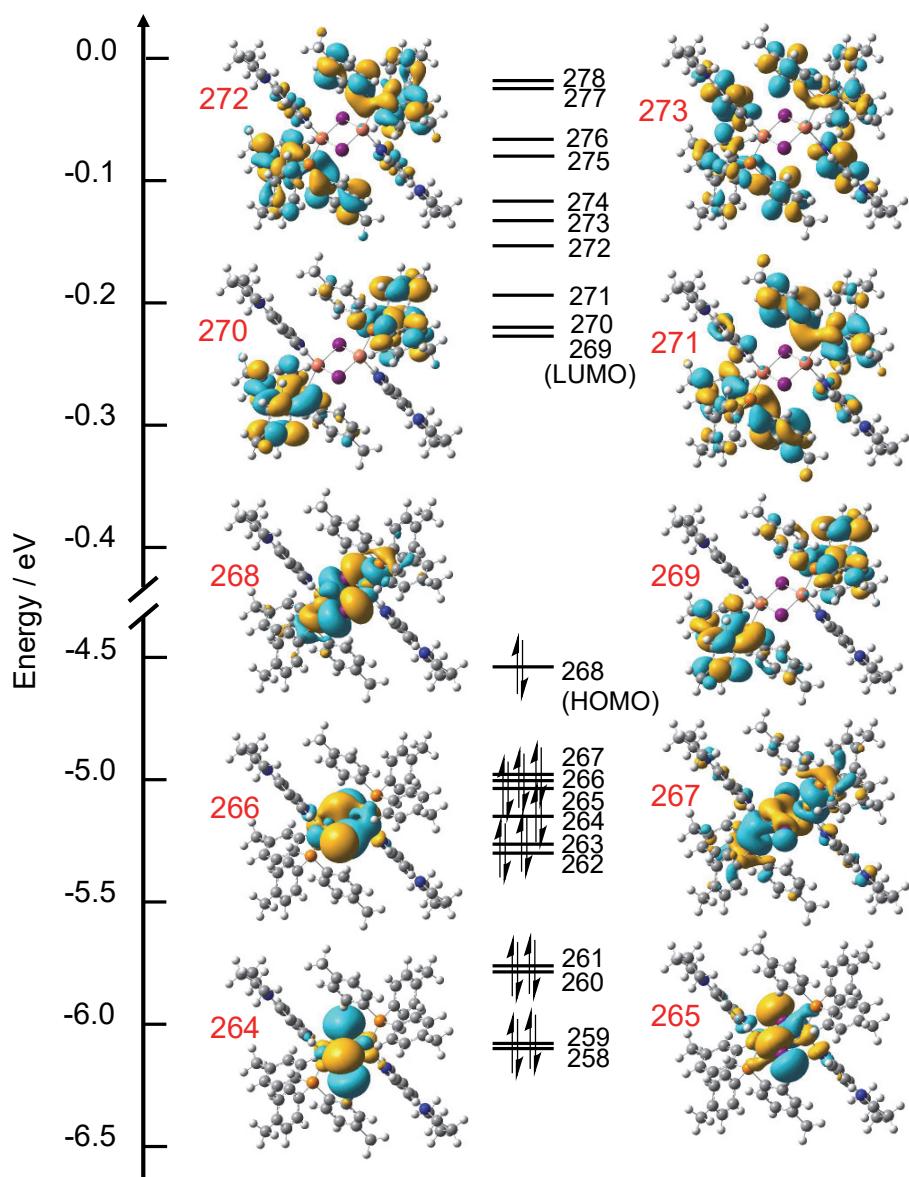


Figure S8. Kohn-Sham orbitals and energies at the frontier region of ground state optimized complex **2**.

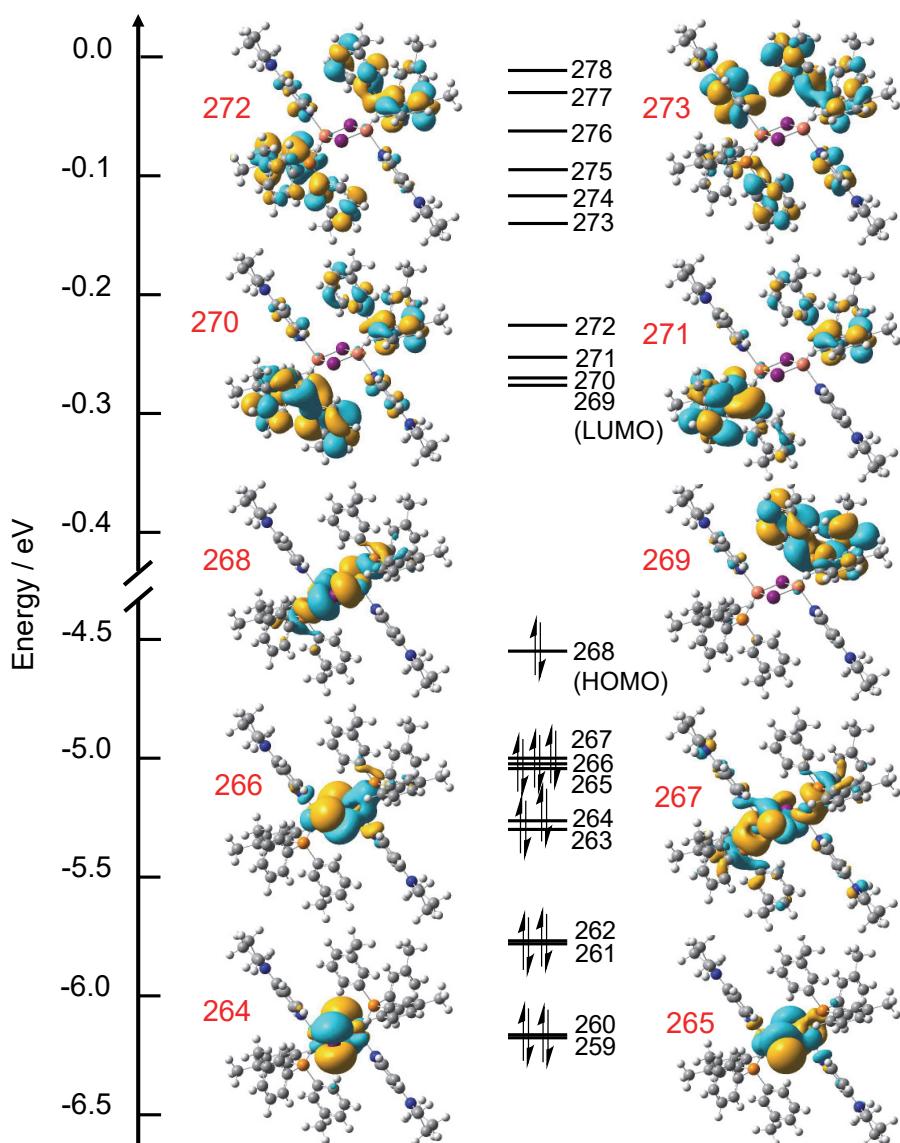


Figure S9. Kohn-Sham orbitals and energies at the frontier region of ground state optimized complex 3.

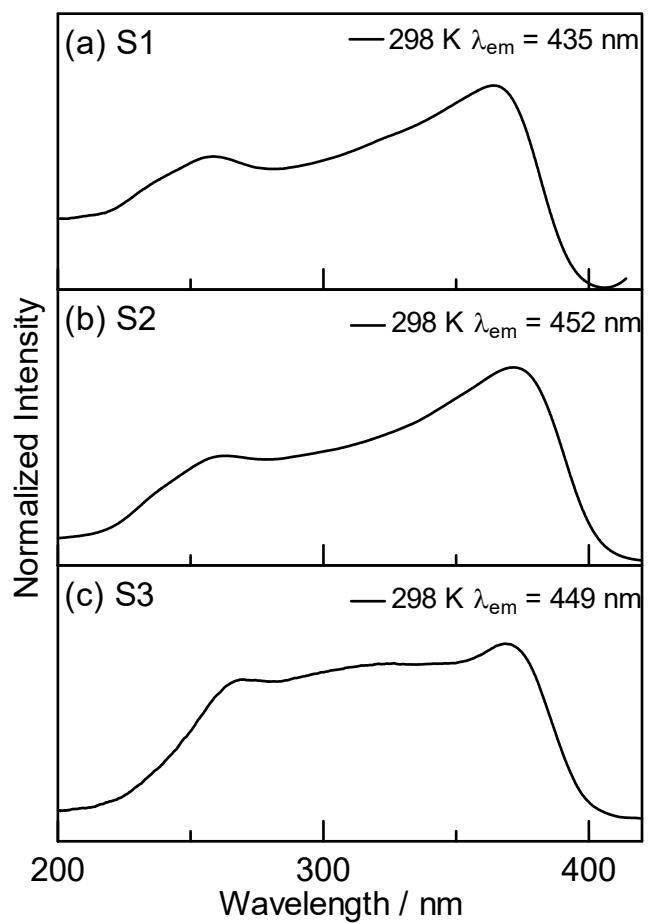


Figure S10. Excitation spectra of the complexes **S1**, **S2** and **S3** in the solid state at 298 K.

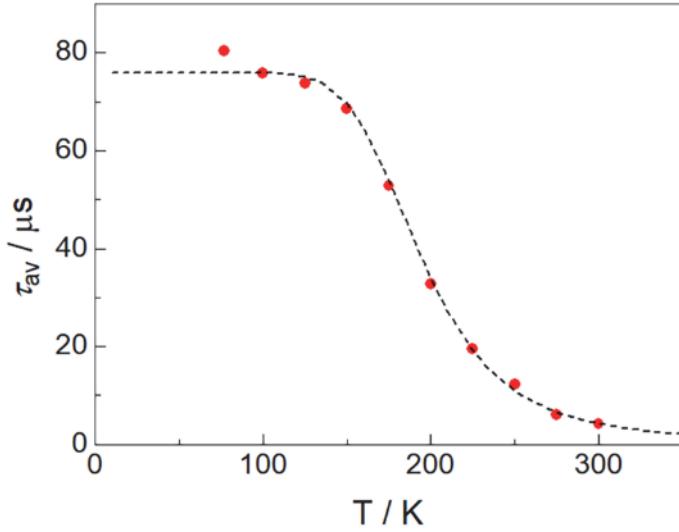


Figure S11. Temperature dependence of the average emission lifetime of complex **3** in the solid state. Assuming the two-state model involving the lowest excited singlet state (S_1) and the lowest excited triplet state (T_1), the observed lifetime can be expressed as a Boltzmann average by using equation (2).^{S1}

$$\tau_{obs} = \frac{3 + \exp(-\Delta E/RT)}{3/\tau_{T_1} + 1/\tau_{S_1} \exp(-\Delta E/RT)} \quad (2)$$

where, ΔE is the energy difference between the singlet and triplet states, τ_{S_1} and τ_{T_1} are the lifetimes of S_1 (fluorescence) and T_1 (phosphorescence) states, R is the ideal gas constant, and T is the absolute temperature. In this two-state model analysis, average lifetime was used instead of τ_{obs} , i.e., $\tau_{obs} = \tau_{av}$. The dotted line was calculated using eq (2). Estimated ΔE , τ_{S_1} , and τ_{T_1} values based on this fitting analysis are 1090 cm^{-1} , 8×10^{-9} and $76 \times 10^{-6} \text{ sec}$, respectively.

Table S1. Selected bond lengths (Å) and bond angles (°) of **1** in S_0 , S_1 and T_1 states after the optimization.

	X-ray	S_0	S_1	T_1
Cu(1)-Cu(2)	3.1538(8)	2.98	2.93	3.12
Cu(1)-I(1)	2.6855(4)	2.73	2.70	2.75
Cu(1)-I(2)	2.7017(5)	2.74	2.68	2.72
Cu(2)-I(1)	2.7017(5)	2.74	2.64	2.65
Cu(2)-I(2)	2.6855(4)	7.73	2.64	2.65
Cu(1)-P(1)	2.2198(6)	2.27	2.33	2.31
Cu(1)-N(1)	2.044(2)	2.09	2.06	2.04
Cu(2)-P(2)	2.2198(6)	2.27	2.34	2.34
Cu(2)-N(2)	2.044(2)	2.09	2.10	2.06
I(1)-Cu(1)-I(2)	108.44(2)	114.8	111.8	106.2
I(1)-Cu(1)-P(1)	111.39(2)	108.9	110.0	108.9
I(2)-Cu(1)-P(1)	108.68(2)	110.1	110.0	111.5
I(1)-Cu(1)-N(1)	104.72(6)	104.5	102.6	103.5
I(2)-Cu(1)-N(1)	102.21(5)	102.6	106.5	107.1
I(1)-Cu(2)-I(2)	108.44(2)	114.8	114.5	111.4
I(1)-Cu(2)-P(1)	108.68(2)	110.1	116.6	119.4
I(2)-Cu(2)-P(2)	111.39(2)	108.9	105.9	103.1
I(1)-Cu(2)-N(2)	102.21(5)	102.6	106.7	109.4
I(2)-Cu(2)-N(2)	104.72(6)	104.5	105.1	112.0

Table S2. Selected bond lengths (\AA) and bond angles ($^\circ$) of **2** in S_0 , S_1 and T_1 states after the optimization.

	X-ray ^a	S_0	S_1	T_1
Cu(1)-Cu(2)	3.002(1)	2.94	2.93	3.07
Cu(1)-I(1)	2.6678(6)	2.73	2.70	2.75
Cu(1)-I(2)	2.6922(5)	2.73	2.67	2.71
Cu(2)-I(1)	2.6922(5)	2.74	2.63	2.64
Cu(2)-I(2)	2.6678(6)	2.73	2.64	2.65
Cu(1)-P(1)	2.234(1)	2.27	2.33	2.31
Cu(1)-N(1)	2.047(4)	2.09	2.06	2.04
Cu(2)-P(2)	2.234(1)	2.27	2.33	2.34
Cu(2)-N(2)	2.047(4)	2.09	2.11	2.07
I(1)-Cu(1)-I(2)	111.89(2)	114.9	111.4	107.2
I(1)-Cu(1)-P(1)	107.13(4)	109.1	110.0	109.1
I(2)-Cu(1)-P(1)	110.47(3)	110.4	110.3	110.4
I(1)-Cu(1)-N(1)	104.85(9)	104.5	102.6	103.1
I(2)-Cu(1)-N(1)	104.16(9)	102.7	106.4	106.9
I(1)-Cu(2)-I(2)	111.89(2)	114.7	114.5	112.8
I(1)-Cu(2)-P(1)	110.47(3)	110.0	116.2	116.9
I(2)-Cu(2)-P(2)	107.13(4)	109.0	106.2	104.3
I(1)-Cu(2)-N(2)	104.16(9)	102.7	107.2	110.4
I(2)-Cu(2)-N(2)	104.85(9)	104.6	105.3	110.3

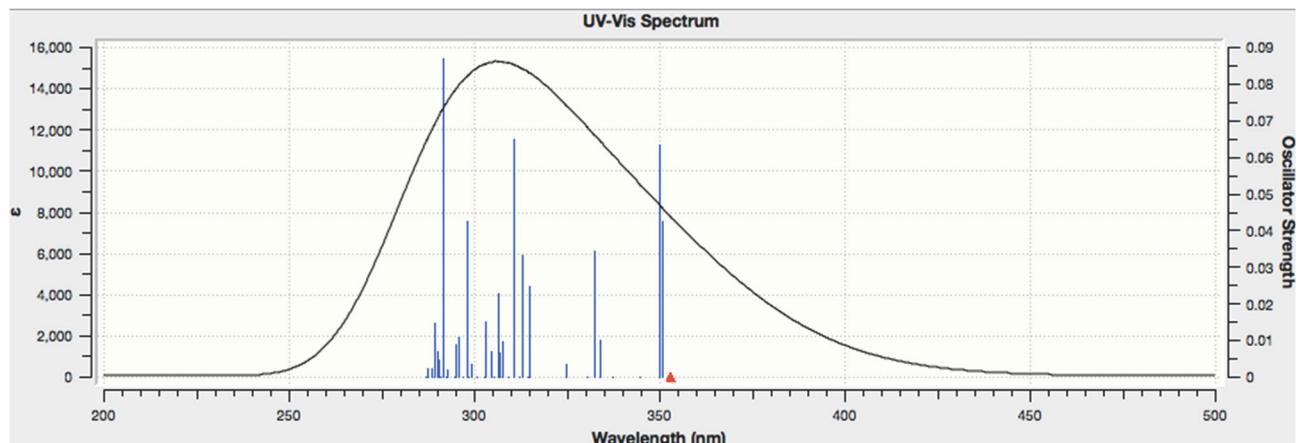
^a Data of symmetric molecule **2S** is shown.

Table S3. Selected bond lengths (\AA) and bond angles ($^\circ$) of **3** in S_0 , S_1 and T_1 states after the optimization.

	X-ray	S_0	S_1	T_1
Cu(1)-Cu(2)	3.3741(9)	2.94	2.95	3.08
Cu(1)-I(1)	2.7450(6)	2.74	2.71	2.76
Cu(1)-I(2)	2.7002(6)	2.74	2.68	2.72
Cu(2)-I(1)	2.7002(6)	2.74	2.63	2.64
Cu(2)-I(2)	2.7450(6)	2.74	2.64	2.65
Cu(1)-P(1)	2.2335(8)	2.27	2.33	2.31
Cu(1)-N(1)	2.053(3)	2.09	2.06	2.04
Cu(2)-P(2)	2.2335(8)	2.27	2.33	2.34
Cu(2)-N(2)	2.053(3)	2.09	2.10	2.06
I(1)-Cu(1)-I(2)	103.42(2)	114.2	110.8	107.0
I(1)-Cu(1)-P(1)	111.06(3)	110.3	110.2	109.0
I(2)-Cu(1)-P(1)	109.79(3)	108.6	110.6	111.4
I(1)-Cu(1)-N(1)	106.67(7)	102.4	102.2	102.7
I(2)-Cu(1)-N(1)	102.71(8)	103.4	106.4	106.8
I(1)-Cu(2)-I(2)	103.42(2)	114.2	114.4	112.8
I(1)-Cu(2)-P(1)	109.79(3)	108.6	116.1	116.2
I(2)-Cu(2)-P(2)	111.06(3)	110.3	105.9	104.8
I(1)-Cu(2)-N(2)	102.71(8)	103.7	107.2	110.5
I(2)-Cu(2)-N(2)	106.67(7)	102.4	105.7	110.3

Scheme S1. Energy, oscillator strength, and transition orbitals of the important excitations for complex **1**.

