Electronic Supplementary Information for

Ethynyl π-Coordinated and Non-Coordinated Mononuclear Cu(I) Halide Diphosphine Complexes: Synthesis and Photophysical Studies

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4. Computational details

1. NMR and mass spectra

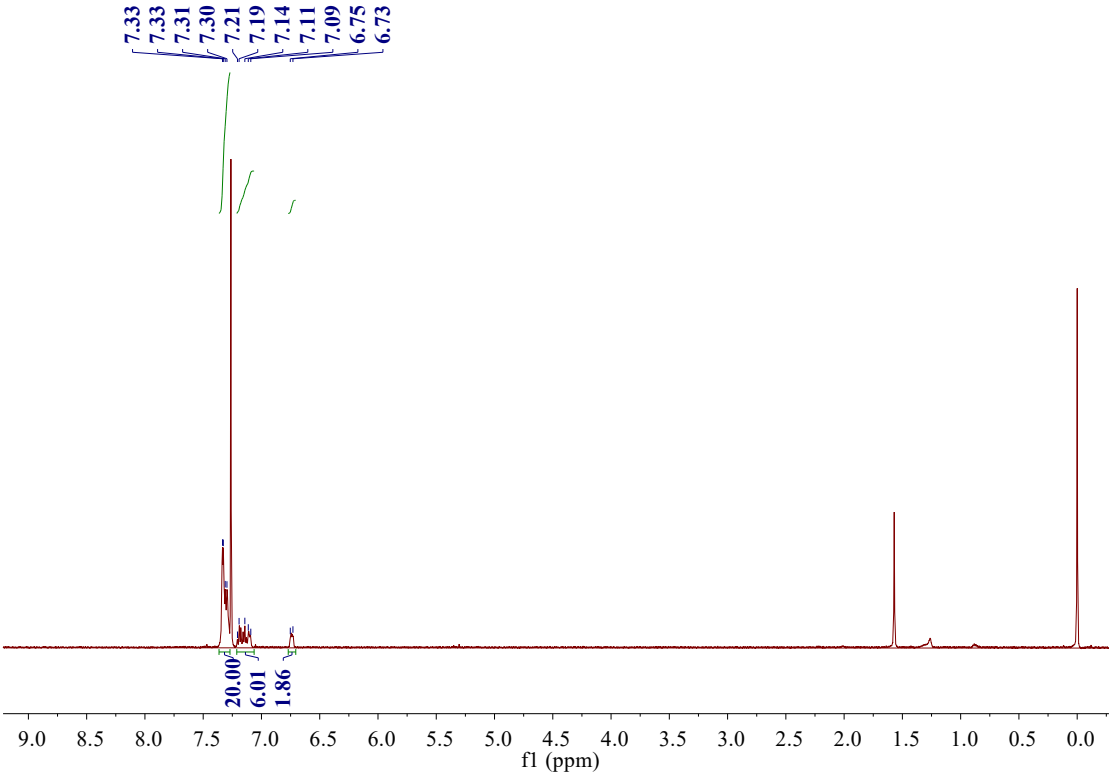


Figure S1. ^{1}H NMR spectrum of **L1** in $CDCl_3$.

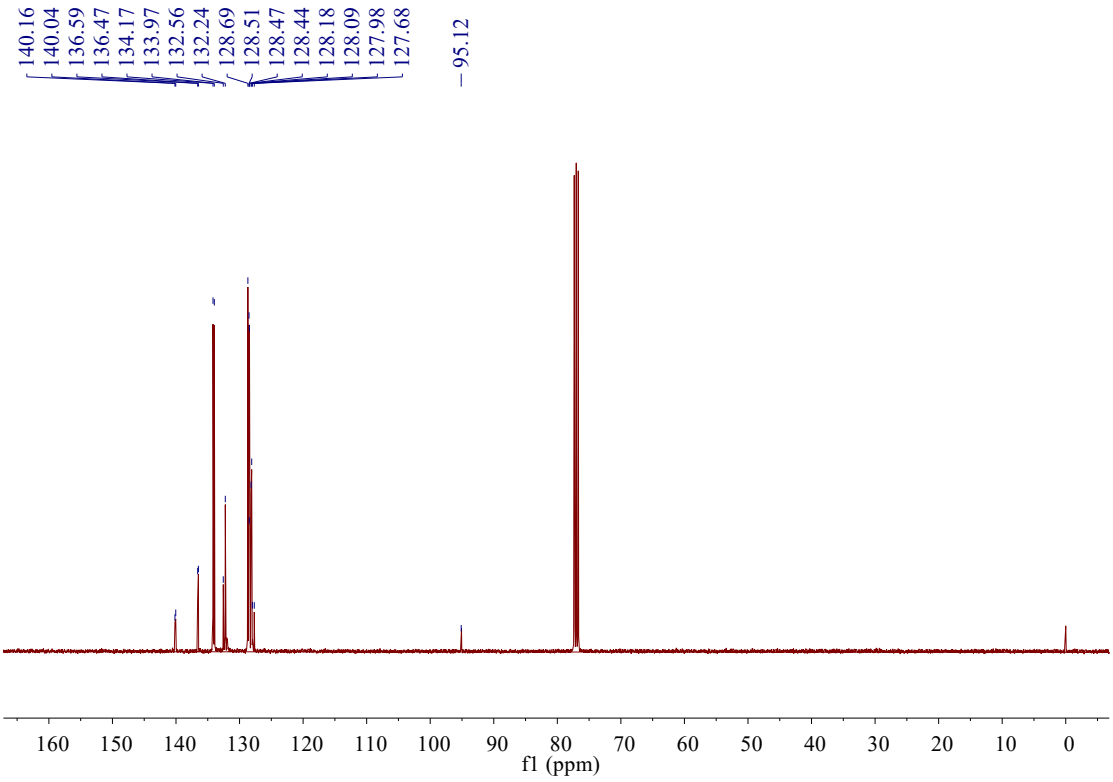


Figure S2. ^{13}C NMR spectrum of **L1** in $CDCl_3$.

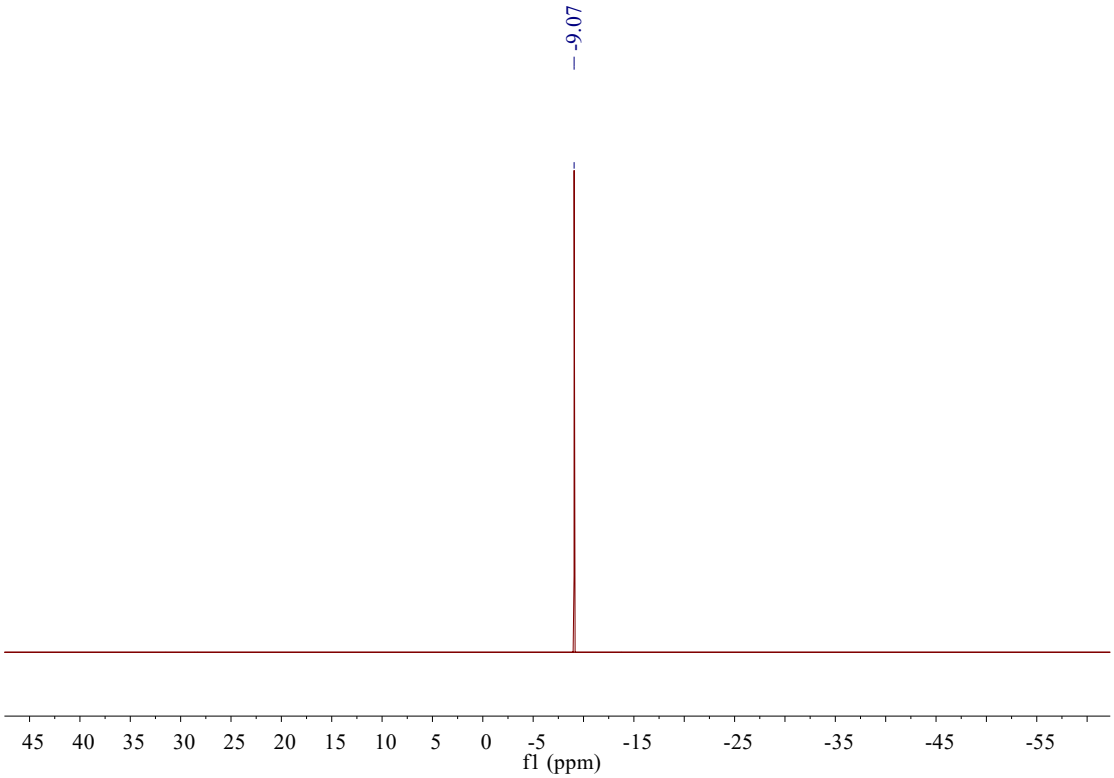


Figure S3. ^{31}P NMR spectrum of **L1** in $CDCl_3$.

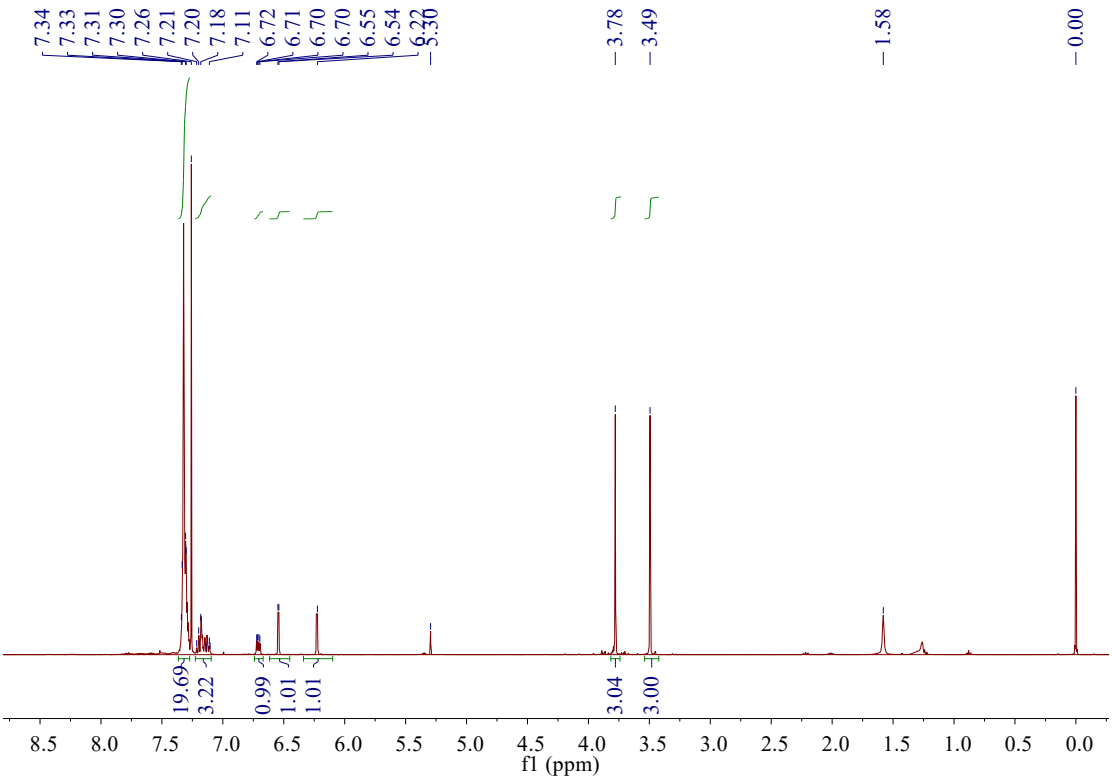


Figure S4. ^{1}H NMR spectrum of **L2** in $CDCl_3$.

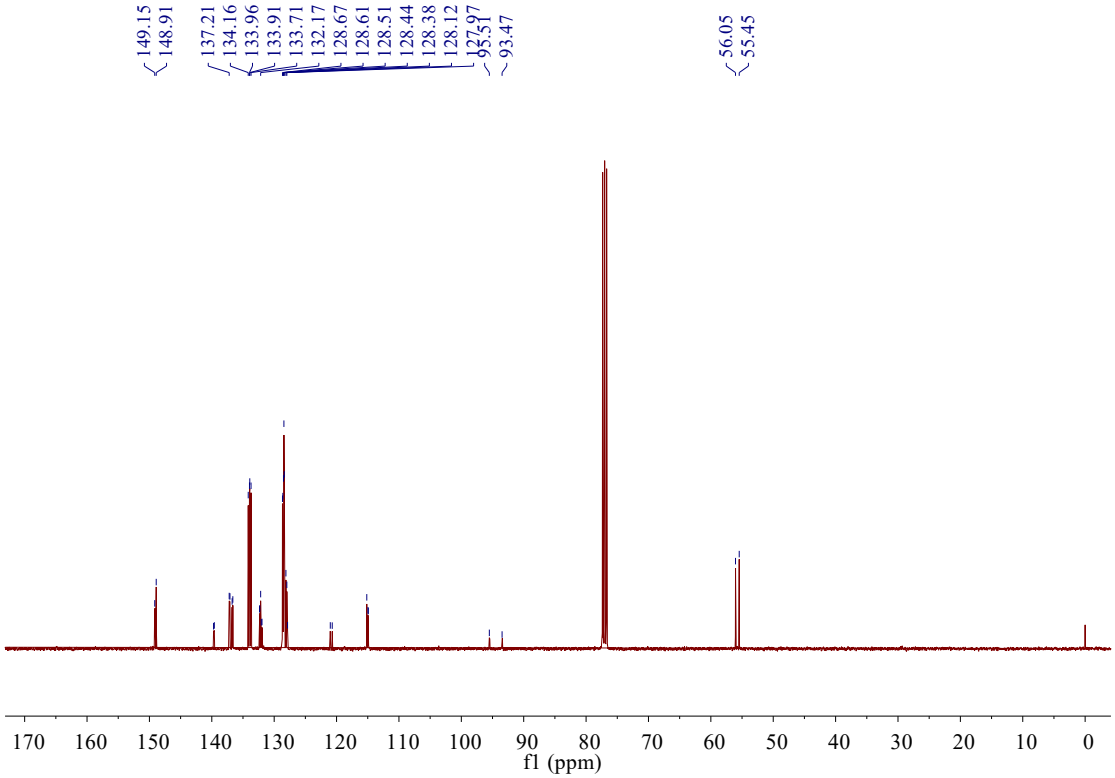


Figure S5. ^{13}C NMR spectrum of **L2** in $CDCl_3$.

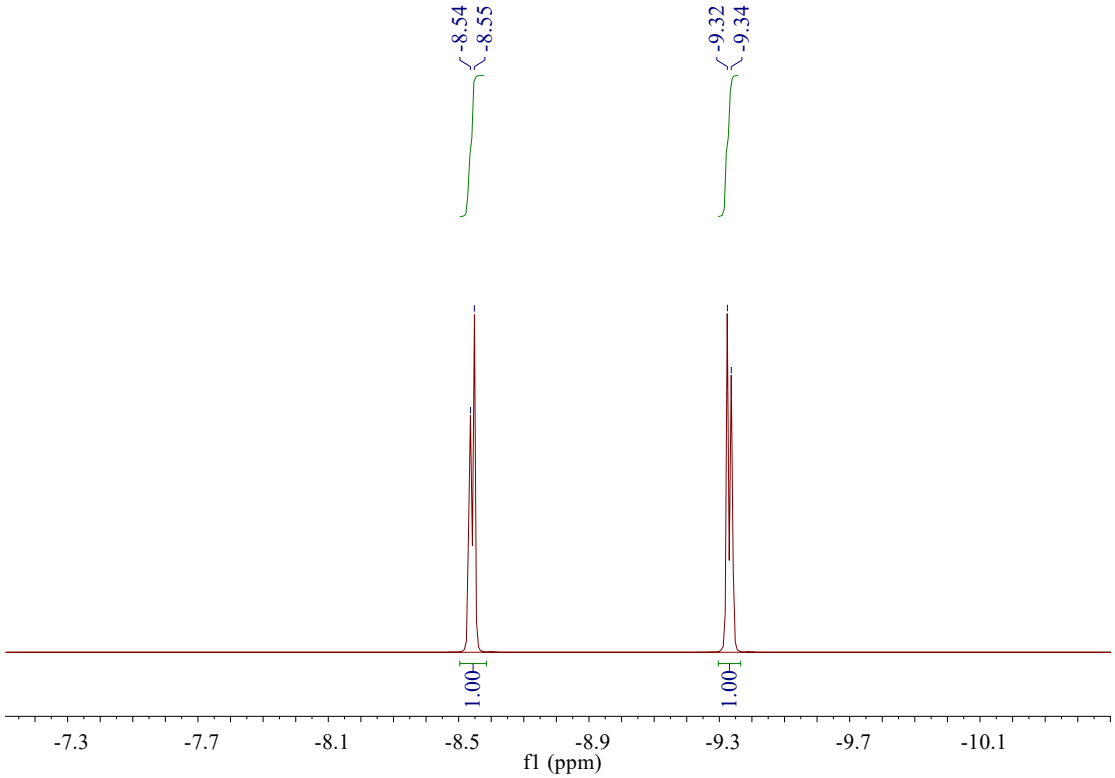


Figure S6. ^{31}P NMR spectrum of **L2** in $CDCl_3$.

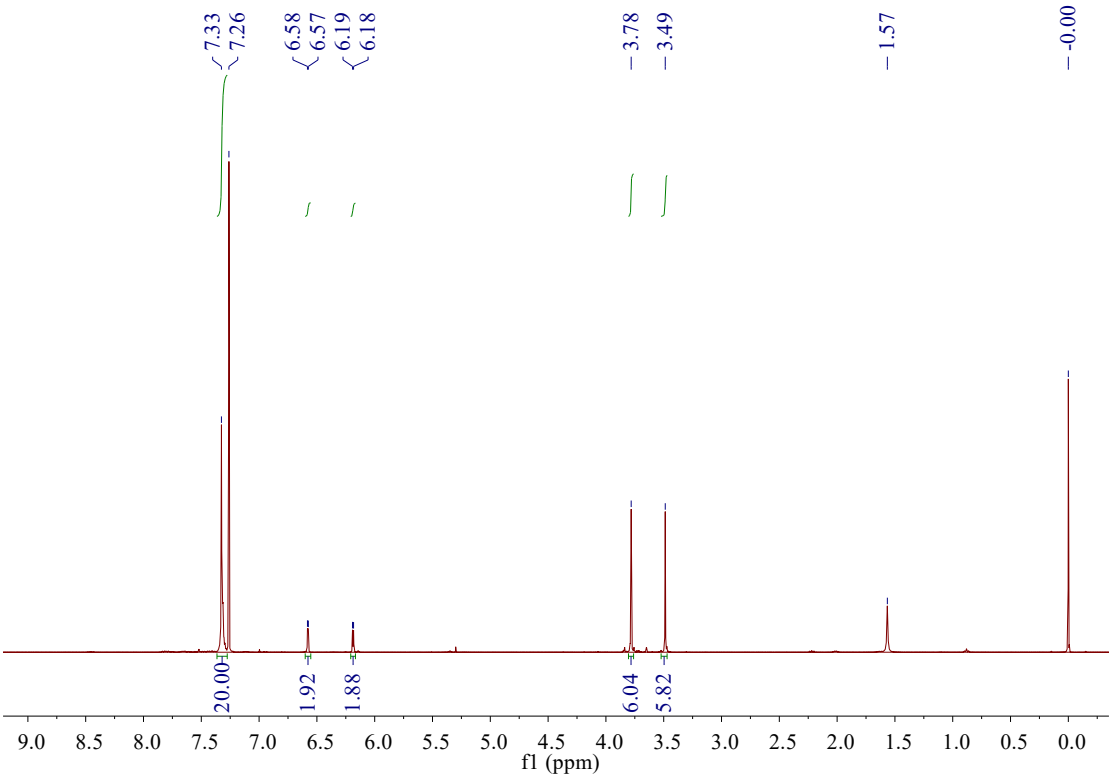


Figure S7. ^{1}H NMR spectrum of **L3** in $CDCl_3$.

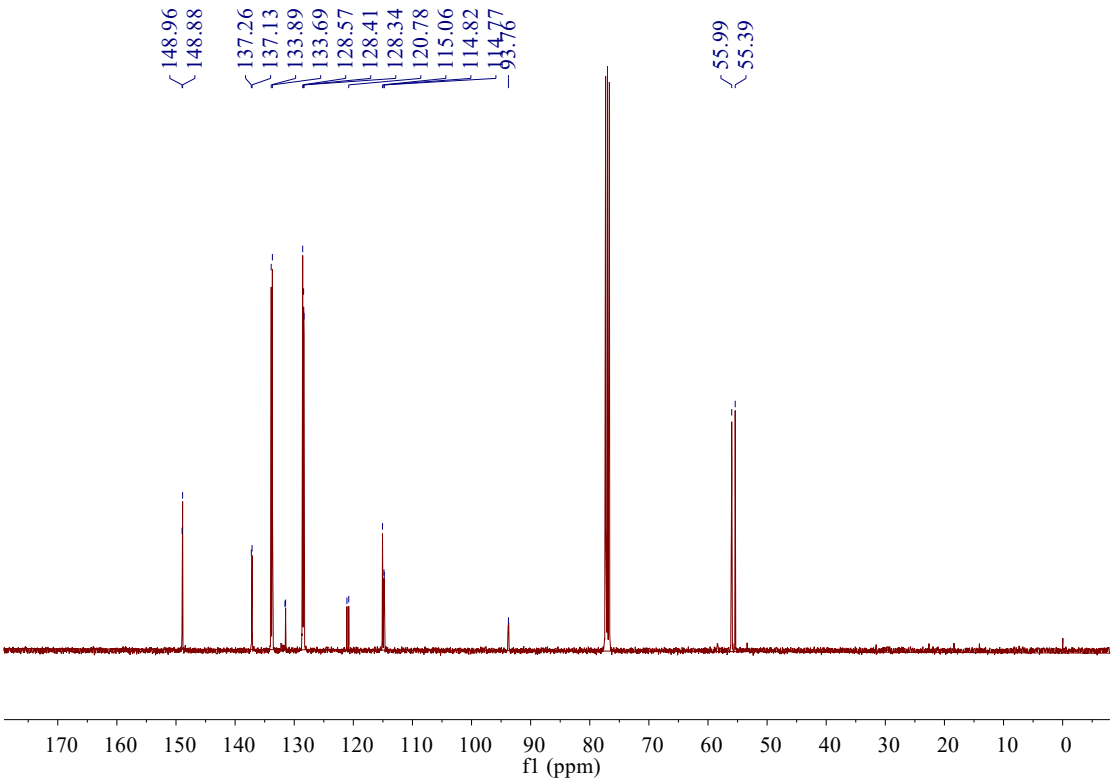


Figure S8. ^{13}C NMR spectrum of **L3** in $CDCl_3$.

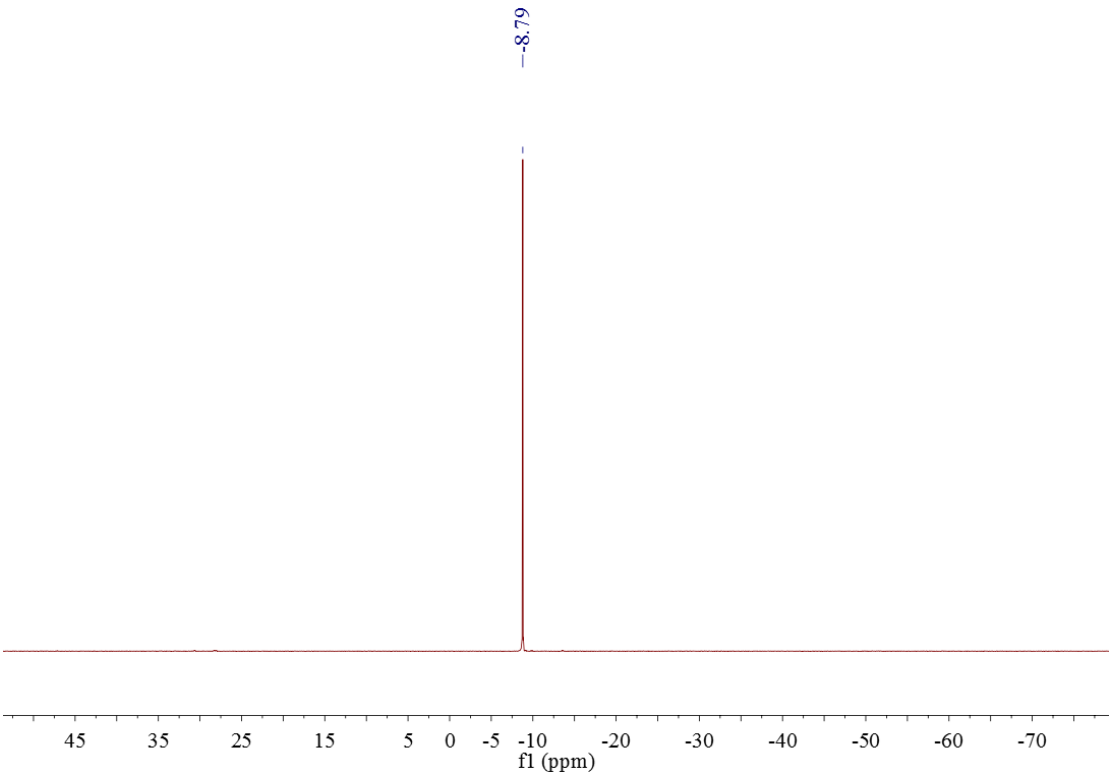


Figure S9. ^{31}P NMR spectrum of **L3** in $CDCl_3$.

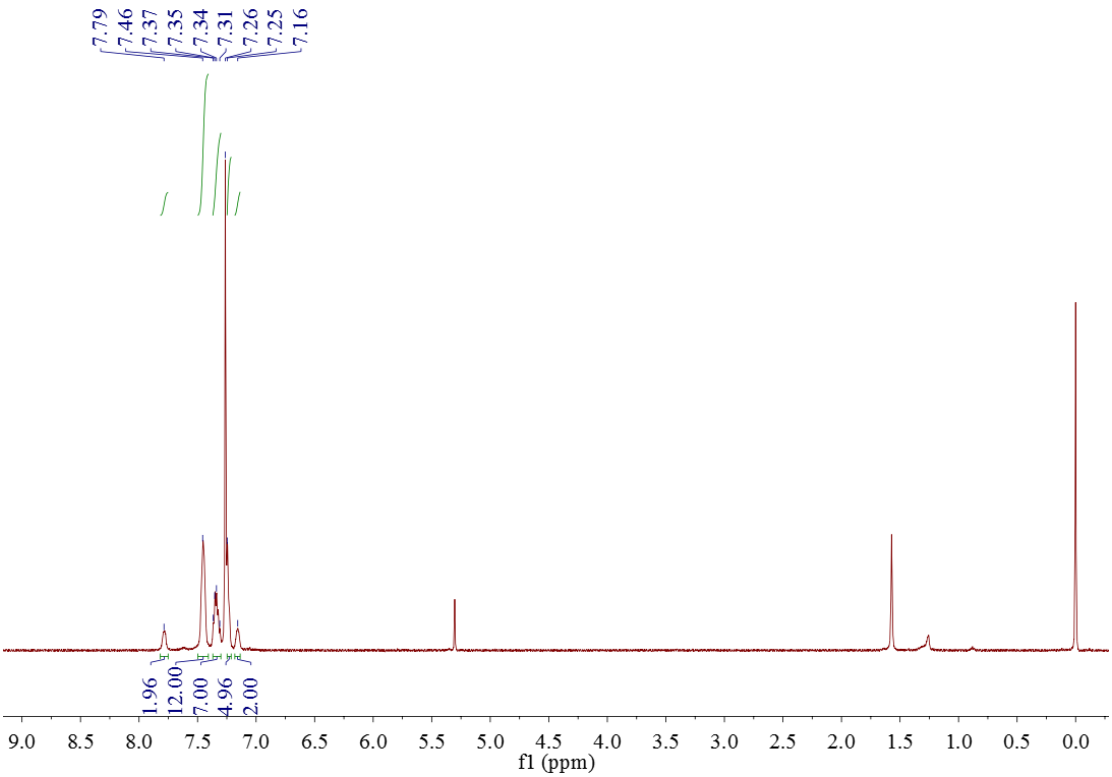


Figure S10. ^{1}H NMR spectrum of **1** in $CDCl_3$.

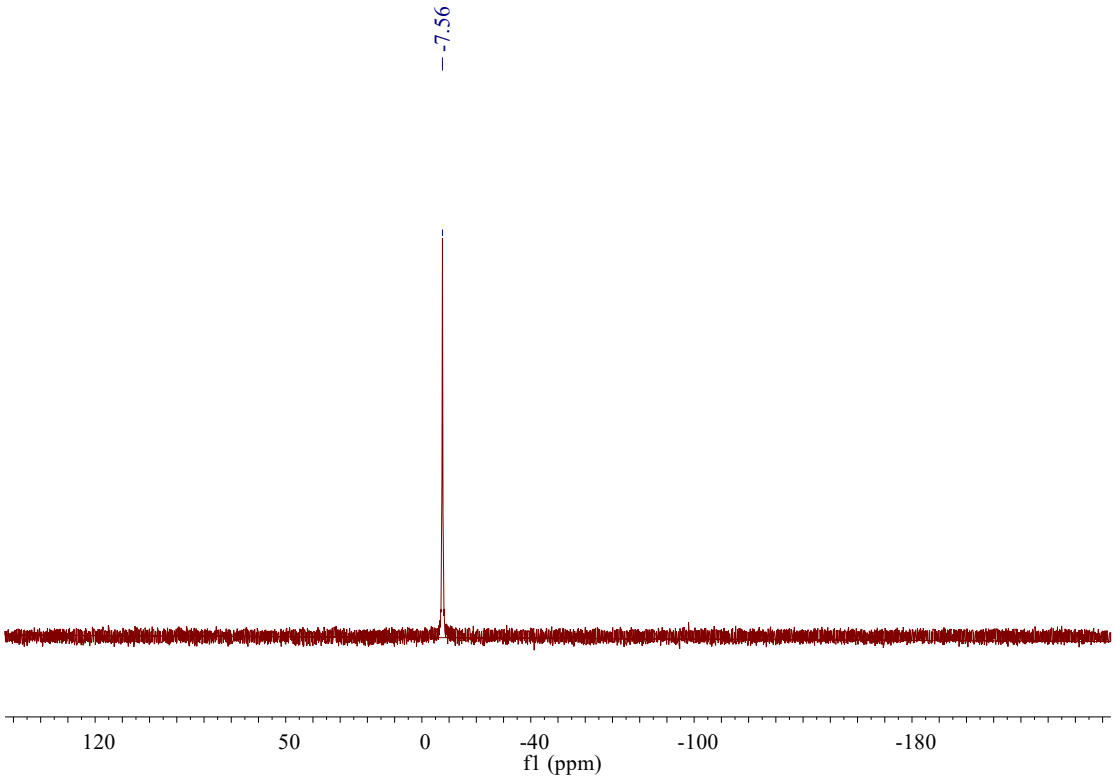


Figure S11. ^{31}P NMR spectrum of **1** in $CDCl_3$.