Simulated UV spectrum:

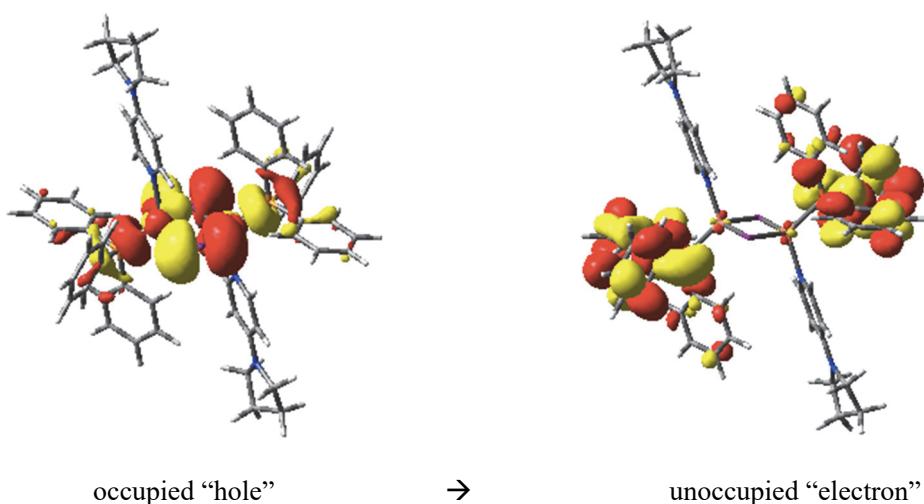


Excited State 1: 3.5112 eV (353.11 nm) f = 0.0000

243 -> 246	0.16456
244 -> 245	0.67616

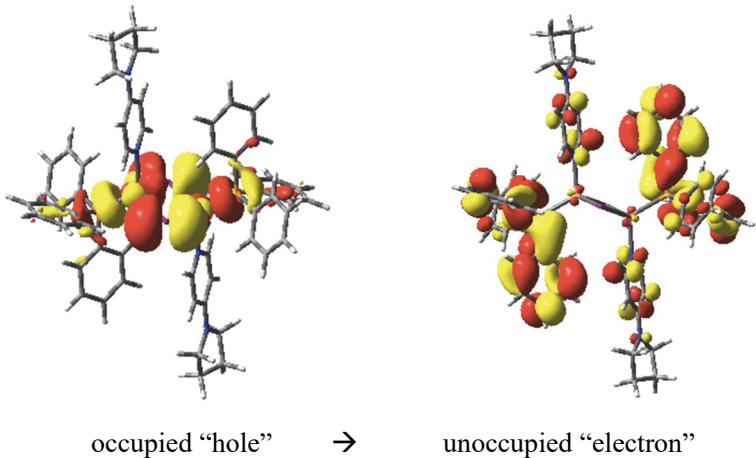
Excited State 2: 3.5365 eV (350.58 nm) f = 0.0426

243 -> 245	0.17398
244 -> 246	0.67620



Excited State 3: 3.5417 eV (350.07 nm) f = 0.0634

243 -> 248	-0.12335
244 -> 247	0.68377



Excited State 4: 3.5956 eV (344.83 nm) f = 0.0000

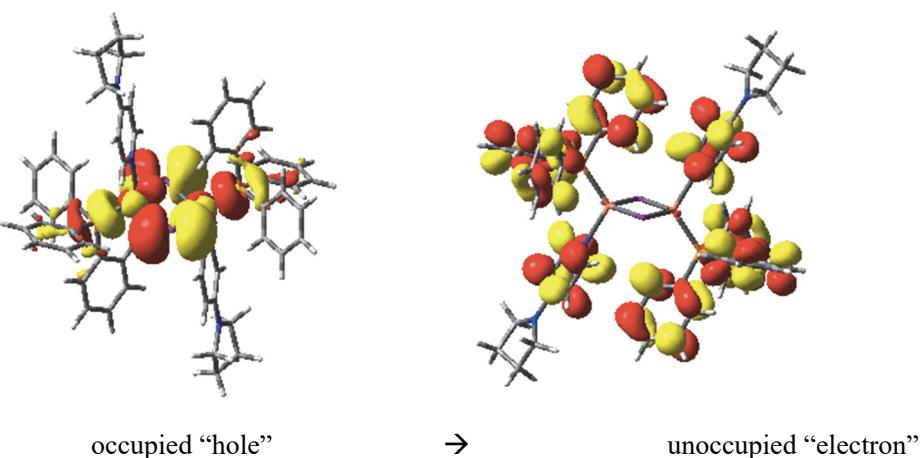
243 -> 247	-0.16836
244 -> 248	0.66513
244 -> 249	-0.10712

Excited State 5: 3.6765 eV (337.24 nm) f = 0.0000

244 -> 248	0.11575
244 -> 249	0.64939
244 -> 252	-0.16530
244 -> 253	-0.13444

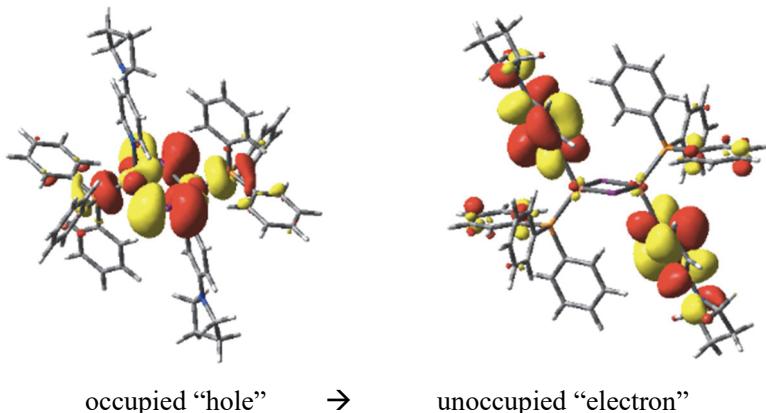
Excited State 6: 3.7110 eV (334.10 nm) f = 0.0102

244 -> 250	0.67453
244 -> 254	0.12928



Excited State 7: 3.7314 eV (332.27 nm) f = 0.0342

244 -> 251 0.68171



Excited State 8: 3.7520 eV (330.45 nm) f = 0.0000

244 -> 249 0.13162

244 -> 252 0.64120

244 -> 253 -0.21204

Excited State 9: 3.8153 eV (324.97 nm) f = 0.0000

243 -> 250 -0.16678

244 -> 249 0.16176

244 -> 252 0.17846

244 -> 253 0.62521

Excited State 10: 3.8193 eV (324.63 nm) f = 0.0033

243 -> 249 0.15507

244 -> 250 -0.11039

244 -> 254 0.65616

244 -> 255 -0.11593

Excited State 11: 3.9394 eV (314.73 nm) f = 0.0247

239 -> 245 0.14848

241 -> 246 0.21668

241 -> 247 0.15032

242 -> 246 -0.34992

242 -> 247 -0.19388

242 -> 251 0.11332

243 -> 245 0.38808

244 -> 246 -0.11548

Excited State 12: 3.9399 eV (314.69 nm) f = 0.0001

239 -> 246	-0.16269
241 -> 245	-0.25172
242 -> 245	0.44233
243 -> 246	-0.37114
244 -> 245	0.11308

Excited State 13: 3.9604 eV (313.06 nm) f = 0.0334

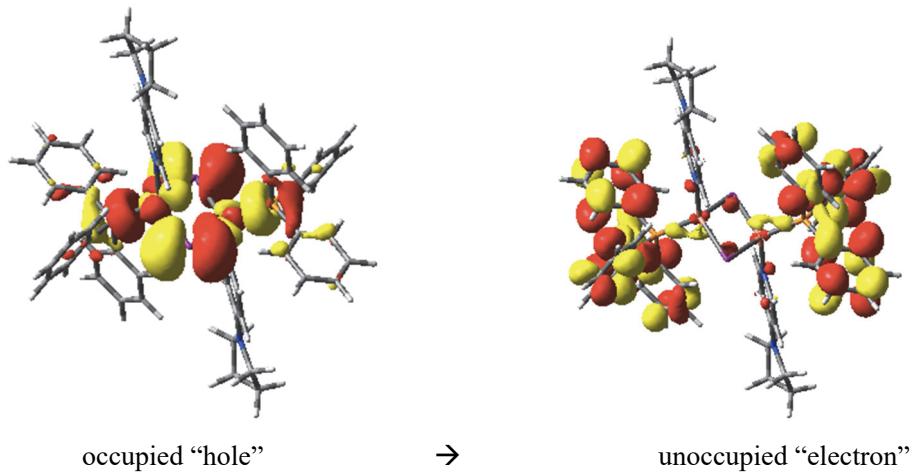
239 -> 252	0.12248
241 -> 247	-0.26807
242 -> 246	-0.19576
242 -> 247	0.42950
242 -> 251	-0.13312
243 -> 245	0.23451
243 -> 248	0.20394

Excited State 14: 3.9696 eV (312.33 nm) f = 0.0000

239 -> 247	0.16716
239 -> 251	-0.10262
241 -> 248	-0.17791
241 -> 252	-0.12223
242 -> 245	0.15321
242 -> 248	0.23908
242 -> 249	-0.10983
242 -> 252	0.16651
243 -> 247	0.48382
244 -> 248	0.12590

Excited State 15: 3.9889 eV (310.82 nm) f = 0.0648

243 -> 256	-0.11608
244 -> 254	0.10337
244 -> 255	0.65090



Excited State 16: 4.0106 eV(309.14 nm) f=0.0000

239 -> 251	-0.14263
241 -> 245	-0.13597
241 -> 249	0.12847
241 -> 252	-0.10624
242 -> 248	-0.11688
242 -> 249	-0.16680
242 -> 252	0.14262
243 -> 251	-0.14133
243 -> 255	-0.11314
244 -> 256	0.54144

Excited State 17: 4.0280 eV (307.80 nm) f=0.0000

241 -> 245	0.50030
242 -> 245	0.38759
242 -> 248	-0.10693
242 -> 249	-0.12256
243 -> 246	0.13546

Excited State 18: 4.0317 eV (307.52 nm) f=0.0097

241 -> 247	0.53126
242 -> 246	0.12556
242 -> 247	0.38548

Excited State 19: 4.0381 eV (307.04 nm) f=0.0000

239 -> 251	0.22377
241 -> 245	0.12607
241 -> 248	-0.11865

241 -> 249	-0.13031
241 -> 252	0.11943
242 -> 245	0.13338
242 -> 248	0.15926
242 -> 249	0.21979
242 -> 252	-0.24668
243 -> 247	0.14081
243 -> 251	0.13456
244 -> 256	0.38576

Excited State 20: 4.0410 eV (306.81 nm) f=0.0064

239 -> 249	0.14748
239 -> 252	-0.18151
241 -> 246	-0.13913
241 -> 251	-0.26101
242 -> 246	-0.11784
242 -> 247	0.12771
242 -> 251	0.38310
243 -> 248	0.28966
243 -> 249	0.13279
243 -> 252	-0.10651
244 -> 255	0.10091

Excited State 21: 4.0458 eV (306.45 nm) f=0.0229

241 -> 246	0.46125
241 -> 247	-0.14709
242 -> 246	0.43625
242 -> 251	0.11833
243 -> 245	0.12191
243 -> 248	0.10888

Excited State 22: 4.0627 eV (305.18 nm) f=0.0000

239 -> 250	0.10087
239 -> 254	0.15895
241 -> 245	-0.22342
241 -> 248	-0.10475
241 -> 249	0.13319
241 -> 252	0.13091

241 -> 253	-0.14879
242 -> 248	0.20002
242 -> 249	-0.20723
242 -> 252	-0.16404
242 -> 253	0.20561
243 -> 246	0.36305
243 -> 250	0.10932
243 -> 254	0.12887

Excited State 23: 4.0688 eV (304.72 nm) f=0.0071

239 -> 253	0.13397
241 -> 246	-0.26857
241 -> 250	-0.13465
241 -> 254	-0.14935
242 -> 246	0.17229
242 -> 250	0.21669
242 -> 254	0.20460
243 -> 245	0.24757
243 -> 248	0.31841
243 -> 249	-0.15157
243 -> 253	0.13430

Excited State 24: 4.0898 eV (303.15 nm) f=0.0000

241 -> 248	0.42044
242 -> 248	0.50244
243 -> 247	-0.16911

Excited State 25: 4.0910 eV (303.07 nm) f=0.0150

239 -> 245	-0.19115
239 -> 253	-0.13438
241 -> 246	-0.26825
241 -> 250	0.14055
241 -> 254	0.13715
242 -> 246	0.16167
242 -> 250	-0.21482
242 -> 254	-0.20002
243 -> 245	0.39122
243 -> 248	-0.13934

Excited State 26: 4.0986 eV (302.50 nm) f=0.0000

239 -> 246	-0.13135
239 -> 247	0.15649
239 -> 254	-0.13624
241 -> 245	-0.18949
241 -> 248	-0.19238
241 -> 252	-0.14665
241 -> 253	0.12825
242 -> 245	0.21641
242 -> 249	0.17029
242 -> 252	0.19629
242 -> 253	-0.18072
243 -> 246	0.29097
243 -> 247	-0.21977
243 -> 254	-0.10078

Excited State 27: 4.1227 eV (300.74 nm) f=0.0000

239 -> 246	-0.11030
239 -> 247	-0.15045
241 -> 245	-0.15605
241 -> 248	0.40093
241 -> 249	-0.12741
242 -> 248	-0.21049
243 -> 246	0.24401
243 -> 247	0.29353
243 -> 250	-0.14793

Excited State 28: 4.1439 eV (299.20 nm) f=0.0036

239 -> 248	-0.14850
239 -> 252	0.11439
241 -> 247	0.21199
242 -> 247	-0.25643
242 -> 250	-0.14250
242 -> 251	-0.23690
242 -> 254	-0.12411
243 -> 248	0.41849
243 -> 252	0.11606

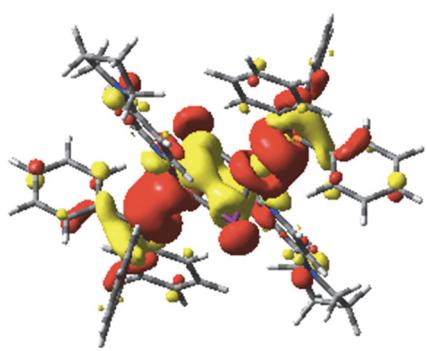
243 -> 253 -0.12943

Excited State 29: 4.1525 eV (298.58 nm) f=0.0000

241 -> 248	0.13424
241 -> 249	0.45490
241 -> 252	-0.20028
241 -> 253	-0.15764
242 -> 249	0.38739
242 -> 252	-0.14597

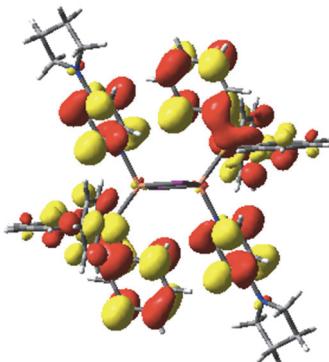
Excited State 30: 4.1571 eV (298.25 nm) f=0.0424

241 -> 250	-0.10301
242 -> 250	0.31901
242 -> 251	-0.10866
243 -> 249	0.54265
244 -> 254	-0.13190



occupied “hole”

→



unoccupied “electron”

Excited State 31: 4.1729 eV (297.12 nm) f=0.0000

241 -> 249	-0.20873
242 -> 249	0.19848
242 -> 252	0.18761
242 -> 253	0.11148
243 -> 250	0.53330
244 -> 253	0.12526

Excited State 32: 4.1917 eV (295.78 nm) f=0.0107

241 -> 247	0.10836
241 -> 250	-0.13579
241 -> 251	0.54737

242 -> 251 0.33562

Excited State 33: 4.2040 eV (294.92 nm) f=0.0088

241 -> 247 0.12189
241 -> 250 0.50395
241 -> 251 0.12957
241 -> 254 0.20132
242 -> 250 0.32927
242 -> 251 0.11319
242 -> 254 0.13462

Excited State 34: 4.2067 eV (294.73 nm) f=0.0000

241 -> 249 -0.19405
241 -> 252 -0.28559
241 -> 253 0.16428
242 -> 252 -0.26021
242 -> 253 0.10355
243 -> 251 -0.22178
244 -> 257 -0.12363
244 -> 259 0.39396

Excited State 35: 4.2075 eV (294.67 nm) f=0.0000

241 -> 252 0.38909
241 -> 253 -0.11216
242 -> 252 0.21923
242 -> 253 -0.15014
243 -> 251 -0.18947
243 -> 254 0.10392
244 -> 257 -0.11880
244 -> 259 0.36929

Excited State 36: 4.2360 eV (292.69 nm) f=0.0018

239 -> 249 0.16383
240 -> 245 0.10426
241 -> 250 -0.11777
241 -> 254 0.11257
242 -> 250 0.16072
242 -> 254 -0.22183

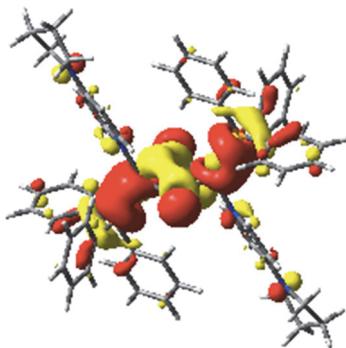
243 -> 252	0.15649
243 -> 253	0.32211
244 -> 261	0.42202

Excited State 37: 4.2388 eV (292.50 nm) f=0.0000

242 -> 252	0.10475
243 -> 251	0.48653
243 -> 254	-0.10284
244 -> 259	0.35621
244 -> 262	-0.21352

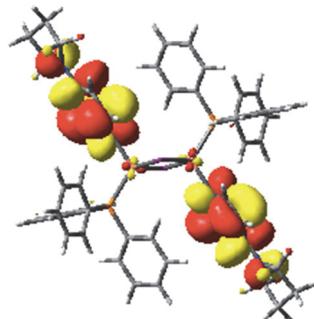
Excited State 38: 4.2530 eV (291.52 nm) f=0.0871

240 -> 245	-0.15681
241 -> 250	-0.13262
242 -> 251	0.10302
243 -> 249	-0.11466
243 -> 252	0.56038
243 -> 253	-0.14626
244 -> 261	-0.15072



occupied "hole"

→



unoccupied "electron"

Excited State 39: 4.2647 eV (290.72 nm) f=0.0000

239 -> 250	-0.14852
240 -> 246	0.14460
240 -> 247	0.18372
242 -> 249	-0.17378
242 -> 253	-0.23856
243 -> 250	0.16095
243 -> 251	0.21379
243 -> 254	0.32867

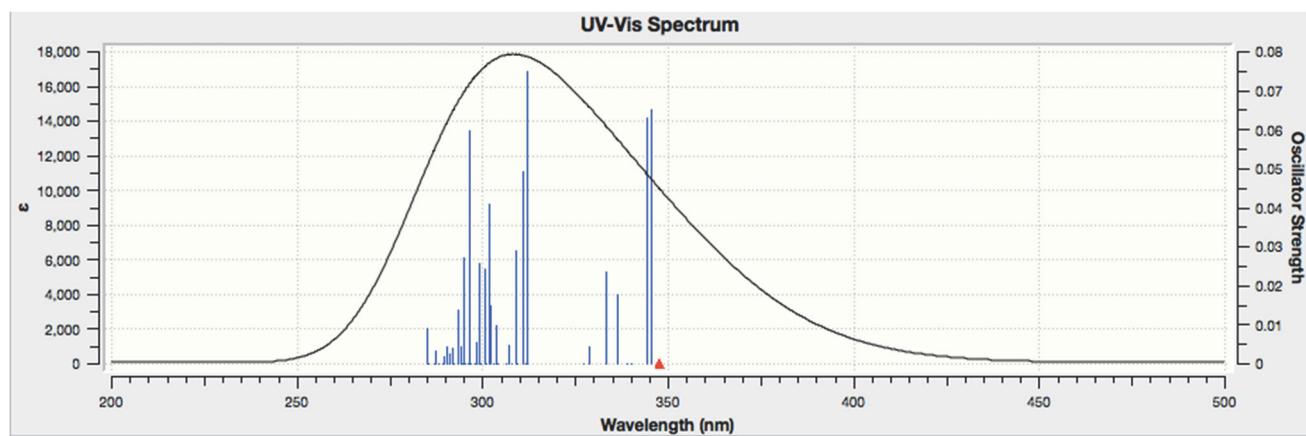
244 -> 257	-0.14812
244 -> 262	0.25670

Excited State 40: 4.2710 eV (290.29 nm) f=0.0047

242 -> 254	-0.18228
243 -> 259	-0.13518
244 -> 258	0.25073
244 -> 260	0.52381
244 -> 261	-0.22623

Scheme S2. Energy, oscillator strength, and transition orbitals for complex **2**.

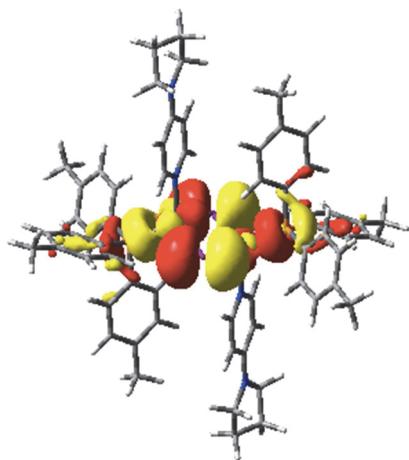
Simulated UV spectrum:



Excited State 1: 3.5652 eV (347.76 nm) f = 0.0000

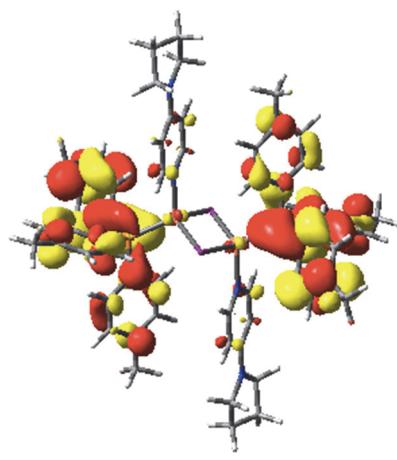
267 -> 270 0.16990

268 -> 269 0.67396



occupied “hole”

→



unoccupied “electron”

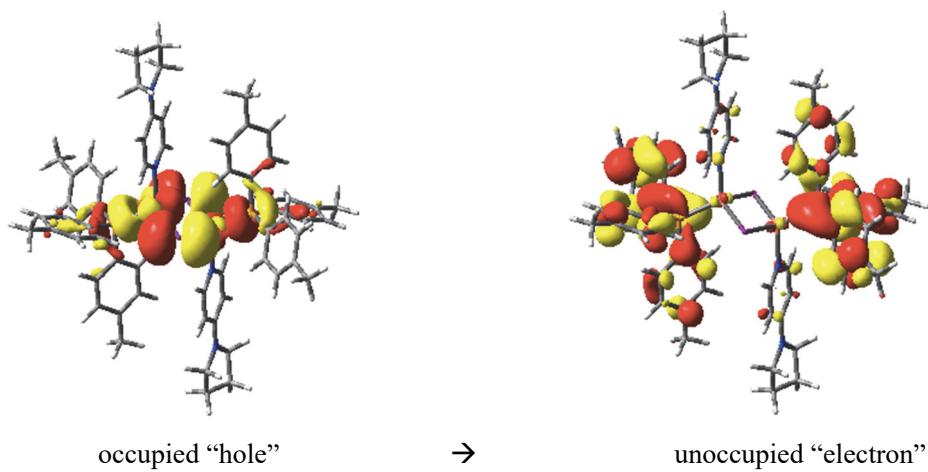
Excited State 2: 3.5875 eV (345.60 nm) f = 0.0651

267 -> 269 0.16808

268 -> 270 0.63815

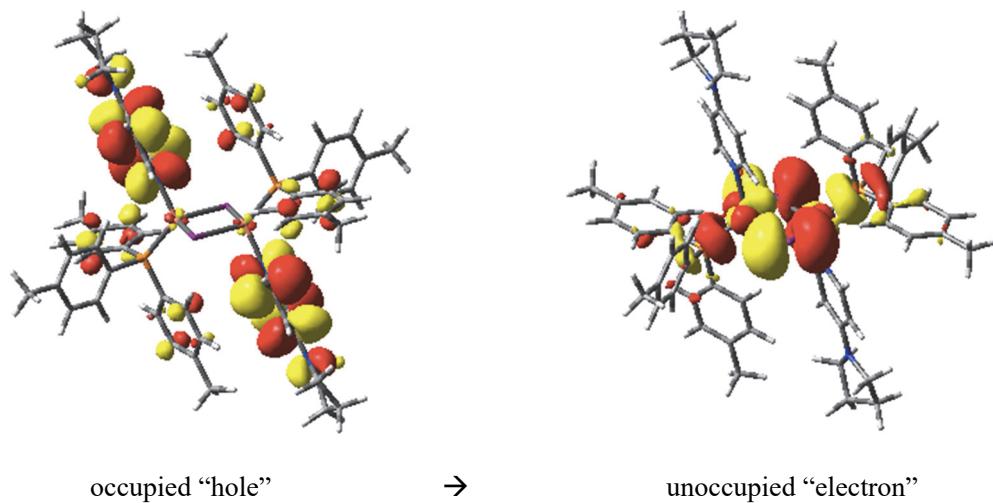
268 -> 271 -0.19741

268 -> 275 -0.11623



Excited State 3: 3.6028 eV (344.14 nm) f = 0.0629

267 -> 272	0.11393
268 -> 270	0.21509
268 -> 271	0.64682
268 -> 275	0.10165



Excited State 4: 3.6455 eV (340.10 nm) f = 0.0000

267 -> 271	0.12678
268 -> 272	0.29415
268 -> 273	0.57871
268 -> 276	-0.18842

Excited State 5: 3.6560 eV (339.12 nm) f = 0.0000

267 -> 271	0.12087
268 -> 272	0.60285
268 -> 273	-0.29728

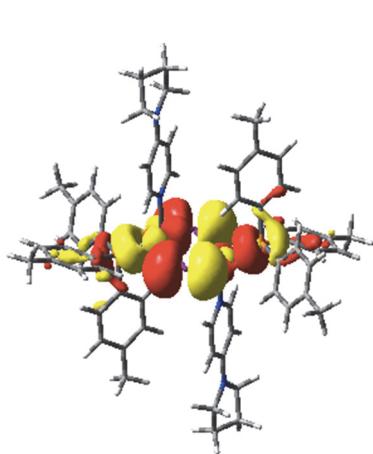
268 -> 277 0.13541

Excited State 6: 3.6859 eV (336.37 nm) f = 0.0176

268 -> 274 0.48171

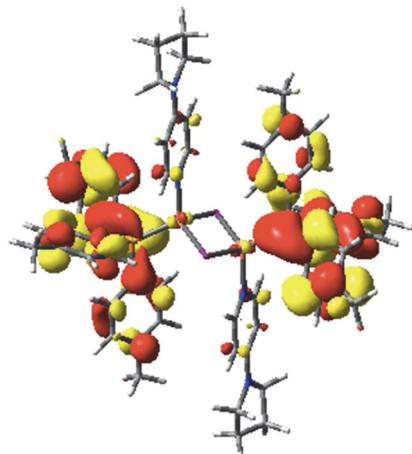
268 -> 275 0.45762

268 -> 278 0.14999



occupied "hole"

→



unoccupied "electron"

Excited State 7: 3.7194 eV (333.34 nm) f = 0.0235

268 -> 274 -0.40577

268 -> 275 0.46603

268 -> 276 -0.17967

268 -> 278 -0.20355

Excited State 8: 3.7196 eV (333.33 nm) f = 0.0021

268 -> 273 0.12504

268 -> 274 -0.12209

268 -> 275 0.13921

268 -> 276 0.60081

268 -> 277 -0.23237

Excited State 9: 3.7716 eV (328.73 nm) f = 0.0045

267 -> 273 0.14631

268 -> 274 -0.24308

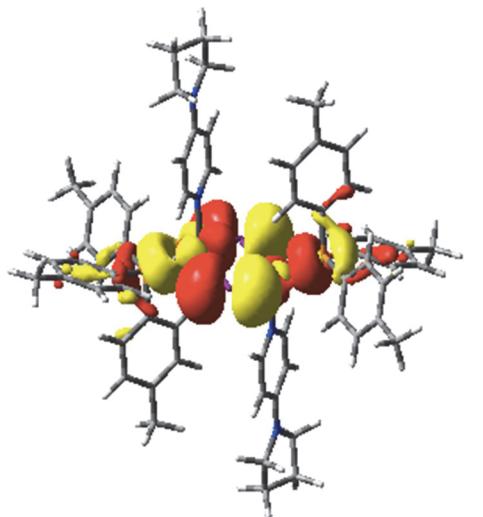
268 -> 278 0.62764

Excited State 10: 3.7874 eV (327.36 nm) f = 0.0000

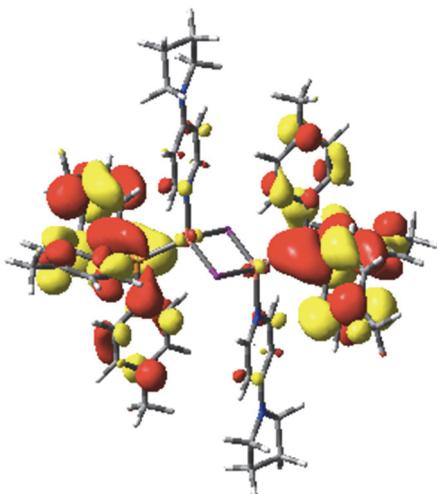
267 -> 274	-0.17263
268 -> 273	0.17708
268 -> 276	0.20894
268 -> 277	0.61354

Excited State 11: 3.9746 eV (311.94 nm) f = 0.0748

263 -> 273	0.14350
263 -> 276	-0.18952
265 -> 270	0.15017
265 -> 271	-0.23131
265 -> 275	-0.29388
266 -> 270	0.11544
266 -> 271	-0.14302
266 -> 275	-0.20409
267 -> 269	0.16351
267 -> 273	-0.10601
267 -> 276	0.14989
268 -> 279	0.30260



occupied “hole”



→

unoccupied “electron”

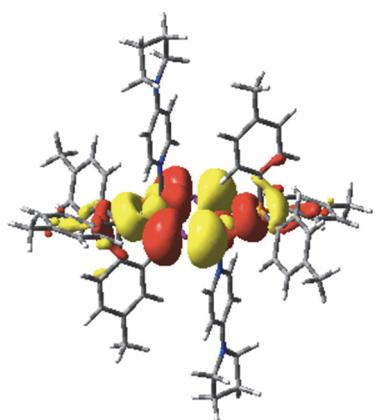
Excited State 12: 3.9791 eV (311.59 nm) f = 0.0000

263 -> 271	0.14745
263 -> 275	0.24938
265 -> 273	-0.27426
265 -> 276	0.29448

266 -> 273	-0.19365
266 -> 276	0.20696
267 -> 270	0.13406
267 -> 271	-0.20620
267 -> 275	-0.19816

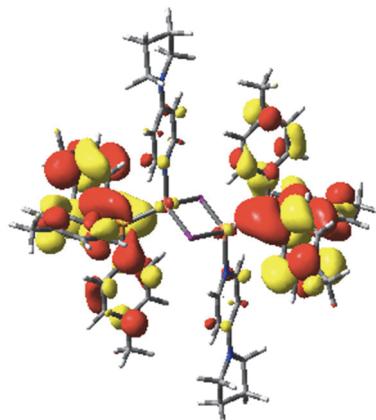
Excited State 13: 3.9901 eV (310.73 nm) f = 0.0491

263 -> 276	0.11160
265 -> 271	0.18105
265 -> 275	0.15421
266 -> 271	0.12279
266 -> 275	0.11060
268 -> 279	0.57296
268 -> 282	0.12834



occupied “hole”

→



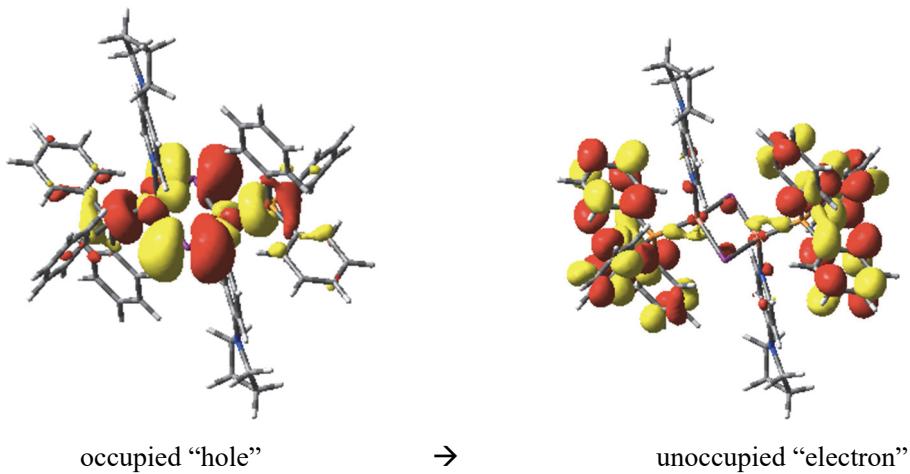
unoccupied “electron”

Excited State 14: 4.0060 eV (309.50 nm) f = 0.0000

263 -> 270	-0.12028
263 -> 278	-0.11041
265 -> 269	0.34878
265 -> 273	0.18614
265 -> 277	-0.16233
266 -> 269	0.29632
266 -> 273	0.13562
266 -> 277	-0.11450
267 -> 270	0.32153

Excited State 15: 4.0140 eV (308.88 nm) f = 0.0291

263 -> 269	-0.14479
265 -> 270	0.27230
265 -> 274	0.13368
265 -> 275	0.14964
265 -> 278	0.10497
266 -> 270	0.20104
266 -> 275	0.11537
267 -> 269	0.45597
267 -> 273	0.10496
268 -> 270	-0.13070



Excited State 16: 4.0289 eV (307.74 nm) f=0.0000

265 -> 272	-0.20477
265 -> 273	0.10918
265 -> 277	-0.14175
266 -> 269	-0.11781
266 -> 272	-0.13974
267 -> 270	-0.19711
267 -> 271	-0.32006
268 -> 280	-0.24797
268 -> 281	0.35760

Excited State 17: 4.0372 eV (307.10 nm) f=0.0046

263 -> 272	-0.12307
263 -> 273	0.13238
263 -> 277	-0.15715

265 -> 270	0.14455
265 -> 271	0.27250
265 -> 274	-0.18645
265 -> 275	-0.12332
265 -> 278	-0.24060
266 -> 270	0.12160
266 -> 271	0.20441
266 -> 274	-0.13856
266 -> 278	-0.16302
267 -> 269	0.13854
267 -> 272	0.22620
267 -> 277	0.11779
268 -> 279	-0.11425

Excited State 18: 4.0474 eV (306.33 nm) f=0.0000

265 -> 269	0.12763
265 -> 272	0.14269
265 -> 273	-0.11699
265 -> 277	0.12837
266 -> 273	-0.13092
266 -> 277	0.10497
267 -> 270	0.18773
267 -> 271	0.18821
267 -> 278	-0.12925
267 -> 279	-0.10821
268 -> 280	-0.27140
268 -> 281	0.41602

Excited State 19: 4.0789 eV (303.96 nm) f=0.0000

263 -> 275	0.10737
263 -> 278	-0.10424
265 -> 269	-0.22324
265 -> 276	0.17405
266 -> 269	0.37887
266 -> 276	0.19471
266 -> 277	-0.15097
267 -> 270	-0.20968
267 -> 271	0.29668

Excited State 20: 4.0826 eV (303.69 nm) f=0.0098

265 -> 271	-0.30229
265 -> 275	-0.16100
266 -> 270	-0.25193
266 -> 271	0.47886
266 -> 275	0.23072

Excited State 21: 4.0921 eV (302.98 nm) f=0.0000

263 -> 278	0.12547
265 -> 269	-0.25617
265 -> 273	-0.11669
265 -> 276	-0.23314
265 -> 277	0.18593
266 -> 269	0.41442
267 -> 271	-0.28370

Excited State 22: 4.1043 eV (302.08 nm) f=0.0147

263 -> 276	-0.12210
263 -> 277	0.11061
265 -> 270	-0.22348
265 -> 274	0.10497
265 -> 275	-0.16768
265 -> 278	0.21861
266 -> 270	0.28988
266 -> 271	0.21578
266 -> 278	0.12154
267 -> 272	0.33379
267 -> 273	0.11412