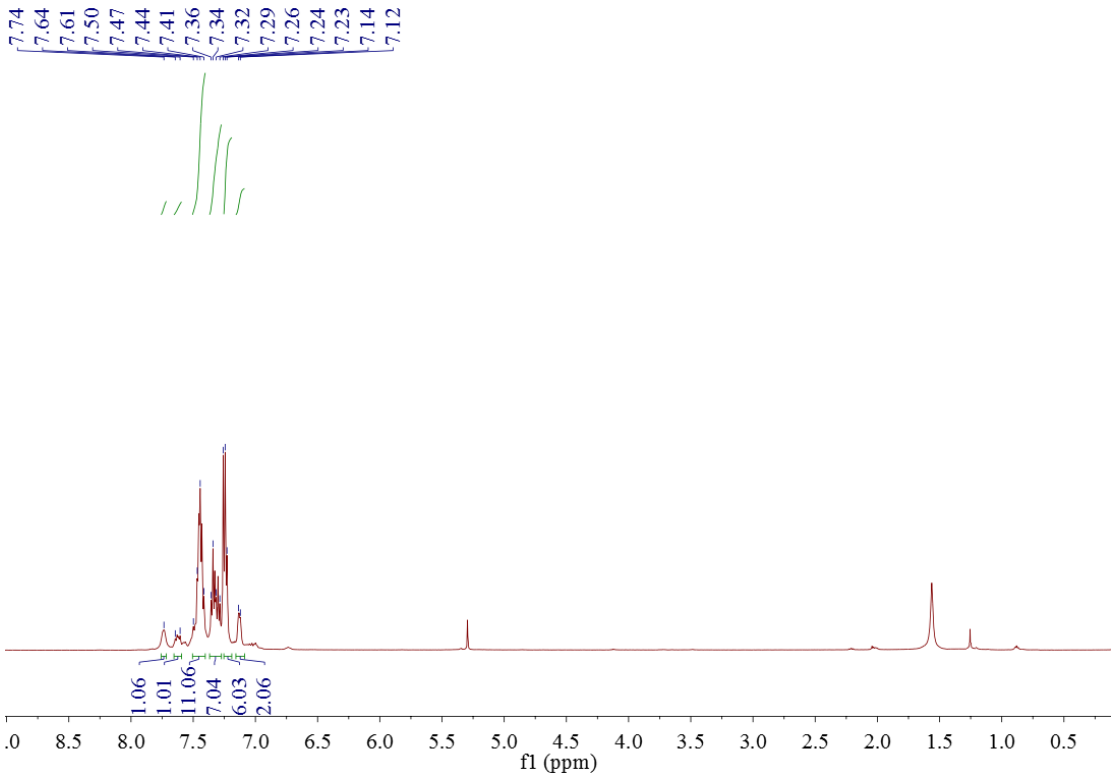


Figure S12. ^{1}H NMR spectrum of **2** in $CDCl_3$.

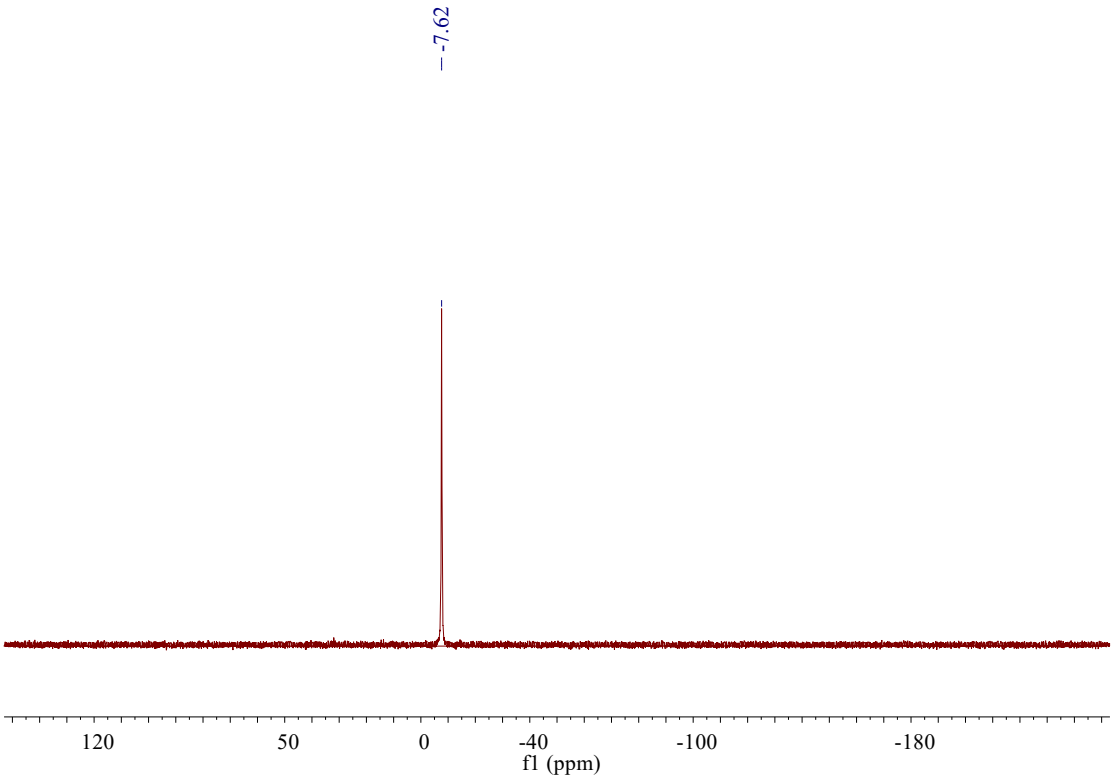


Figure S13. ^{31}P NMR spectrum of **2** in $CDCl_3$.

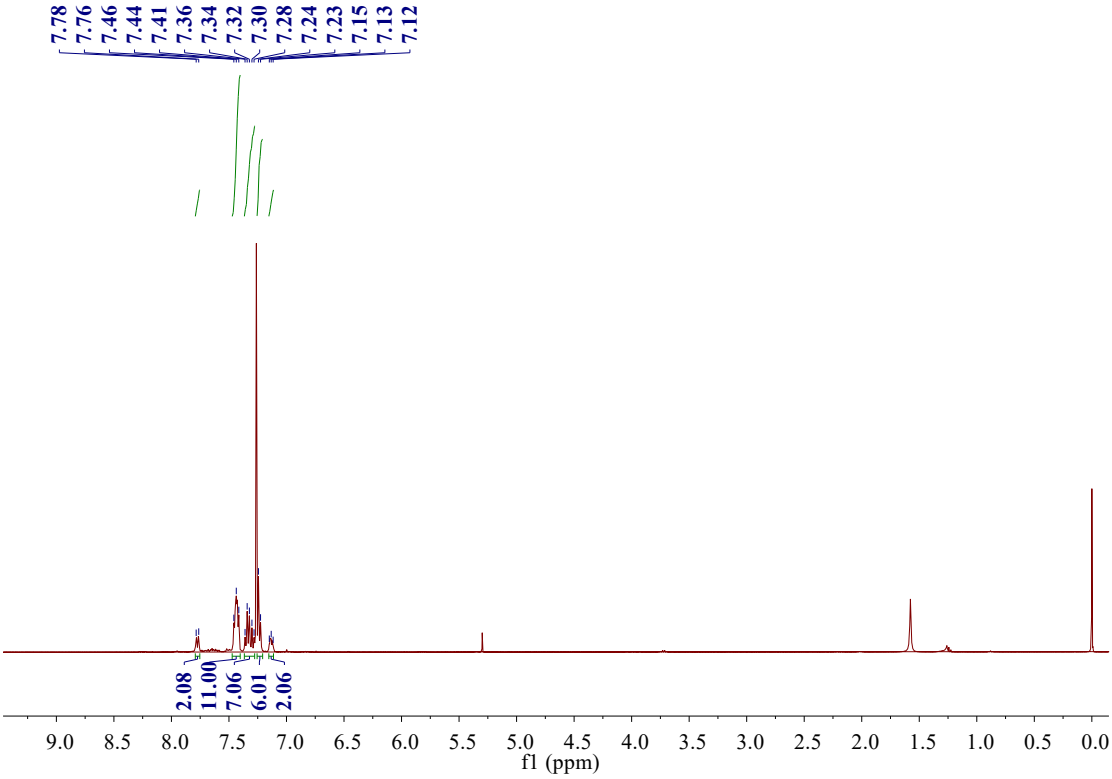


Figure S14. ^{1}H NMR spectrum of **3** in $CDCl_3$.

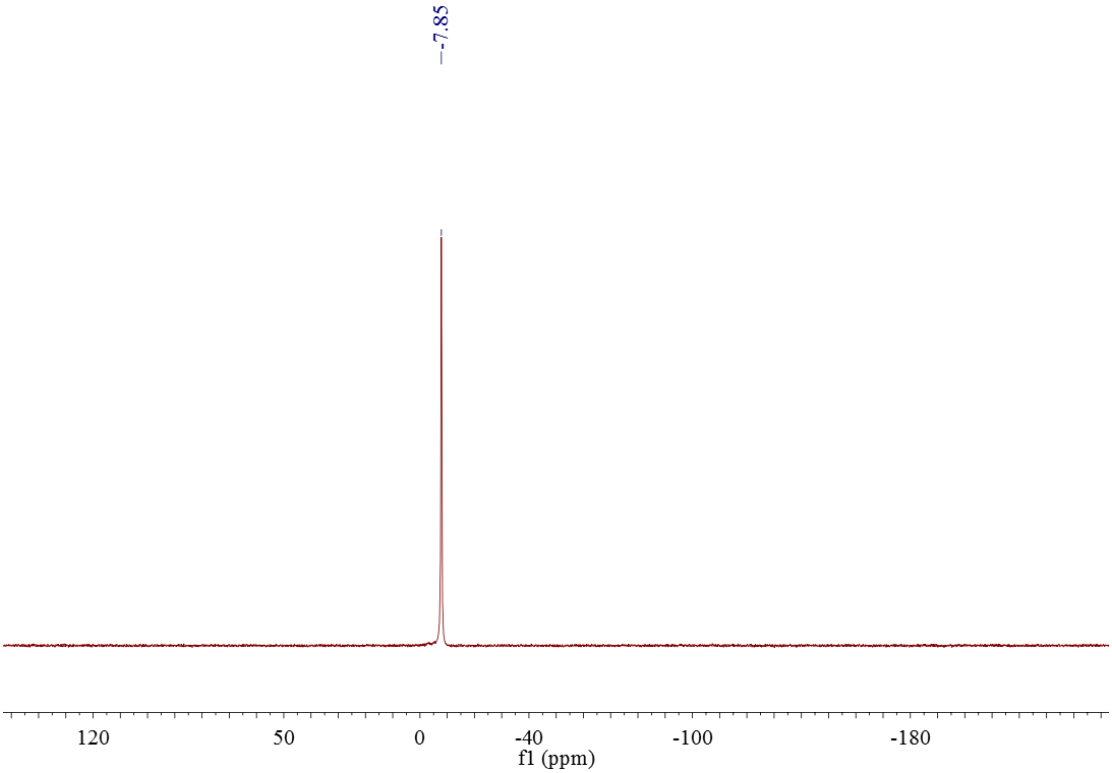


Figure S15. ^{31}P NMR spectrum of **3** in $CDCl_3$.

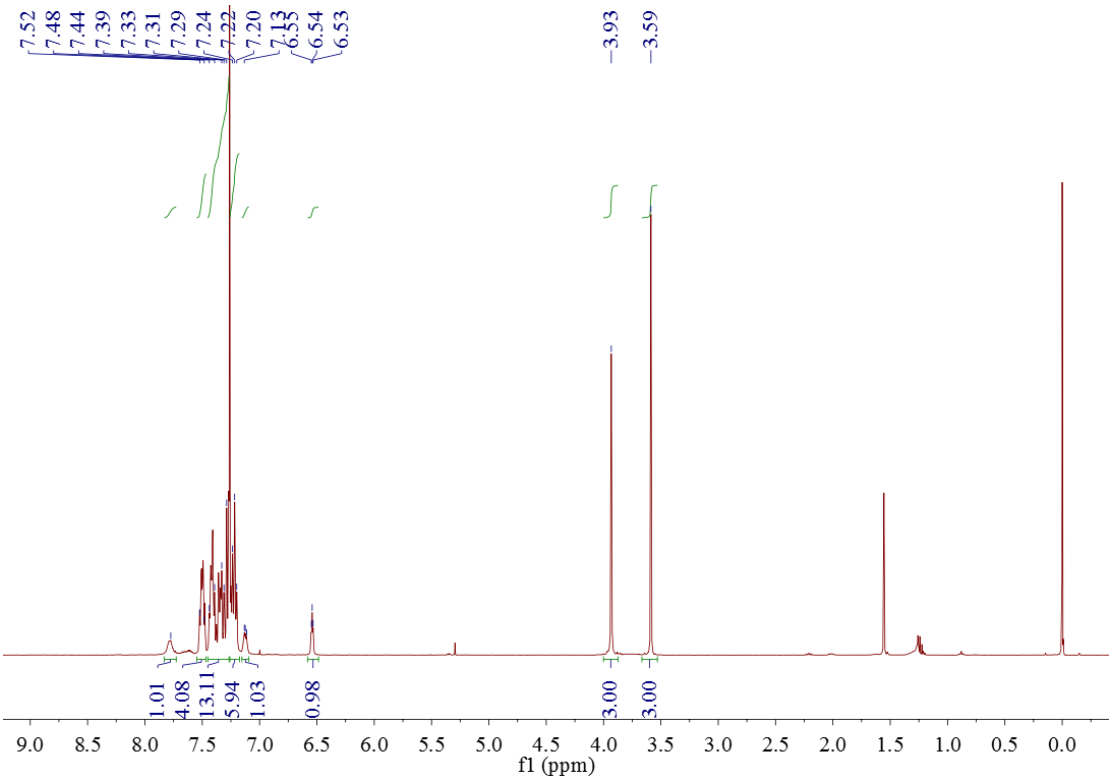


Figure S16. ^{1}H NMR spectrum of **4** in $CDCl_3$.

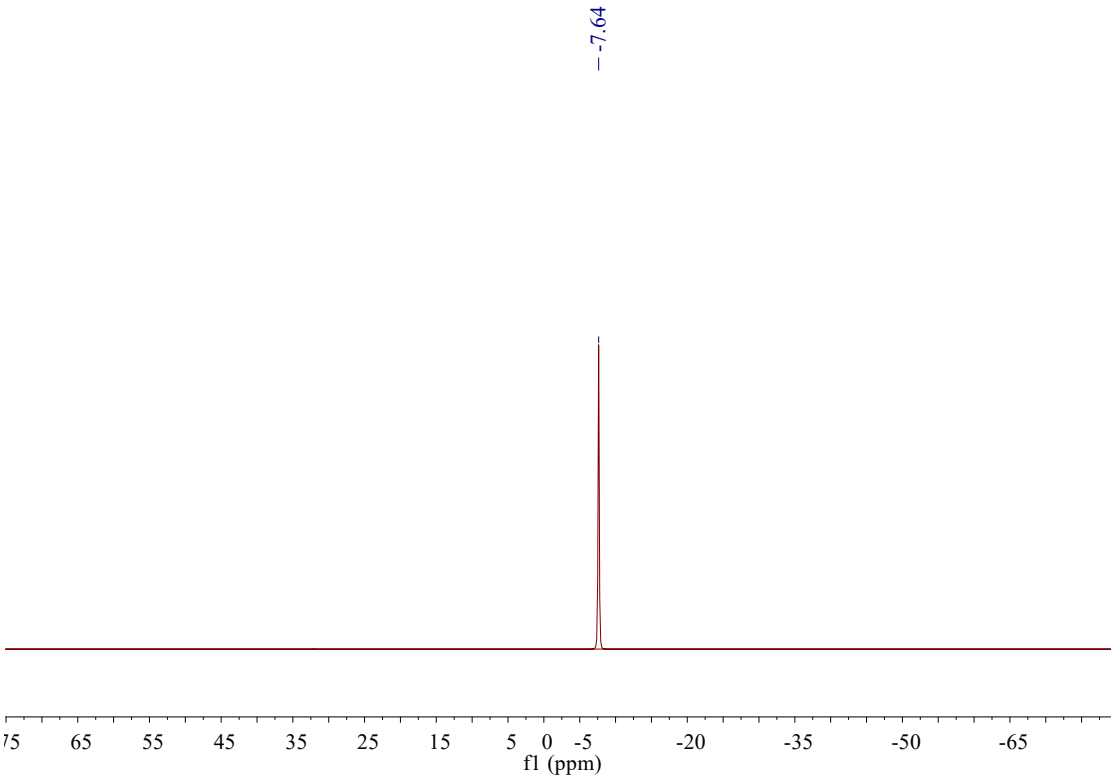


Figure S17. ^{31}P NMR spectrum of **4** in $CDCl_3$.

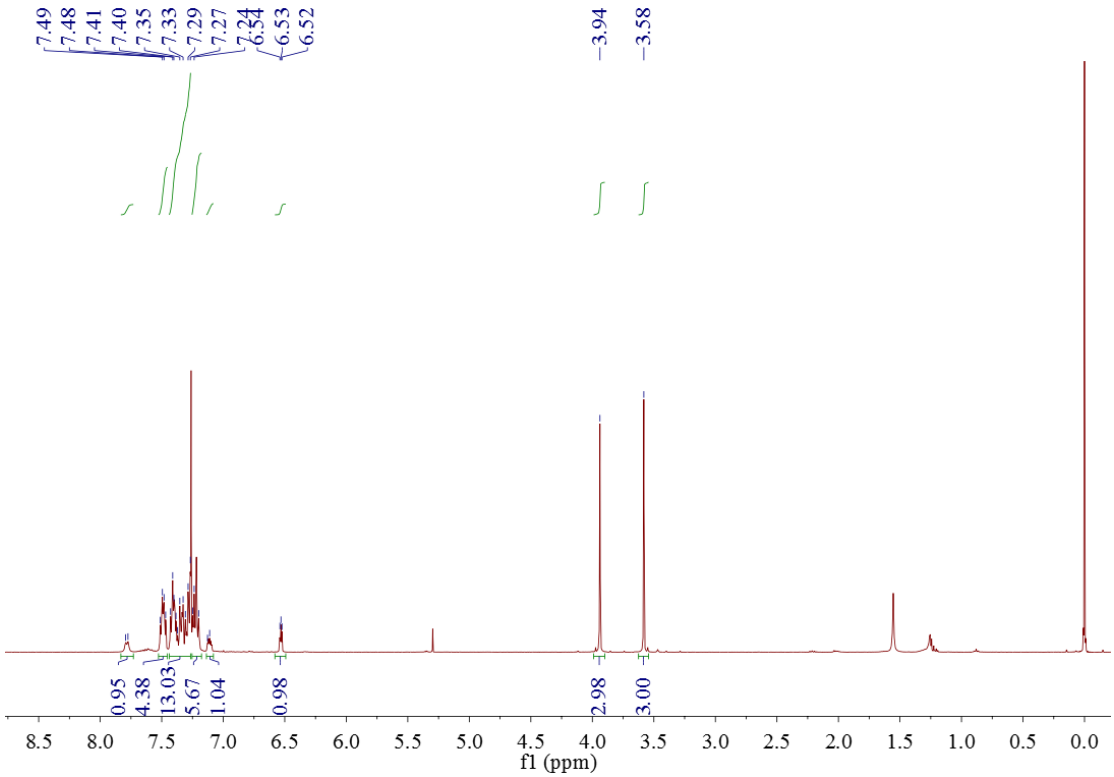


Figure S18. ^{1}H NMR spectrum of **5** in $CDCl_3$.

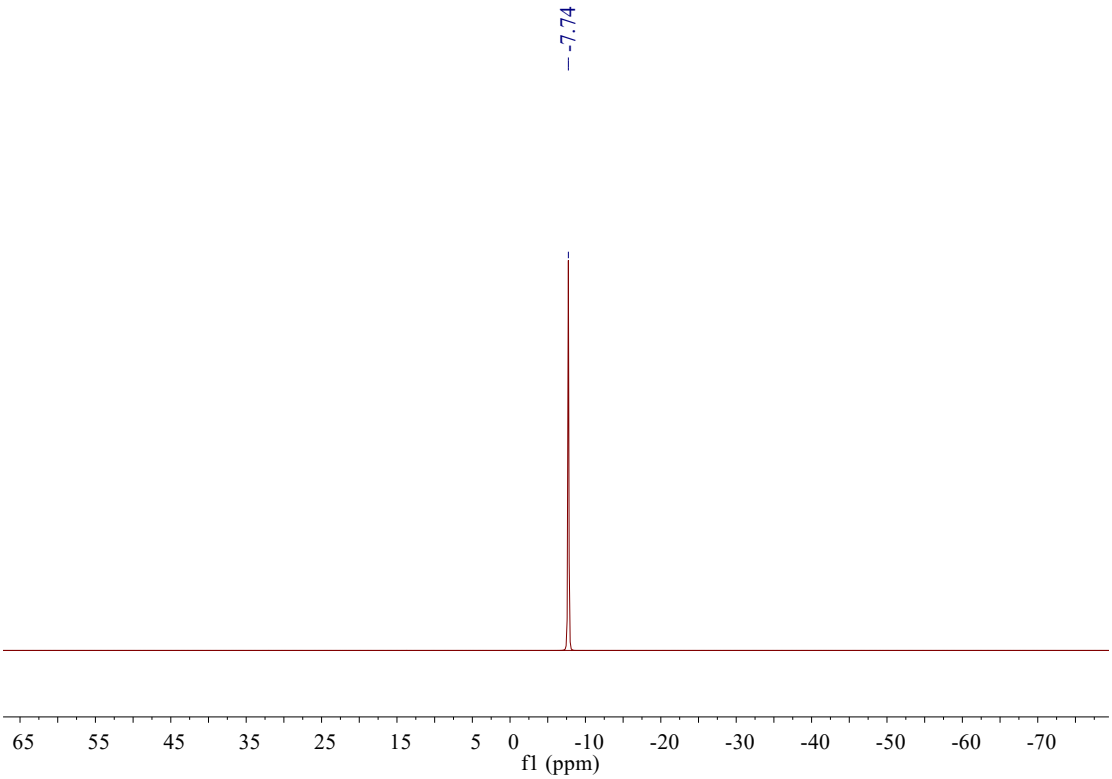


Figure S19. ^{31}P NMR spectrum of **5** in $CDCl_3$.

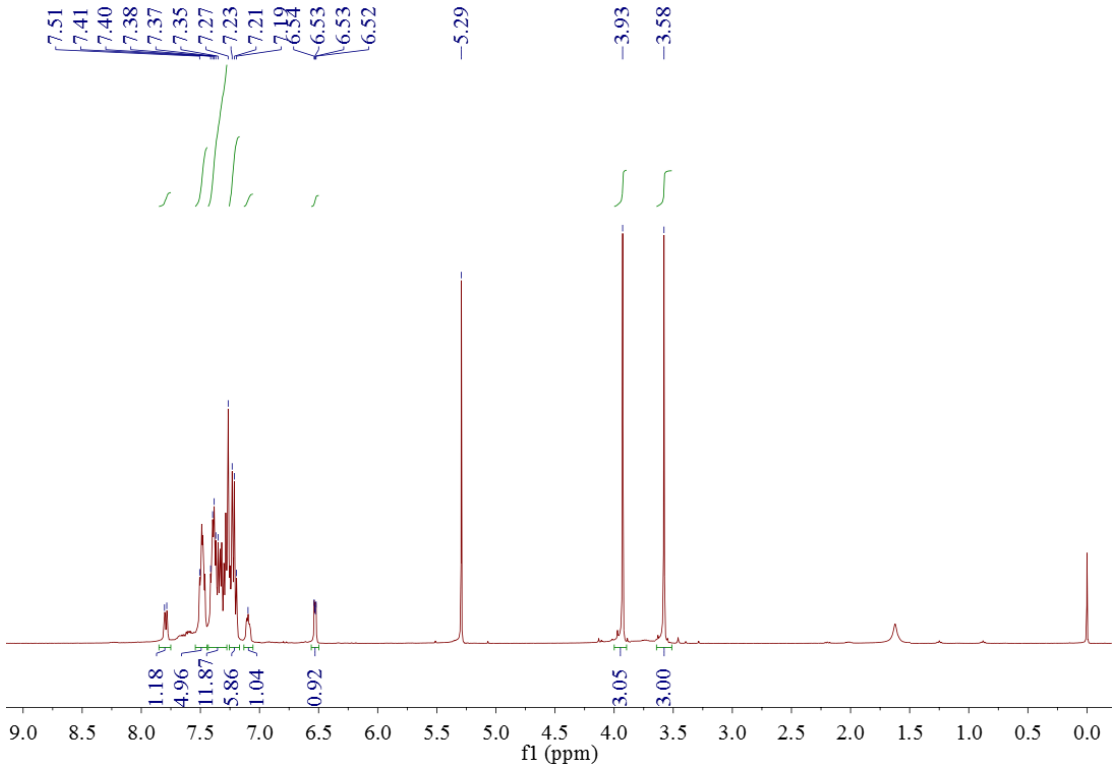


Figure S20. ^{1}H NMR spectrum of **6** in $CDCl_3$.

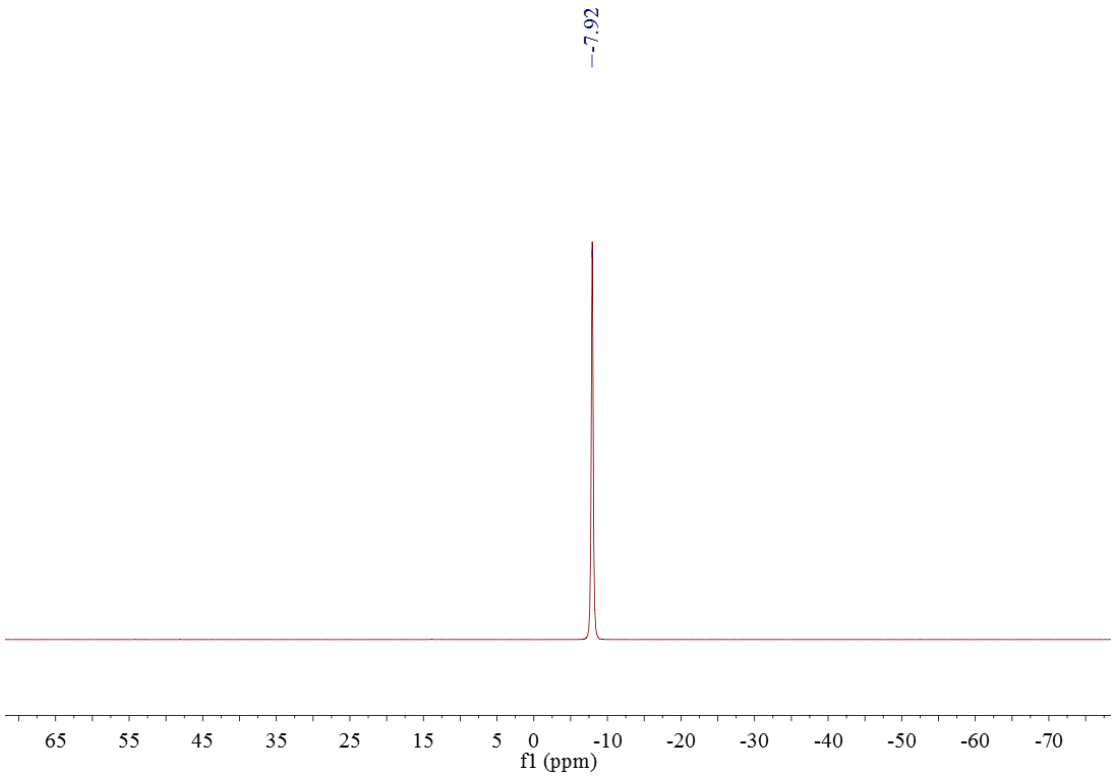


Figure S21. ^{31}P NMR spectrum of **6** in $CDCl_3$.