Excited State 23: 4.1071 eV (301.88 nm) f=0.0409

265 -> 270	-0.16408
265 -> 271	-0.21486
265 -> 275	0.11929
265 -> 278	-0.10862
266 -> 270	0.48326
266 -> 271	0.13917
266 -> 278	-0.11542
267 -> 272	-0.24985

267 -> 273 -0.10099

Excited State 24: 4.1178 eV (301.10 nm) f=0.0000

265 -> 273 -0.30879
265 -> 276 0.18673
266 -> 273 0.49210
266 -> 276 -0.27705

Excited State 25: 4.1236 eV (300.67 nm) f=0.0241

263 -> 269 0.16882
265 -> 270 -0.32659
265 -> 274 -0.11510
266 -> 274 -0.18557
266 -> 275 -0.13364
267 -> 269 0.27649
267 -> 272 -0.12407
267 -> 273 0.36613
267 -> 277 -0.13215
268 -> 278 -0.11027

Excited State 26: 4.1388 eV (299.56 nm) f=0.0000

263 -> 270 0.16319
263 -> 271 0.10391
265 -> 269 -0.33706
265 -> 272 -0.17210
266 -> 269 -0.17028
266 -> 272 -0.22681
267 -> 270 0.40150
267 -> 271 0.16257

Excited State 27: 4.1466 eV (299.00 nm) f=0.0258

263 -> 269 -0.13528
265 -> 270 0.31406
265 -> 271 0.11031
265 -> 278 0.12281
266 -> 271 0.18333
266 -> 274 -0.21243
266 -> 275 -0.20973

267 -> 269	-0.27688
267 -> 272	-0.21103
267 -> 273	0.24538

Excited State 28: 4.1471 eV (298.96 nm) f=0.0001

265 -> 269	-0.17316
265 -> 272	-0.25694
265 -> 276	0.11359
265 -> 277	-0.12042
266 -> 272	0.51217
266 -> 276	-0.12275
266 -> 277	0.12030
267 -> 270	0.11436
267 -> 274	0.16582

Excited State 29: 4.1537 eV (298.49 nm) f=0.0053

265 -> 274	-0.28213
265 -> 275	-0.23451
266 -> 270	0.10331
266 -> 271	-0.13798
266 -> 274	0.17683
266 -> 275	0.34079
266 -> 278	0.11581
267 -> 269	-0.11679
267 -> 273	0.31091

Excited State 30: 4.1615 eV (297.93 nm) f=0.0000

265 -> 269	-0.10312
265 -> 272	0.30124
265 -> 273	-0.14997
266 -> 277	-0.11980
267 -> 270	0.12025
267 -> 274	0.47292
267 -> 278	0.19747
268 -> 277	0.13031

Excited State 31: 4.1753 eV (296.95 nm) f=0.0000

263 -> 271	0.10685
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265 -> 269	0.10564
265 -> 272	-0.19492
265 -> 273	-0.14341
266 -> 272	-0.21065
266 -> 273	-0.18650
266 -> 276	-0.12939
267 -> 270	-0.10503
267 -> 271	0.13382
267 -> 274	0.13457
267 -> 275	0.44751
268 -> 283	0.16476

Excited State 32: 4.1831 eV (296.39 nm) f=0.0598

265 -> 271	0.29436
265 -> 275	-0.10381
266 -> 271	0.11803
266 -> 274	0.15648
267 -> 272	-0.30617
267 -> 273	-0.22763
267 -> 276	0.36065
267 -> 277	-0.18579

Excited State 33: 4.1873 eV (296.10 nm) f=0.0000

265 -> 277	0.16081
266 -> 272	0.16109
266 -> 273	0.18734
266 -> 276	0.29429
267 -> 271	-0.10160
267 -> 274	-0.20383
267 -> 275	0.22853
267 -> 278	0.13872
268 -> 280	-0.17396
268 -> 281	-0.13335
268 -> 283	0.31330
268 -> 286	-0.11181

Excited State 34: 4.1960 eV (295.48 nm) f=0.0000

265 -> 272	-0.17073
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265 -> 273	-0.16342
265 -> 276	-0.21978
266 -> 272	0.13899
266 -> 273	0.10075
266 -> 276	0.32215
266 -> 277	-0.18116
267 -> 274	0.13010
267 -> 275	0.15947
267 -> 278	-0.12089
268 -> 280	0.20411
268 -> 281	0.11780
268 -> 283	-0.27767

Excited State 35: 4.2040 eV (294.92 nm) f=0.0272

265 -> 278	0.15048
266 -> 271	-0.16972
266 -> 274	-0.33275
266 -> 275	0.31352
266 -> 278	-0.25501
267 -> 272	0.12500
267 -> 276	0.34020

Excited State 36: 4.2095 eV (294.53 nm) f=0.0000

265 -> 272	-0.22216
265 -> 273	-0.14941
265 -> 276	-0.22869
266 -> 277	-0.14505
267 -> 271	0.14963
267 -> 274	0.10705
267 -> 275	-0.29394
267 -> 278	-0.13698
268 -> 280	-0.17762
268 -> 281	-0.12497
268 -> 283	0.31966

Excited State 37: 4.2129 eV (294.29 nm) f=0.0043

263 -> 273	-0.10724
265 -> 274	-0.30023

265 -> 275	0.23706
266 -> 278	0.26840
267 -> 276	0.32294
267 -> 277	0.24845
268 -> 282	0.10658
268 -> 285	0.15140

Excited State 38: 4.2262 eV (293.37 nm) f=0.0137

263 -> 276	-0.12421
265 -> 270	-0.10492
265 -> 271	0.19910
265 -> 275	-0.14363
265 -> 278	0.24684
266 -> 274	-0.12831
267 -> 269	0.10569
267 -> 272	-0.20692
267 -> 276	-0.18637
267 -> 277	0.34229
268 -> 285	0.26091

Excited State 39: 4.2394 eV (292.46 nm) f=0.0000

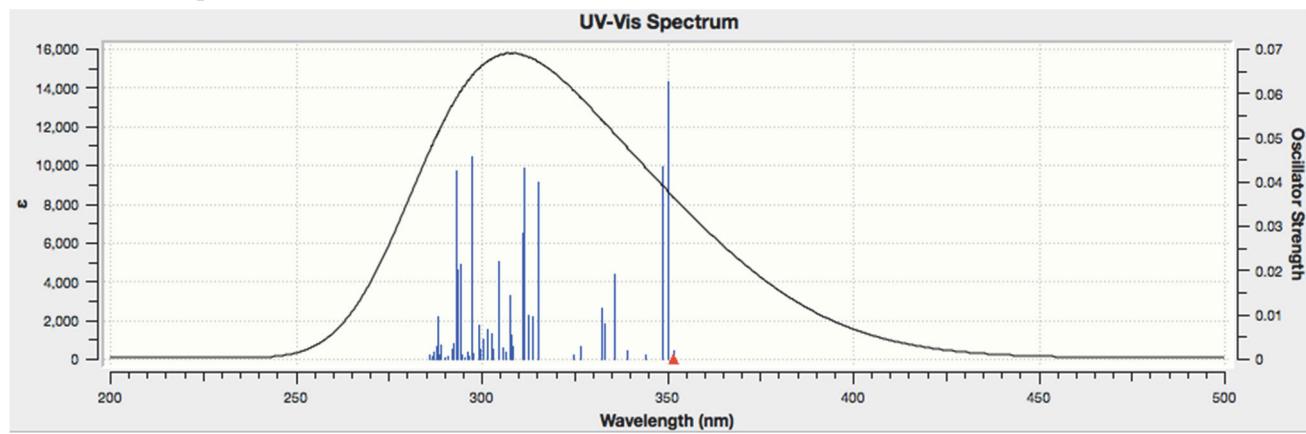
265 -> 272	0.14095
267 -> 271	-0.12077
267 -> 278	-0.27590
268 -> 280	0.33443
268 -> 281	0.18631
268 -> 283	0.34635
268 -> 286	0.23735

Excited State 40: 4.2409 eV (292.36 nm) f=0.0000

265 -> 272	-0.12357
265 -> 277	0.15394
266 -> 277	0.10527
267 -> 275	-0.18281
267 -> 278	0.40955
268 -> 280	0.32067
268 -> 281	0.23306
268 -> 283	0.15912

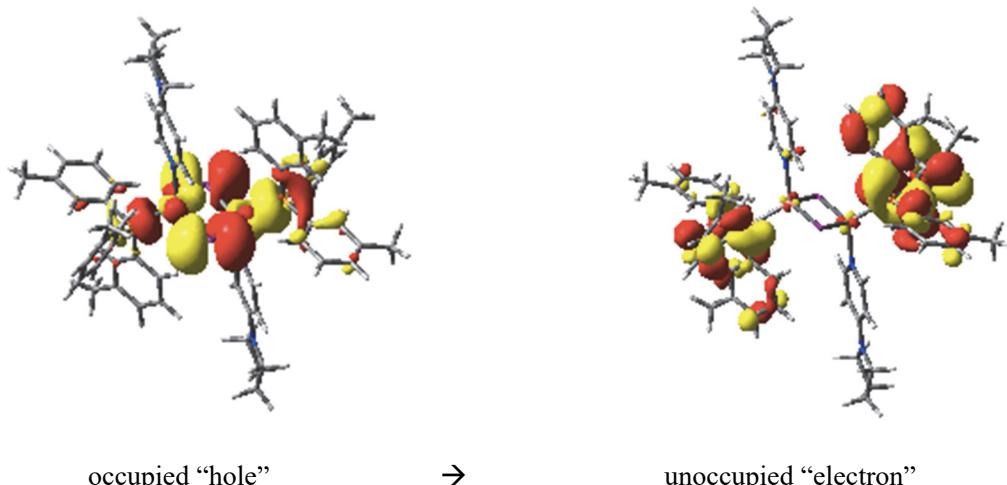
Scheme S3. Energy, oscillator strength, and transition orbitals for complex **3**.

Simulated UV spectrum:



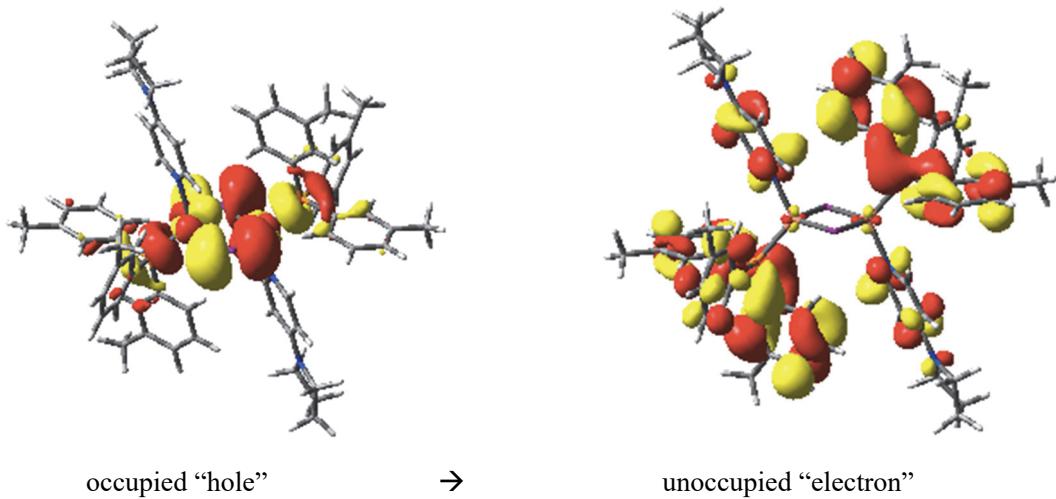
Excited State 1: 3.5261 eV (351.62 nm) f = 0.0019

267 -> 269	-0.11585
268 -> 269	0.58497
268 -> 270	0.27140
268 -> 271	-0.21622



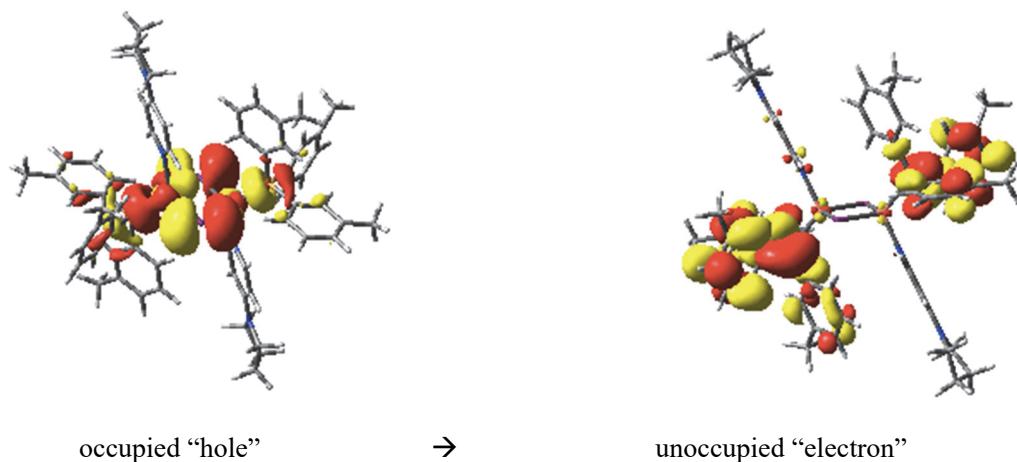
Excited State 2: 3.5395 eV (350.29 nm) f = 0.0628

268 -> 269	-0.24524
268 -> 270	0.62614
268 -> 271	0.13550



Excited State 3: 3.5577 eV (348.50 nm) f = 0.0435

267 -> 270	-0.10341
268 -> 269	0.25053
268 -> 271	0.62411



Excited State 4: 3.6033 eV (344.08 nm) f = 0.0009

267 -> 270	-0.12207
267 -> 271	-0.10558
268 -> 272	0.66896

Excited State 5: 3.6544 eV (339.27 nm) f = 0.0019

268 -> 272	0.10057
268 -> 273	0.64073
268 -> 274	0.10212
268 -> 275	-0.10241
268 -> 276	-0.12590

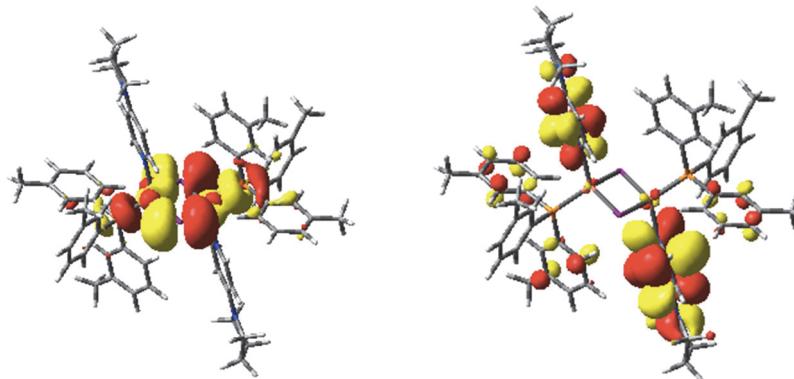
268 -> 277 -0.12332

Excited State 6: 3.6947 eV (335.58 nm) f = 0.0191

268 -> 274 0.31665

268 -> 275 0.58801

268 -> 276 -0.11789



occupied “hole”

→

unoccupied “electron”

Excited State 7: 3.7209 eV (333.21 nm) f = 0.0080

268 -> 273 0.16455

268 -> 274 -0.35094

268 -> 275 0.27532

268 -> 276 0.44011

268 -> 277 -0.21293

Excited State 8: 3.7308 eV (332.32 nm) f = 0.0116

268 -> 274 0.40874

268 -> 275 -0.14890

268 -> 276 0.47659

268 -> 278 0.23725

Excited State 9: 3.7958 eV (326.64 nm) f = 0.0029

267 -> 273 -0.13763

268 -> 273 0.10188

268 -> 274 -0.24278

268 -> 277 0.40095

268 -> 278 0.45582

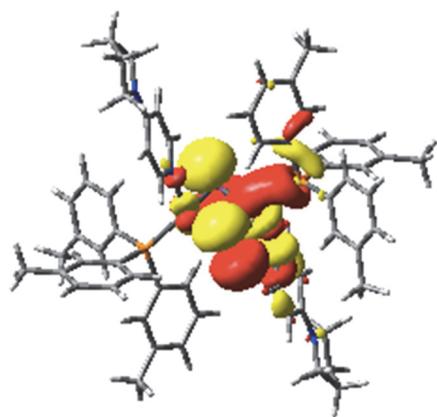
268 -> 279 0.11826

Excited State 10: 3.8192 eV (324.63 nm) f = 0.0008

267 -> 274	0.16537
268 -> 273	0.13295
268 -> 276	0.14893
268 -> 277	0.48114
268 -> 278	-0.40922

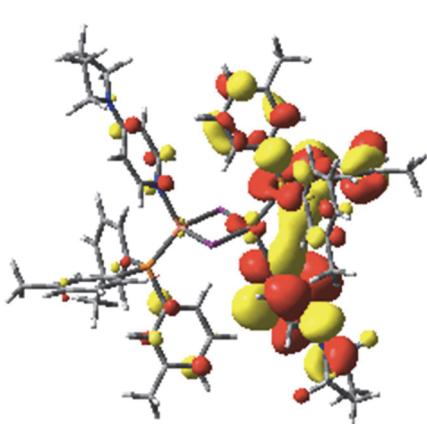
Excited State 11: 3.9343 eV (315.14 nm) f = 0.0399

263 -> 273	0.10206
263 -> 276	-0.15534
265 -> 270	-0.16842
265 -> 271	-0.14406
265 -> 275	0.13687
266 -> 269	-0.10166
266 -> 270	0.21858
266 -> 271	0.18111
266 -> 275	-0.18290
267 -> 269	-0.15369
267 -> 270	0.16745
267 -> 271	0.20856
267 -> 272	-0.14090
267 -> 273	0.12332
267 -> 275	-0.17240
267 -> 276	-0.16092



occupied “hole”

→



unoccupied “electron”

Excited State 12: 3.9515 eV (313.76 nm) f = 0.0095

263 -> 270	-0.12198
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263 -> 271	-0.12098
263 -> 275	0.11859
265 -> 269	-0.14806
265 -> 270	-0.18573
265 -> 276	-0.14757
266 -> 269	0.25887
266 -> 270	0.29322
266 -> 271	0.10553
266 -> 272	0.10524
266 -> 276	0.22112
267 -> 270	-0.12066
267 -> 271	-0.20196

Excited State 13: 3.9650 eV (312.70 nm) f = 0.0098

265 -> 270	-0.11177
265 -> 271	0.13913
266 -> 269	-0.14096
266 -> 270	0.16576
266 -> 271	-0.18688
267 -> 269	0.10368
267 -> 270	0.39793
267 -> 271	-0.36798
268 -> 271	0.10722

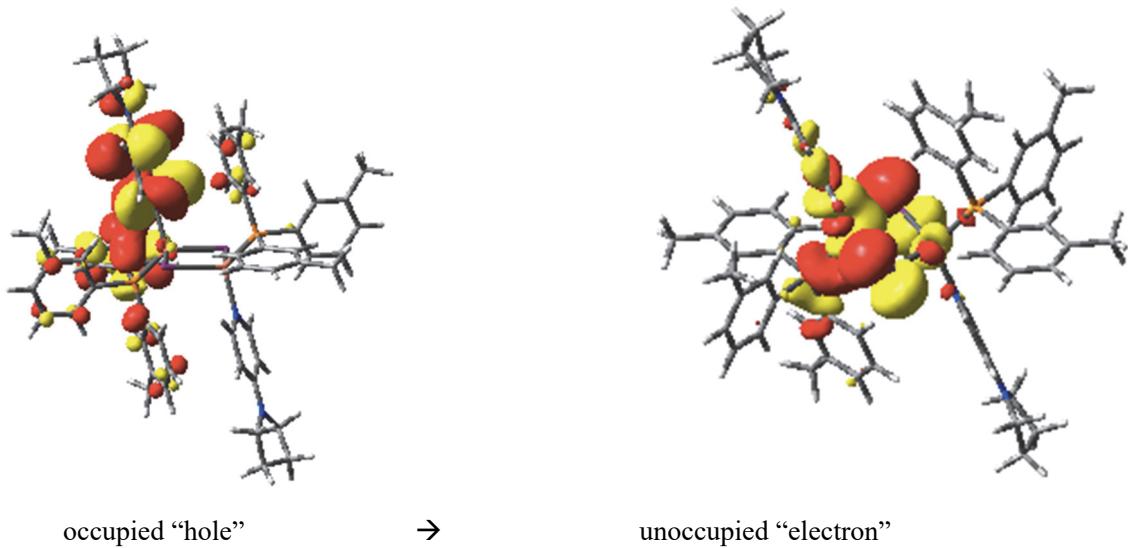
Excited State 14: 3.9673 eV (312.52 nm) f = 0.0037

263 -> 269	-0.11869
265 -> 269	-0.21026
265 -> 276	0.10018
266 -> 269	0.43890
266 -> 273	0.13134
266 -> 276	-0.13293
267 -> 269	-0.24001
267 -> 270	0.20376

Excited State 15: 3.9833 eV (311.26 nm) f = 0.0430

263 -> 273	-0.11766
265 -> 272	0.10518
265 -> 273	0.11324

266 -> 272	-0.13126
266 -> 273	-0.15132
266 -> 275	0.11687
267 -> 269	-0.10297
267 -> 270	0.12879
267 -> 272	-0.21035
267 -> 273	-0.18052
267 -> 275	0.12146
267 -> 277	0.14689
268 -> 279	0.29742
268 -> 280	0.22539
268 -> 281	0.15971



Excited State 16: 3.9846 eV (311.16 nm) f=0.0283

263 -> 275	-0.11054
265 -> 272	-0.10690
265 -> 273	-0.11424
266 -> 272	0.15624
266 -> 273	0.15013
267 -> 270	-0.17257
267 -> 272	0.12068
267 -> 273	0.12378
267 -> 275	-0.12726
268 -> 279	0.41775
268 -> 280	0.28065

Excited State 17: 4.0195 eV (308.46 nm) f=0.0030

263 -> 273	0.11247
265 -> 275	0.18984
266 -> 270	-0.10461
266 -> 272	-0.14459
266 -> 274	-0.14552
266 -> 275	-0.28888
266 -> 278	-0.10711
267 -> 272	0.15924
268 -> 281	0.36694

Excited State 18: 4.0277 eV (307.83 nm) f=0.0053

263 -> 275	-0.13501
265 -> 269	0.12751
265 -> 271	-0.10853
266 -> 272	0.15503
266 -> 273	0.11807
266 -> 274	0.10725
266 -> 275	0.14483
266 -> 276	-0.10400
268 -> 279	-0.12898
268 -> 281	0.50609

Excited State 19: 4.0301 eV (307.65 nm) f=0.0145

265 -> 269	-0.25897
265 -> 270	0.43898
265 -> 271	0.18206
265 -> 275	-0.12859
266 -> 269	-0.16080
266 -> 270	0.31520
266 -> 271	0.16828

Excited State 20: 4.0464 eV (306.40 nm) f=0.0015

265 -> 269	0.37148
265 -> 270	0.26251
266 -> 269	0.26755
266 -> 270	0.19674
266 -> 276	0.17307

267 -> 269	0.16327
267 -> 271	0.14611

Excited State 21: 4.0557 eV (305.71 nm) f=0.0025

263 -> 277	0.11011
263 -> 278	0.10393
265 -> 269	0.25920
265 -> 270	0.12790
265 -> 273	0.10877
265 -> 276	0.16477
265 -> 277	-0.11830
266 -> 269	0.12236
266 -> 273	-0.15237
266 -> 276	-0.15437
266 -> 277	0.13697
267 -> 271	-0.13482
267 -> 272	0.26863
267 -> 273	-0.16134
267 -> 276	-0.11843
267 -> 277	0.16937
267 -> 278	0.10374

Excited State 22: 4.0692 eV (304.69 nm) f=0.0219

265 -> 269	0.14685
265 -> 271	0.30563
265 -> 278	0.10427
266 -> 269	0.17474
266 -> 271	0.42757
266 -> 276	-0.10913
266 -> 278	-0.13459
267 -> 269	0.15093
267 -> 272	-0.13975

Excited State 23: 4.0711 eV (304.55 nm) f=0.0049

263 -> 276	-0.11003
263 -> 278	-0.12591
265 -> 270	-0.11293
265 -> 271	0.34930

265 -> 274	-0.10813
265 -> 276	-0.12627
265 -> 278	-0.16378
266 -> 272	-0.12209
266 -> 274	0.18601
266 -> 276	0.14931
266 -> 278	0.24390
267 -> 271	0.13177
267 -> 272	0.24160

Excited State 24: 4.0931 eV (302.91 nm) f=0.0023

263 -> 269	0.14516
265 -> 269	0.12614
265 -> 272	0.18966
266 -> 270	-0.10902
266 -> 272	0.38874
267 -> 269	-0.38508
267 -> 270	0.10307

Excited State 25: 4.0979 eV (302.55 nm) f=0.0056

263 -> 269	-0.12856
265 -> 269	-0.18175
265 -> 272	0.39009
266 -> 272	0.30275
267 -> 269	0.35064

Excited State 26: 4.1115 eV (301.55 nm) f=0.0067

263 -> 270	-0.18294
265 -> 270	0.17546
265 -> 271	-0.28800
265 -> 272	-0.22689
266 -> 270	-0.25499
266 -> 271	0.23503
267 -> 270	0.28829
267 -> 271	-0.11378

Excited State 27: 4.1271 eV (300.41 nm) f=0.0045

265 -> 272	-0.14875
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265 -> 273	0.43548
265 -> 275	-0.13577
265 -> 276	-0.16115
266 -> 273	0.36951
266 -> 275	-0.14218
266 -> 276	-0.10247

Excited State 28: 4.1377 eV (299.65 nm) f=0.0021

263 -> 271	-0.12822
265 -> 270	-0.14734
265 -> 272	-0.19573
265 -> 274	0.10352
265 -> 278	0.10421
266 -> 270	0.16916
266 -> 275	0.20608
266 -> 276	-0.11801
266 -> 278	-0.11351
267 -> 270	0.14391
267 -> 271	0.30773
267 -> 272	0.27551

Excited State 29: 4.1420 eV (299.33 nm) f=0.0076

265 -> 271	-0.11642
265 -> 272	0.27429
265 -> 273	0.19687
266 -> 271	0.13453
266 -> 272	-0.21756
266 -> 274	0.16670
266 -> 275	0.11502
267 -> 271	-0.17440
267 -> 272	0.15858
267 -> 273	0.29057
267 -> 277	-0.11503

Excited State 30: 4.1629 eV (297.83 nm) f=0.0012

265 -> 270	0.10397
265 -> 274	0.23292
265 -> 275	0.46281

265 -> 276	-0.13247
266 -> 273	0.14841
266 -> 275	0.23920
267 -> 272	-0.10809
267 -> 273	-0.18746

Excited State 31: 4.1699 eV (297.33 nm) f=0.0457

265 -> 271	0.16842
265 -> 276	-0.10883
266 -> 271	-0.15901
266 -> 272	0.12225
266 -> 273	-0.21010
266 -> 274	0.21750
267 -> 272	-0.20460
267 -> 273	0.32769
267 -> 274	0.23817

Excited State 32: 4.1784 eV (296.73 nm) f=0.0006

265 -> 276	0.28189
265 -> 277	-0.11677
266 -> 273	0.22994
266 -> 276	0.25096
267 -> 274	0.36566
267 -> 275	0.24075
267 -> 278	0.10408

Excited State 33: 4.1881 eV (296.04 nm) f=0.0016

265 -> 273	0.25531
265 -> 275	0.13121
265 -> 276	0.32592
265 -> 277	-0.13391
266 -> 275	0.15707
266 -> 276	0.25784
266 -> 277	-0.11064
267 -> 274	-0.15696
267 -> 275	-0.23935
268 -> 280	-0.13550
268 -> 283	0.11978

Excited State 34: 4.1962 eV (295.47 nm) f=0.0004

266 -> 277	-0.10177
267 -> 274	-0.24750
268 -> 279	-0.32373
268 -> 280	0.47339
268 -> 283	-0.11269
268 -> 286	-0.15388

Excited State 35: 4.2064 eV (294.75 nm) f=0.0009

263 -> 275	-0.10359
265 -> 276	0.16267
266 -> 274	0.16069
266 -> 275	-0.20314
267 -> 274	-0.21643
267 -> 275	0.40262
268 -> 279	0.15200
268 -> 280	-0.16713
268 -> 283	-0.12631

Excited State 36: 4.2116 eV (294.39 nm) f=0.0215

265 -> 270	-0.10602
265 -> 274	0.35611
265 -> 275	-0.16538
265 -> 277	0.11107
265 -> 278	0.27660
266 -> 274	0.24461
266 -> 275	-0.11530
266 -> 277	0.14309
266 -> 278	0.19694
267 -> 275	-0.11834
267 -> 276	0.20927

Excited State 37: 4.2226 eV (293.62 nm) f=0.0200

265 -> 274	-0.12291
267 -> 276	0.25515
268 -> 282	0.51418
268 -> 283	0.22949

Excited State 38: 4.2309 eV (293.05 nm) f=0.0425

265 -> 274	-0.18540
265 -> 275	0.10247
265 -> 278	-0.10321
266 -> 276	-0.10553
267 -> 276	0.49963
268 -> 282	-0.27323
268 -> 283	-0.14754

Excited State 39: 4.2413 eV (292.32 nm) f=0.0035

263 -> 273	0.12329
266 -> 274	0.18298
266 -> 277	-0.14225
266 -> 278	-0.10989
267 -> 277	0.17335
267 -> 278	-0.17979
268 -> 282	-0.30440
268 -> 283	0.35080
268 -> 285	0.19989

Excited State 40: 4.2444 eV (292.12 nm) f=0.0023

263 -> 273	-0.10580
266 -> 274	-0.13166
266 -> 277	0.14616
266 -> 278	0.12268
267 -> 275	0.13637
267 -> 277	-0.22502
267 -> 278	0.14851
268 -> 280	0.10175
268 -> 282	-0.13200
268 -> 283	0.43802
268 -> 285	-0.15722
268 -> 286	-0.10235

Cartesian coordinates of the optimized structures

Complex 1 in the S₀ state

I	6.52553600	1.56791000	0.26677300
Cu	3.95532400	0.83012300	0.80997000
P	3.65785600	0.80496200	3.06517500
N	0.32643400	4.92904600	-2.24813700
N	2.78258500	2.19616400	-0.25184300
C	0.82323200	6.12382100	-2.91214900
C	-0.37699100	6.60306800	-3.72228600
C	-1.56610500	6.15145000	-2.87786300
C	-1.11808400	4.79247300	-2.34932800
C	1.12213300	4.04487400	-1.59827500
C	0.61410200	2.85203200	-1.04551600
C	1.46841200	1.98387700	-0.39871400
C	3.27161600	3.32440300	-0.78155400
C	2.50561600	4.26014200	-1.44447400
C	1.90808000	0.64685900	3.60347400
C	1.15315200	-0.39240300	3.04771100
C	-0.18094600	-0.55391900	3.39564900
C	-0.78407300	0.32707400	4.28802000
C	-0.04411000	1.36860400	4.83259700
C	1.29646900	1.52798400	4.49609700
C	4.50331200	-0.52486700	4.00426200
C	3.91497100	-1.19978500	5.07485700
C	4.62458400	-2.18129800	5.75803900
C	5.92579500	-2.49151900	5.38149500
C	6.51439100	-1.82532800	4.31192000
C	5.80604900	-0.85208900	3.61958200
C	4.21967800	2.32667800	3.92401900
C	4.68881900	2.33235200	5.23873400
C	5.08562300	3.52279000	5.83593800
C	5.01583200	4.71726900	5.12818000
C	4.55611300	4.71803500	3.81643600
C	4.16795200	3.52790400	3.21434600
H	1.68608800	5.89067200	-3.54482100
H	1.14139800	6.87950000	-2.17900700
H	-0.35648700	7.67945300	-3.90262500

H	-0.39361000	6.09859500	-4.69375500
H	-2.50042400	6.09400600	-3.43937100
H	-1.71657600	6.84234600	-2.04214900
H	-1.55931700	4.55981400	-1.37451800
H	-1.39065500	3.98206500	-3.04118500
H	-0.43414800	2.59454200	-1.12838500
H	1.09058400	1.05550600	0.01884200
H	4.34282200	3.46840900	-0.66888200
H	2.98508700	5.14662100	-1.83955200
H	1.61486700	-1.06892600	2.33355300
H	-0.75277100	-1.36735400	2.96047000
H	-1.82893500	0.20321700	4.55436900
H	-0.50855900	2.06205100	5.52665200
H	1.86729800	2.34256500	4.92892000
H	2.89843200	-0.96254300	5.37136300
H	4.15768100	-2.70288700	6.58764500
H	6.47869500	-3.25595600	5.91875900
H	7.52515400	-2.07053900	4.00222600
H	6.25928500	-0.34523500	2.77203600
H	4.75355600	1.40165300	5.79305500
H	5.45452900	3.51585400	6.85667600
H	5.33027300	5.64512200	5.59522000
H	4.51481700	5.64477600	3.25342500
H	3.83460800	3.52061200	2.18113200
I	3.19795800	-1.56811700	-0.26643300
Cu	5.76813600	-0.83028700	-0.80979800
P	6.06552100	-0.80487000	-3.06502000
N	9.39728500	-4.92930400	2.24782100
N	6.94092800	-2.19637400	0.25183100
C	8.90055900	-6.12415000	2.91176000
C	10.10082900	-6.60340200	3.72182500
C	11.28989600	-6.15166800	2.87739800
C	10.84179800	-4.79267300	2.34897400
C	8.60152400	-4.04512300	1.59804700
C	9.10947100	-2.85220000	1.04538900
C	8.25509600	-1.98403300	0.39869000
C	6.45198100	-3.32469700	0.78144500
C	7.21805200	-4.26045800	1.44425000

C	7.81531500	-0.64688100	-3.60328600
C	8.57030400	0.39231600	-3.04748800
C	9.90441800	0.55375100	-3.39540500
C	10.50749400	-0.32725400	-4.28779700
C	9.76746700	-1.36871800	-4.83241400
C	8.42687400	-1.52801800	-4.49593400
C	5.22017600	0.52509600	-4.00398300
C	5.80852700	1.20000000	-5.07458100
C	5.09898400	2.18163700	-5.75765700
C	3.79783700	2.49199200	-5.38100200
C	3.20923000	1.82581100	-4.31142700
C	3.91750400	0.85245000	-3.61919000
C	5.50357500	-2.32648300	-3.92396700
C	5.03449700	-2.33201200	-5.23870900
C	4.63758200	-3.52235900	-5.83601800
C	4.70719500	-4.71689500	-5.12833500
C	5.16684900	-4.71780500	-3.81657100
C	5.55512400	-3.52776200	-3.21437700
H	8.03771100	-5.89108100	3.54447100
H	8.58240700	-6.87979200	2.17857300
H	10.08038200	-7.67980200	3.90208200
H	10.11745500	-6.09900400	4.69333300
H	12.22423200	-6.09422400	3.43887900
H	11.44037000	-6.84249600	2.04162800
H	11.28299000	-4.55992300	1.37416700
H	11.11435700	-3.98230300	3.04088200
H	10.15771100	-2.59466200	1.12823800
H	8.63286400	-1.05559700	-0.01877600
H	5.38078100	-3.46875500	0.66879800
H	6.73863900	-5.14700600	1.83924400
H	8.10862600	1.06884900	-2.33331600
H	10.47629400	1.36713500	-2.96019300
H	11.55236700	-0.20345700	-4.55413400
H	10.23187600	-2.06217300	-5.52648800
H	7.85599700	-2.34255200	-4.92878300
H	6.82501800	0.96265300	-5.37116800
H	5.56589100	2.70322000	-6.58726500
H	3.24499600	3.25653400	-5.91817700

H	2.19851700	2.07112400	-4.00165300
H	3.46426900	0.34559900	-2.77164200
H	4.96988800	-1.40126600	-5.79296900
H	4.26872900	-3.51530900	-6.85677400
H	4.39266700	-5.64468000	-5.59545300
H	5.20800100	-5.64458800	-3.25361900
H	5.88842300	-3.52058100	-2.18115000