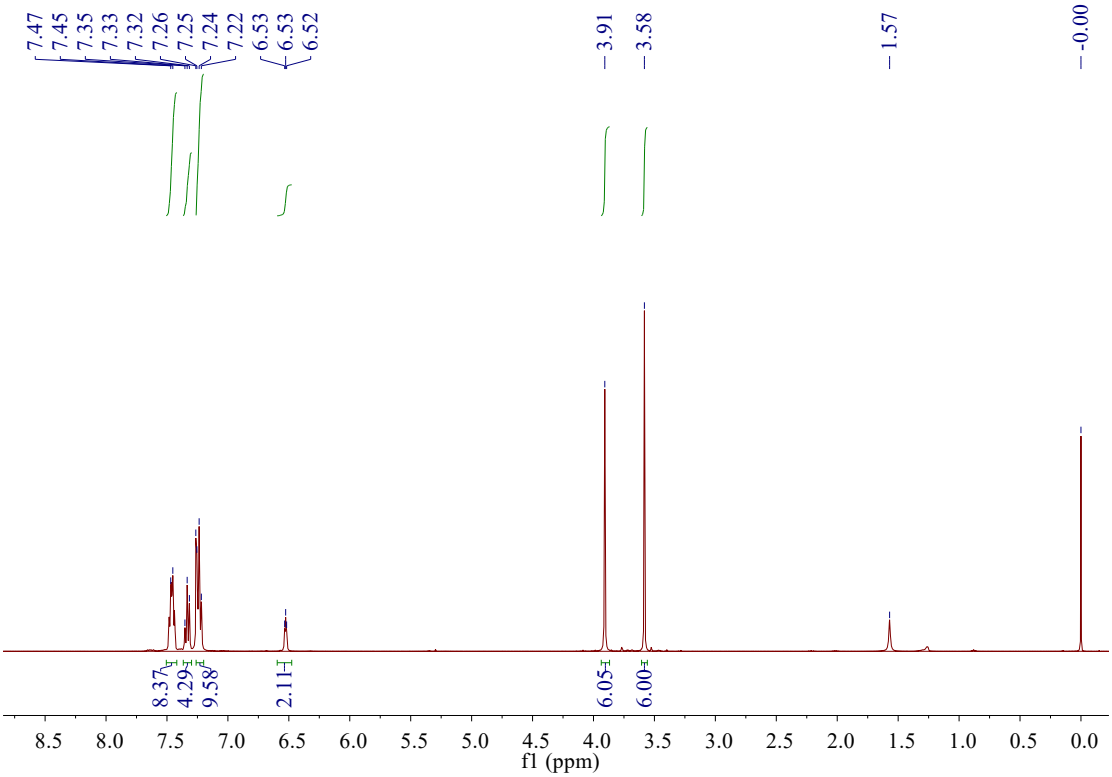


Figure S22. ^{1}H NMR spectrum of **7** in $CDCl_3$.

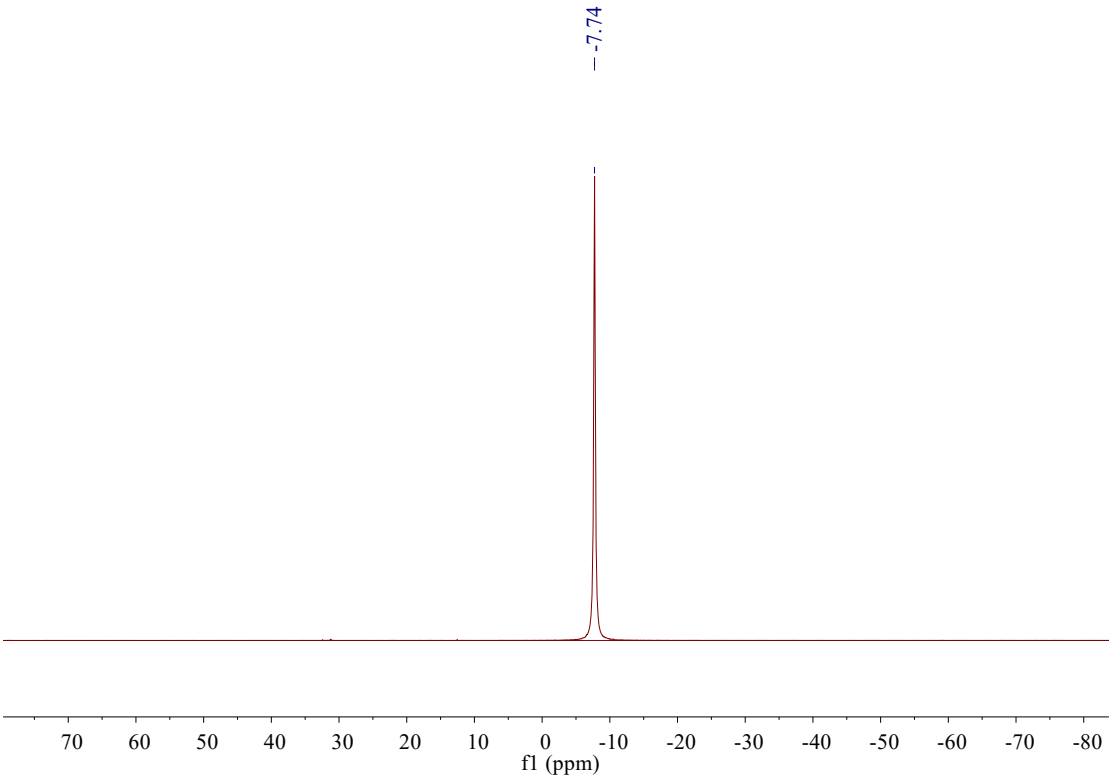


Figure S23. ^{31}P NMR spectrum of **7** in $CDCl_3$.

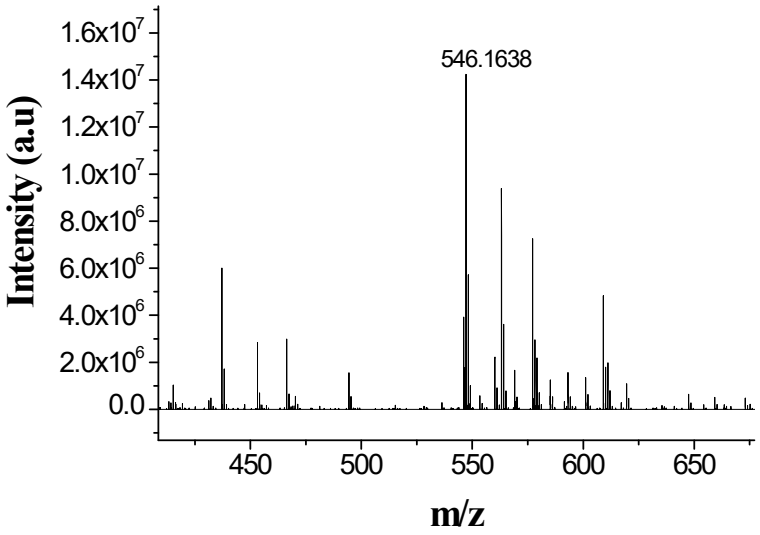


Figure 24. Mass spectrum of **L1**.

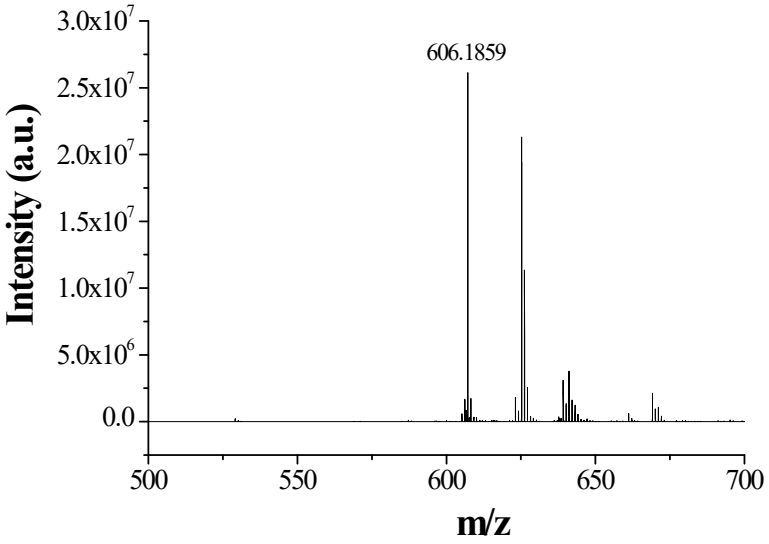


Figure 25. Mass spectrum of **L2**.

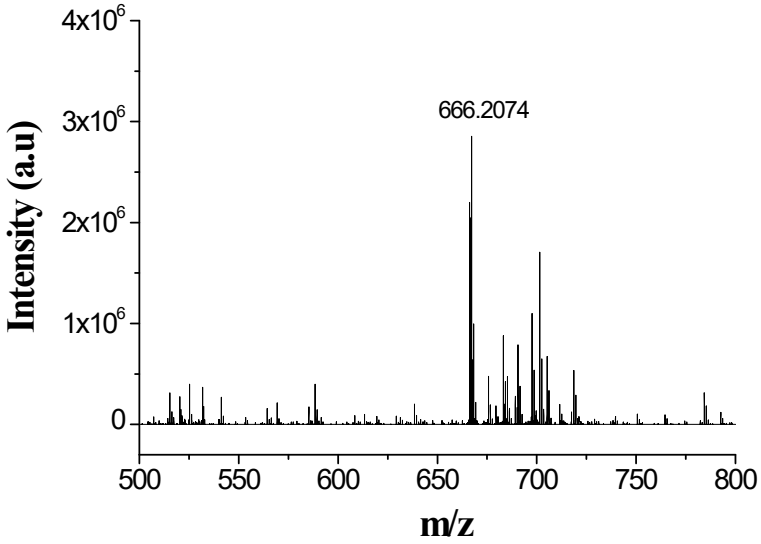


Figure 26. Mass spectrum of **L3**.

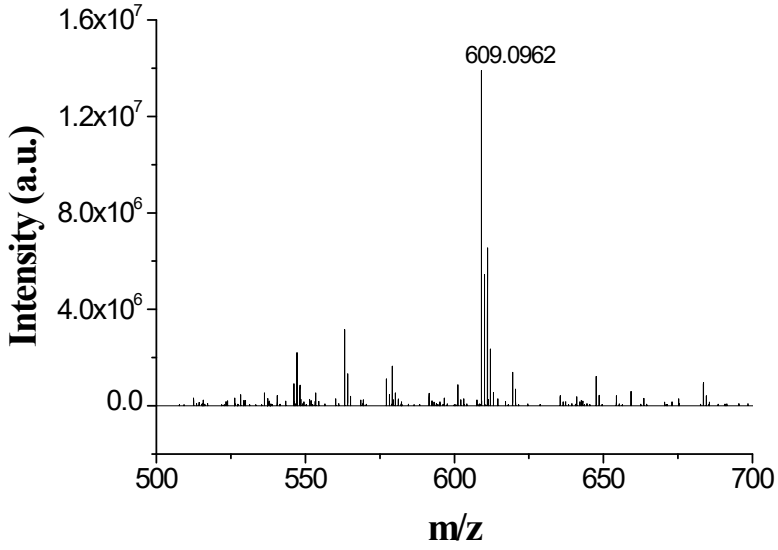


Figure 27. Mass spectrum of complex **1**.

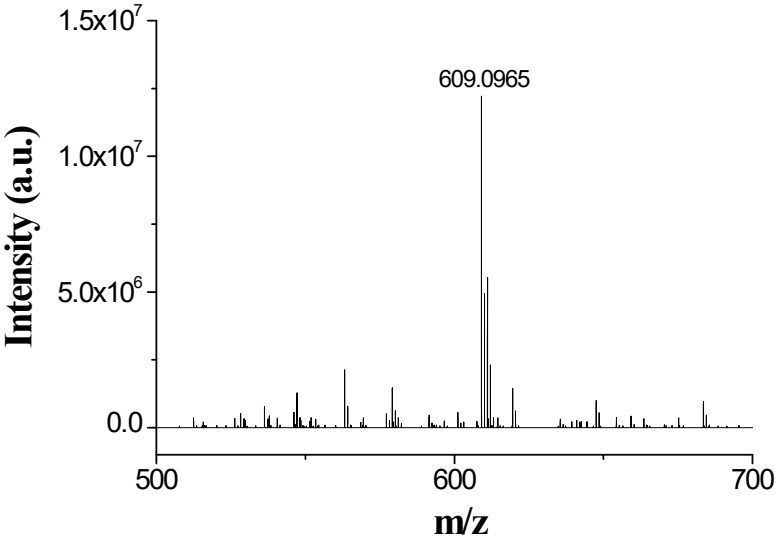


Figure 28. Mass spectrum of complex **2**.

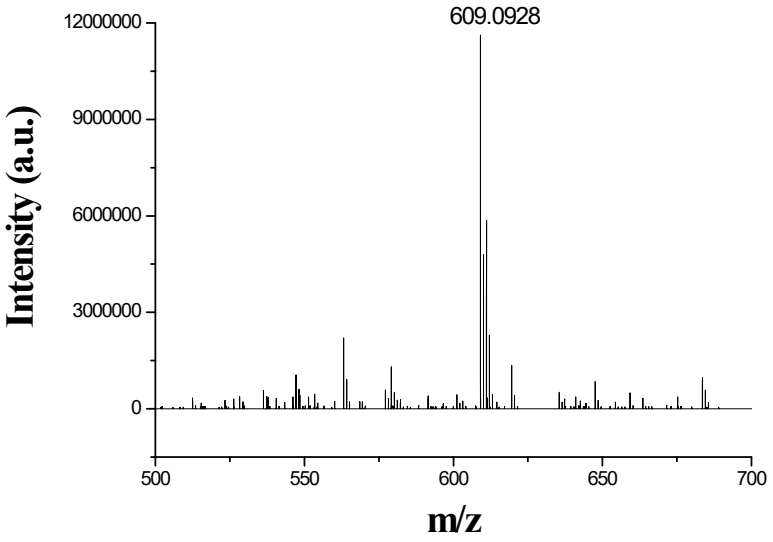


Figure 29. Mass spectrum of complex **3**.

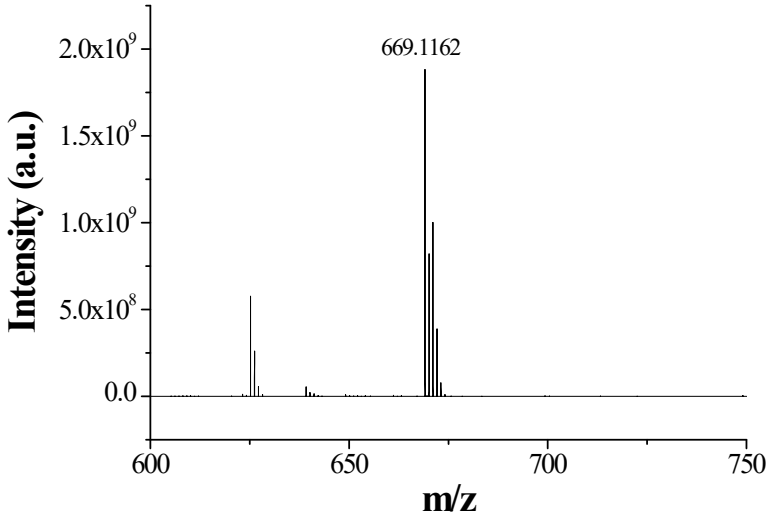


Figure 30. Mass spectrum of complex **4**.

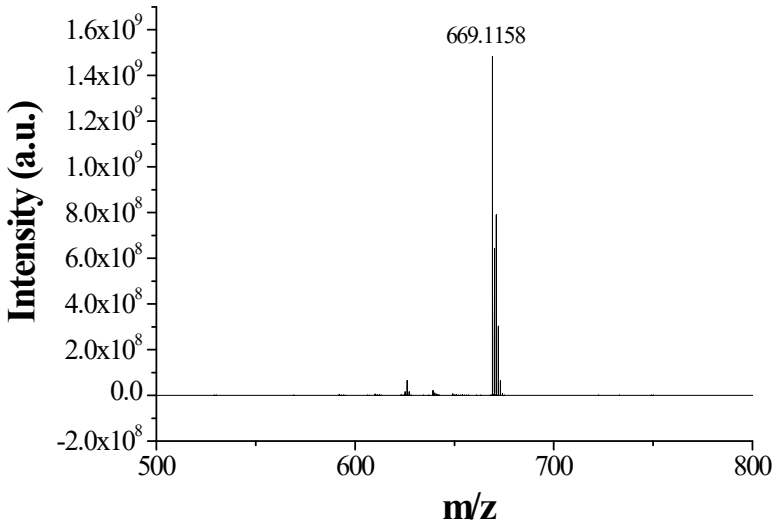


Figure 31. Mass spectrum of complex **5**.

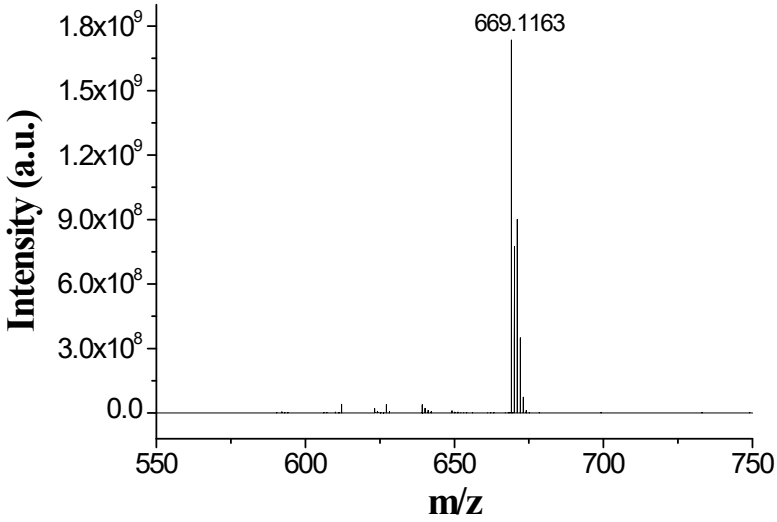


Figure 32. Mass spectrum of complex **6**.

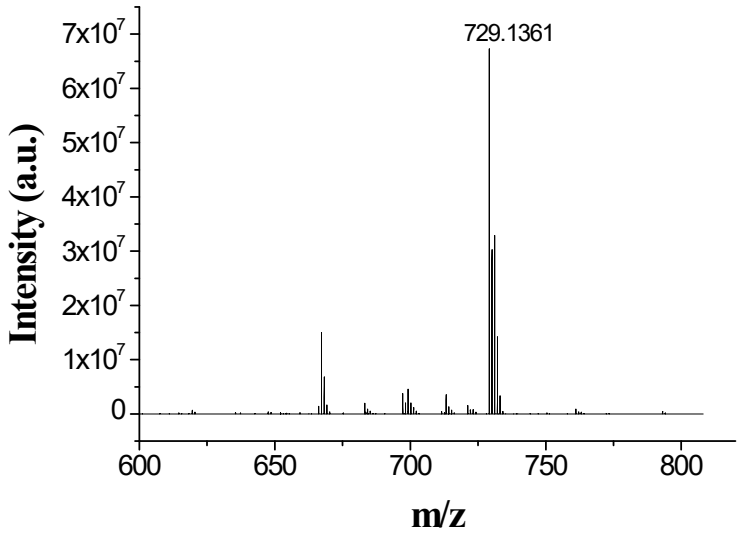


Figure S33. Mass spectrum of complex **7**.

2. Molecular structures

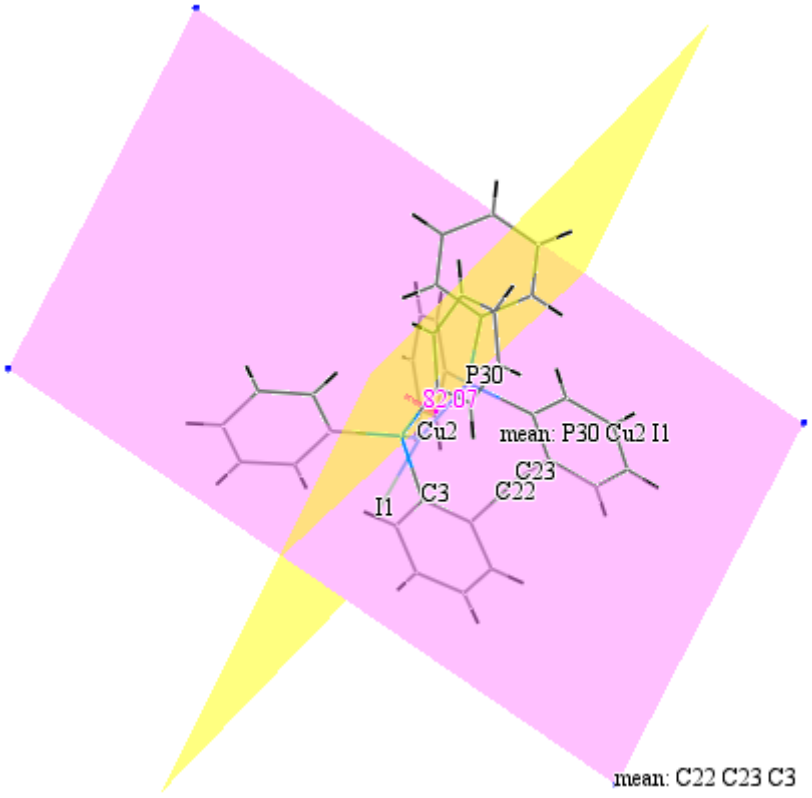


Figure S34. The dihedral angles between the Cu-X-P plane and the plane of C≡C and its connected phenyl ring in complex **1**.

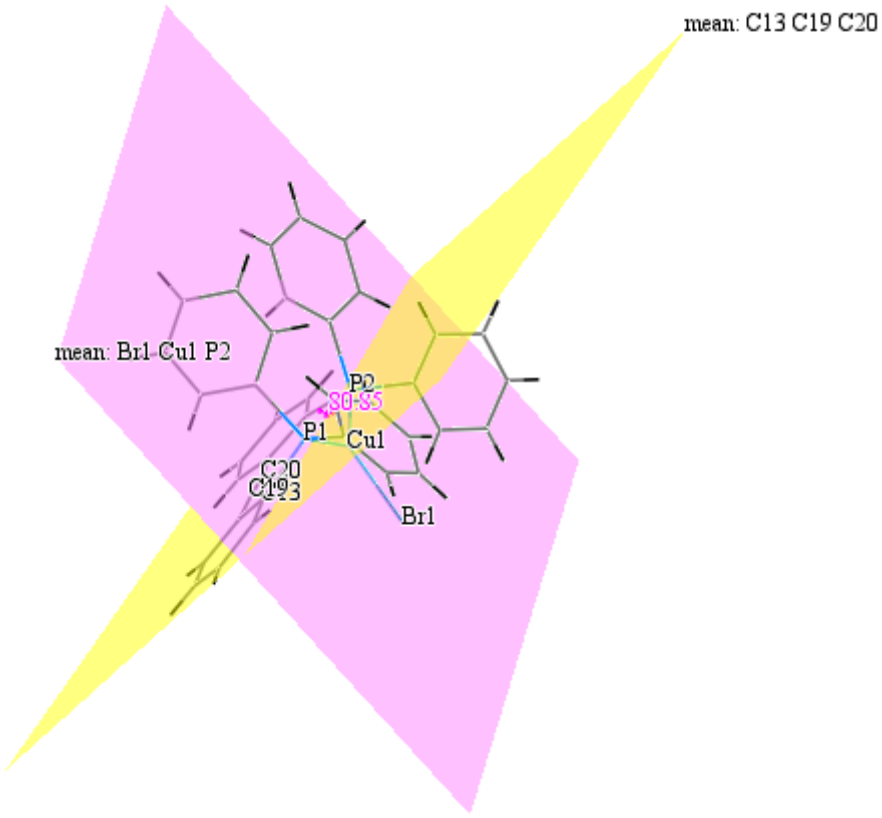


Figure S35. The dihedral angles between the Cu-X-P plane and the plane of C≡C and its connected phenyl ring in complex **2**.

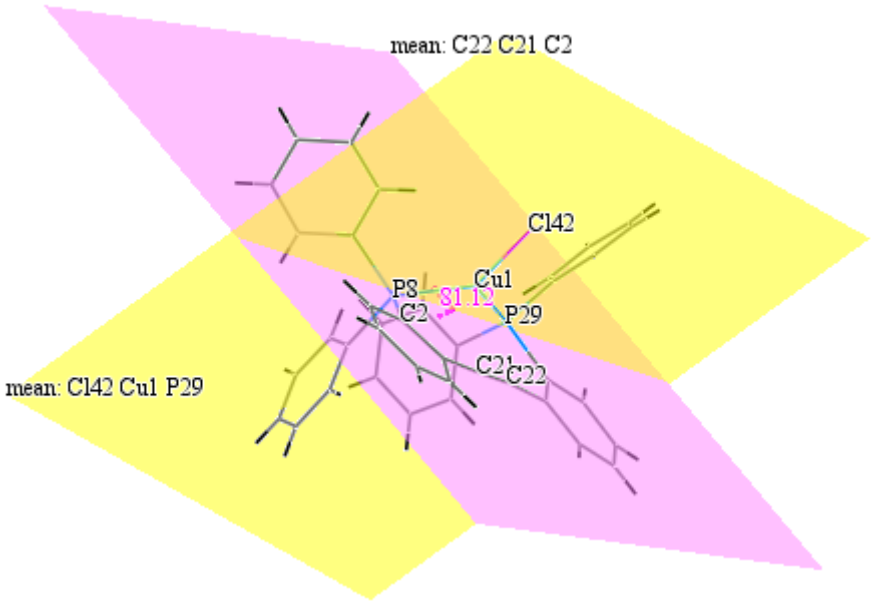


Figure S36. The dihedral angles between the Cu-X-P plane and the plane of C≡C and its connected phenyl ring in complex **3**.

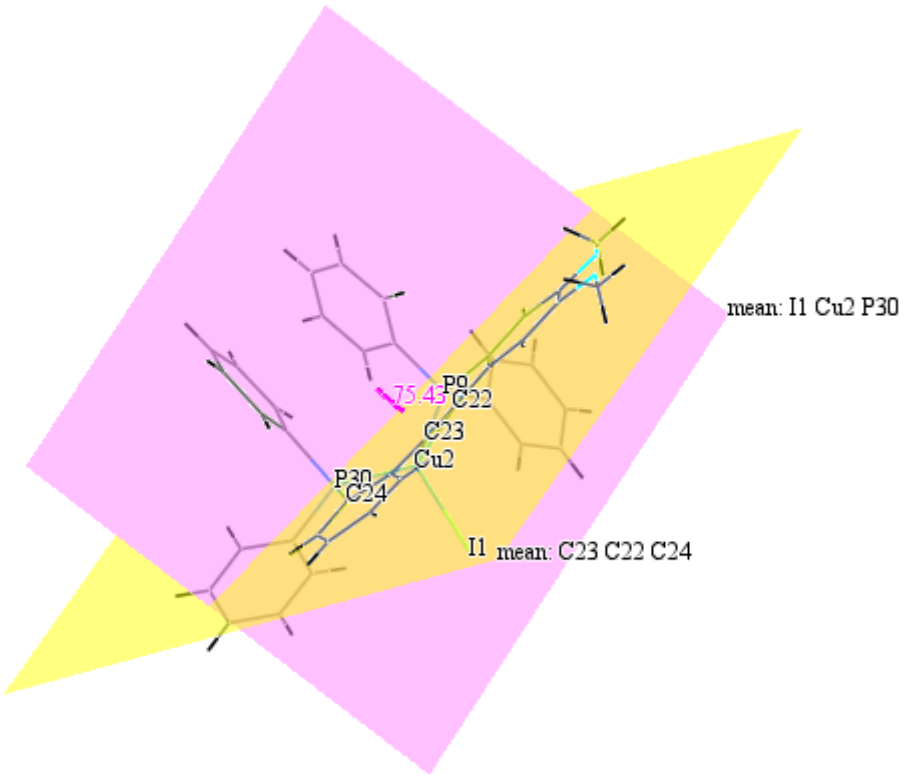


Figure S37. The dihedral angles between the Cu-X-P plane and the plane of C≡C and its connected phenyl ring in complex **4**.

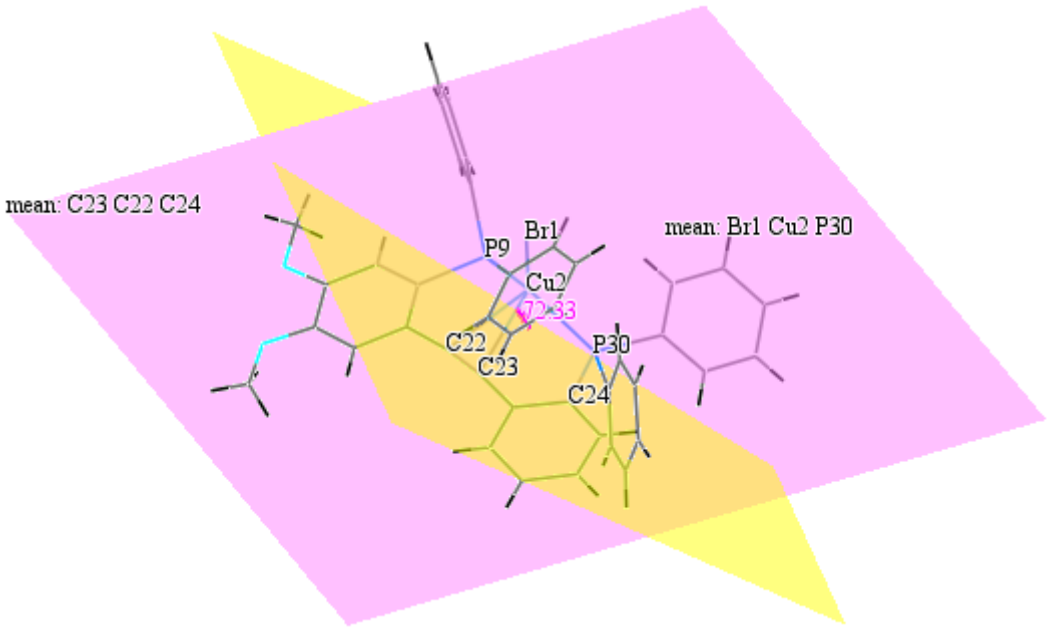


Figure S38. The dihedral angles between the Cu-X-P plane and the plane of C≡C and its connected phenyl ring in complex **5**.

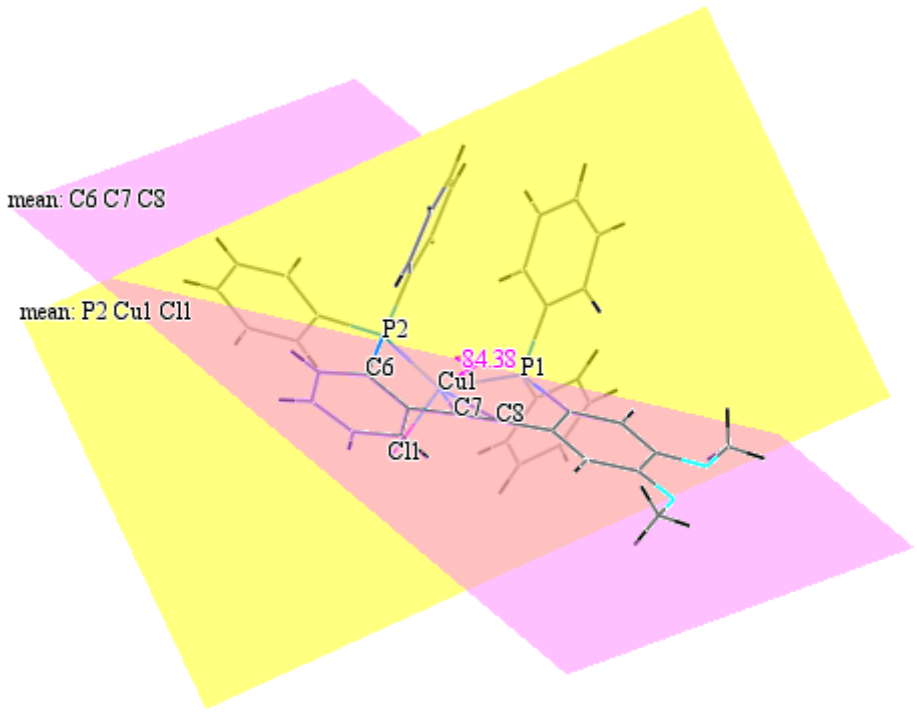


Figure S39.The dihedral angles between the Cu-X-P plane and the plane of C≡C and its connected phenyl ring in complex **6**.

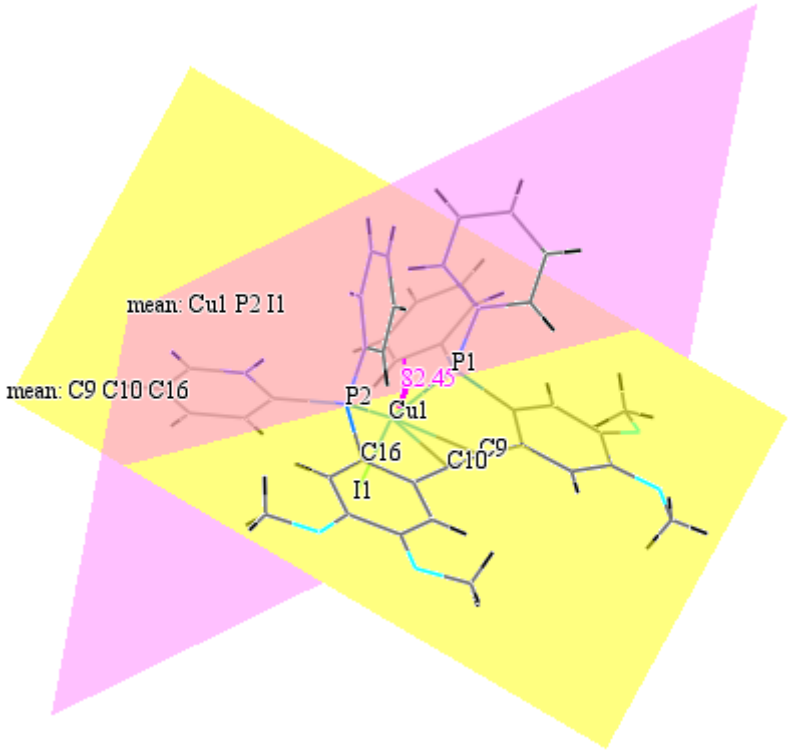


Figure S40. The dihedral angles between the Cu-X-P plane and the plane of C≡C and its connected phenyl ring in complex **7**.

3. Photophysical properties

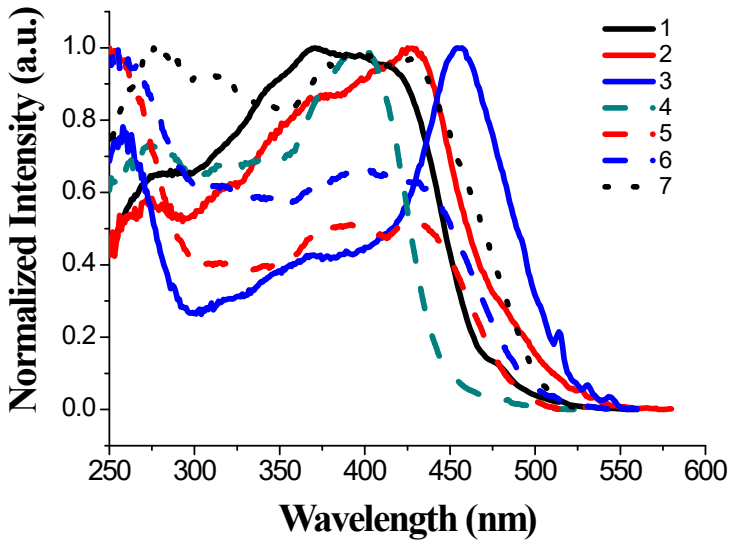
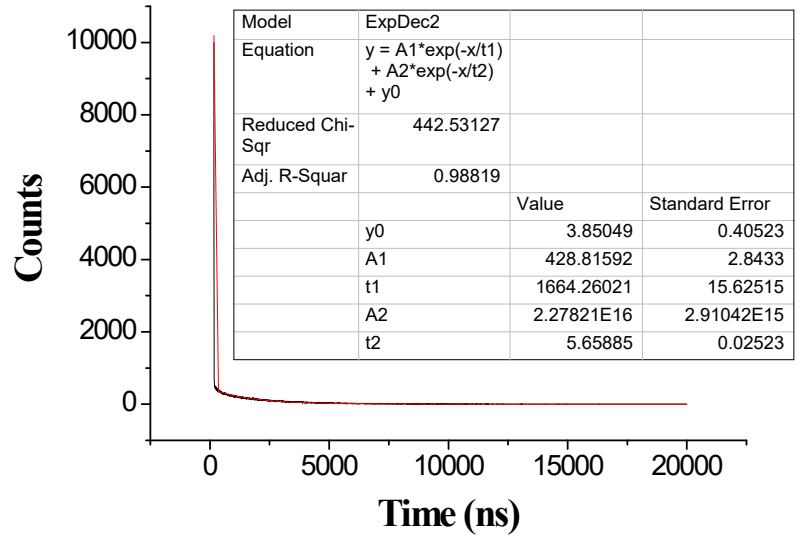


Figure S41. Normalized excitation spectra of **1-7** in solid state at 298 K (λ_{em} = 582 nm for **1**, λ_{em} = 607 nm for **2**, λ_{em} = 580 nm for **3**, λ_{em} = 540 nm for **4**, λ_{em} = 545 nm for **5**, λ_{em} = 574 nm for **6**, λ_{em} = 550 nm for **7**).



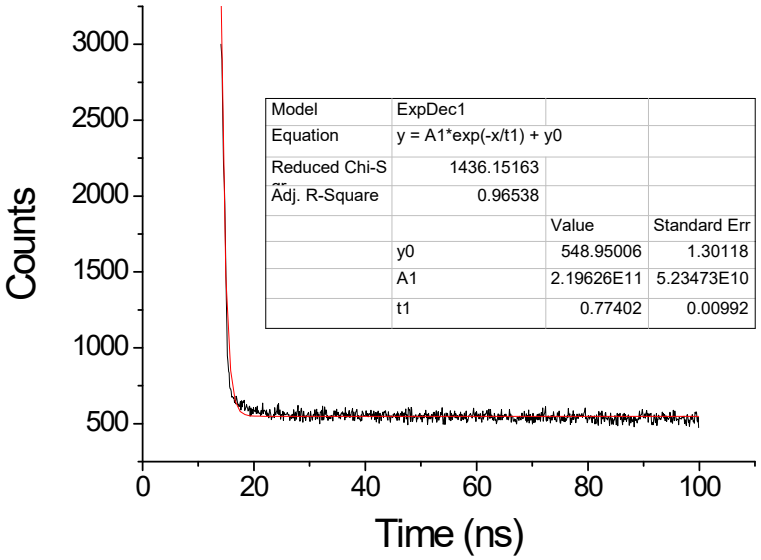
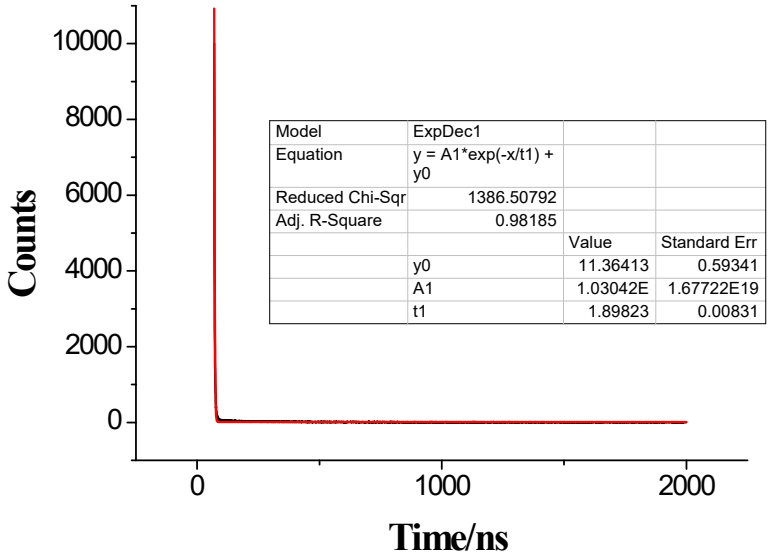


Figure S42. Time profiles of luminescence decay and exponential fit spectrum of **1** at 297 K (λ_{em} = 582 nm (up) and λ_{em} =753 nm (down)).



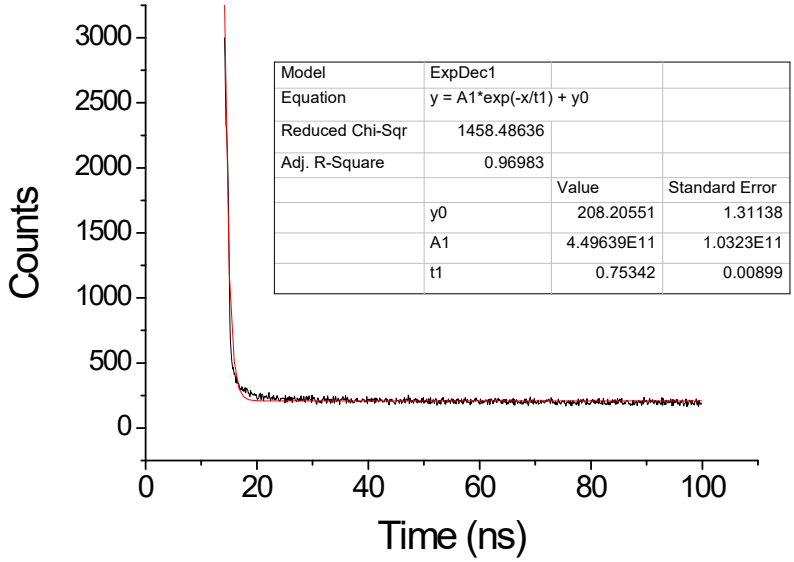


Figure S43. Time profiles of luminescence decay and exponential fit spectrum of **2** at 297 K (λ_{em} = 607 nm (up) and λ_{em} = 694 nm (down)).

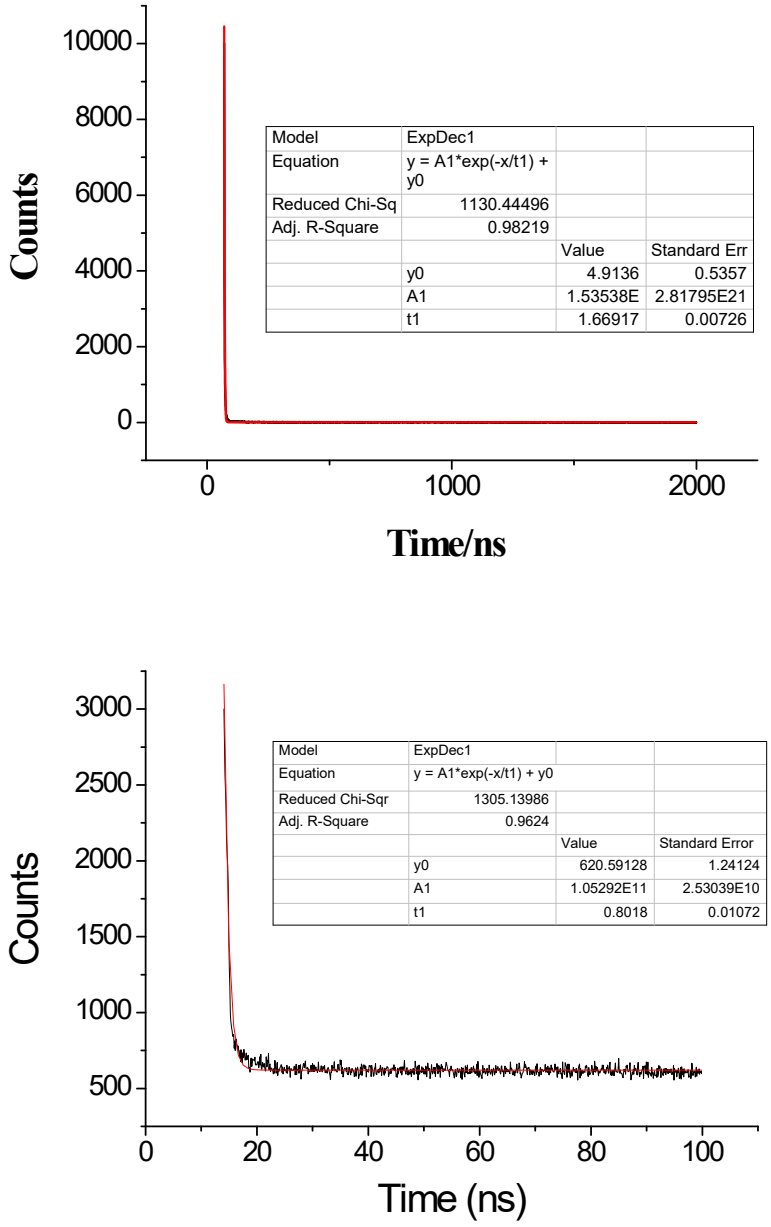


Figure S44. Time profiles of luminescence decay and exponential fit spectrum of **3** at 297 K (λ_{em} = 572 nm (up) and λ_{em} = 685 nm (down)).

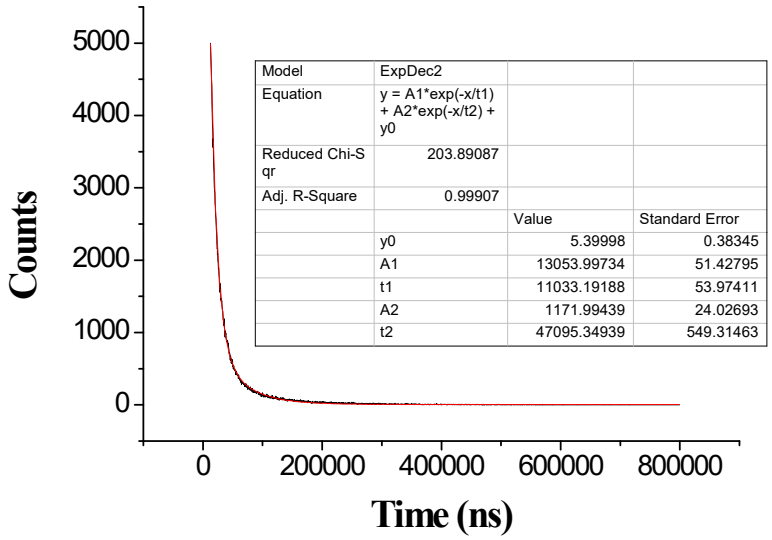


Figure S45. Time profiles of luminescence decay and exponential fit spectrum of **4** at 297 K (λ_{em} = 540 nm).

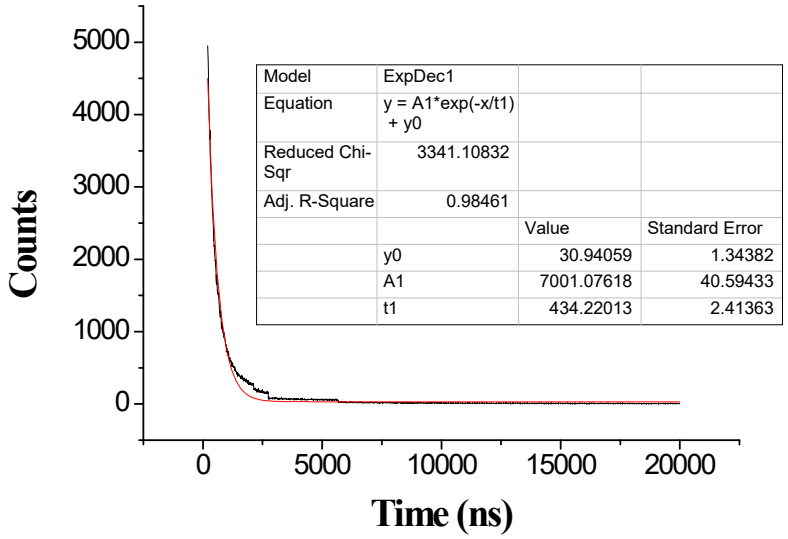
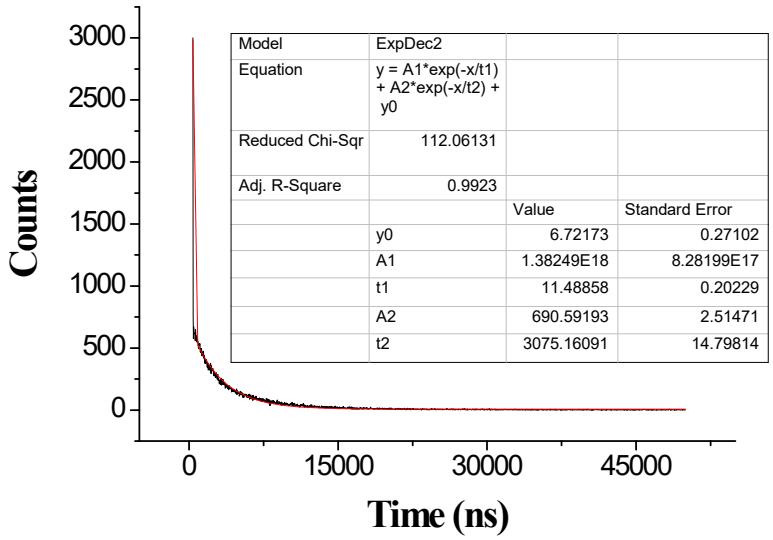
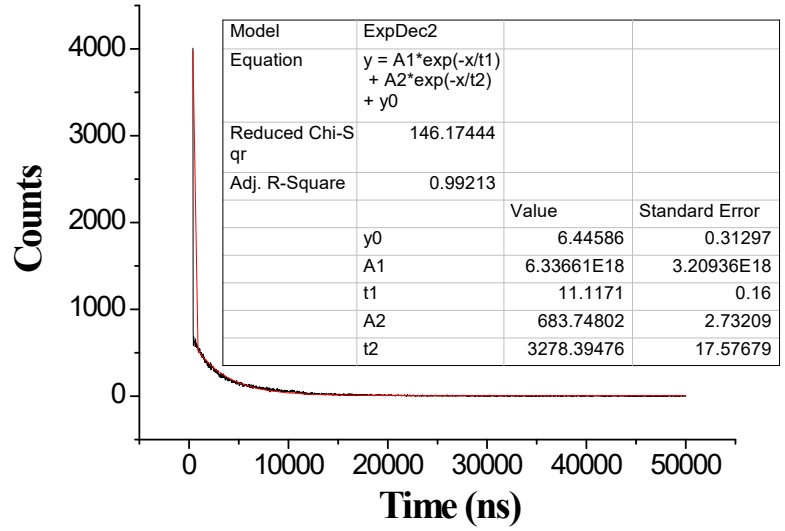


Figure S46. Time profiles of luminescence decay and exponential fit spectrum of **5** at 297 K (λ_{em} = 545 nm).



Model	ExpDec2		
Equation	y = A1*exp(-x/t1) + A2*exp(-x/t2) + y0		
Reduced Chi-Sqr	112.06131		
Adj. R-Square	0.9923		
		Value	Standard Error
	y0	6.72173	0.27102
	A1	1.38249E18	8.28199E17
	t1	11.48858	0.20229
	A2	690.59193	2.51471
	t2	3075.16091	14.79814

Figure S47. Time profiles of luminescence decay and exponential fit spectrum of **6** at 297 K (λ_{em} = 574 nm).



Model	ExpDec2		
Equation	y = A1*exp(-x/t1) + A2*exp(-x/t2) + y0		
Reduced Chi-Sqr	146.17444		
Adj. R-Square	0.99213		
		Value	Standard Error
	y0	6.44586	0.31297
	A1	6.33661E18	3.20936E18
	t1	11.1171	0.16
	A2	683.74802	2.73209
	t2	3278.39476	17.57679

Figure S48. Time profiles of luminescence decay and exponential fit spectrum of **7** at 297 K (λ_{em} = 550 nm).

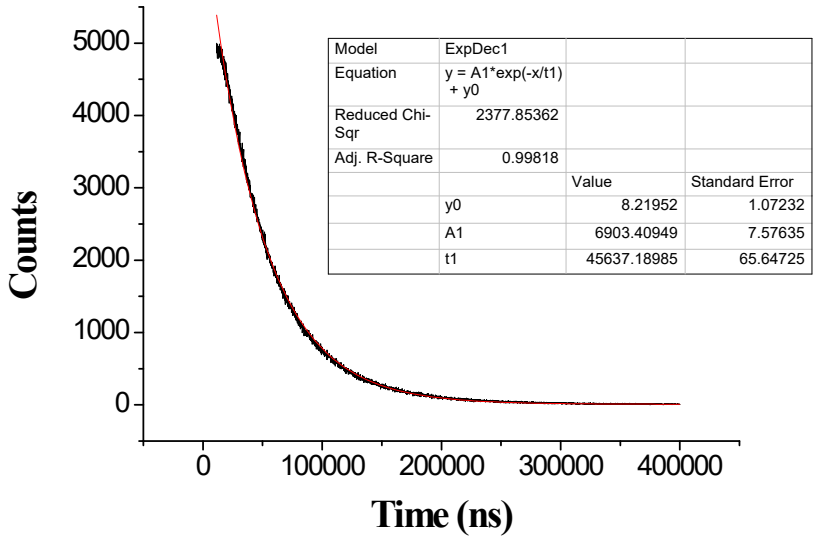


Figure S49. Time profiles of luminescence decay and exponential fit spectrum of **1** at 77 K (λ_{em} = 517 nm).

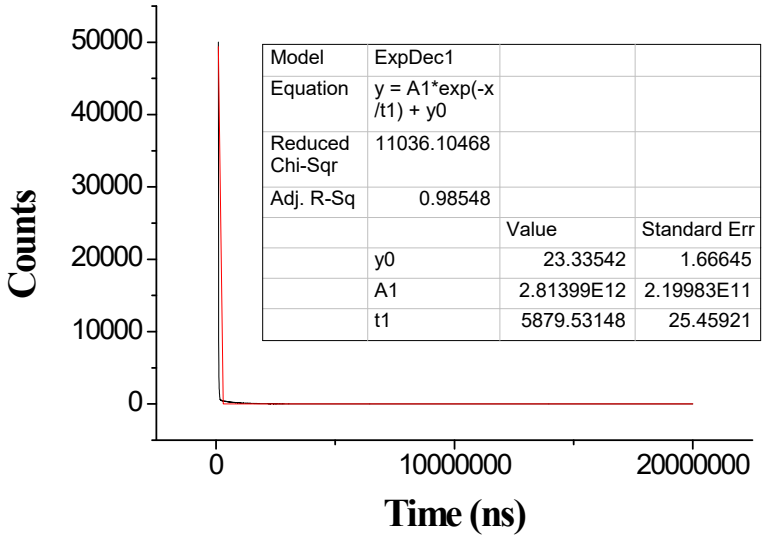


Figure S50. Time profiles of luminescence decay and exponential fit spectrum of **2** at 77 K (λ_{em} = 510 nm).

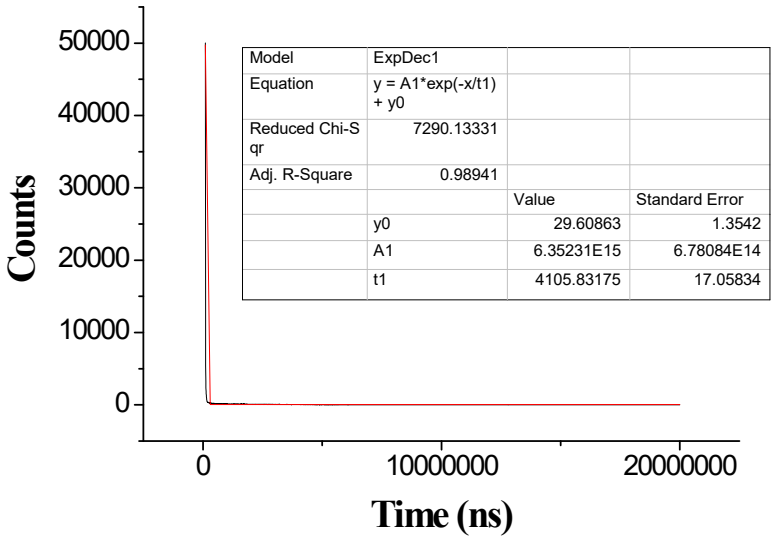


Figure S51. Time profiles of luminescence decay and exponential fit spectrum of **3** at 77 K (λ_{em} = 580 nm).

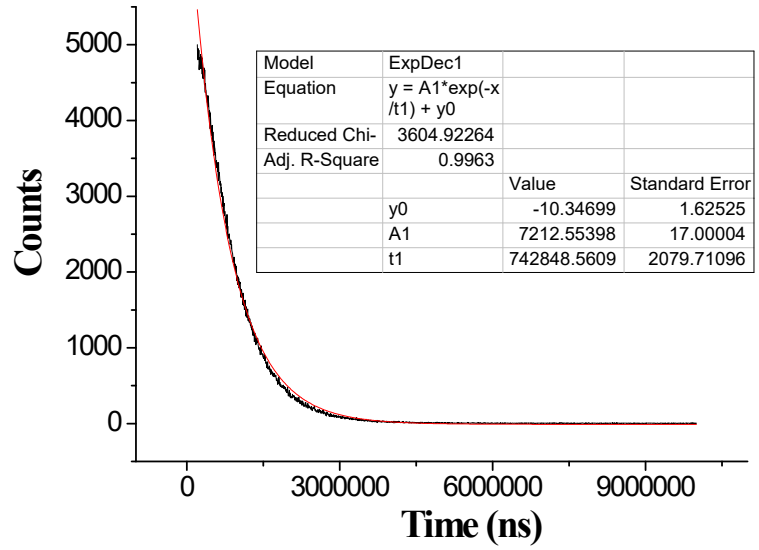


Figure S52. Time profiles of luminescence decay and exponential fit spectrum of **4** at 77 K (λ_{em} = 538 nm).

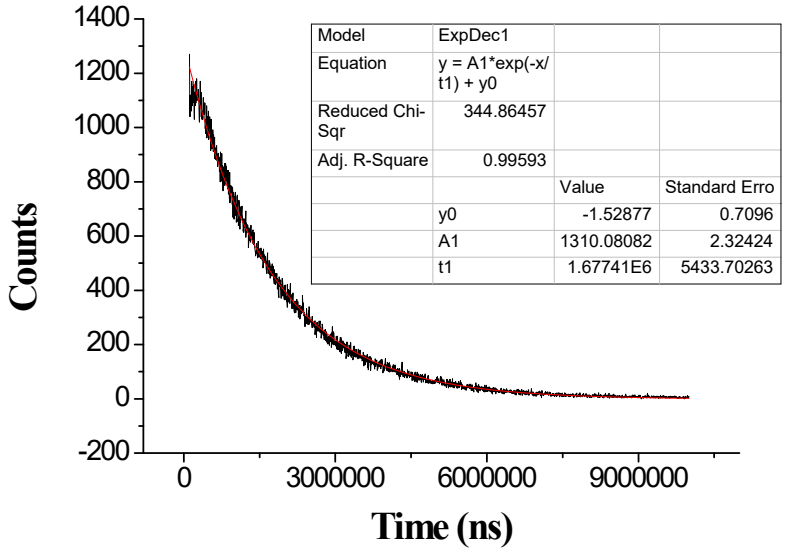


Figure S53. Time profiles of luminescence decay and exponential fit spectrum of **5** at 77 K (λ_{em} = 537 nm).