Complex 1 in the S₁ state

I	-1.36899900	1.05606800	1.50166700
Cu	0.18023600	1.02766900	-0.63020700
P	-0.62618500	2.13285900	-2.52455200
N	1.98200800	1.96465600	-0.08248800
N	5.45256300	4.18841900	0.62505500
C	3.07539600	1.81335900	-0.84813700
C	4.24973100	2.51621400	-0.64989400
C	4.32950700	3.45955200	0.40131900
C	3.17587300	3.60138100	1.20645900
C	2.05174000	2.84715600	0.92728100
C	6.62698500	4.15986700	-0.24153000
C	7.44047700	5.36329600	0.22224100
C	7.08944800	5.47187300	1.70341700
C	5.60527900	5.12510700	1.73412200
C	-0.70571900	3.95197900	-2.27865600
C	-0.88482400	4.49577000	-0.98489000
C	-1.21973900	5.82869500	-0.81002300
C	-1.41739900	6.67165200	-1.91937000
C	-1.26499200	6.13861700	-3.20525100
C	-0.91798700	4.80847900	-3.39445500
C	0.66792500	1.93102700	-3.85798200
C	1.73208200	2.83379000	-3.94451800
C	2.74392500	2.64021800	-4.88477500
C	2.70347000	1.54104400	-5.74219800
C	1.64402700	0.63626900	-5.65549100
C	0.63308000	0.82793400	-4.71602100
C	-2.16152900	1.46573400	-3.26991300
C	-3.11791400	0.82542800	-2.44518900
C	-4.40327600	0.58345000	-2.89992700
C	-4.80148100	0.99065000	-4.18912700
C	-3.86910200	1.64494900	-5.00422700
C	-2.57526300	1.88723400	-4.56556700
H	2.99607800	1.08724400	-1.66170700
H	5.09304300	2.33171400	-1.31449300
H	3.14500000	4.30713800	2.03561600
H	1.15157900	2.94461200	1.54003000
H	6.33631200	4.23263400	-1.30211700

H	7.18843600	3.21418900	-0.11468700
H	8.51614400	5.24219700	0.03381900
H	7.10655900	6.26685100	-0.31280700
H	7.29904700	6.46145100	2.13232700
H	7.65926000	4.72800300	2.28364900
H	5.30010600	4.66263400	2.68700300
H	4.97371000	6.02127400	1.58214900
H	-0.76189300	3.85448000	-0.10891600
H	-1.32721800	6.22551200	0.20352700
H	-1.41191600	6.77970000	-4.07989000
H	-0.78474100	4.42722200	-4.40997800
H	1.75156500	3.69945400	-3.27617200
H	3.56563600	3.35851200	-4.95256100
H	1.60350600	-0.22574800	-6.32655900
H	-0.19929300	0.12225500	-4.64480500
H	-2.83989900	0.52806100	-1.43083300
H	-5.11284500	0.07209700	-2.24262000
H	-4.15823700	1.96555800	-6.00990600
H	-1.86394000	2.37824300	-5.23473400
I	0.88191100	-1.38725800	-1.44332900
Cu	-0.56421000	-1.41554500	0.79773800
P	0.66511300	-2.37955500	2.52995100
N	-2.33600900	-2.35188200	0.33791400
N	-6.16643300	-3.78939000	-0.53646000
C	-3.17383000	-2.74907500	1.31245000
C	-4.44320700	-3.24168700	1.07688400
C	-4.92026000	-3.33503800	-0.25231800
C	-4.02876600	-2.92200600	-1.26796900
C	-2.77675600	-2.44611300	-0.92895600
C	-7.09920800	-4.29002800	0.46761900
C	-8.21434700	-4.91399200	-0.36404200
C	-8.22152200	-4.06165600	-1.62997000
C	-6.74128400	-3.79532600	-1.87953100
C	1.41227300	-4.01482900	2.05338800
C	0.73510400	-4.79268400	1.10835300
C	1.24334900	-6.03417800	0.73023800
C	2.43557600	-6.49945500	1.28432400
C	3.11868900	-5.72079200	2.21772300

C	2.60918900	-4.48149300	2.60395100
C	-0.35287200	-2.78495200	4.03696300
C	-0.38744000	-4.06278200	4.60148300
C	-1.19322300	-4.31540200	5.71290500
C	-1.96163400	-3.29512200	6.26965000
C	-1.92849100	-2.01752600	5.70857400
C	-1.13312400	-1.76304200	4.59376100
C	2.09888600	-1.41897800	3.21838300
C	2.87331400	-0.67593100	2.32173600
C	3.97320000	0.04520800	2.78186500
C	4.29924200	0.03546100	4.13798300
C	3.52246700	-0.69680500	5.03473100
C	2.42390300	-1.42481300	4.57788500
H	-2.80271400	-2.65519200	2.33663600
H	-5.06361500	-3.52877300	1.92515500
H	-4.30757800	-2.95309200	-2.32031400
H	-2.08390100	-2.11284200	-1.70528500
H	-6.61024700	-5.02077400	1.13261700
H	-7.47706300	-3.46420700	1.10083400
H	-9.17779500	-4.92368700	0.16416800
H	-7.95696600	-5.95688900	-0.61050500
H	-8.71096200	-4.54921400	-2.48428000
H	-8.74494700	-3.11015700	-1.44316700
H	-6.56562900	-2.83374600	-2.38797200
H	-6.28261800	-4.58882500	-2.50001200
H	-0.18660200	-4.41470200	0.65636600
H	0.71050800	-6.63419500	-0.01129700
H	4.05806100	-6.07758300	2.64740500
H	3.15103500	-3.87104200	3.33062800
H	0.21424100	-4.86657500	4.17087300
H	-1.21588700	-5.31854500	6.14612400
H	-2.53109200	-1.21262200	6.13660300
H	-1.12358500	-0.76458500	4.14659700
H	2.60694000	-0.65330000	1.26150900
H	4.56788400	0.62710800	2.07337600
H	3.77068500	-0.70270600	6.09908000
H	1.81457000	-1.99379600	5.28449700
H	-2.59039200	-3.49501700	7.14082900

H	5.15857100	0.60596800	4.49946300
H	2.83879300	-7.46867700	0.98052900
H	-1.69235700	7.71922500	-1.78054700
H	3.49548500	1.38958900	-6.48028600
H	-5.81978900	0.81341300	-4.54148000

Complex 1 in the T₁ state

I	-1.35424000	1.03005100	1.51835000
Cu	0.21058000	1.07926900	-0.61761700
P	-0.49730600	2.21770400	-2.53216000
N	1.94279200	2.09659000	-0.17235900
N	5.44870000	4.24637200	0.55121300
C	3.05147700	1.87938500	-0.89895900
C	4.23814300	2.55718100	-0.69249300
C	4.31200800	3.54231200	0.32108300
C	3.13873000	3.75245900	1.08250000
C	2.00215600	3.01897500	0.80235900
C	6.65135500	4.14136600	-0.26975500
C	7.48992400	5.33510400	0.17368200
C	7.09239400	5.51657300	1.63582100
C	5.59681500	5.22130700	1.62798400
C	-0.60597800	4.02036500	-2.20148600
C	-0.96544300	4.48811200	-0.90996800
C	-1.37087900	5.79635700	-0.71350100
C	-1.47297300	6.69318000	-1.79493100
C	-1.15588600	6.23275400	-3.08045900
C	-0.73291200	4.92978300	-3.29330500
C	0.82074000	2.06989900	-3.83566000
C	1.86405700	3.00219200	-3.89123200
C	2.90260000	2.84150300	-4.80654500
C	2.91941500	1.74039000	-5.66403400
C	1.89027300	0.79940900	-5.59926500
C	0.85003900	0.95841400	-4.68683500
C	-1.99557900	1.46323500	-3.31812400
C	-2.93724700	0.78576800	-2.51536600
C	-4.19978900	0.48613200	-3.00688600
C	-4.57400200	0.87156600	-4.30382100
C	-3.65307200	1.56216400	-5.09846000
C	-2.38245300	1.85920800	-4.62111600
H	2.97235300	1.11889800	-1.68082500
H	5.09636100	2.31964700	-1.31994000
H	3.10397400	4.49340200	1.88004900
H	1.08674300	3.16327700	1.38146900
H	6.40110100	4.17849800	-1.34239000

H	7.17394600	3.18350300	-0.08290700
H	8.56648200	5.17013800	0.02876100
H	7.20640100	6.22638400	-0.40895500
H	7.32158200	6.51546600	2.03180300
H	7.61575300	4.77877400	2.26540600
H	5.24393100	4.80750800	2.58663800
H	5.00212800	6.13098200	1.41901900
H	-0.93264400	3.80342700	-0.05888500
H	-1.61552800	6.13254700	0.29826300
H	-1.23271300	6.91217800	-3.93493800
H	-0.48131800	4.60512000	-4.30653600
H	1.84592700	3.86232000	-3.21645500
H	3.70291100	3.58503900	-4.85290400
H	1.89835300	-0.06850400	-6.26364500
H	0.04755200	0.21843000	-4.62997300
H	-2.67084600	0.49953700	-1.49389800
H	-4.90496500	-0.05586800	-2.37011000
H	-3.92914800	1.86855200	-6.11176400
H	-1.67431800	2.38946700	-5.26385000
I	0.69665800	-1.36168100	-1.51436500
Cu	-0.68387900	-1.54621700	0.81665900
P	0.61159400	-2.46503100	2.49584500
N	-2.48237800	-2.40601800	0.38172500
N	-6.33043800	-3.83342200	-0.43751200
C	-3.34012200	-2.71490100	1.37062900
C	-4.61760500	-3.19577300	1.15359900
C	-5.08000400	-3.37698600	-0.17105000
C	-4.16925600	-3.05235100	-1.20171200
C	-2.91049800	-2.57887900	-0.88062900
C	-7.28020700	-4.24975300	0.58876300
C	-8.39033900	-4.92551300	-0.20845000
C	-8.37319200	-4.17169800	-1.53531300
C	-6.88730200	-3.93628800	-1.78321500
C	1.39005500	-4.08992200	2.03063300
C	0.72612000	-4.88544400	1.09110900
C	1.25595200	-6.11963300	0.71841900
C	2.45735400	-6.56025300	1.27268800
C	3.12803300	-5.76392600	2.20036600

C	2.59666000	-4.53201500	2.58060600
C	-0.35859900	-2.86999000	4.03494400
C	-0.35663400	-4.13868200	4.62040300
C	-1.13371800	-4.38886300	5.75276700
C	-1.90977100	-3.37468300	6.30998300
C	-1.91342400	-2.10596500	5.72786100
C	-1.14719800	-1.85423200	4.59210400
C	2.03964700	-1.46351000	3.14096500
C	2.77508800	-0.71473600	2.21654300
C	3.86341600	0.04471100	2.64074800
C	4.21779700	0.06739200	3.98975700
C	3.48089200	-0.67118000	4.91433600
C	2.39365200	-1.43688500	4.49273100
H	-2.97719400	-2.55781700	2.38990000
H	-5.25363600	-3.40940500	2.01193700
H	-4.43554000	-3.15971500	-2.25257600
H	-2.19910400	-2.31449900	-1.66739100
H	-6.80624200	-4.93278600	1.31267100
H	-7.65845200	-3.37614000	1.15396500
H	-9.36073200	-4.88707000	0.30554100
H	-8.13969500	-5.98621700	-0.37181600
H	-8.85538500	-4.71891100	-2.35705300
H	-8.89084700	-3.20481600	-1.42826600
H	-6.69748100	-3.01689000	-2.36047400
H	-6.42733100	-4.77728000	-2.33687600
H	-0.20270000	-4.52458700	0.63945700
H	0.73290000	-6.73327400	-0.01901700
H	4.07459600	-6.10130200	2.63011900
H	3.12886800	-3.90756800	3.30259400
H	0.25131000	-4.93777900	4.18969600
H	-1.12768700	-5.38520800	6.20211200
H	-2.52180500	-1.30561600	6.15648600
H	-1.16541800	-0.86320300	4.12827100
H	2.48500400	-0.71962800	1.16204900
H	4.42680900	0.63117200	1.91048100
H	3.75099700	-0.65200000	5.97324700
H	1.81457000	-2.00933300	5.22169900
H	-2.51544300	-3.57236100	7.19794500

H	5.06756700	0.66835300	4.32359400
H	2.87761400	-7.52369900	0.97341900
H	-1.80712900	7.72052500	-1.63757500
H	3.73582400	1.61264400	-6.37955500
H	-5.57306800	0.64651600	-4.68407700

Complex 2 in the S₀ state

I	1.42055200	2.09779400	3.87994800
I	1.33835100	4.90364300	7.52807200
Cu	2.47366800	4.29402300	5.11122000
Cu	0.30447300	2.69780300	6.29982400
P	0.46115400	0.91702000	7.70869000
P	2.31701300	6.07548700	3.70572500
N	8.33989900	2.72448300	6.67570700
N	4.41077000	3.71903200	5.64610300
C	7.06690000	3.04841200	6.33973600
C	9.14212600	3.48066700	7.62396500
H	8.57708700	3.68891700	8.53858500
H	9.45318700	4.44551200	7.19710300
C	10.33965600	2.57096700	7.87879000
H	11.23143000	3.12700200	8.17404600
H	10.10312100	1.86314000	8.67975500
C	2.13680900	0.23926700	8.01956700
C	6.43611800	4.20540000	6.83922500
H	6.95302700	4.88727400	7.50239200
C	2.94259500	5.75798800	2.00982200
C	-0.40390000	5.83474500	3.25408200
H	-0.20720100	4.77061200	3.34913400
C	10.49766900	1.82887200	6.55398300
H	11.06855200	0.90248200	6.64067600
H	11.00267700	2.46908700	5.82352100
C	5.00299200	2.61511400	5.17384300
H	4.38841900	1.99502900	4.52680600
C	0.63851200	6.75143200	3.40558400
C	4.00224000	4.86118600	1.86963600
H	4.39682100	4.35658100	2.74597000
C	-0.49626700	-0.55878100	7.17680500
C	3.27461300	7.55394400	4.23045200
C	6.29583100	2.24368000	5.47860200
H	6.68784200	1.32198600	5.06792100
C	9.05568100	1.58770500	6.11872500
H	8.95098200	1.55365800	5.02919000
H	8.66608200	0.64086200	6.52053700
C	-0.16957800	1.23554300	9.40245800

C	4.53406600	4.61100300	0.61187000
H	5.35988800	3.91508700	0.50384700
C	2.41312900	6.37341000	0.87574200
H	1.57698300	7.05894800	0.98081700
C	-1.41324100	-1.21141300	7.99890200
H	-1.56626200	-0.86012600	9.01509500
C	2.92826900	6.11754300	-0.39468000
C	0.37329100	8.11708500	3.30914200
H	1.18219900	8.83071700	3.43785200
C	-0.30712400	-1.01330500	5.86700400
H	0.38973700	-0.49897600	5.21113900
C	-0.91601600	8.58771000	3.05732600
C	4.16723100	8.22220700	3.39404300
H	4.30320100	7.87914600	2.37261500
C	0.31459200	0.57971700	10.53497000
H	1.11911300	-0.14239300	10.44318100
C	5.13718600	4.48537100	6.46972500
H	4.63837800	5.36949400	6.85495300
C	-2.14281300	-2.31187700	7.54317900
C	-1.74462700	2.47103900	10.78486300
C	-1.92688500	-2.75920300	6.24188900
H	-2.47916200	-3.61966300	5.87393000
C	2.40199000	-1.12655000	8.11268500
H	1.59477400	-1.84021200	7.97386400
C	4.00184300	5.23444800	-0.50945100
H	4.41816400	5.02565900	-1.49124000
C	-1.25538300	1.79551400	11.90213800
H	-1.67390400	2.01075500	12.88157000
C	3.10747400	7.99734200	5.54678000
H	2.42867000	7.47152500	6.21248300
C	-1.68631900	6.29323300	2.98719500
H	-2.49484000	5.57930200	2.86643200
C	-1.93969200	7.65637400	2.88928500
H	-2.94846000	8.00530100	2.68398100
C	-1.18635000	2.17957800	9.54113800
H	-1.53718600	2.70785500	8.65855800
C	3.81381000	9.10348500	5.99575600
H	3.67489900	9.45148600	7.01459500

C	-1.19364200	10.06310600	2.99681300
H	-2.04231300	10.28322500	2.34401700
H	-0.32707600	10.61717900	2.62762200
H	-1.43221800	10.45673600	3.99121800
C	-1.01585700	-2.11499000	5.41120400
H	-0.85983000	-2.47151900	4.39780900
C	-2.80905200	3.52224100	10.91636400
H	-3.44833200	3.55318500	10.03054400
H	-2.35849400	4.51457000	11.02818900
H	-3.44075300	3.34464600	11.79041800
C	4.45734500	0.69739300	8.46086900
H	5.26410300	1.41140100	8.59236200
C	3.68936500	-1.59730100	8.37408600
C	4.71079900	-0.66600400	8.55501500
H	5.71787600	-1.01512400	8.76812300
C	4.89449700	9.32700700	3.84247200
C	4.70070700	9.76292100	5.15124300
H	5.25166900	10.62642500	5.51402300
C	3.17707900	1.15605800	8.18465600
H	2.98034000	2.22044200	8.09295500
C	-0.23234500	0.86296100	11.77967100
H	0.14291000	0.35399600	12.66208300
C	5.87790400	10.01030600	2.93505400
H	6.84587600	9.49708100	2.95052800
H	6.04931600	11.04553800	3.24012600
H	5.52888800	10.01306800	1.89927100
C	-3.15077800	-2.97873800	8.43578400
H	-2.81435100	-2.99258900	9.47568200
H	-3.33905700	-4.00911200	8.12440600
H	-4.10800000	-2.44608500	8.41104200
C	2.31936400	6.75373700	-1.61177700
H	3.07072400	6.93957100	-2.38375200
H	1.83918500	7.70403200	-1.36660500
H	1.55382100	6.10299800	-2.04871100
C	3.96733500	-3.07273600	8.43164400
H	4.81062400	-3.29461400	9.09077000
H	4.21439400	-3.46277700	7.43788400
H	3.09809500	-3.62852300	8.79183800