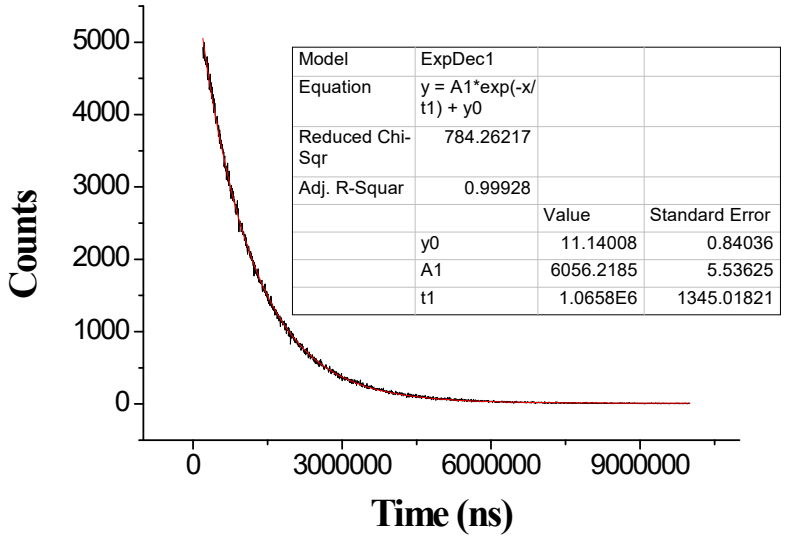


Figure S54. Time profiles of luminescence decay and exponential fit spectrum of **6** at 77 K (λ_{em} = 543 nm).

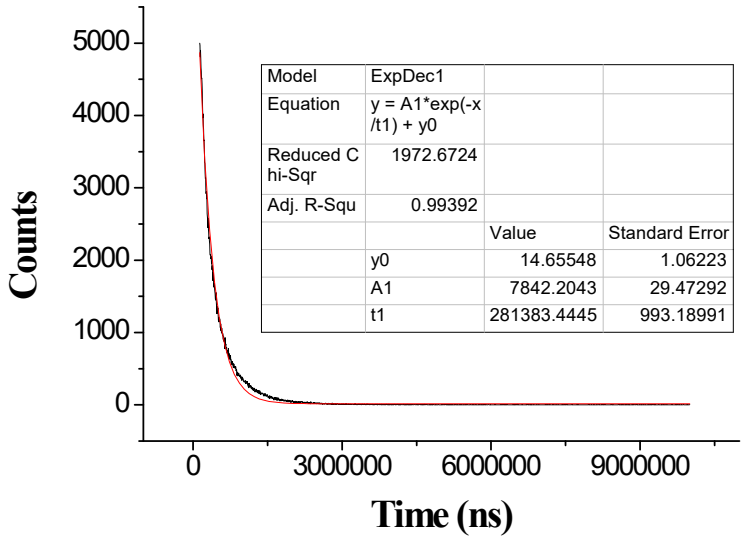


Figure S55. Time profiles of luminescence decay and exponential fit spectrum of **7** at 77 K (λ_{em} = 556 nm).

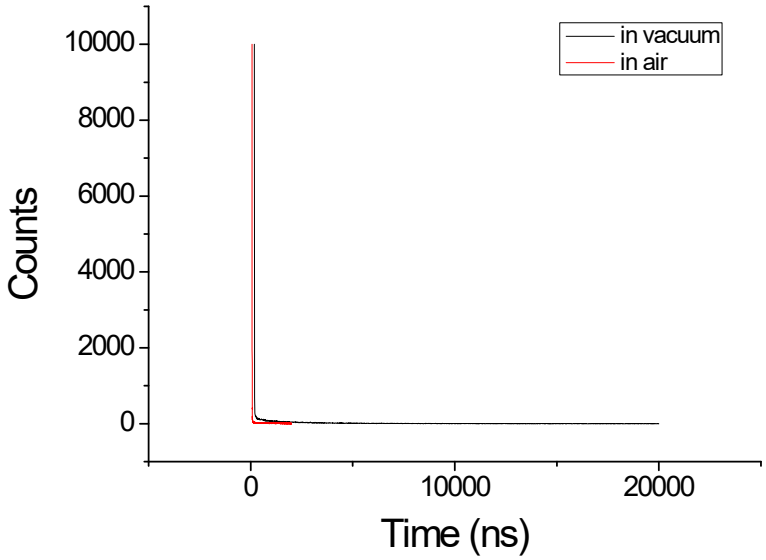


Figure S56. Luminescence decay of **2** at 298 K in air and under vacuum (λ_{em} = 607 nm).

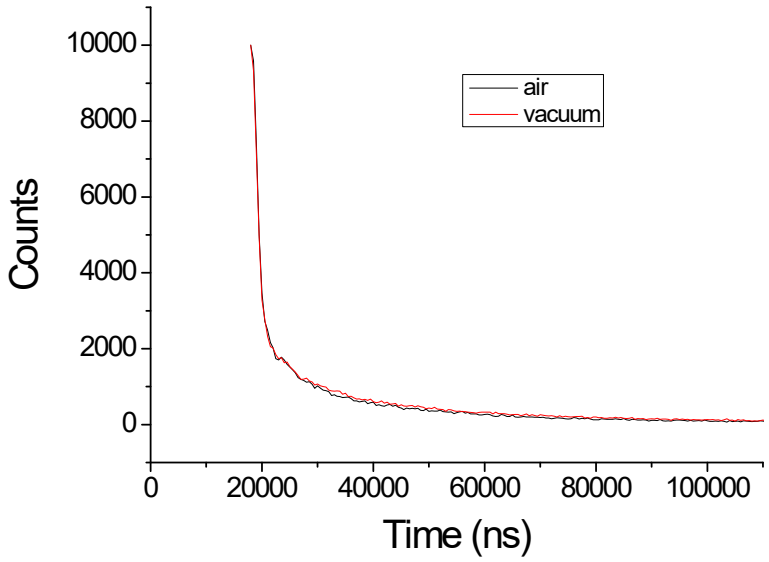


Figure S57. Luminescence decay of **4** at 298 K in air and under vacuum (λ_{em} = 540 nm).

4.Computational details

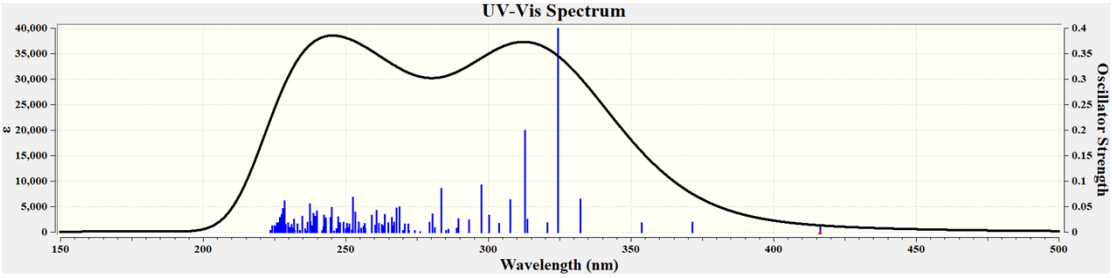


Figure S58. The absorption spectrum of complex **1** in CH_2Cl_2.

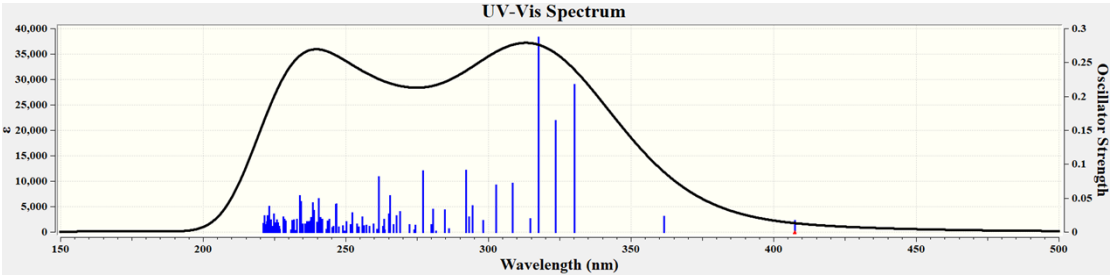


Figure S59. The absorption spectrum of complex **2** in CH_2Cl_2.

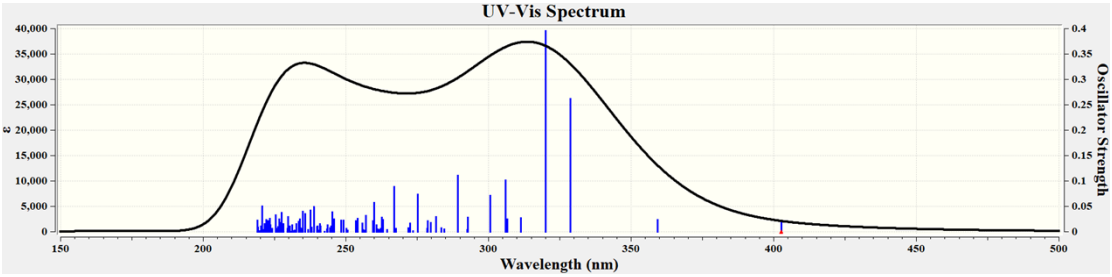


Figure S60. The absorption spectrum of complex **3** in CH_2Cl_2.

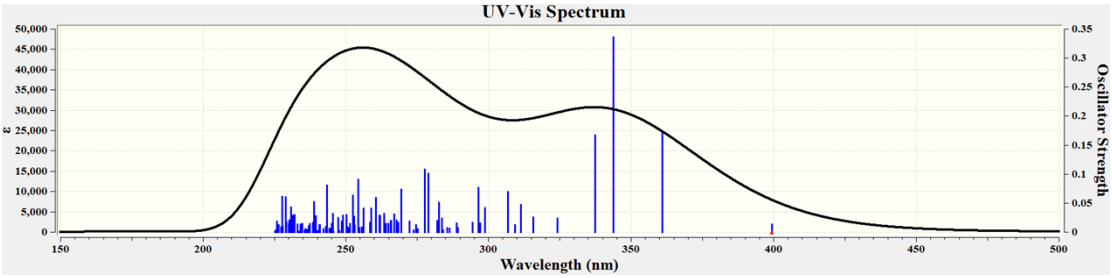


Figure S61. The absorption spectrum of complex **4** in CH_2Cl_2.

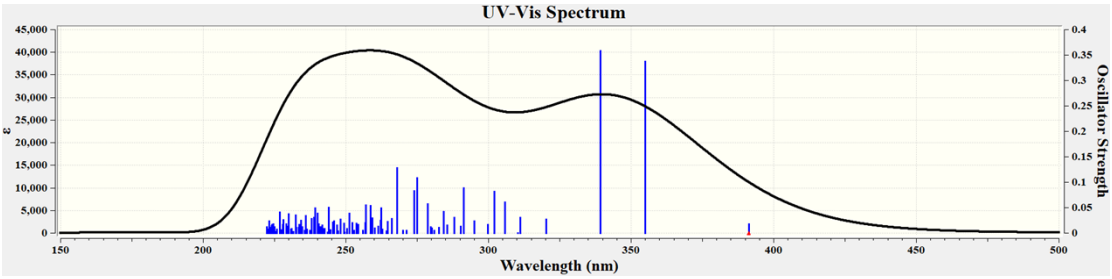


Figure S62. The absorption spectrum of complex **5** in CH_2Cl_2.

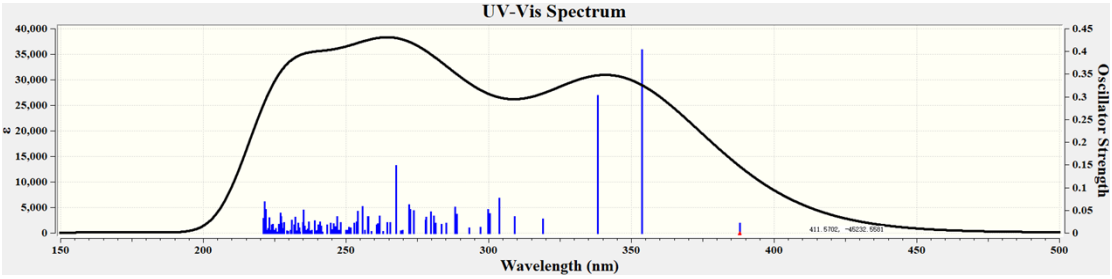


Figure S63. The absorption spectrum of complex **6** in CH_2Cl_2.

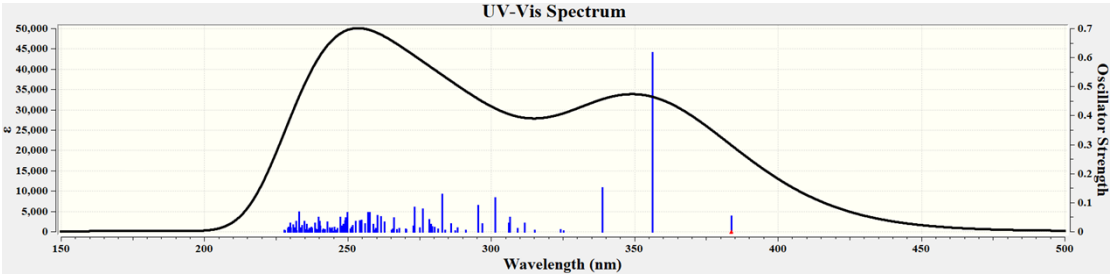
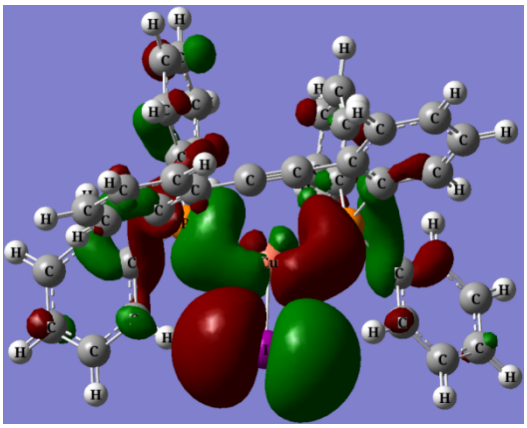
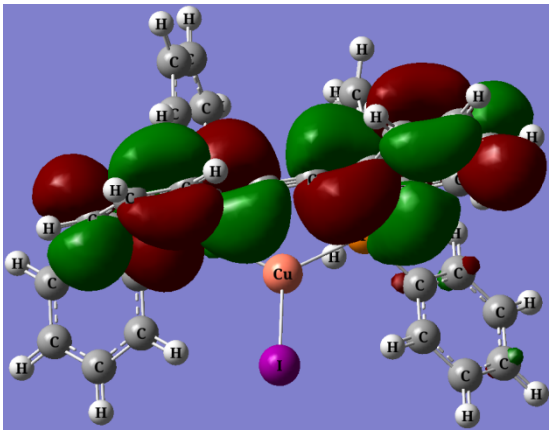


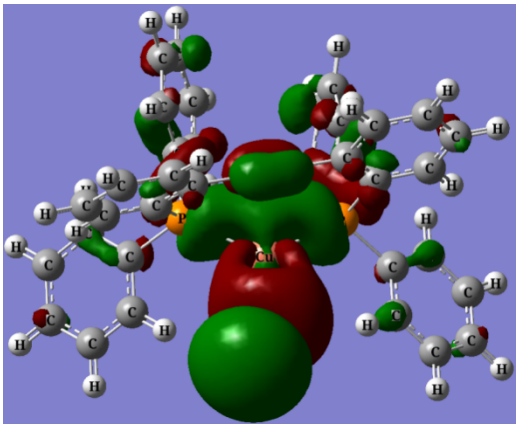
Figure S64. The absorption spectrum of complex **7** in CH_2Cl_2.



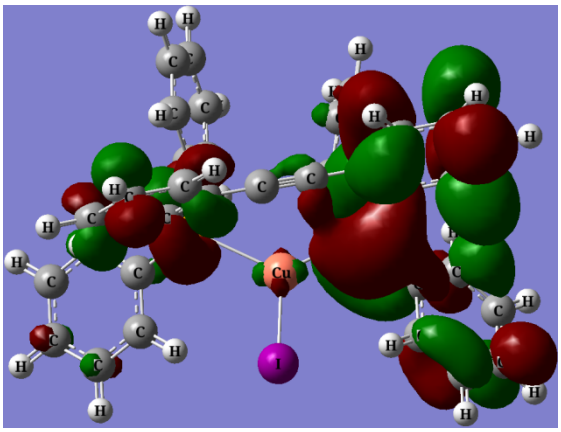
HOMO



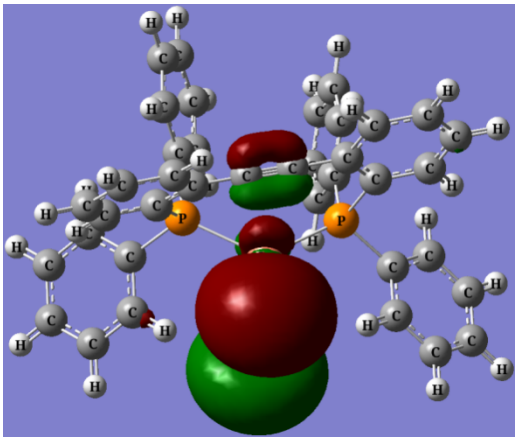
LUMO



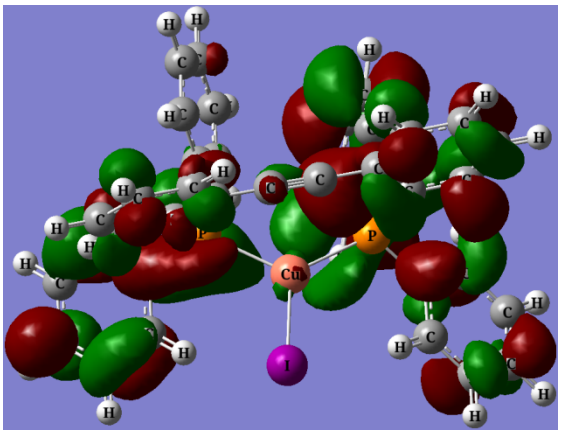
HOMO–1



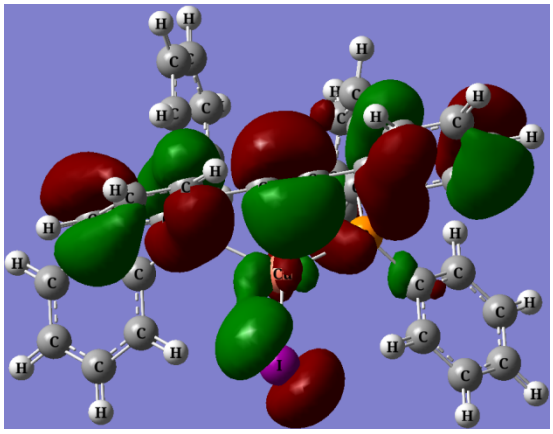
LUMO+1



HOMO–2



LUMO+2



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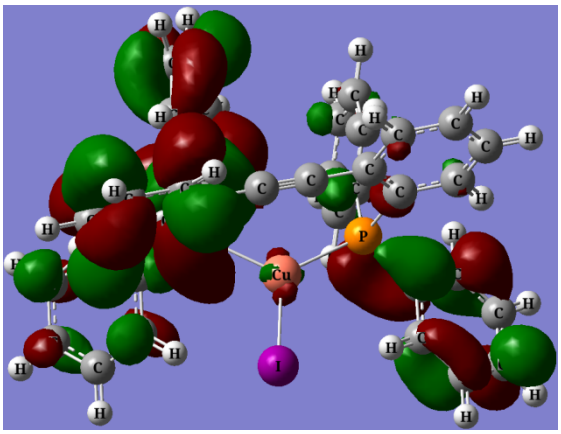
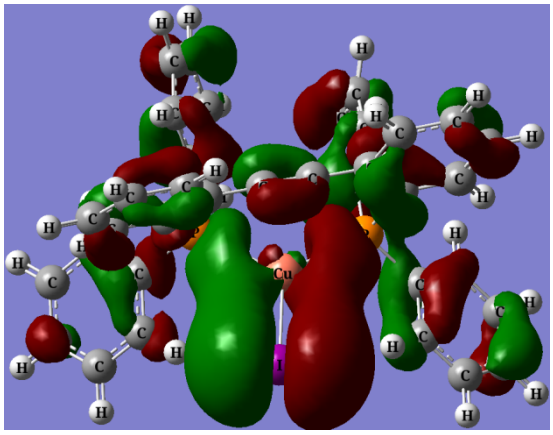
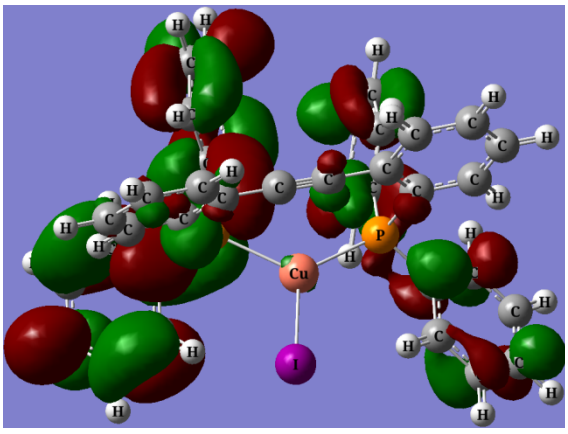


LUMO+3



HOMO–4



LUMO+4

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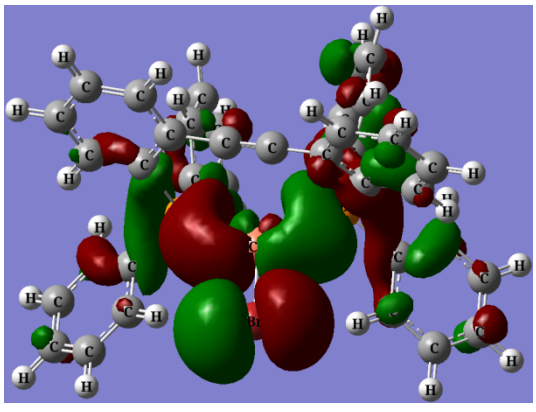
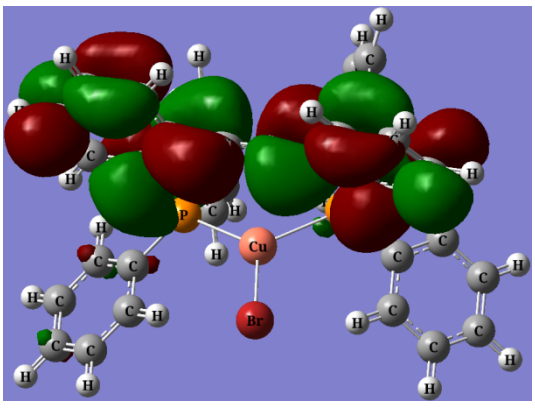
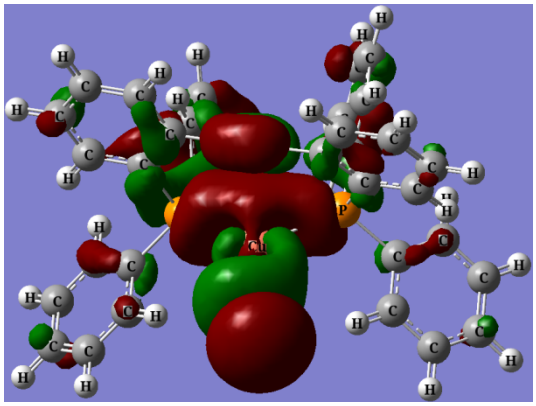


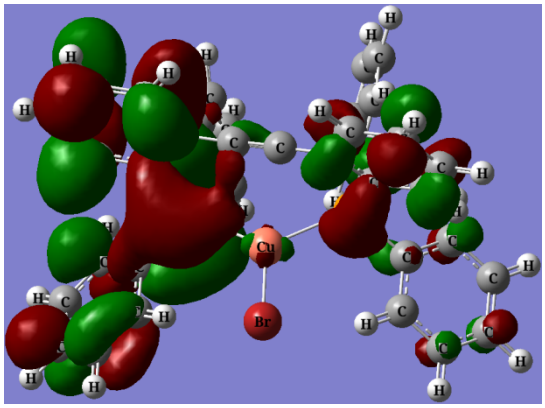
HOMO



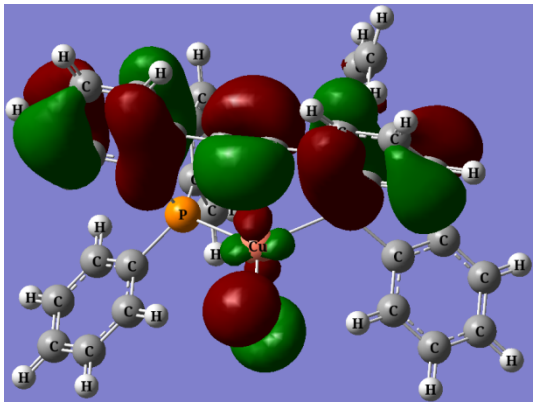
LUMO



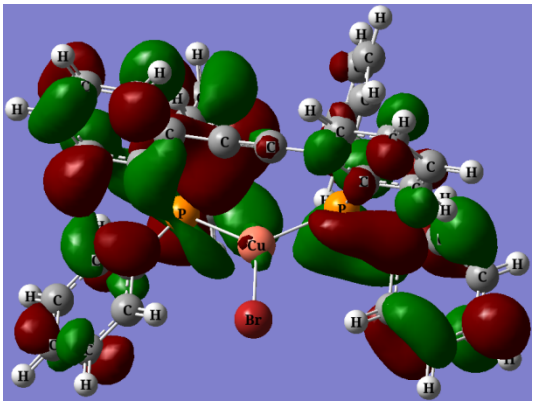
HOMO–1



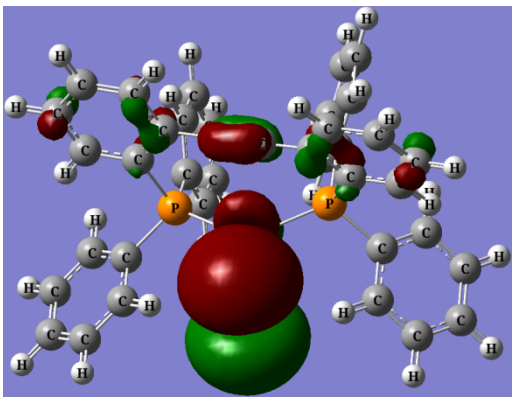
LUMO+1



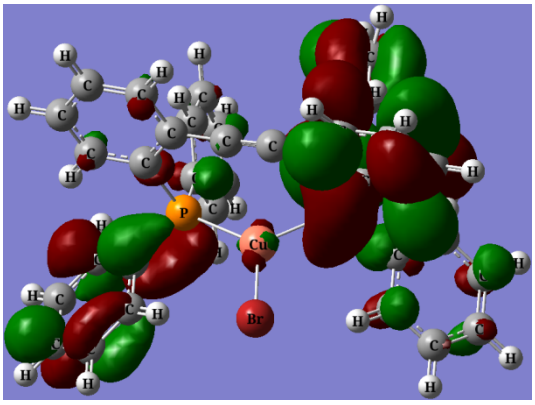
HOMO–2



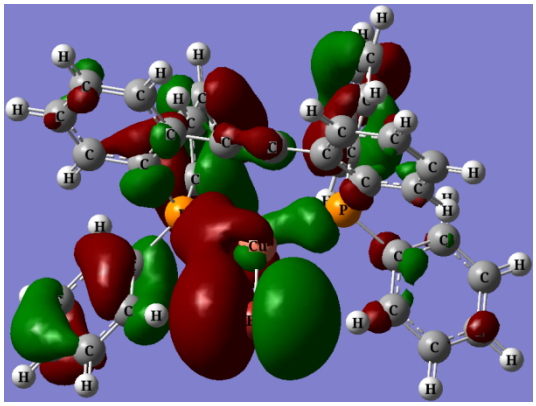
LUMO+2



HOMO–3



LUMO+3



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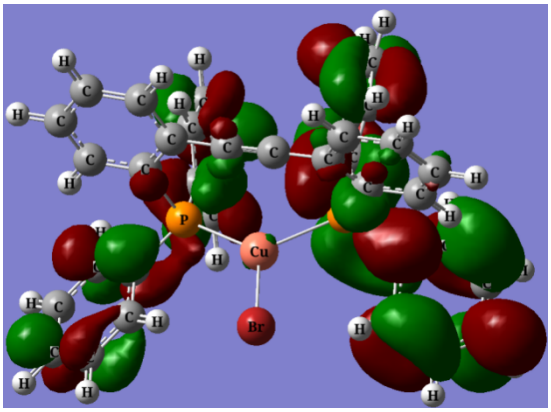

LUMO+4

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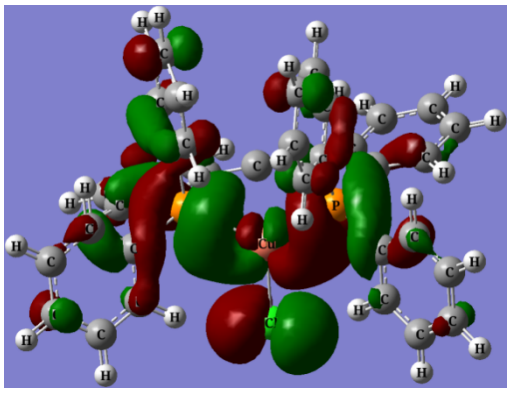
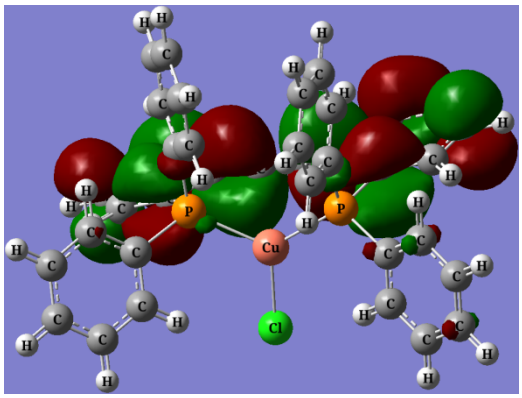


HOMO



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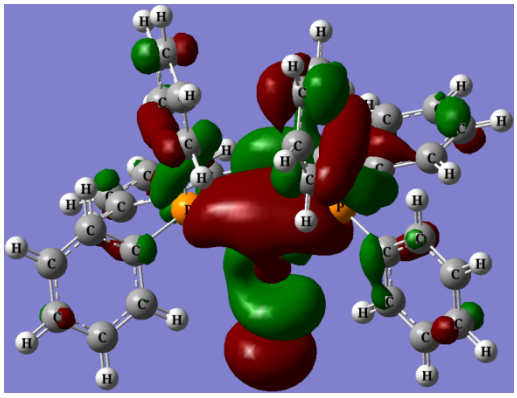

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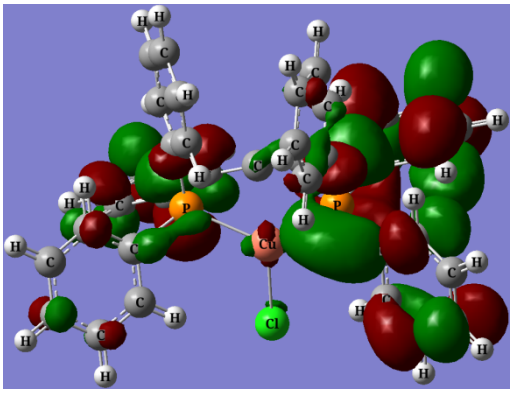

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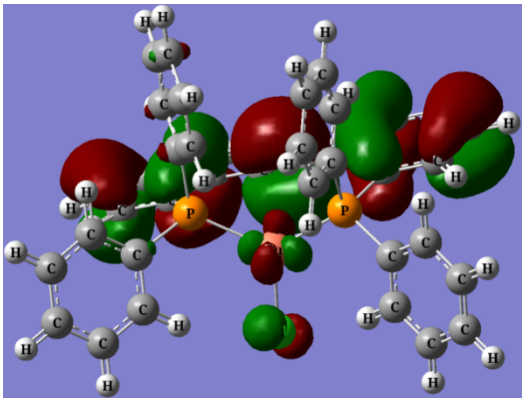

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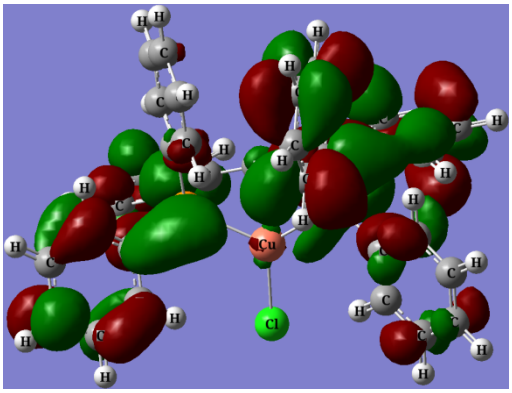

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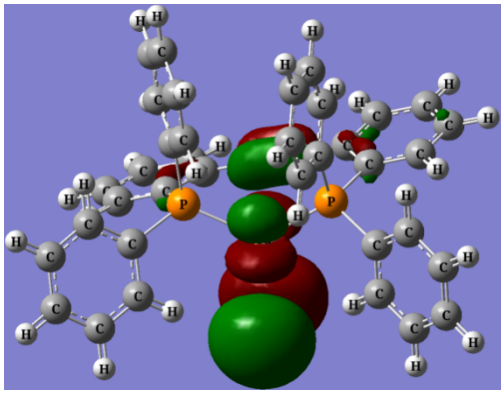

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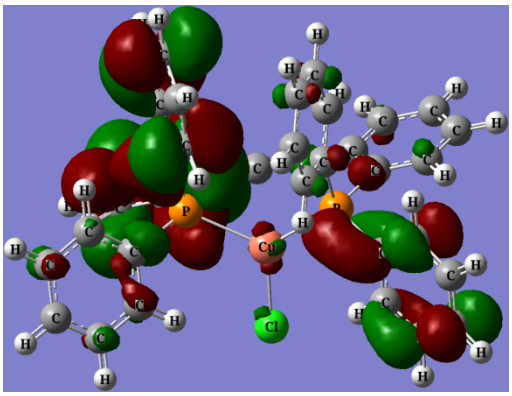

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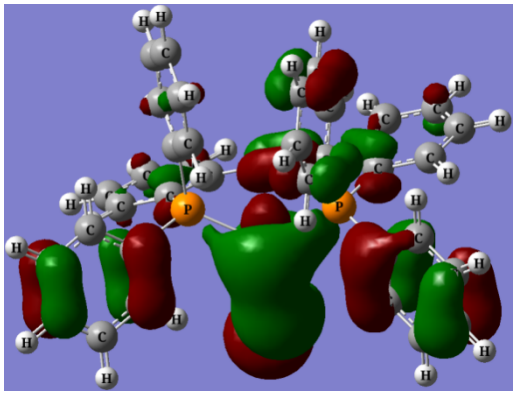

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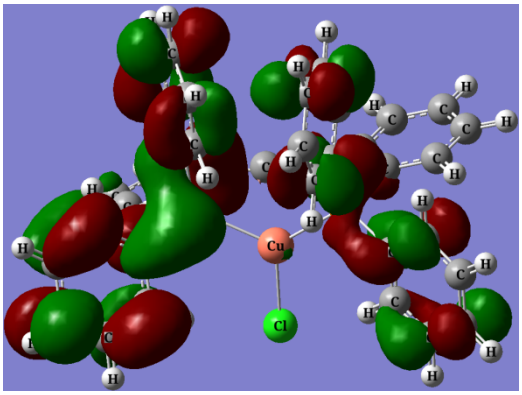

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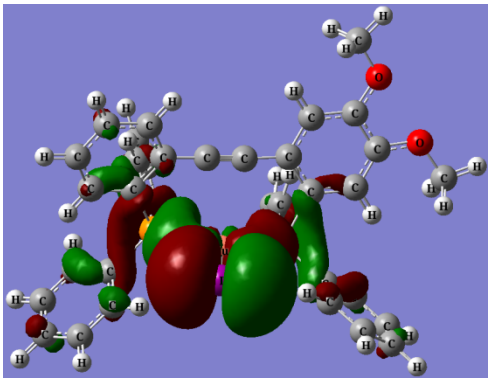
3



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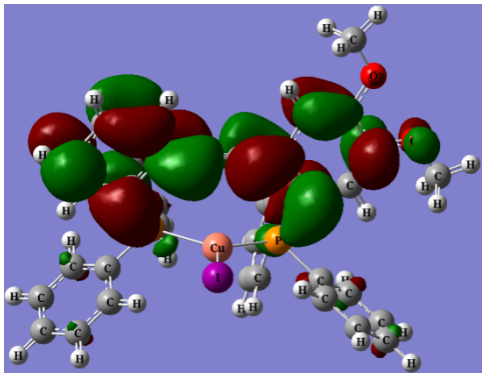
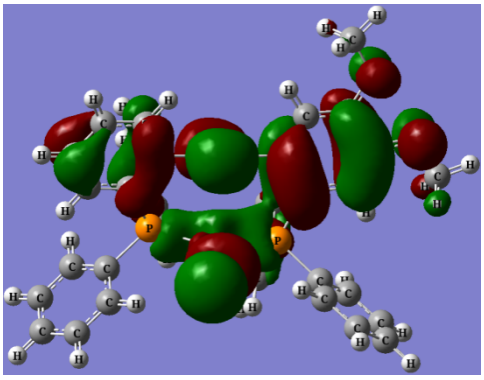


LUMO



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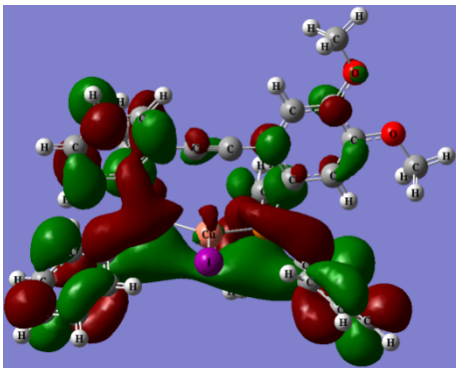

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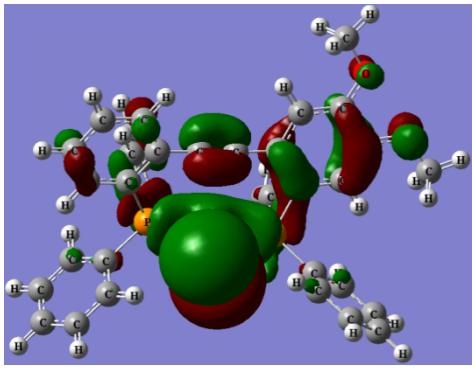

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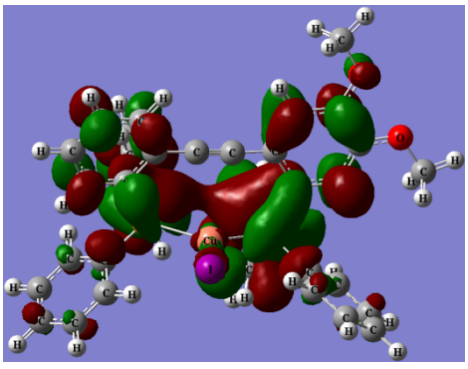

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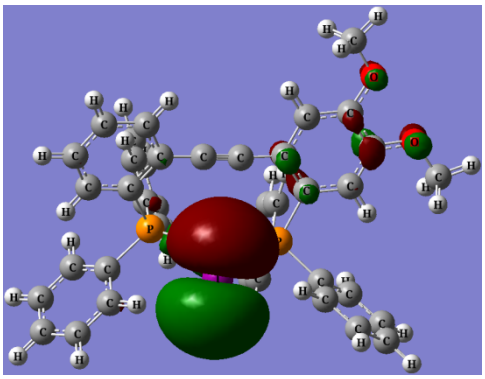

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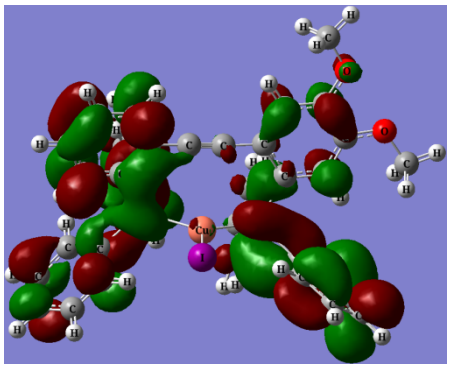

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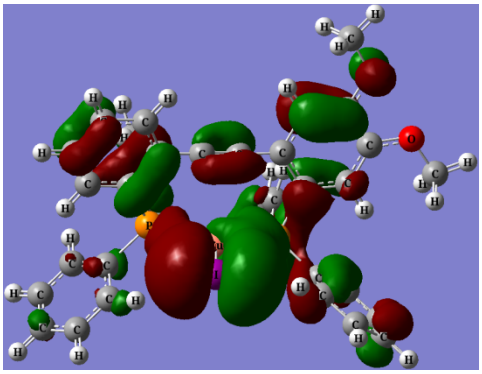

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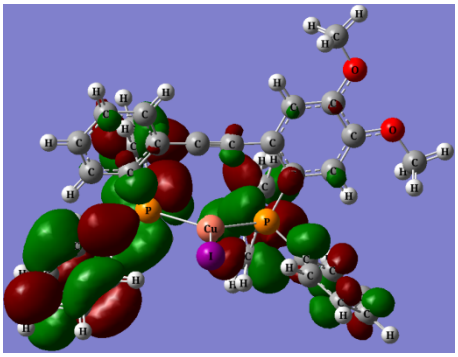

LUMO+4

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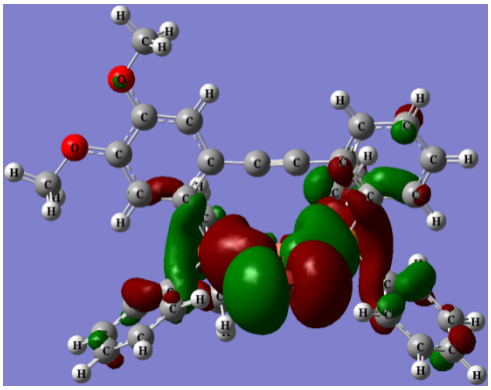

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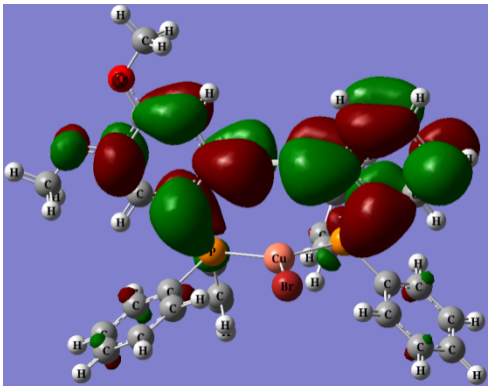

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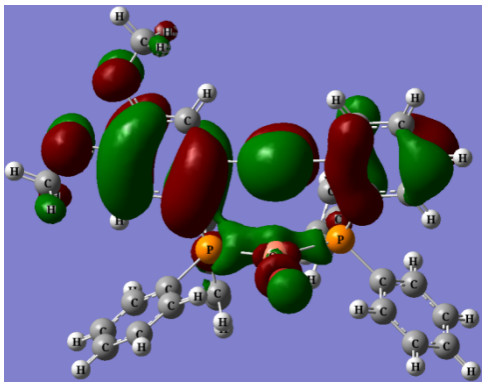

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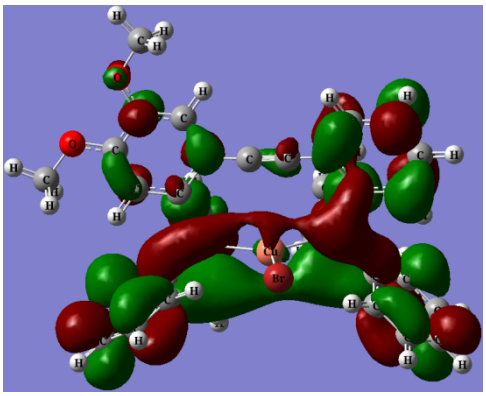

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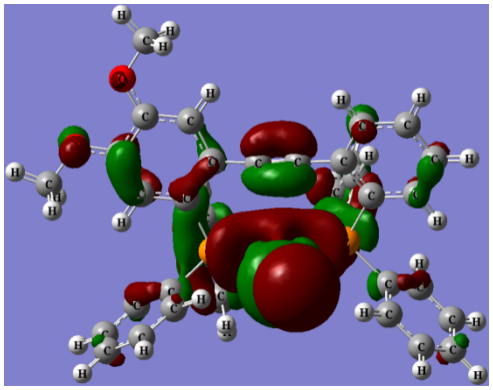

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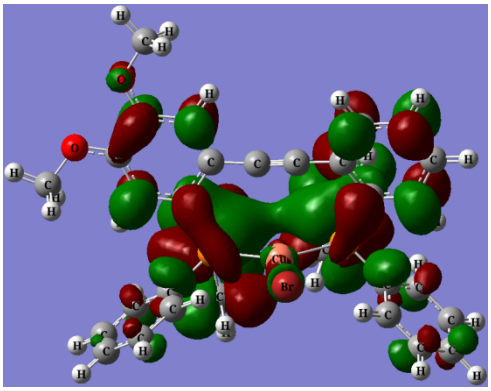

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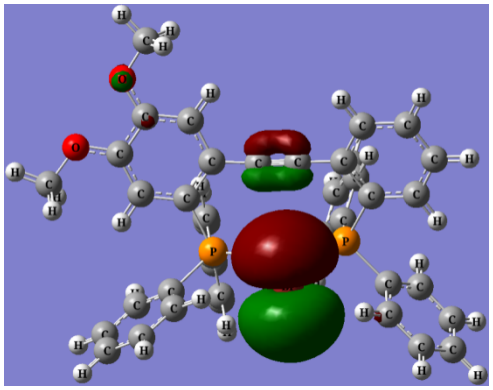

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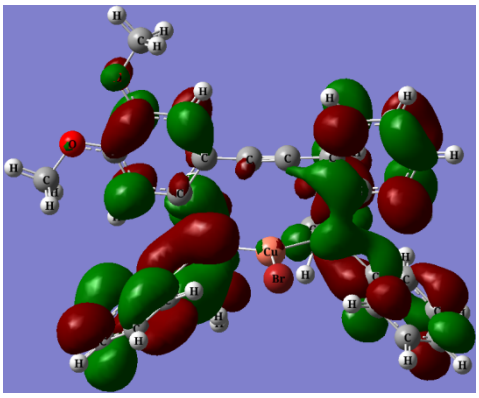

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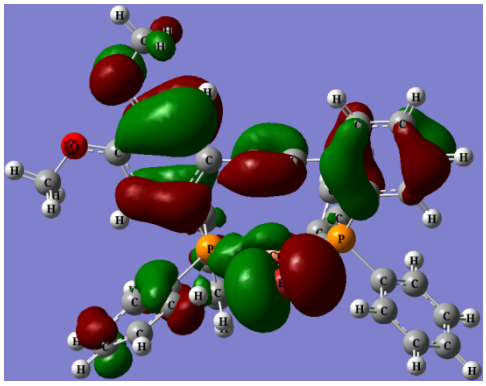

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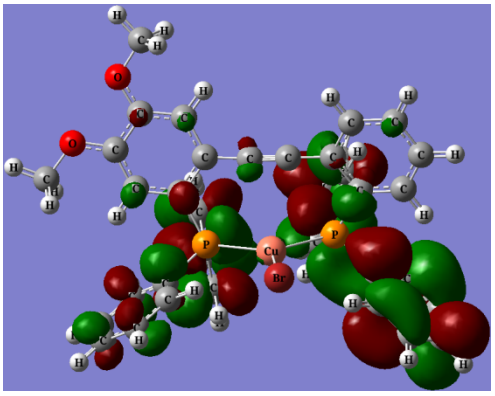

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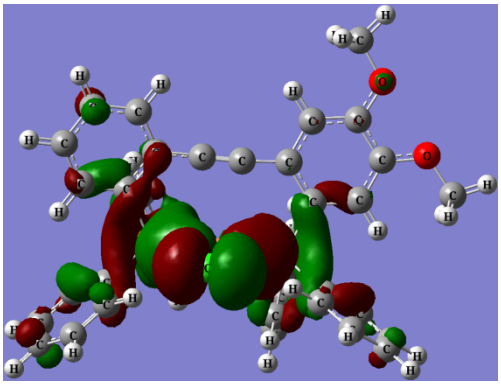

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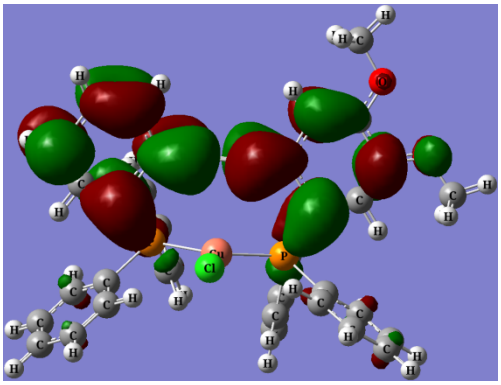

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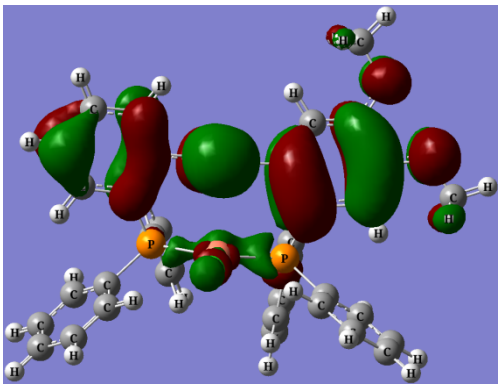

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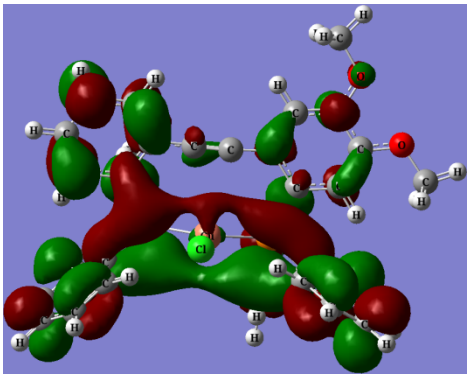

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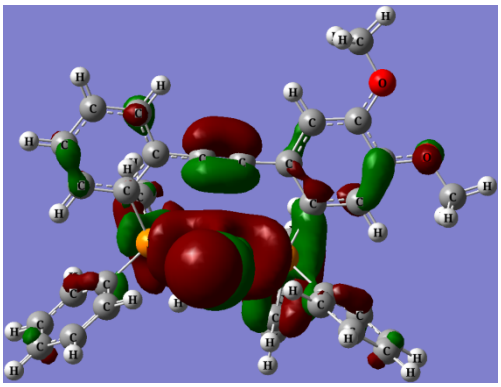

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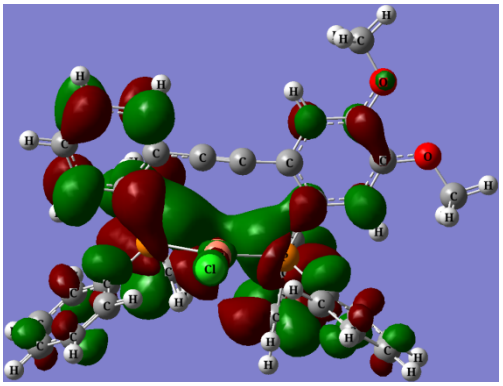
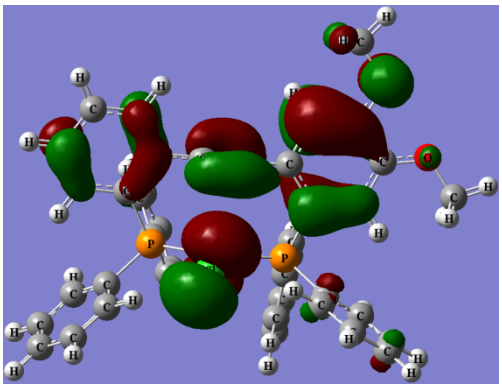
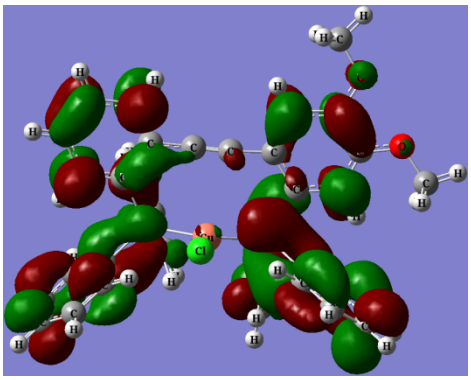


LUMO+2





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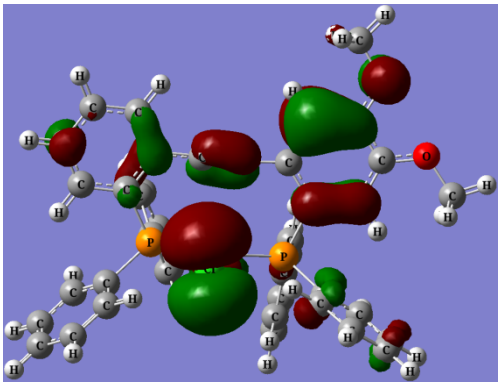
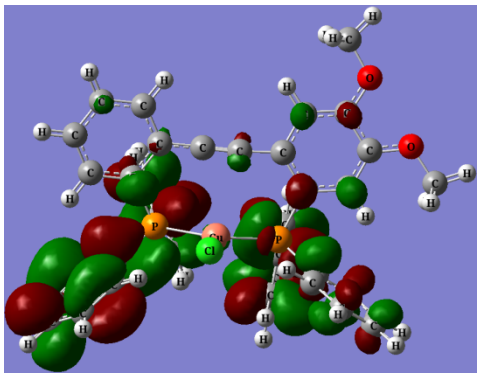


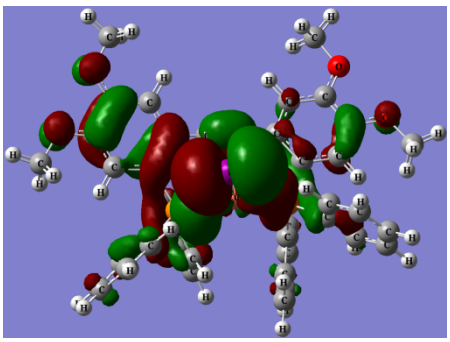
LUMO+3



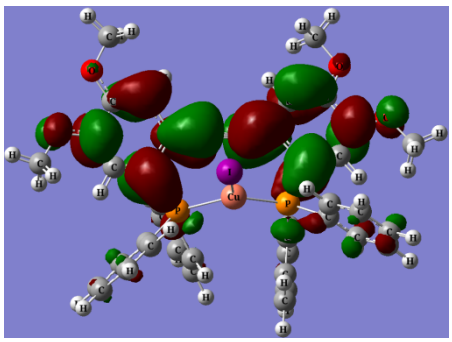
HOMO–4

LUMO+4

6



HOMO



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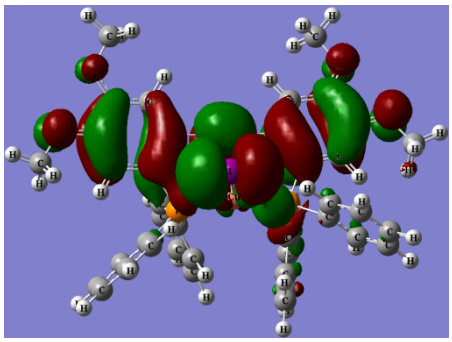

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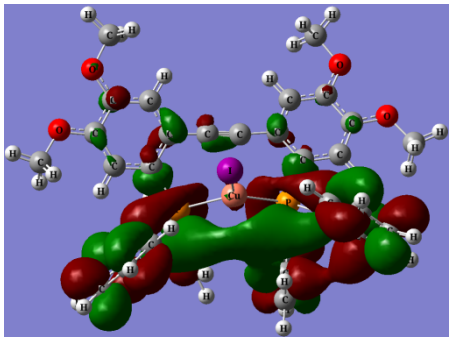

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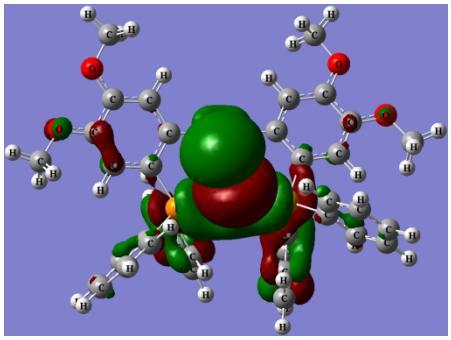

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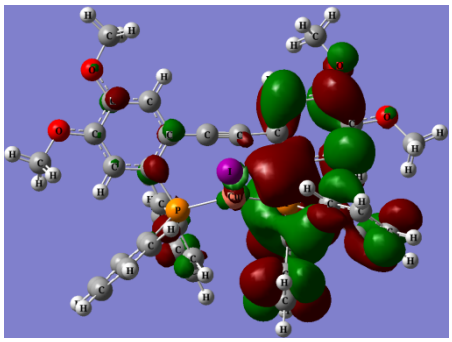
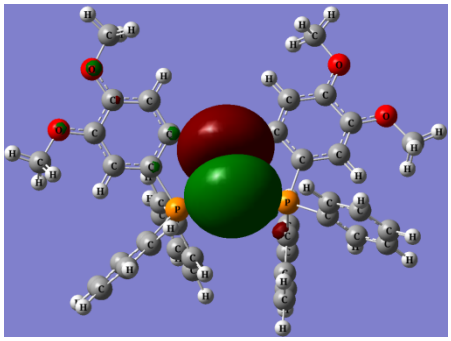
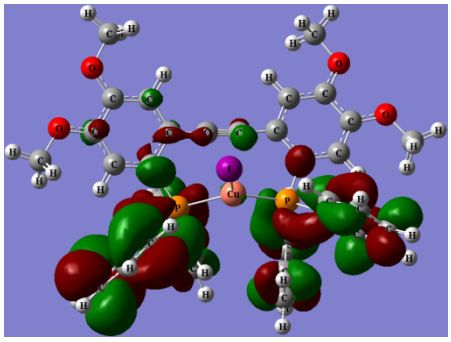


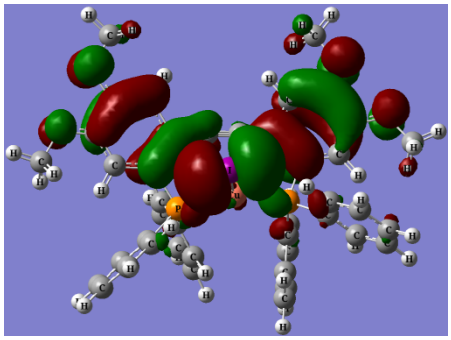
LUMO+2



HOMO–3



LUMO+3



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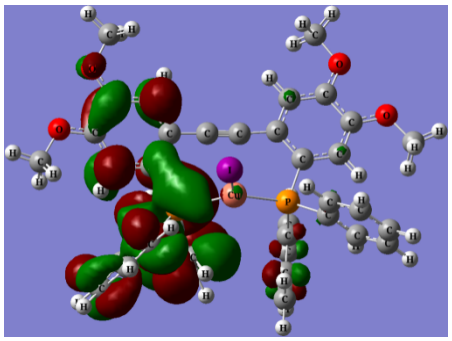
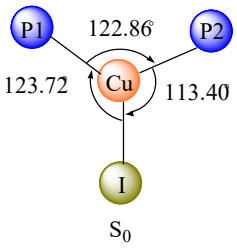


LUMO+4

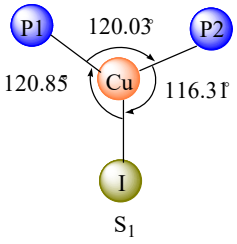
7

Figure S65. Contour plots of frontier molecular orbitals of complexes **1–7** in CH_2Cl_2.