N	-1.64820000	3.25194000	5.78296900
N	-5.60918400	4.17523100	4.80995900
C	-2.38278800	2.45574700	4.99558500
H	-1.88269200	1.56599300	4.62518000
C	-3.69199500	2.71180100	4.64549100
H	-4.21480100	2.00641000	4.01223100
C	-4.32548600	3.87507200	5.12666700
C	-2.24244900	4.36240800	6.23629200
H	-1.62151200	5.00650600	6.85322900
C	-3.54562900	4.71179600	5.94872000
H	-3.93902400	5.64079200	6.34135500
C	-6.32630900	5.31866600	5.35120000
H	-5.95661000	6.25863400	4.91577400
H	-6.19900000	5.38358200	6.43694800
C	-7.77417200	5.04965800	4.95344500
H	-8.25595800	4.42328500	5.71108500
H	-8.35779600	5.96685300	4.85470800
C	-7.63513800	4.27464400	3.64547100
H	-7.42385400	4.96374100	2.82145300
H	-8.52624800	3.70098400	3.38387900
C	-6.42181100	3.38557200	3.89844100
H	-6.71239800	2.42866200	4.35639000
H	-5.87324700	3.16013900	2.97789000

Complex 2 in the S₁ state

I	-1.37224300	1.05278800	1.50816000
Cu	0.16874700	1.02461100	-0.62559500
P	-0.63122200	2.14917000	-2.50887700
N	1.97582200	1.96917000	-0.10261900
N	5.45228900	4.19675100	0.56053500
C	3.07056300	1.79391200	-0.86040300
C	4.24751400	2.49683600	-0.67535700
C	4.32699800	3.46616300	0.35194800
C	3.17160500	3.63242600	1.14960400
C	2.04530300	2.87584000	0.88536300
C	6.62694700	4.14502900	-0.30415900
C	7.44373000	5.35651100	0.13229800
C	7.09075100	5.50141800	1.60993200
C	5.60550700	5.15992200	1.64639500
C	-0.73119600	3.96268600	-2.24393700
C	-0.93066100	4.49227400	-0.94825700
C	-1.28069300	5.82210800	-0.77912200
C	-1.47094900	6.66579200	-1.88624000
C	-1.30211700	6.15672500	-3.18833700
C	-0.93891900	4.82534500	-3.35645900
C	0.68057500	1.96614100	-3.82622700
C	1.73799700	2.87513300	-3.88047900
C	2.78523600	2.72133100	-4.79862600
C	2.75251100	1.62236100	-5.66282200
C	1.69955100	0.70686100	-5.61290500
C	0.66552600	0.87197400	-4.69664400
C	-2.15619200	1.47355300	-3.27000900
C	-3.10917400	0.81739100	-2.45827500
C	-4.38424300	0.56710300	-2.93909500
C	-4.76476100	0.97680200	-4.22891100
C	-3.83971500	1.65170200	-5.04773200
C	-2.55740200	1.89563100	-4.56728400
H	2.99066100	1.04696000	-1.65486600
H	5.09396300	2.28944300	-1.32927000
H	3.14083000	4.35884800	1.96071500
H	1.14345200	2.99176300	1.49231200
H	6.33706400	4.19441100	-1.36659200

H	7.18572700	3.20083200	-0.15608800
H	8.51929900	5.22757400	-0.05150800
H	7.11358500	6.24825000	-0.42448600
H	7.30279900	6.50031800	2.01542700
H	7.65733000	4.76978000	2.20859500
H	5.29720400	4.72180500	2.60971300
H	4.97691100	6.05403800	1.47147500
H	-0.81345100	3.84880700	-0.07362700
H	-1.40564700	6.21852100	0.23274900
H	-0.78781100	4.44587900	-4.37119200
H	1.73225000	3.72924200	-3.19535200
H	1.68789200	-0.14557000	-6.29730700
H	-0.16084700	0.15778600	-4.65044600
H	-2.84180200	0.51703200	-1.44219100
H	-5.10163400	0.04384400	-2.29972000
H	-1.83792300	2.39888700	-5.21991400
I	0.85776400	-1.38921000	-1.44959900
Cu	-0.57306100	-1.42755100	0.80618000
P	0.66516100	-2.38541800	2.53206200
N	-2.34936100	-2.35747600	0.35055200
N	-6.18357800	-3.79287200	-0.51213300
C	-3.18450300	-2.75335900	1.32771600
C	-4.45524100	-3.24481200	1.09591000
C	-4.93596500	-3.33868200	-0.23171700
C	-4.04726900	-2.92692200	-1.25008700
C	-2.79364300	-2.45190500	-0.91489000
C	-7.11343400	-4.29245800	0.49484600
C	-8.23093100	-4.91712000	-0.33316400
C	-8.24155300	-4.06583100	-1.59978400
C	-6.76196600	-3.79948800	-1.85339900
C	1.44051900	-4.00540900	2.04841000
C	0.76931000	-4.79719800	1.11269500
C	1.30585600	-6.02934600	0.74501000
C	2.51036700	-6.46301400	1.29434000
C	3.20544900	-5.67554100	2.22041700
C	2.64932900	-4.44569900	2.59217700
C	-0.35481700	-2.81637800	4.03104000
C	-0.36644000	-4.09573400	4.58657400

C	-1.16809600	-4.39856400	5.69748200
C	-1.95267800	-3.37991400	6.24517300
C	-1.94563300	-2.09649000	5.69639000
C	-1.15572900	-1.81020500	4.58776900
C	2.07859600	-1.40310000	3.23202400
C	2.84862500	-0.65004900	2.34180000
C	3.93336300	0.07900000	2.82298200
C	4.24170200	0.06754700	4.18190200
C	3.47258500	-0.66995700	5.08976800
C	2.39109700	-1.40831700	4.59336000
H	-2.81001600	-2.65934000	2.35068000
H	-5.07361500	-3.53053900	1.94615100
H	-4.32887000	-2.95895700	-2.30170200
H	-2.10252500	-2.11977800	-1.69329300
H	-6.62274100	-5.02273900	1.15913200
H	-7.48960600	-3.46627800	1.12867800
H	-9.19297400	-4.92642100	0.19765000
H	-7.97418700	-5.96020400	-0.57956500
H	-8.73327400	-4.55411600	-2.45239600
H	-8.76458400	-3.11424600	-1.41225400
H	-6.58797400	-2.83807100	-2.36282400
H	-6.30495200	-4.59302400	-2.47514200
H	-0.16359900	-4.44226000	0.66573200
H	0.78356500	-6.65207400	0.01457700
H	3.17659300	-3.81651600	3.31492100
H	0.25735400	-4.87972600	4.14822500
H	-2.56749800	-1.31206000	6.13502200
H	-1.16335700	-0.80832100	4.14899700
H	2.59466500	-0.62873100	1.27879800
H	4.53574900	0.66911400	2.12772900
H	1.77957600	-1.99284700	5.28665600
H	-2.58148900	-3.59439300	7.11396600
H	5.09395200	0.64693200	4.54920300
H	2.92562800	-7.42907900	0.99282900
H	-1.75685700	7.71080100	-1.74152500
H	3.56137200	1.48102600	-6.38587400
H	-5.77751100	0.78631100	-4.59396300
C	-1.17924400	-5.78878800	6.26668300

H	-1.64427200	-6.50043900	5.56513900
H	-0.15775000	-6.15104300	6.46047200
H	-1.74072100	-5.83446100	7.21038200
C	4.52742700	-6.12232900	2.77645200
H	4.56014900	-7.21322800	2.91444000
H	5.35038000	-5.85582200	2.09223800
H	4.74085000	-5.64668000	3.74443000
C	3.77771300	-0.64838600	6.56067800
H	4.85591700	-0.53797200	6.74844400
H	3.27186600	0.19824200	7.05461800
H	3.43500900	-1.56684700	7.05881500
C	-4.24190600	2.10274000	-6.42437100
H	-4.64548500	1.26699600	-7.01959400
H	-5.03215800	2.87030100	-6.37408300
H	-3.39252300	2.53195200	-6.97513700
C	-1.51521200	7.05009700	-4.37859200
H	-2.56683200	7.37528300	-4.44566800
H	-0.90255500	7.96426600	-4.31001300
H	-1.26152900	6.54067600	-5.31949800
C	3.89826400	3.72998200	-4.85466200
H	4.71680900	3.39455000	-5.50787000
H	3.53765000	4.69778300	-5.24005700
H	4.31448300	3.92180800	-3.85265000

Complex 2 in the T₁ state

I	-1.38077800	1.03198300	1.49928400
Cu	0.19543500	1.04855500	-0.61745800
P	-0.56376600	2.21699000	-2.49161800
N	1.95162000	2.05167600	-0.19754100
N	5.46673700	4.20797400	0.46603300
C	3.05800500	1.81286600	-0.92014800
C	4.24778200	2.49219000	-0.73282100
C	4.32677800	3.50176000	0.25571500
C	3.15575300	3.73477000	1.01366900
C	2.01627700	2.99815800	0.75337300
C	6.66469200	4.08236600	-0.35823300
C	7.50901900	5.28279600	0.05564400
C	7.11728400	5.49834700	1.51476300
C	5.62081700	5.20764500	1.51863000
C	-0.67107700	4.01620000	-2.14748000
C	-1.02945100	4.47846000	-0.85481400
C	-1.43625300	5.78754800	-0.66689100
C	-1.53784200	6.68067600	-1.74871500
C	-1.22147200	6.23744000	-3.04895200
C	-0.79682900	4.92846900	-3.23802700
C	0.75069200	2.07930500	-3.80081200
C	1.80436100	2.99682200	-3.82323100
C	2.86185000	2.87050800	-4.73228800
C	2.85198700	1.78438300	-5.61445700
C	1.81156000	0.85358800	-5.58813600
C	0.76494800	0.99198000	-4.68254900
C	-2.06782000	1.47175800	-3.27243400
C	-2.99528300	0.77341900	-2.47506600
C	-4.25549600	0.47594000	-2.97503300
C	-4.63279200	0.88144800	-4.26200700
C	-3.73111700	1.59861000	-5.06711400
C	-2.46280600	1.88534400	-4.56685500
H	2.97471300	1.03236600	-1.68163100
H	5.10547700	2.23368500	-1.35286700
H	3.12464200	4.49587800	1.79218100
H	1.10180900	3.16192300	1.32883900
H	6.40912500	4.09797200	-1.43048900

H	7.18574100	3.12696700	-0.15497900
H	8.58451300	5.11098200	-0.08936400
H	7.22649700	6.16193700	-0.54564200
H	7.35109200	6.50516600	1.88734300
H	7.64051300	4.77310100	2.15888300
H	5.26967900	4.81778200	2.48790200
H	5.02833100	6.11420200	1.29031300
H	-0.99377900	3.79563200	-0.00296200
H	-1.68128100	6.13024900	0.34273900
H	-0.53905800	4.59990500	-4.24945400
H	1.78665400	3.83422800	-3.11852100
H	1.82141200	0.00746900	-6.28013500
H	-0.04561400	0.25979700	-4.65136900
H	-2.72339600	0.47075500	-1.46031900
H	-4.95849200	-0.08417400	-2.35150600
H	-1.75597800	2.43096600	-5.19943000
I	0.71899600	-1.38187800	-1.52307800
Cu	-0.67045200	-1.53543100	0.80342800
P	0.61526900	-2.45051400	2.49477800
N	-2.46505300	-2.40819500	0.36567000
N	-6.30617800	-3.84958900	-0.46164200
C	-3.32716500	-2.71009100	1.35275400
C	-4.60256700	-3.19568400	1.13306200
C	-5.05730200	-3.38939400	-0.19233700
C	-4.14155600	-3.07306600	-1.22086600
C	-2.88551200	-2.59381900	-0.89725600
C	-7.26128200	-4.25673800	0.56305500
C	-8.36756000	-4.93885000	-0.23415000
C	-8.34320700	-4.19618700	-1.56719000
C	-6.85592900	-3.96324800	-1.80922900
C	1.41212500	-4.06737000	2.03290100
C	0.75387600	-4.87610100	1.10263000
C	1.30505200	-6.10600400	0.74910300
C	2.51200900	-6.52109800	1.30728300
C	3.19486800	-5.71652400	2.22781100
C	2.62389700	-4.48921200	2.58487900
C	-0.36863700	-2.86839700	4.02212700
C	-0.35488700	-4.13626800	4.60321900

C	-1.13494000	-4.42737700	5.73248800
C	-1.92372200	-3.40831600	6.27326500
C	-1.94224600	-2.13612100	5.69900600
C	-1.17431700	-1.86185600	4.57192600
C	2.02745500	-1.43619000	3.15474200
C	2.77758600	-0.69782200	2.23504400
C	3.85540300	0.06155900	2.68247400
C	4.17790700	0.09511700	4.03823100
C	3.42998600	-0.62729000	4.97472100
C	2.35475300	-1.39663000	4.51149000
H	-2.96984900	-2.54304700	2.37246200
H	-5.24298900	-3.40256300	1.98981500
H	-4.40207800	-3.19027300	-2.27211200
H	-2.17007700	-2.33493300	-1.68218200
H	-6.79146100	-4.93379300	1.29529000
H	-7.64223400	-3.37833800	1.11903600
H	-9.34062900	-4.89582300	0.27443500
H	-8.11641300	-6.00096300	-0.38738900
H	-8.82137800	-4.75009000	-2.38682400
H	-8.86105200	-3.22827400	-1.47084300
H	-6.66279600	-3.04860400	-2.39295900
H	-6.39345000	-4.80881500	-2.35385100
H	-0.18064700	-4.53389900	0.64902800
H	0.79255400	-6.74169700	0.02283000
H	3.14167200	-3.84693500	3.30306100
H	0.27233500	-4.92079700	4.17066600
H	-2.56644400	-1.35073500	6.13279900
H	-1.20094900	-0.86904800	4.11314300
H	2.51129500	-0.71348500	1.17470800
H	4.44164300	0.64039000	1.96406000
H	1.75928700	-1.96934600	5.22831300
H	-2.53500700	-3.61345200	7.15677900
H	5.02426500	0.69854600	4.37956900
H	2.93902000	-7.48559700	1.01718300
H	-1.87315300	7.70828300	-1.58772500
H	3.67237500	1.66205700	-6.32779600
H	-5.63246400	0.65082500	-4.64076100
C	-1.12090800	-5.80679100	6.32759500

H	-1.61271900	-6.53176500	5.65848900
H	-0.09210000	-6.16482600	6.48713900
H	-1.64477700	-5.83557700	7.29343400
C	4.51957100	-6.14316700	2.79341500
H	4.56524000	-7.23265000	2.93906300
H	5.34289400	-5.87094000	2.11183400
H	4.72203100	-5.65843000	3.75928600
C	3.74770800	-0.55899900	6.44162000
H	4.81539400	-0.36027800	6.61558200
H	3.17988700	0.25106700	6.92954900
H	3.48455100	-1.49440300	6.95678600
C	-4.13764400	2.05421400	-6.44079100
H	-3.28357300	2.45943200	-7.00218100
H	-4.56938800	1.22771400	-7.02801300
H	-4.90514600	2.84408600	-6.38440900
C	-1.34404400	7.17996400	-4.21379600
H	-2.39246200	7.48572900	-4.36703800
H	-0.76466500	8.10303200	-4.04596600
H	-0.98829600	6.72107400	-5.14769800
C	3.96521900	3.89075500	-4.75759400
H	4.79282700	3.57628100	-5.40974200
H	3.59931800	4.86287200	-5.12669100
H	4.37013500	4.06542500	-3.74780500

Complex 3 in the S₀ state

I	-1.14206400	1.38295200	1.44102300
Cu	0.44857900	1.18469500	-0.78007800
P	-0.61138000	2.19020100	-2.52328100
N	2.27219400	1.99870200	-0.15953700
N	5.94257100	3.66142600	0.96274400
C	3.37511900	1.83255800	-0.90036800
C	4.60819400	2.36045900	-0.57804700
C	4.75106000	3.12656500	0.59612600
C	3.58837100	3.29547800	1.37201700
C	2.40452600	2.71995900	0.96061400
C	7.13937100	3.60611600	0.13750300
C	8.07606200	4.61171500	0.80051300
C	7.66146900	4.55740000	2.26882700
C	6.14565400	4.40972700	2.19288400
C	-1.17660100	3.89864300	-2.17311800
C	-0.42724100	4.66646700	-1.28018700
C	-0.79150600	5.97451300	-0.99540600
C	-1.92255900	6.54956500	-1.57563300
C	-2.67356900	5.77355700	-2.45810600
C	-2.30961400	4.46667000	-2.75566500
C	-2.34098300	7.94862100	-1.22739000
C	0.39955000	2.39016400	-4.04277800
C	0.52420600	3.59460900	-4.73268200
C	1.32715700	3.67845500	-5.86584700
C	2.02025500	2.56995600	-6.34476600
C	1.89142800	1.36575000	-5.64738700
C	1.10346200	1.27435300	-4.51107100
C	2.89370400	2.66125300	-7.56260100
C	-2.13403800	1.37623700	-3.13890000
C	-3.02637000	0.87404500	-2.18913300
C	-4.20633100	0.26478100	-2.58926900
C	-4.52516200	0.12337800	-3.94005000
C	-3.62165900	0.61258600	-4.88264600
C	-2.44224200	1.23524900	-4.49199800
C	-5.81270000	-0.52293400	-4.36462900
H	3.25604600	1.22925000	-1.79530500
H	5.45080400	2.16478200	-1.22909000

H	3.60286600	3.86511900	2.29239600
H	1.50323400	2.82548000	1.55815700
H	6.91312500	3.87268200	-0.90036600
H	7.57062600	2.59453200	0.13523500
H	9.12864300	4.37284200	0.63735200
H	7.89104900	5.61210500	0.39624500
H	7.96772600	5.43635600	2.83912400
H	8.09609500	3.67509400	2.75000100
H	5.73644400	3.86983200	3.05314400
H	5.64789000	5.38969600	2.14642300
H	0.44195000	4.22701200	-0.79999200
H	-0.19460400	6.55528800	-0.29757700
H	-3.56098500	6.19861900	-2.91935700
H	-2.91550100	3.88184700	-3.44046500
H	-1.47538400	8.58829500	-1.03688100
H	-2.93000500	8.40053800	-2.02917400
H	-2.95802300	7.95548100	-0.32190900
H	-0.00587100	4.47519000	-4.38526700
H	1.41167200	4.62732200	-6.38875800
H	2.42410900	0.48477500	-5.99583700
H	1.03462500	0.33202400	-3.97411400
H	2.65070200	1.87605100	-8.28485600
H	2.78169300	3.62628600	-8.06176600
H	3.95013500	2.54207900	-7.29926300
H	-2.78755800	0.95224700	-1.13213900
H	-4.88253900	-0.12507400	-1.83355700
H	-3.84100400	0.50368900	-5.94159400
H	-1.75349600	1.60335100	-5.24557000
H	-6.17964900	-1.21036000	-3.59764900
H	-6.59334400	0.22808000	-4.53127300
H	-5.69270800	-1.08027900	-5.29757700
I	1.14231800	-1.38326100	-1.44089300
Cu	-0.44853500	-1.18506100	0.78012700
P	0.61141500	-2.19047500	2.52339200
N	-2.27216700	-1.99879200	0.15948700
N	-5.94263200	-3.66112400	-0.96307900
C	-3.37509300	-1.83267000	0.90032100
C	-4.60819600	-2.36045300	0.57791400