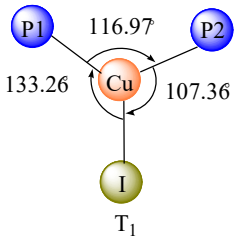
1



S_0

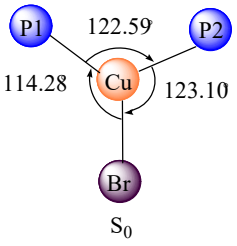


S_1

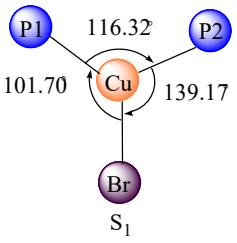


T_1

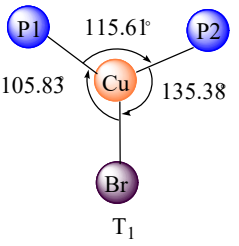
2



S_0



S_1



T_1

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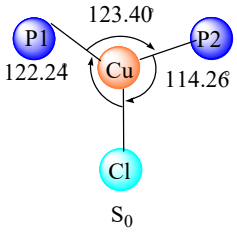
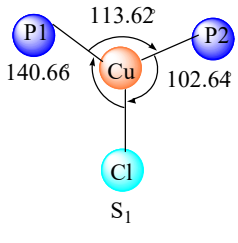
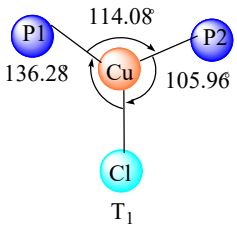


S_0

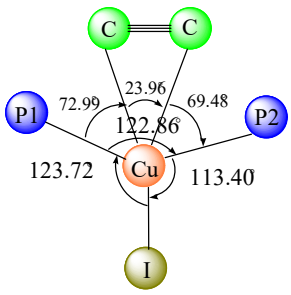


S_1

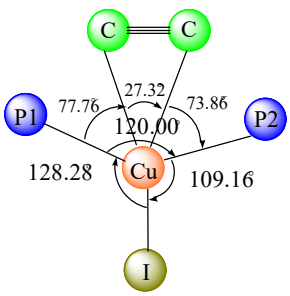


T_1

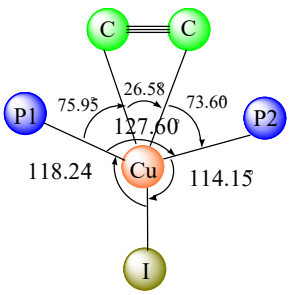
4



S_0

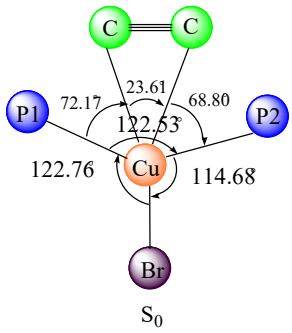


S_1

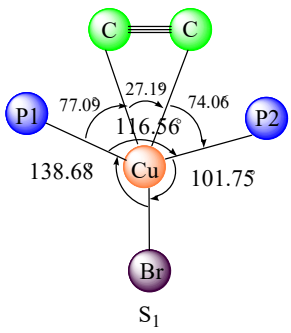


T_1

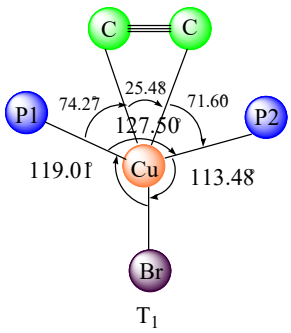
5



S_0

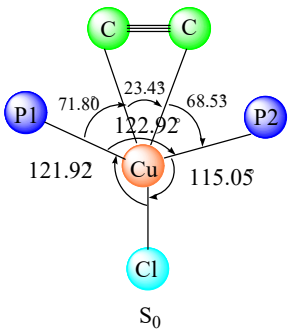


S_1

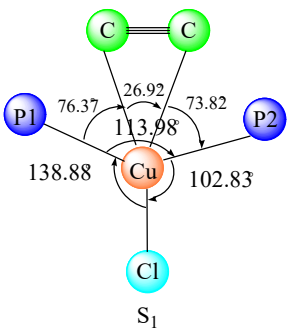


T_1

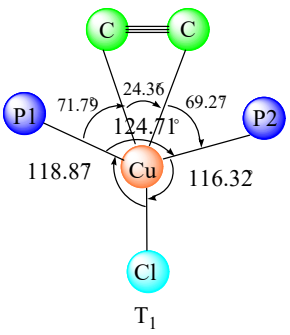
6



S_0



S_1



T_1

7

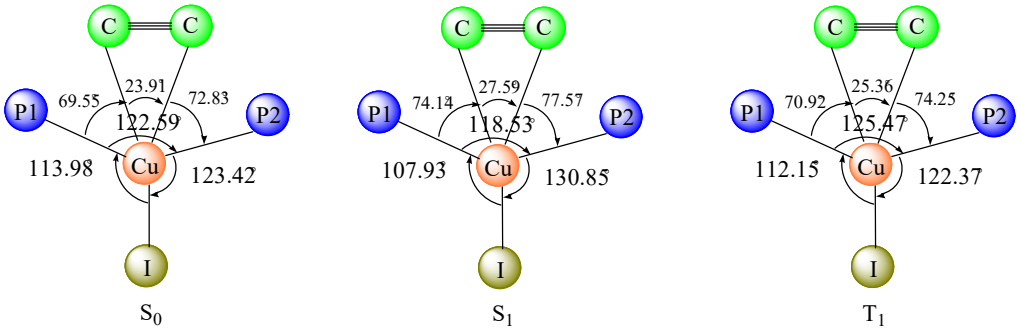


Figure S66. The core structures in the optimized S_0, S_1, and T_1 geometries for complexes **1-7**.

Table S1. Computed excitation states for complex **1** in CH_2Cl_2.

State	λ(nm)/*E*(eV)	Configurations	*f*
1	416.3 / 2.98	H→L (99)	0.0113
4	332.3 / 3.73	H-3→L (14); H→L+1 (78); H→L+2 (5)	0.0636
5	324.4 / 3.82	H-4→L (6); H-3→L (74); H→L+1 (14)	0.3989
8	312.9 / 3.96	H-4→L (57); H-3→L (5); H→L+3 (32)	0.1992
9	307.7 / 4.03	H→L+4 (92)	0.0623
12	297.6 / 4.17	H-1→L+1 (3); H→L+5 (91)	0.0913
18	283.4 / 4.37	H-3→L+1 (6); H-2→L+2 (4); H-1→L+3 (19); H→L+7 (2); H→L+8 (59)	0.0847
48	252.6 / 4.91	H-16→L (3); H-14→L (2); H-5→L+1 (47); H-4→L+1 (3); H-4→L+2 (5); H-4→L+3 (14); H-2→L+8 (7)	0.0670
72	237.3 / 5.22	H-18→L (3); H-16→L (4); H-15→L (3); H-14→L(3); H-4→L+6 (11); H-3→L+6 (2); H-3→L+7 (9); H-3→L+8 (14); H-3→L+9 (4); H-2→L+10 (14); H-2→L+11 (5)	0.0546
88	228.5 / 5.43	H-9→L+2 (6); H-8→L+2 (7); H-7→L+1 (2); H-7→L+2 (4); H-7→L+3 (2); H-7→L+4 (5); H-6→L+1 (4); H-6→L+2 (4); H-6→L+3 (5); H-6→L+4 (2); H-5→L+6 (2); H-4→L+7 (14); H-4→L+8 (9); H-3→L+10 (4); H-1→L+12 (4)	0.0605

Table S2. Computed excitation states for complex **2** in CH_2Cl_2.

State	λ(nm)/*E*(eV)	Configurations	*f*
1	407.4 / 3.04	H→L (99)	0.0162
3	330.1 / 3.76	H-2→L (43); H→L+1 (51)	0.2168
4	323.5 / 3.83	H-3→L (26); H-2→L (33); H-1→L (2); H→L+1 (35)	0.1642
5	317.6 / 3.90	H-3→L (70); H-2→L (18); H→L+1 (9)	0.2873
7	308.4 / 4.02	H→L+2 (3); H→L+3 (90)	0.0717

8	302.7 / 4.10	H→L+4 (94)	0.0685
12	292.2 / 4.24	H-4→L (11); H-1→L+1 (9); H→L+5 (75)	0.0906
18	277.1 / 4.47	H-1→L+3 (53); H-1→L+4 (3); H→L+8 (32)	0.0897
25	265.5 / 4.67	H-8→L (11); H-7→L (2); H-3→L+1 (57); H-2→L+1 (3); H-1→L+5 (15)	0.0531
31	261.5 / 4.74	H-2→L+2 (2); H-2→L+3 (4); H-1→L+6 (64); H-1→L+7 (2); H→L+10 (14)	0.0813
71	233.9 / 5.30	H-5→L+4 (25); H-3→L+7 (28); H-3→L+8 (29)	0.0533

Table S3. Computed excitation states for complex **3** in CH_2Cl_2.

State	λ(nm)/*E*(eV)	Configurations	*f*
1	402.7 / 3.08	H→L (99)	0.0190
3	328.7 / 3.77	H-2→L (46); H→L+1 (49)	0.2616
4	320.0 / 3.88	H-2→L (46); H-1→L (3); H→L+1 (45)	0.3949
7	306.0 / 4.05	H-3→L (13); H-2→L (2); H→L+2 (5); H→L+3 (74)	0.1012
8	300.5 / 4.13	H→L+4 (94)	0.0709
11	289.2 / 4.29	H-4→L (3); H→L+5 (91)	0.1109
18	275.2 / 4.50	H-1→L+3 (45); H-1→L+4 (5); H→L+8 (39)	0.0736
23	267.0 / 4.64	H-8→L (50); H-7→L (8); H-2→L+1 (23); H-2→L+2 (4); H-2→L+3 (4)	0.0887
31	260.0 / 4.77	H-15→L (2); H-10→L (5); H-2→L+3 (3); H-1→L+6 (58); H-1→L+7 (3); H→L+10 (13); H→L+11 (4)	0.0573

Table S4. Computed excitation states for complex **4** in CH_2Cl_2.

State	λ(nm)/*E*(eV)	Configurations	*f*
1	399.3 / 3.10	H→L (99)	0.0129
2	361.0 / 3.43	H-2→L (27); H-1→L (69)	0.1707
3	343.9 / 3.61	H-3→L (10); H-2→L (66); H-1→L (21)	0.3359
4	337.5 / 3.67	H-3→L (88); H-2→L (4); H-1→L (6)	0.1664
9	306.8 / 4.04	H→L+2 (2); H→L+3 (13); H→L+4 (79)	0.0694
12	296.5 / 4.18	H→L+5 (89); H→L+6 (2)	0.0763
20	282.7 / 4.39	H-6→L (4); H-3→L+1 (27); H-2→L+2 (6); H-2→L+4 (5); H-1→L+4 (13); H→L+6 (3); H→L+8 (32)	0.0506
22	279.0 / 4.44	H-3→L+1 (23); H-2→L+2 (33); H-2→L+3 (25); H→L+8 (6)	0.1008
23	277.7 / 4.47	H-6→L (12); H-5→L (5); H-2→L+2 (18); H-2→L+3 (33); H-1→L+2 (4); H-1→L+3 (5); H-1→L+5 (9); H-1→L+6 (5); H-1→L+7 (2)	0.1081
28	269.5 / 4.60	H-6→L (7); H-3→L+4 (5); H-2→L+5 (4); H-1→L+6 (68)	0.0733
40	260.5 / 4.76	H-4→L+1 (8); H-3→L+5 (13); H-2→L+6 (54); H-2→L+8 (4); H-1→L+8 (7)	0.0586
46	254.4 / 4.87	H-17→L (2); H-14→L (5); H-13→L (4); H-12→L (4);	0.0903

		H-11→L (20); H-10→L (13); H-4→L-2 (35)	
49	252.4 / 4.91	H-15→L (2); H-14→L (4); H-12→L (22); H-11→L (5); H-9→L (2); H-5→L+1 (5); H-4→L+3 (40); H-4→L+4 (3); H-3→L+6 (3); H-1→L+10 (3)	0.0628
65	243.4 / 5.09	H-18→L (2); H-17→L (8); H-16→L (11); H-6→L+2 (7); H-5→L+2 (27); H-4→L+4 (5); H-4→L+5 (12); H-2→L+9 (4)	0.0800
72	238.8 / 5.19	H-18→L (5); H-15→L (7); H-6→L+1 (20); H-6→L+3 (8); H-6→L+4 (6); H-5→L+4 (35)	0.0515
92	229.0 / 5.41	H-10→L+1 (6); H-9→L+1 (5); H-8→L+1 (4); H-8→L+2 (2); H-7→L+1 (14); H-7→L+3 (3); H-6→L+3 (7); H-6→L+4 (6); H-5→L+8 (2); H-4→L+6 (3); H-2→L+12 (9); H-1→L+14 (2)	0.0603
94	227.6 / 5.45	H-20→L (5); H-3→L+12 (32); H-3→L+13 (4); H-3→L+15 (11); H-2→L+12 (9); H-2→L+13 (3); H-2→L+15 (4); H-1→L+14 (7)	0.0614

Table S5. Computed excitation states for complex **5** in CH_2Cl_2.

State	λ(nm)/*E*(eV)	Configurations	*f*
1	391.3 / 3.17	H→L (99)	0.0180
2	354.9 / 3.49	H-2→L (23); H-1→L (73)	0.3370
3	339.2 / 3.66	H-2→L (74); H-1→L (22)	0.3578
7	305.8 / 4.05	H-1→L+1 (3); H→L+3 (78); H→L+4 (15)	0.0601
8	302.1 / 4.10	H→L+3 (13); H→L+4 (80)	0.0811
11	291.2 / 4.26	H-6→L (3); H-1→L+2 (5); H→L+5 (82)	0.0882
20	278.8 / 4.45	H-6→L (13); H-5→L (18); H-2→L+2 (3); H-2→L+3 (7); H-1→L+2 (3); H-1→L+3 (6); H-1→L+4 (3); H-1→L+6 (3); H-1→L+7 (4); H→L+8 (35)	0.0564
21	275.1 / 4.51	H-2→L+2 (59); H-2→L+3 (8); H→L+7 (4); H→L+8 (14)	0.1076
22	274.0 / 4.53	H-6→L (3); H-2→L+2 (5); H-2→L+3 (68); H-2→L+4 (3); H-1→L+5 (4); H-1→L+6 (2); H→L+7 (3)	0.0822
25	267.9 / 4.63	H-6→L (10); H-5→L (2); H-4→L (5); H-1→L+3 (2); H-1→L+5 (11); H-1→L+6 (52); H-1→L+7 (3)	0.1276
35	258.7 / 4.79	H-9→L (50); H-7→L (2); H-2→L+8 (4); H-1→L+8 (22); H→L+9 (2); H→L+11 (3)	0.0534
36	257.1 / 4.82	H-10→L (5); H-9→L (3); H-2→L+6 (73); H-1→L+8 (2)	0.0548
54	244.1 / 5.08	H-17→L (4); H-16→L (2); H-15→L (7); H-13→L (3); H-6→L+1 (8); H-5→L+1 (38); H-4→L+2 (6); H-4→L+3 (5); H-3→L+5 (3); H-1→L+10 (3); H→L+12 (2)	0.0501

Table S6. Computed excitation states for complex **6** in CH_2Cl_2.

State	λ(nm)/*E*(eV)	Configurations	*f*
1	388.0 / 3.20	H→L (99)	0.0204
2	353.7 / 3.51	H-2→L (20); H-1→L (76); H→L+1 (2)	0.4029

3	338.2 / 3.67	H-2→L (78); H-1→L (19)	0.3028
6	303.7 / 4.08	H-1→L+1 (8); H→L+3 (75); H→L+4 (12)	0.0761
8	299.9 / 4.13	H-3→L (19); H→L+3 (13); H→L+4 (60)	0.0511
12	288.3 / 4.30	H-4→L (4); H-1→L+2 (31); H-1→L+3 (6); H→L+5 (50)	0.0561
21	272.4 / 4.55	H-6→L (63); H-2→L+2 (19); H→L+8 (9)	0.0504
22	272.0 / 4.56	H-6→L (10); H-2→L+2 (4); H-2→L+3 (61); H-2→L+4 (5); H-1→L+5 (3); H-1→L+6 (3); H→L+7 (4); H→L+8 (2)	0.0618
25	267.5 / 4.63	H-5→L (7); H-4→L (4); H-3→L (5); H-2→L+3 (3); H-1→L+3 (2); H-1→L+5 (21); H-1→L+6 (37); H-1→L+7 (6)	0.1474
36	255.9 / 4.85	H-2→L+6 (78)	0.0572
65	235.2 / 5.27	H-18→L (4); H-17→L (24); H-6→L+1 (7); H-5→L+3 (11); H-4→L+2 (3); H-4→L+3 (14); H-3→L+3 (5); H-3→L+4 (2)	0.0502
96	221.9 / 5.59	H-16→L+1 (4); H-13→L+1 (2); H-12→L+1 (2); H-11→L+1 (5); H-8→L+4 (2); H-5→L+5 (5); H-4→L+7 (6); H-1→L+15 (13); H-1→L+18 (3); H→L+16 (4); H→L+18 (12); H→L+21 (2)	0.0508
98	221.4 / 5.60	H-6→L+5 (3); H-5→L+5 (34); H-4→L+5 (3); H-4→L+6 (5); H-3→L+5 (4); H-3→L+6 (3); H-2→L+13 (3); H→L+18 (12); H→L+21 (3)	0.0679

Table S7. Computed excitation states for complex **7** in CH_2Cl_2.

State	λ(nm)/*E*(eV)	Configurations	*f*
1	383.7 / 3.23	H-1→L (8); H→L (90)	0.0539
2	356.2 / 3.48	H-2→L (6); H-1→L (83); H→L (7)	0.6159
3	338.8 / 3.66	H-2→L (92); H-1→L (6)	0.1498
11	301.5 / 4.11	H-6→L (3); H-5→L (3); H-4→L (24); H-1→L+2 (53); H-1→L+4 (3); H→L+2 (5)	0.1165
13	295.4 / 4.20	H-6→L (5); H-4→L (3); H-1→L+3 (35); H-1→L+4 (19); H-1→L+5 (2); H→L+3 (2); H→L+5 (25)	0.0888
20	283.0 / 4.38	H-7→L (4); H-6→L (3); H-5→L (2); H-3→L+1 (7); H-2→L+2 (61); H→L+6 (6); H→L+8 (9)	0.1290
26	276.1 / 4.49	H-3→L+1 (8); H-2→L+2 (2); H-2→L+4 (68); H-1→L+6 (5); H-1→L+8 (4)	0.0776
28	273.2 / 4.54	H-8→L (4); H-7→L (7); H-3→L+2 (12); H-2→L+4 (6); H-1→L+7 (17); H-1→L+8 (38)	0.0832
38	261.5 / 4.74	H-4→L+2 (39); H-2→L+6 (6); H-2→L+7 (7); H→L+11 (33)	0.0506
39	260.3 / 4.76	H-8→L (5); H-4→L+2 (18); H-2→L+8 (2); H-1→L+8 (6); H-1→L+9 (26); H-1→L+10 (5); H→L+11 (20)	0.0552
43	257.5 / 4.81	H-9→L (15); H-8→L (35); H-7→L (4); H-4→L+2 (3); H-4→L+4 (7); H-2→L+7 (4); H-2→L+8 (3); H-1→L+9 (6); H-1→L+10 (8)	0.0641

45	256.9 / 4.83	H-8→L (3); H-7→L (6); H-6→L (2); H-4→L+2 (3); H-4→L+3 (48); H-1→L+8 (2); H-1→L+9 (2); H-1→L+10 (20)	0.0657
53	249.8 / 4.96	H-14→L (2); H-10→L (4); H-9→L (2); H-8→L (7); H-7→L+1 (2); H-6→L+1 (17); H-4→L+4 (3); H-1→L+11 (34); H→L+12 (5)	0.0660
90	232.9 / 5.32	H-14→L (2); H-10→L+2 (3); H-7→L+1 (9); H-6→L+5 (13); H-5→L+6 (2); H-4→L+8 (14); H-1→L+14 (4); H-1→L+15 (5); H-1→L+21 (2); H→L+21 (3)	0.0680

Table S8. Selected bond lengths (Å) and angles (°) in the optimized S_0, S_1, and T_1 geometries for complexes **1-7**.

Complex	Geometry	Cu–X	Cu–P	Cu–C≡	P–Cu–X	P–Cu–P	P–Cu–C≡	≡C–Cu–C≡
1	S_0	2.5725	2.2873	2.9088	123.72	122.86	/	/
			2.3101	2.9037	113.40			
	S_1	2.5930	2.3016	2.6527	120.85	120.03	/	/
			2.3158	2.6452	116.31			
	T_1	2.5478	2.3139	2.6420	133.26	116.97	/	/
			2.3386	2.5825	107.36			
2	S_0	2.3887	2.3074	2.9459	114.28	122.59	/	/
			2.2870	2.9454	123.10			
	S_1	2.3386	2.3236	2.6664	101.70	116.32	/	/
			2.3295	2.6567	139.17			
	T_1	2.3501	2.3412	2.6394	105.83	115.61	/	/
			2.3114	2.5859	135.38			
3	S_0	2.2714	2.2822	2.9627	122.24	123.40	/	/
			2.3020	2.9590	114.26			
	S_1	2.2092	2.3303	2.6922	140.66	113.62	/	/
			2.3296	2.6829	102.64			
	T_1	2.2248	2.3095	2.6494	136.28	114.08	/	/
			2.3431	2.6122	105.96			
4	S_0	2.5736	2.2877	2.9196	123.45	122.77	72.99	23.96
			2.3088	2.9176	113.78		69.48	
	S_1	2.5783	2.3124	2.6178	128.28	120.00	77.76	27.32
			2.3149	2.6517	109.16		73.86	
	T_1	2.5959	2.2943	2.7402	118.24	127.60	75.95	26.58
			2.2988	2.7507	114.15		73.60	
5	S_0	2.3900	2.2872	2.9592	122.76	122.53	72.17	23.61
			2.3065	2.9638	114.68		62.80	
	S_1	2.3392	2.3321	2.6311	138.68	116.56	77.09	27.19
			2.3232	2.6599	101.75		74.06	
	T_1	2.3985	2.2868	2.8536	119.01	127.50	74.27	25.48
			2.2954	2.8610	113.48		71.60	
6	S_0	2.2718	2.2832	2.9782	121.92	122.92	71.80	23.43
			2.2996	2.9873	115.05		68.53	
	S_1	2.2101	2.3336	2.6660	139.88	113.98	76.37	26.92

			2.3293	2.6761	102.83		73.82	
	T_1	2.2751	2.2934	2.9753	118.87	124.71	71.20	24.36
			2.2968	2.9883	116.32		69.27	
7	S_0	2.5760	2.3085	2.9236	113.98	122.69	69.55	23.91
			2.2873	2.9269	123.42		72.83	
	S_1	2.5660	2.3182	2.6428	107.93	118.53	74.14	27.29
			2.3166	2.6347	130.85		77.57	
	T_1	2.5878	2.3071	2.8867	112.15	125.47	70.92	25.36
			2.2925	2.8482	122.37		74.25	

Table S9. Cartesian coordinates of the optimized S_0 geometry for complex **1**.

Atom	x	y	z
I	-0.38423354	-3.40592653	-0.2703049
Cu	-0.0076503	-0.86186999	-0.21084816
P	2.05987576	0.11487742	-0.1558457
P	-1.97055027	0.3553321	-0.16416402
C	3.31901651	-2.10843774	-1.21827017
H	2.47320099	-2.6430057	-0.79941129
C	-1.87211452	2.17097504	0.06921294
C	-4.24832195	-0.46773148	1.32355675
H	-4.81873981	-0.3134247	0.41657277
C	2.35336596	2.92814288	0.13754448
H	2.49687704	2.74877225	1.19547145
C	1.87449989	0.12745208	2.66556987
C	2.15058481	1.85438415	-0.73159388
C	2.74214304	0.19743334	1.55108075
C	-2.32521269	2.81696377	1.22192952
H	-2.79287765	2.24721679	2.01452668
C	-2.78784491	-0.89043867	3.65990094
H	-2.20839583	-1.06280065	4.55813836
C	-3.17236226	0.14399888	-1.5264903
C	2.41786459	0.21035829	3.9623988
H	1.74714283	0.15273705	4.81032566
C	-2.87779731	-0.2182413	1.3226377
C	4.11636237	0.32629492	1.76665071
H	4.78602392	0.3557961	0.91678036
C	-0.72820637	-0.22127808	2.52813334
C	-4.07742453	1.14346193	-1.89980328
H	-4.06877731	2.09912493	-1.39007761
C	0.46989993	-0.04363801	2.53937772
C	-4.88691778	-0.92160512	2.47557387
H	-5.95275525	-1.11612099	2.45813603
C	-4.15584639	-1.12964887	3.64362179

H	-4.64936291	-1.48778827	4.53922584
C	1.95167058	2.10706607	-2.0958494
H	1.78064493	1.28148238	-2.77824834
C	-3.18122664	-1.08692531	-2.19418359
H	-2.47835291	-1.86173983	-1.90615891
C	-4.98616189	0.91158519	-2.92946614
H	-5.68422775	1.68969471	-3.21658532
C	3.39030327	-0.71523814	-1.1053128
C	4.32133508	-2.80362867	-1.88989843
H	4.25553807	-3.88184757	-1.97623906
C	-4.99925847	-0.31785975	-3.58692524
H	-5.70797982	-0.4964473	-4.38750206
C	-2.13103637	-0.4420288	2.50335339
C	5.39234802	-2.11688821	-2.45809556
H	6.16810801	-2.66017548	-2.98543542
C	4.46359536	-0.02691881	-1.68334923
H	4.51688532	1.05274384	-1.6154774
C	-1.26864468	2.92444322	-0.94526421
H	-0.895051	2.43169611	-1.83471269
C	2.38043826	4.23273268	-0.35281193
H	2.53572691	5.05836283	0.33185127
C	4.63900127	0.40587256	3.05246326
H	5.70848581	0.50513728	3.19520451
C	2.21336422	4.47527289	-1.71272154
H	2.24583567	5.48974796	-2.09296964
C	3.78370566	0.35080183	4.15299827
H	4.18319067	0.407589	5.1586648
C	-4.09761972	-1.31474645	-3.21725383
H	-4.10159312	-2.27078826	-3.7276397
C	1.9954907	3.40763239	-2.58429708
H	1.8567618	3.58899555	-3.64404277
C	-1.59876889	4.94318712	0.33354531
H	-1.49360441	6.01712797	0.43565087
C	5.46008784	-0.72766711	-2.35747319
H	6.28761554	-0.18910749	-2.80513479
C	-2.18281092	4.19766622	1.35386896
H	-2.5357919	4.68886312	2.25350844
C	-1.14549967	4.30234764	-0.81941526
H	-0.68018264	4.87243619	-1.61317958

Table S10. Cartesian coordinates of the optimized S_1 geometry for complex **1**.

Atom	x	y	z
I	-0.08360233	-3.39165373	-0.75900118

Cu	0.00014802	-0.902137	-0.03854795
P	1.98032948	0.27044394	-0.07293498
P	-2.01861522	0.23246502	-0.02997068
C	3.70316424	-1.81276653	-0.71075579
H	3.13385264	-2.35310392	0.04088488
C	-1.81671148	2.00597811	0.38661399
C	-4.32294278	-0.68186224	1.34999536
H	-4.90170963	-0.37553224	0.48364812
C	2.14038391	3.10035839	-0.07260796
H	2.47265194	3.01727863	0.95709119
C	1.76820773	-0.05621389	2.69936435
C	1.81763528	1.9444201	-0.79173096
C	2.60144975	0.40582303	1.61250933
C	-1.79989389	2.4249022	1.72420881
H	-1.96179938	1.70676565	2.51976449
C	-2.84444113	-1.49571552	3.58830102
H	-2.2680506	-1.81463569	4.45165406
C	-3.11650522	0.23031258	-1.4875741
C	2.36080651	-0.08060206	4.00406855
H	1.75979766	-0.44405582	4.83239705
C	-2.93953684	-0.51006199	1.34570422
C	3.91056113	0.83623478	1.86327224
H	4.52805486	1.15715298	1.02732141
C	-0.76238578	-0.75719347	2.49800977
C	-4.19108071	1.12754872	-1.60382503
H	-4.36605851	1.86421514	-0.82555859
C	0.44643547	-0.46425827	2.5316988
C	-4.97912558	-1.25046327	2.44663267
H	-6.05557259	-1.38804412	2.42960929
C	-4.21965963	-1.64822125	3.5659308
H	-4.71792644	-2.0898523	4.42557333
C	1.35766928	2.06069063	-2.11379654
H	1.08078231	1.16798072	-2.67009502
C	-2.88773759	-0.70172723	-2.50981401
H	-2.04974595	-1.38757687	-2.43433929
C	-5.02788797	1.0809365	-2.71936826
H	-5.858374	1.77725861	-2.79916047
C	3.37282682	-0.48073404	-1.00860107
C	4.76585923	-2.44066347	-1.35608961
H	5.01185553	-3.47061788	-1.11238327
C	-4.79928563	0.14178036	-3.73054345
H	-5.45142146	0.10848992	-4.5990632
C	-2.14761107	-0.92780322	2.47829449
C	5.51335451	-1.74656603	-2.31542432

H	6.33946364	-2.23731252	-2.82263205
C	4.12962903	0.21165837	-1.96197546
H	3.89755139	1.24497848	-2.19684039
C	-1.59694949	2.94545584	-0.63182237
H	-1.59586705	2.63202553	-1.67086925
C	2.03396054	4.354788	-0.67940778
H	2.28095482	5.24759618	-0.11157561
C	4.44854871	0.83388559	3.14782179
H	5.46667129	1.167866	3.31988802
C	1.61361605	4.46242843	-2.00625035
H	1.5409655	5.43891319	-2.4777062
C	3.65241174	0.35551752	4.21685418
H	4.06306583	0.3277351	5.22324628
C	-3.72796544	-0.74886354	-3.62475064
H	-3.54150462	-1.47563835	-4.41058179
C	1.26955162	3.3114385	-2.72293877
H	0.92581505	3.38921097	-3.75108069
C	-1.37443036	4.70235514	1.01639978
H	-1.20417875	5.74767742	1.26021918
C	5.19383127	-0.42159213	-2.61338327
H	5.77331474	0.12755128	-3.35089537
C	-1.5751298	3.76801366	2.03488906
H	-1.56111015	4.08138704	3.07523687
C	-1.38963875	4.28785513	-0.31813168
H	-1.22646342	5.00583239	-1.11588148

Table S11. Cartesian coordinates of the optimized T_1 geometry for complex **1**.