C	-4.75109200	-3.12639800	-0.59636000
C	-3.58840200	-3.29528800	-1.37225400
C	-2.40452400	-2.71990500	-0.96075600
C	-7.13945900	-3.60582400	-0.13788100
C	-8.07618100	-4.61129300	-0.80104000
C	-7.66157000	-4.55677900	-2.26934200
C	-6.14574700	-4.40917200	-2.19337000
C	1.17688400	-3.89885900	2.17336600
C	0.42791000	-4.66669100	1.28011600
C	0.79236800	-5.97469800	0.99541200
C	1.92324000	-6.54970100	1.57604500
C	2.67386800	-5.77368400	2.45883200
C	2.30971700	-4.46683100	2.75630900
C	2.34186400	-7.94872100	1.22789900
C	-0.39962000	-2.39046400	4.04281600
C	-0.52449600	-3.59497900	4.73256200
C	-1.32755000	-3.67886000	5.86564900
C	-2.02055100	-2.57033000	6.34464300
C	-1.89149000	-1.36605200	5.64743500
C	-1.10341800	-1.27461800	4.51119200
C	-2.89425400	-2.66172600	7.56228700
C	2.13392100	-1.37628000	3.13908900
C	3.02621900	-0.87393300	2.18936700
C	4.20609500	-0.26455400	2.58955800
C	4.52487900	-0.12318700	3.94036100
C	3.62140800	-0.61253300	4.88290600
C	2.44207000	-1.23531900	4.49219800
C	5.81237000	0.52320300	4.36496100
H	-3.25599600	-1.22947900	1.79533300
H	-5.45080400	-2.16479800	1.22896500
H	-3.60292300	-3.86480100	-2.29271200
H	-1.50322800	-2.82541400	-1.55829500
H	-6.91327100	-3.87251300	0.89996800
H	-7.57066000	-2.59421600	-0.13552500
H	-9.12875600	-4.37240700	-0.63785500
H	-7.89120400	-5.61174700	-0.39691400
H	-7.96785300	-5.43564200	-2.83976900
H	-8.09616300	-3.67439100	-2.75039400

H	-5.73652500	-3.86911300	-3.05352200
H	-5.64801300	-5.38916400	-2.14710600
H	-0.44112000	-4.22725900	0.79960500
H	0.19577100	-6.55548000	0.29732700
H	3.56114000	-6.19870800	2.92039200
H	2.91531300	-3.88199300	3.44135500
H	1.47634300	-8.58863000	1.03781500
H	2.93127700	-8.40036000	2.02955100
H	2.95857000	-7.95560200	0.32219100
H	0.00551800	-4.47557900	4.38510300
H	-1.41221000	-4.62777500	6.38845000
H	-2.42405800	-0.48504300	5.99596900
H	-1.03440000	-0.33222400	3.97437400
H	-2.65282600	-1.87533200	8.28375900
H	-2.78084500	-3.62603800	8.06253500
H	-3.95079500	-2.54461700	7.29843400
H	2.78744100	-0.95211900	1.13236500
H	4.88227200	0.12542200	1.83388000
H	3.84071500	-0.50365400	5.94186400
H	1.75334300	-1.60352600	5.24573700
H	6.17839400	1.21195900	3.59872800
H	6.59354700	-0.22763900	4.52988600
H	5.69276400	1.07909400	5.29881800

Complex 3 in the S₁ state

I	-1.40357300	1.04310200	1.45532300
Cu	0.16866700	1.02217600	-0.65637600
P	-0.62540700	2.14267100	-2.54309000
N	1.96490200	1.96163100	-0.10113100
N	5.44791900	4.14441100	0.66615700
C	3.05591700	1.82618600	-0.87260200
C	4.23363200	2.51826100	-0.65669300
C	4.31932300	3.42995700	0.42144500
C	3.16740100	3.55577200	1.23125600
C	2.03901800	2.81506000	0.93241900
C	6.62163000	4.13359400	-0.20144100
C	7.44537000	5.31452100	0.30041100
C	7.09693000	5.37681900	1.78486300
C	5.61003200	5.04075300	1.80621300
C	-0.71909600	3.95579400	-2.27757400
C	-0.89499300	4.48960500	-0.98120300
C	-1.23264400	5.81778600	-0.79230300
C	-1.44836800	6.68936600	-1.88588600
C	-1.29354400	6.15181200	-3.17120300
C	-0.93845100	4.82516400	-3.38023300
C	-1.85063000	8.11668000	-1.66574800
C	0.67239700	1.96063400	-3.87212300
C	1.72709600	2.87105300	-3.96115000
C	2.73938800	2.68919100	-4.90339000
C	2.73002700	1.59630600	-5.77618600
C	1.66847700	0.68516600	-5.67246800
C	0.65664800	0.85994500	-4.73470900
C	3.80799500	1.40375500	-6.80420000
C	-2.15329900	1.47435400	-3.29677600
C	-3.10525700	0.81384100	-2.48709600
C	-4.38357300	0.55958900	-2.94868800
C	-4.80404600	0.97561700	-4.23679300
C	-3.86358200	1.64867900	-5.02831400
C	-2.57032500	1.90220700	-4.58779900
C	-6.20511800	0.72526300	-4.70659300
H	2.97148100	1.12271900	-1.70538700
H	5.07523100	2.34898900	-1.32749500

H	3.14085000	4.23851500	2.07966500
H	1.13947500	2.89881500	1.54825300
H	6.33128000	4.24278900	-1.25898100
H	7.17538300	3.17968000	-0.10548400
H	8.51984200	5.19121800	0.10661400
H	7.11797300	6.23787300	-0.20398900
H	7.31501600	6.34987200	2.24615500
H	7.66140700	4.60947100	2.33923500
H	5.30334200	4.54750900	2.74347500
H	4.98477300	5.94640900	1.68809600
H	-0.76631300	3.84289800	-0.10972600
H	-1.33182300	6.20214800	0.22801100
H	-1.44723700	6.80042600	-4.04046500
H	-0.80267500	4.46232700	-4.40190300
H	-1.18938000	8.62217300	-0.94075500
H	-1.81981400	8.69236800	-2.60307100
H	-2.87731400	8.20027600	-1.26516100
H	1.74311900	3.73672700	-3.29270400
H	3.55219600	3.41936100	-4.96609300
H	1.63453300	-0.17939300	-6.34253400
H	-0.16402800	0.14023700	-4.66771300
H	3.41027500	1.52614600	-7.82523900
H	4.62337300	2.13011300	-6.67634900
H	4.24140300	0.39258600	-6.74862300
H	-2.82919400	0.50663300	-1.47487300
H	-5.08554400	0.02688800	-2.29853400
H	-4.15309800	1.97798300	-6.03229700
H	-1.86509800	2.40222400	-5.25638200
H	-6.49966500	-0.33219100	-4.57960400
H	-6.94565700	1.32542100	-4.14653100
H	-6.32352700	0.97549600	-5.77170500
I	0.85214400	-1.39243600	-1.48272400
Cu	-0.57776700	-1.44501000	0.78017500
P	0.66782500	-2.37648800	2.51306800
N	-2.34889800	-2.38268800	0.32491200
N	-6.18946400	-3.80423700	-0.53207300
C	-3.17810600	-2.79025300	1.30226300
C	-4.45046600	-3.27855300	1.07214000

C	-4.93936400	-3.35577300	-0.25353100
C	-4.05604800	-2.93352400	-1.27233800
C	-2.80027800	-2.46327500	-0.93886600
C	-7.11394100	-4.31515500	0.47415400
C	-8.23749300	-4.92756900	-0.35483000
C	-8.25452600	-4.06023600	-1.61043000
C	-6.77612800	-3.79295700	-1.86981800
C	1.41735400	-4.01556300	2.06241300
C	0.75419600	-4.81270500	1.12411400
C	1.26790200	-6.05711300	0.77097200
C	2.46010500	-6.53468900	1.33069200
C	3.11794700	-5.72410700	2.26312300
C	2.60713300	-4.47980600	2.62742400
C	3.03056800	-7.85895700	0.91290000
C	-0.33098500	-2.75312400	4.03807600
C	-0.33771400	-4.00796400	4.64848500
C	-1.12970700	-4.23869000	5.77440800
C	-1.92570900	-3.22926600	6.32304000
C	-1.91067700	-1.97223000	5.70026500
C	-1.13248300	-1.73524000	4.57284700
C	-2.77247400	-3.47120800	7.53897100
C	2.10598900	-1.39719400	3.16057000
C	2.90315400	-0.71550800	2.23430300
C	4.00046900	0.02173600	2.66421300
C	4.32746500	0.11134300	4.02454400
C	3.51927900	-0.56943200	4.94004600
C	2.42041900	-1.31831300	4.51784000
C	5.50072600	0.93269100	4.47572100
H	-2.79725700	-2.70836700	2.32400400
H	-5.06387600	-3.57468400	1.92241900
H	-4.34373000	-2.95307300	-2.32258400
H	-2.11317100	-2.12306900	-1.71739300
H	-6.62034300	-5.05453800	1.12612000
H	-7.48495900	-3.49646100	1.12064100
H	-9.19627200	-4.94217800	0.18174500
H	-7.98387700	-5.96782000	-0.61598600
H	-8.75224900	-4.53683000	-2.46616300
H	-8.77478100	-3.11026600	-1.40768400

H	-6.60414400	-2.82529000	-2.36824600
H	-6.32421400	-4.57924100	-2.50436100
H	-0.16590600	-4.44841600	0.65770900
H	0.73583000	-6.66629800	0.03474600
H	4.05202500	-6.07228500	2.71347600
H	3.14422800	-3.86396700	3.35337100
H	2.23951100	-8.60612600	0.75079200
H	3.72878600	-8.25452300	1.66433200
H	3.58593600	-7.76418300	-0.03528500
H	0.27527400	-4.81648900	4.24315900
H	-1.12424400	-5.22990400	6.23692600
H	-2.52715400	-1.16289900	6.10246500
H	-1.15243100	-0.75033200	4.09688000
H	-2.45809400	-2.82735600	8.37616300
H	-2.70860600	-4.51536700	7.87564500
H	-3.83160400	-3.24300300	7.34008200
H	2.65523500	-0.75405400	1.16994600
H	4.60707500	0.55182300	1.92411900
H	3.75097800	-0.51426400	6.00764900
H	1.80296800	-1.83753700	5.25508700
H	5.33567900	2.00278400	4.26696000
H	6.42147200	0.63976500	3.94712100
H	5.68002200	0.82651400	5.55486100

Complex 3 in the T₁ state

I	-1.39273100	1.03072300	1.46239800
Cu	0.20884100	1.03586800	-0.63650600
P	-0.54982800	2.21063000	-2.50862300
N	1.96243000	2.03266300	-0.20451500
N	5.49329200	4.14282000	0.52092500
C	3.06341100	1.81635500	-0.94251500
C	4.25676300	2.48357900	-0.73805400
C	4.34706700	3.45358000	0.28811000
C	3.18131400	3.66477200	1.06034500
C	2.03659500	2.94343000	0.77969100
C	6.68903100	4.03696800	-0.30934500
C	7.54561200	5.21174800	0.14997000
C	7.16053300	5.37055700	1.61808100
C	5.66133000	5.09356000	1.61549300
C	-0.64589100	4.01276600	-2.16375600
C	-0.98257800	4.47855800	-0.86786400
C	-1.37915800	5.78568600	-0.65885600
C	-1.50581800	6.70622200	-1.72708300
C	-1.20130400	6.23473900	-3.01363100
C	-0.78087000	4.93236500	-3.24339100
C	-1.98021300	8.10749900	-1.48665400
C	0.75110200	2.07287100	-3.82678600
C	1.80277000	2.99271700	-3.88576800
C	2.82922900	2.83376300	-4.81503500
C	2.84755400	1.74889000	-5.69916400
C	1.79807400	0.82096600	-5.61728600
C	0.77036400	0.97287600	-4.69414800
C	3.94803600	1.57444400	-6.70557700
C	-2.05556400	1.46719400	-3.28153600
C	-2.99683200	0.79073300	-2.47732100
C	-4.26250900	0.50037300	-2.95858200
C	-4.67073600	0.89116000	-4.25204100
C	-3.73725000	1.57896000	-5.03985700
C	-2.45782800	1.86617900	-4.57891000
C	-6.06026600	0.60826700	-4.74082500
H	2.97203300	1.06496100	-1.73173800
H	5.10810300	2.24775200	-1.37550500

H	3.15821600	4.39711500	1.86633700
H	1.12624400	3.08869400	1.36687700
H	6.43264900	4.09636700	-1.37956600
H	7.20079500	3.06935500	-0.14321500
H	8.61904800	5.03639400	-0.00568800
H	7.26902700	6.11722700	-0.41381700
H	7.40503000	6.35882100	2.03126100
H	7.67896100	4.61439400	2.22977300
H	5.31111700	4.66419200	2.56869600
H	5.07576700	6.01449800	1.43124100
H	-0.93601300	3.79200200	-0.01874600
H	-1.60091700	6.11590100	0.36130000
H	-1.28689600	6.91920300	-3.86461500
H	-0.53807000	4.62025900	-4.26253900
H	-1.44434300	8.58316000	-0.64741100
H	-1.83585600	8.73931500	-2.37611100
H	-3.05556200	8.14386500	-1.23298400
H	1.80508200	3.84600200	-3.20207600
H	3.63452500	3.57354600	-4.85608400
H	1.78887000	-0.04162500	-6.29045800
H	-0.03303700	0.23362000	-4.63992400
H	3.55814400	1.62739800	-7.73535700
H	4.71933100	2.35079600	-6.60058800
H	4.43783000	0.59308000	-6.59965700
H	-2.72516600	0.49464100	-1.46016500
H	-4.96014700	-0.04685600	-2.31604700
H	-4.01930600	1.89151800	-6.05084800
H	-1.75571800	2.38920000	-5.23387000
H	-6.37013100	-0.42591600	-4.51304200
H	-6.80557100	1.27302000	-4.26819700
H	-6.14241800	0.75014700	-5.82888700
I	0.73346300	-1.40088200	-1.53369200
Cu	-0.66710900	-1.54906100	0.79178600
P	0.61702800	-2.43754600	2.49681600
N	-2.46020500	-2.41779200	0.34502800
N	-6.31168600	-3.81829000	-0.50416700
C	-3.32091300	-2.73785000	1.32754000
C	-4.59942100	-3.21208800	1.10057000

C	-5.05885500	-3.37299000	-0.22757900
C	-4.14378600	-3.03987800	-1.25121400
C	-2.88454000	-2.57435700	-0.92050500
C	-7.26680300	-4.24325200	0.51313800
C	-8.37924500	-4.89957900	-0.29700800
C	-8.35387300	-4.12545900	-1.61201100
C	-6.86586700	-3.89547400	-1.85253500
C	1.40120000	-4.06724200	2.06859200
C	0.76185200	-4.88271500	1.12984300
C	1.30052100	-6.12058700	0.79045200
C	2.49522600	-6.57310000	1.36492300
C	3.12990000	-5.74433100	2.29764900
C	2.59378200	-4.50671200	2.64770400
C	3.09393200	-7.88960400	0.96188700
C	-0.35576500	-2.81073400	4.04026700
C	-0.34018600	-4.05689300	4.66771400
C	-1.11966400	-4.28351800	5.80335300
C	-1.92494400	-3.27799600	6.34525100
C	-1.93251200	-2.02937500	5.70551100
C	-1.16726000	-1.79681500	4.56823500
C	-2.75794300	-3.51526700	7.57176100
C	2.04132500	-1.41932500	3.11870900
C	2.81284600	-0.73244700	2.17459400
C	3.89316400	0.04164800	2.58203600
C	4.22891400	0.16339400	3.93779900
C	3.44770700	-0.52395300	4.87137000
C	2.36577300	-1.30911000	4.47124900
C	5.38239400	1.02493900	4.36484000
H	-2.95999900	-2.59510800	2.34972700
H	-5.23868200	-3.43518600	1.95412400
H	-4.40743800	-3.13230300	-2.30411300
H	-2.16956000	-2.30260500	-1.70145200
H	-6.79948900	-4.94019100	1.22812300
H	-7.64100700	-3.37576000	1.09050200
H	-9.35073700	-4.86294600	0.21509800
H	-8.13479500	-5.95918800	-0.47617700
H	-8.83741000	-4.65680100	-2.44335000
H	-8.86576500	-3.15712100	-1.49124100

H	-6.66912200	-2.96766900	-2.41426600
H	-6.40994100	-4.72991900	-2.41934400
H	-0.15938000	-4.53602300	0.65225200
H	0.78655500	-6.74425400	0.05341700
H	4.06556100	-6.07296700	2.75944100
H	3.11313200	-3.87612200	3.37398200
H	2.31739100	-8.64617900	0.77527300
H	3.77457200	-8.27812600	1.73302500
H	3.67636200	-7.78631900	0.03089400
H	0.28058400	-4.86236600	4.26812100
H	-1.09660900	-5.26829700	6.27906900
H	-2.55621100	-1.22296500	6.10266100
H	-1.20359200	-0.81872900	4.07876200
H	-2.44764700	-2.85417800	8.39701300
H	-2.67434200	-4.55321600	7.92321500
H	-3.82240500	-3.30758700	7.37849600
H	2.55624800	-0.79745300	1.11332900
H	4.47894000	0.57577000	1.82796200
H	3.68661800	-0.44433100	5.93590200
H	1.76821000	-1.83127800	5.22272400
H	5.18755200	2.08575400	4.13528700
H	6.30795400	0.74565900	3.83703900
H	5.57040600	0.94571500	5.44487500

Reference

S1. Q. Zhang, T. Komino, S. Huang, S. Matsunami, K. Goushi and C. Adachi, *Adv. Funct. Mater.*, **2012**, *22*, 2327.