Atom	x	y	z
I	6.102909	3.165607	11.957891
Cu	4.224119	4.885611	12.013763
P	3.496036	6.488202	10.511861
P	2.708453	4.210183	13.661596
C	5.307966	5.49857	8.637949
H	5.810773	5.070655	9.500344
C	1.314547	5.384961	13.800489
C	3.638604	3.397201	16.193175
H	2.954071	2.557935	16.115023
C	1.070905	7.950807	10.66823
H	1.643828	8.732501	11.156162
C	4.873081	8.149298	12.296466
C	1.704926	6.769223	10.268147
C	4.217126	8.077614	11.014359
C	1.371785	6.481731	14.672333

H	2.23963	6.626816	15.306021
C	5.425379	5.566039	16.427679
H	6.126655	6.391702	16.499277
C	1.944744	2.558574	13.646263
C	5.533535	9.375975	12.634263
H	6.049202	9.436852	13.587669
C	3.685098	4.340192	15.164561
C	4.208398	9.190983	10.17302
H	3.723323	9.119347	9.203163
C	4.80846	6.300471	14.167146
C	0.779746	2.283829	14.382366
H	0.296312	3.07452	14.947928
C	4.883727	7.086948	13.19194
C	4.435851	3.531995	17.329501
H	4.36838	2.804712	18.132301
C	5.321716	4.639102	17.436763
H	5.939031	4.745659	18.325002
C	0.94836	5.75434	9.657898
H	1.430998	4.828915	9.353009
C	2.561654	1.533118	12.913936
H	3.465664	1.74108	12.349336
C	0.243797	0.995642	14.387272
H	-0.654991	0.788422	14.961875
C	4.111885	6.212168	8.805242
C	5.847165	5.322015	7.362447
H	6.772209	4.764375	7.245251
C	0.863432	-0.024934	13.65811
H	0.443176	-1.02708	13.662559
C	4.642352	5.439043	15.226716
C	5.194753	5.848469	6.244334
H	5.612679	5.705541	5.251473
C	3.456678	6.735012	7.679238
H	2.521859	7.275148	7.793796
C	0.1878	5.212204	12.980966
H	0.139791	4.376658	12.28959
C	-0.294803	8.128939	10.431695
H	-0.776886	9.050497	10.746118
C	4.838496	10.383969	10.535959
H	4.834154	11.232705	9.859139
C	-1.035651	7.131722	9.795537
H	-2.095375	7.277426	9.60378
C	5.509358	10.457656	11.776327
H	6.015231	11.376359	12.061929
C	2.021456	0.245335	12.924121

H	2.506369	-0.54379	12.356349
C	-0.411618	5.93844	9.415033
H	-0.983806	5.153092	8.92823
C	-0.825013	7.190137	13.936532
H	-1.656264	7.887808	13.992003
C	3.99764	6.552788	6.405302
H	3.482596	6.96005	5.539164
C	0.306702	7.382498	14.73326
H	0.359178	8.228523	15.413191
C	-0.882776	6.100497	13.063622
H	-1.752766	5.950399	12.432611

Table S12. Cartesian coordinates of the optimized S_0 geometry for complex **2**.

Atom	x	y	z
Br	0.26487448	-3.44178748	-0.24066835
Cu	0.00681264	-1.06844504	-0.15956926
P	1.99474079	0.10288753	-0.16251234
P	-2.03264255	-0.03391004	-0.13725955
C	3.19117396	-0.26693668	-1.49479448
C	-2.72609582	0.13339418	1.55989573
C	-1.86402494	0.11650373	2.68086042
C	2.89138534	-0.34779255	1.37282768
C	-0.459355	-0.06384941	2.56969827
C	2.14140462	-0.46339437	2.56694338
C	0.73883007	-0.24012637	2.57101867
C	1.93885427	1.93366109	-0.10029644
C	-2.09492295	1.68235361	-0.78253834
C	4.26180151	-0.59933408	1.40029876
H	4.83454066	-0.52811886	0.48447594
C	-4.10054878	0.27748897	1.76307692
H	-4.76709817	0.26643375	0.91057338
C	-2.41234992	0.2665478	3.96956232
H	-1.74520797	0.25008803	4.82212603
C	-3.36161556	-0.88895064	-1.06526667
C	4.89728618	-0.94725518	2.5900504
H	5.96303716	-1.14307392	2.59304014
C	-3.26782384	-2.28167307	-1.16943734
H	-2.406169	-2.79870912	-0.75889236
C	4.12077964	0.66763615	-1.96330107
H	4.13627554	1.66911383	-1.55080386
C	3.16645398	-1.55831266	-2.03667831
H	2.43880223	-2.28010467	-1.67817114
C	2.79554656	-0.80605698	3.76128835

H	2.2139408	-0.89429648	4.67032748
C	4.16314378	-1.04680629	3.77062516
H	4.65416368	-1.32125742	4.69666985
C	-2.21874719	2.79354313	0.05410182
H	-2.32158527	2.65771175	1.12330227
C	2.406718	2.67475833	0.98733933
H	2.85933467	2.17156323	1.83206974
C	-3.778461	0.42059712	4.14700343
H	-4.18213489	0.52938907	5.14669674
C	1.35483602	2.60188804	-1.18370223
H	0.9691019	2.03556382	-2.02301045
C	-1.94837113	1.87874669	-2.16250081
H	-1.8393812	1.02390735	-2.82093479
C	-4.45131759	-0.22145467	-1.63783432
H	-4.51905871	0.85814186	-1.57989535
C	-4.26756563	-2.99725164	-1.82437725
H	-4.18581358	-4.07489445	-1.90407713
C	5.00389867	-0.97738068	-3.49462898
H	5.70718145	-1.25257031	-4.27234126
C	-4.62845164	0.42241924	3.04109984
H	-5.69826492	0.53190104	3.17367082
C	4.07690684	-1.90927072	-3.03003025
H	4.05532215	-2.91043408	-3.44448149
C	5.02290195	0.31143887	-2.9628583
H	5.7402999	1.03907539	-3.3249695
C	1.73530959	4.72421514	-0.10187
H	1.65714958	5.80528461	-0.10287405
C	-5.35526238	-2.33170155	-2.38549403
H	-6.12825101	-2.89105086	-2.9000353
C	-2.22125412	4.079836	-0.48251521
H	-2.31559561	4.93445568	0.17720937
C	-2.10808864	4.26742695	-1.85665167
H	-2.12167878	5.26822677	-2.27257808
C	-5.44369981	-0.94254708	-2.29566963
H	-6.283953	-0.42071733	-2.73945964
C	-1.96837651	3.16208288	-2.69633299
H	-1.8720496	3.30016685	-3.7672858
C	2.2985683	4.0649278	0.9870417
H	2.66257799	4.63060393	1.8371947
C	1.26688869	3.98805888	-1.19002143
H	0.8167339	4.49182598	-2.03566157

Table S13. Cartesian coordinates of the optimized S_1 geometry for complex **2**.

Atom	x	y	z
Br	0.98181101	-2.85930923	-1.62972555
Cu	0.06774651	-1.07134507	-0.4309906
P	1.95023778	0.22341215	-0.0077889
P	-1.99292237	-0.03264616	-0.11265726
C	3.01701067	0.760085	-1.3819739
C	-2.66761359	-0.5944577	1.46043226
C	-1.80789157	-1.33529361	2.35554204
C	2.92434142	-0.80508141	1.1159236
C	-0.44068592	-1.50134819	2.14093076
C	2.18906535	-1.62775477	2.0431304
C	0.79472513	-1.62059099	2.07491178
C	1.51451135	1.75069742	0.8862561
C	-2.10356348	1.7912541	-0.16424479
C	4.31838397	-0.80427706	1.11159687
H	4.85121788	-0.18541176	0.39566006
C	-4.01957195	-0.41275027	1.77594408
H	-4.65461187	0.13565711	1.08474598
C	-2.41779983	-1.89789656	3.52366855
H	-1.79475257	-2.47919585	4.19685753
C	-3.18423281	-0.56099873	-1.40278775
C	5.0405294	-1.60435085	2.00207197
H	6.12539758	-1.61040939	1.9760652
C	-2.98256338	-1.79703209	-2.03571364
H	-2.10390352	-2.39116691	-1.80181101
C	3.9071941	1.83544541	-1.21256639
H	3.94068558	2.3694854	-0.26823147
C	2.97777312	0.08155484	-2.60872284
H	2.29647588	-0.75166238	-2.74424761
C	2.9528171	-2.43146886	2.94155158
H	2.4221494	-3.06735648	3.64360721
C	4.33674185	-2.41423967	2.91557913
H	4.88664292	-3.0456889	3.60913806
C	-2.44383135	2.53941482	0.96792022
H	-2.62333062	2.03434131	1.91143678
C	1.48298954	1.76392013	2.28879153
H	1.74847257	0.87266766	2.84549082
C	-3.75429938	-1.70067926	3.80313283
H	-4.17885031	-2.13824263	4.70334657
C	1.15388851	2.90566627	0.17288025
H	1.15625502	2.89909537	-0.91245822
C	-1.85761398	2.45061861	-1.38019381
H	-1.58828307	1.87585836	-2.26303174
C	-4.31167143	0.20588236	-1.73655574

H	-4.47084563	1.17229582	-1.26805647
C	-3.90344339	-2.26669758	-2.97356554
H	-3.73539993	-3.22510338	-3.45690847
C	4.70683602	1.53824087	-3.47788474
H	5.36068566	1.84096608	-4.29122773
C	-4.57778578	-0.94075635	2.93724498
H	-5.62994062	-0.79380585	3.15879999
C	3.82121444	0.47170103	-3.65100118
H	3.78304898	-0.0594145	-4.59787703
C	4.74921287	2.21840938	-2.25656808
H	5.43822113	3.04662757	-2.11513919
C	0.79201324	4.08438303	2.25258545
H	0.51498927	4.99172545	2.78245527
C	-5.02824883	-1.5026535	-3.29650576
H	-5.74225309	-1.86643825	-4.03035084
C	-2.56520802	3.92879594	0.87823336
H	-2.83175482	4.50139171	1.76231304
C	-2.35009736	4.57752991	-0.33879725
H	-2.45668773	5.6568659	-0.40794468
C	-5.22826175	-0.26476398	-2.67810639
H	-6.09837282	0.33642875	-2.92845428
C	-1.98897838	3.83524476	-1.46883436
H	-1.81237588	4.33480251	-2.41775826
C	1.11862386	2.9289645	2.96627695
H	1.09735056	2.93256592	4.05244729
C	0.81299952	4.07105416	0.85471062
H	0.54694879	4.96183533	0.29518819

Table S14. Cartesian coordinates of the optimized T_1 geometry for complex **2**.

Atom	x	y	z
Br	-0.489946	5.112303	4.347068
Cu	1.185948	3.46482	4.344873
P	2.736415	4.133252	2.722997
P	1.934976	1.877982	5.849376
C	3.455871	5.801816	2.776
C	1.217661	0.283077	5.367757
C	0.566329	0.193352	4.084902
C	1.760244	4.005643	1.224046
C	0.559321	1.245427	3.175079
C	0.810039	2.901253	1.148482
C	0.647599	2.02601	2.198605
C	4.142708	2.97833	2.593855
C	3.719227	1.596493	6.130397

C	1.808835	4.958695	0.202046
H	2.490315	5.799461	0.291618
C	1.232761	-0.822477	6.221093
H	1.718975	-0.739741	7.189338
C	-0.086878	-1.039424	3.760164
H	-0.599212	-1.114177	2.805921
C	1.29242	2.225582	7.531881
C	1.019242	4.829549	-0.937782
H	1.087923	5.562341	-1.735439
C	0.158631	3.042091	7.658662
H	-0.282851	3.50426	6.779826
C	4.669527	6.10177	2.135002
H	5.219768	5.320831	1.619487
C	2.747291	6.817117	3.43816
H	1.803382	6.587238	3.924461
C	0.031622	2.784192	-0.055488
H	-0.66715	1.957335	-0.137351
C	0.136792	3.719621	-1.056416
H	-0.477597	3.618687	-1.947382
C	4.359805	0.420909	5.722106
H	3.795241	-0.351879	5.210764
C	4.112917	1.90112	1.696216
H	3.260385	1.765973	1.039741
C	-0.060226	-2.111115	4.630613
H	-0.561217	-3.035255	4.354035
C	5.248632	3.140984	3.443653
H	5.27317	3.959729	4.155975
C	4.464004	2.600147	6.772745
H	3.975731	3.519346	7.086845
C	1.873924	1.665681	8.680845
H	2.766348	1.052712	8.597123
C	-0.397258	3.277093	8.918085
H	-1.274074	3.912678	9.004846
C	4.460525	8.414557	2.819299
H	4.851522	9.428352	2.837465
C	0.60834	-2.021039	5.871403
H	0.615917	-2.862401	6.557327
C	3.251959	8.118659	3.456345
H	2.698875	8.900059	3.969931
C	5.167524	7.405207	2.157794
H	6.104565	7.632377	1.656518
C	6.297978	1.193133	2.466213
H	7.135935	0.503305	2.413649
C	0.177631	2.709502	10.057868

H	-0.253648	2.897404	11.037441
C	5.720436	0.237448	5.981289
H	6.207541	-0.679572	5.661495
C	6.450149	1.224214	6.646296
H	7.506074	1.07458	6.855195
C	1.31647	1.906391	9.937133
H	1.772983	1.469138	10.821256
C	5.819702	2.411324	7.03561
H	6.383206	3.187727	7.546258
C	5.185962	1.009802	1.639846
H	5.155811	0.178695	0.940499
C	6.328011	2.263177	3.364626
H	7.182464	2.405326	4.018209

Table S15. Cartesian coordinates of the optimized S_0 geometry for complex **3**.

Atom	x	y	z
Cu	-0.00169466	-1.23881395	0.16476822
P	2.02552216	-0.19117912	0.13226316
P	-2.00978314	-0.11340034	0.16689428
Cl	-0.19662252	-3.49579	0.33024551
C	-3.18902075	-0.54930022	1.49348817
C	-2.14855577	-0.62492762	-2.57420893
C	-0.74725826	-0.39227042	-2.57474144
C	2.08523308	1.52290485	0.78315176
C	0.45047265	-0.21281444	-2.57356062
C	-1.99870771	1.71890413	0.15002173
C	1.85482209	-0.02800349	-2.68467273
C	2.71815204	-0.01540097	-1.56449726
C	-2.89959131	-0.54492512	-1.37778756
C	3.34810009	-1.0537642	1.06111481
C	-4.14334256	0.34544436	1.98895824
H	-4.1902942	1.356107	1.60161118
C	-4.90034695	-1.13432356	-2.60899122
H	-5.96423004	-1.33993186	-2.61677738
C	-4.26760783	-0.80948663	-1.41135936
H	-4.84040251	-0.76560877	-0.49376901
C	3.22865749	-2.44284139	1.18821009
H	2.3532891	-2.95006657	0.7939566
C	-2.8002873	-0.94458599	-3.77652323
H	-2.2182587	-1.00513577	-4.68757915
C	-4.16559293	-1.19744713	-3.79183161
H	-4.65435247	-1.4531868	-4.72441896
C	-3.11956341	-1.85185046	2.00451729

H	-2.36787107	-2.53995518	1.62886207
C	-1.38108729	2.37264393	1.22351033
H	-0.9390317	1.79393663	2.02579217
C	2.17226214	2.63727011	-0.05420403
H	2.25601538	2.5046462	-1.12552537
C	4.09205712	0.13188227	-1.76858359
H	4.75970223	0.11681011	-0.91707479
C	4.45317195	-0.3968846	1.6164878
H	4.53841769	0.68066749	1.54333932
C	-2.53727939	2.47628419	-0.89285758
H	-3.01499852	1.98351887	-1.7300105
C	2.40148404	0.13068157	-3.97313352
H	1.73339894	0.1180534	-4.82503917
C	4.22049516	-3.16565824	1.84772164
H	4.11981415	-4.24018351	1.94578686
C	5.32409437	-2.51124277	2.39036952
H	6.09052263	-3.07643326	2.90837367
C	-1.8682823	4.51251097	0.22208016
H	-1.81788572	5.59488183	0.25008235
C	-5.02866472	-0.06217607	2.98392308
H	-5.76554329	0.63423569	3.36768657
C	5.43711779	-1.12531846	2.27856862
H	6.28947962	-0.61208663	2.7091019
C	1.9633646	1.71520661	2.16609519
H	1.88381133	0.85801992	2.82558849
C	4.61834511	0.28478474	-3.04633909
H	5.68783774	0.39667416	-3.17947393
C	3.76710967	0.28810421	-4.15129011
H	4.16944762	0.40357127	-5.15077466
C	2.07136979	4.10701682	1.86026171
H	2.07405936	5.10750147	2.27715392
C	-4.01371536	-2.25368786	2.99346287
H	-3.95821356	-3.26265835	3.38522596
C	-1.32871781	3.76009638	1.26528161
H	-0.85071748	4.25255367	2.10225069
C	1.96944419	2.99838718	2.70098043
H	1.89173624	3.13357169	3.77381006
C	-4.96694669	-1.36232956	3.48402173
H	-5.65705211	-1.67765352	4.25832823
C	2.16183507	3.92277203	0.48392516
H	2.22781516	4.77963103	-0.17635763
C	-2.46578407	3.86836202	-0.8576884
H	-2.88426913	4.44714335	-1.67325322

Table S16. Cartesian coordinates of the optimized S_1 geometry for complex **3**.

Atom	x	y	z
Cu	-0.06392577	-0.68646886	1.18872489
P	1.92342218	0.00528266	0.18767863
P	-1.97457009	0.0679917	0.09008231
Cl	-0.8558542	-1.33295693	3.14720385
C	-3.02118783	1.29890508	0.92633935
C	-2.19788025	-2.65601312	-0.40262126
C	-0.80441115	-2.65562288	-0.47620356
C	1.95340617	1.51740289	-0.83602361
C	0.42014385	-2.57413294	-0.66871716
C	-1.61816275	0.75845589	-1.55708935
C	1.7716696	-2.52166811	-1.00206981
C	2.59652733	-1.35513368	-0.7782536
C	-2.935811	-1.4460971	-0.14577297
C	3.14440908	0.3615181	1.5081453
C	-3.95852192	2.05329245	0.19848419
H	-4.03916905	1.93021437	-0.87690799
C	-5.04719484	-2.63742194	-0.30105192
H	-6.1308969	-2.63585971	-0.24405329
C	-4.32922962	-1.45461965	-0.10116895
H	-4.8643009	-0.53296635	0.10758941
C	2.99789435	-0.27843286	2.74869945
H	2.1413249	-0.92025065	2.93565955
C	-2.95687397	-3.84667332	-0.60432617
H	-2.42315241	-4.77369073	-0.79004564
C	-4.34041071	-3.82938749	-0.55349216
H	-4.88681081	-4.75724893	-0.70391529
C	-2.92243448	1.46830911	2.31540918
H	-2.20864473	0.87975702	2.88237795
C	-1.32529897	2.12423776	-1.70542044
H	-1.33136916	2.78038263	-0.8411803
C	2.24780766	1.47280427	-2.20308676
H	2.43691455	0.5171913	-2.6810092
C	3.92910425	-1.3439841	-1.20952182
H	4.53866038	-0.46368327	-1.02102591
C	4.24334174	1.20920504	1.29675502
H	4.35958036	1.72401186	0.34793387
C	-1.57984298	-0.08485562	-2.67815252
H	-1.79189463	-1.14215761	-2.56886389
C	2.39991652	-3.65109025	-1.62073531
H	1.8060785	-4.547538	-1.77251642
C	3.94509095	-0.08601233	3.75566897
H	3.81927721	-0.58565534	4.7121058

C	5.04092195	0.75355111	3.53777211
H	5.77506774	0.90688583	4.32399044
C	-1.02013856	1.80621892	-4.08285141
H	-0.79262322	2.21435427	-5.06388424
C	-4.78813273	2.96084375	0.85712735
H	-5.51360444	3.53629305	0.28859018
C	5.1860749	1.40211224	2.30761622
H	6.03355046	2.05994198	2.13381343
C	1.69176124	2.75500251	-0.22451132
H	1.45799667	2.79622354	0.83656662
C	4.50143472	-2.44223994	-1.84499605
H	5.53817551	-2.41507438	-2.16452707
C	3.71601442	-3.6066889	-2.03110753
H	4.15492024	-4.48191207	-2.50371891
C	2.07796764	3.88636428	-2.32713617
H	2.13716256	4.80542049	-2.90410799
C	-3.755988	2.37917449	2.96774382
H	-3.67431786	2.50302243	4.04387919
C	-1.04623063	2.64656104	-2.96593526
H	-0.83305918	3.70518615	-3.07266529
C	1.7609798	3.93367485	-0.96490901
H	1.5714969	4.88776951	-0.48026986
C	-4.68714485	3.12654938	2.24220733
H	-5.33274922	3.83604701	2.75262189
C	2.30987215	2.65591142	-2.94405
H	2.54173415	2.61215692	-4.00458877
C	-1.27742467	0.44115388	-3.93522168
H	-1.25087076	-0.21711747	-4.79900473

Table S17. Cartesian coordinates of the optimized T_1 geometry for complex **3**.

Atom	x	y	z
Cu	1.177998	3.518614	4.315446
P	1.939578	1.923209	5.801536
P	2.753008	4.148796	2.699115
Cl	-0.359704	5.126363	4.330719
C	3.472636	5.815718	2.766037
C	0.813875	2.941502	1.11976
C	0.641669	2.063157	2.167622
C	3.724927	1.666165	6.092717
C	0.561088	1.271907	3.134137
C	4.1525	2.986214	2.574921
C	0.576133	0.224139	4.048796
C	1.237718	0.322411	5.325993

C	1.776016	4.034031	1.200344
C	1.28284	2.284546	7.475306
C	4.684091	6.125299	2.125346
H	5.237308	5.350649	1.603537
C	1.058352	4.867142	-0.965859
H	1.139764	5.599082	-1.76311
C	1.841937	4.987372	0.177998
H	2.532539	5.820163	0.271801
C	0.140328	3.091828	7.584679
H	-0.299748	3.540977	6.698143
C	0.04059	2.834655	-0.087255
H	-0.667739	2.01635	-0.17303
C	0.162913	3.768336	-1.088364
H	-0.447611	3.6741	-1.982735
C	2.75907	6.822779	3.435763
H	1.815781	6.584728	3.919756
C	5.275905	3.163431	3.398525
H	5.318576	3.998132	4.090947
C	4.379446	0.493163	5.699353
H	3.825514	-0.289657	5.191711
C	1.267251	-0.780211	6.184185
H	1.761225	-0.690383	7.147959
C	1.861821	1.743301	8.634409
H	2.760066	1.137243	8.563603
C	4.099245	1.887383	1.704556
H	3.23242	1.739923	1.069825
C	-0.075157	-1.012648	3.736693
H	-0.596897	-1.094047	2.78807
C	-0.425445	3.337277	8.837685
H	-1.308258	3.966114	8.911357
C	0.147535	2.788744	9.987797
H	-0.291354	2.984982	10.962321
C	6.296653	1.187857	2.446433
H	7.130428	0.493051	2.393055
C	5.174533	7.431451	2.155115
H	6.109589	7.666901	1.65395
C	1.294079	1.994274	9.88403
H	1.748633	1.571829	10.776313
C	4.455534	2.683823	6.729361
H	3.955947	3.600796	7.031922
C	0.64709	-1.983005	5.844882
H	0.666061	-2.822004	6.533463
C	-0.033917	-2.080704	4.61074
H	-0.533291	-3.008298	4.342893

C	6.456149	1.327219	6.626849
H	7.512403	1.190499	6.842792
C	3.256025	8.127279	3.459463
H	2.698695	8.902948	3.977087
C	6.349325	2.27823	3.318782
H	7.217468	2.431529	3.951613
C	5.811844	2.511927	7.000467
H	6.364811	3.299264	7.505806
C	4.462643	8.433041	2.823297
H	4.847753	9.448991	2.845998
C	5.740165	0.326087	5.968392
H	6.238396	-0.589013	5.660553
C	5.166877	0.989976	1.647799
H	5.118554	0.142374	0.969631

Table S18. Cartesian coordinates of the optimized S_0 geometry for complex **4**.

Atom	x	y	z
I	1.07885603	3.07762821	1.5225557
Cu	0.60833309	0.96760437	0.12612565
P	2.42975321	-0.43583149	-0.0825112
P	-1.43252348	0.49216671	-0.79165205
O	-5.19282462	-2.21773424	3.01965923
O	-6.15369475	-0.94559627	0.96405638
C	-1.91588955	-1.94161622	-2.17605633
H	-2.33099876	-2.31779903	-1.24954281
C	2.18803483	-2.05243243	-0.91268202
C	-0.63697802	-1.06066259	1.81717538
C	0.52434834	-1.12599127	2.15647632
C	1.85131639	-2.04073592	-2.27191503
H	1.75939481	-1.09792096	-2.79749391
C	-2.43771569	1.91552621	-1.36686317
C	2.22439996	-1.53500174	3.86511069
H	1.43008482	-1.75089444	4.56858225
C	-3.93464719	-0.31307478	0.21013264
H	-4.33038267	0.22529422	-0.6378649
C	3.55380101	-1.58090317	4.26412033
H	3.79879885	-1.8398875	5.28736048
C	1.88798496	-1.18617143	2.54743174
C	6.05846947	-0.03325274	-2.01229539
H	6.77218807	-0.66514117	-2.52859405
C	-2.02402635	-1.01114245	1.52029054
C	-1.43670625	-0.63186566	-2.24225469
C	-3.3444652	1.83278529	-2.43045034

H	-3.43869061	0.91213425	-2.99341424
C	3.96727506	0.22079226	-0.82464213
C	4.8934879	-0.58976304	-1.4897923
H	4.70256221	-1.65009809	-1.60124374
C	2.27665627	-3.27435188	-0.24181199
H	2.53498046	-3.29816929	0.8090333
C	1.63345969	-3.23169675	-2.95292647
H	1.37675226	-3.20735783	-4.00415622
C	-2.54656954	-0.34072224	0.40237395
C	-4.80591882	-0.94029822	1.08707258
C	-2.91179176	-1.65568789	2.41102524
H	-2.49247406	-2.16267433	3.26734432
C	6.30647309	1.33133028	-1.86989068
H	7.21409473	1.76234012	-2.27682107
C	-0.88597786	-0.16520331	-3.44349401
H	-0.49843995	0.84624819	-3.50233867
C	4.21433022	1.59269078	-0.69031712
H	3.49516471	2.22243057	-0.17690399
C	-4.28107741	-1.63147651	2.20976047
C	-2.30611757	3.11726892	-0.66201737
H	-1.58277392	3.19606614	0.14247493
C	4.24739419	-0.94207786	2.04232244
H	5.03632339	-0.70412238	1.34027748
C	1.72255257	-4.44962644	-2.27894782
H	1.54281178	-5.37829689	-2.80824386
C	-0.85280352	-0.98301681	-4.56715916
H	-0.43833755	-0.60570648	-5.4951243
C	2.03890142	-4.46727992	-0.92335217
H	2.10826956	-5.41013833	-0.39277365
C	4.56692356	-1.28170497	3.35496345
H	5.60437956	-1.30779287	3.66660035
C	-6.72524238	-0.22646867	-0.12340908
H	-6.461283	0.83471818	-0.07834863
H	-7.80189233	-0.34141665	-0.01767326
H	-6.40472649	-0.64178265	-1.08452124
C	-3.08690772	4.21679416	-1.00942259
H	-2.97423889	5.14453579	-0.46077086
C	-4.72249649	-2.89616571	4.17794289
H	-4.19027661	-2.21292332	4.84752102
H	-4.06731905	-3.73135278	3.90935621
H	-5.61132982	-3.27664262	4.67680922
C	2.91951259	-0.89708726	1.62269758
C	-4.11994518	2.93689963	-2.77531839
H	-4.81743168	2.86750908	-3.60251005

C	-3.99533733	4.12901111	-2.06250513
H	-4.59733817	4.98852922	-2.33445047
C	-1.8676602	-2.76459515	-3.3000565
H	-2.23958352	-3.78059553	-3.23596683
C	-1.347641	-2.28591807	-4.49884208
H	-1.32024975	-2.92451697	-5.37425053
C	5.38452001	2.14109698	-1.20825092
H	5.57108293	3.20299086	-1.09806452

Table S19. Cartesian coordinates of the optimized S_1 geometry for complex **4**.

Atom	x	y	z
I	1.39463929	-0.61804137	3.3376714
Cu	0.57587293	-0.11900787	0.94427319
P	2.38153356	-0.17380963	-0.5032189
P	-1.40379698	0.87866735	0.28627336
O	-5.27803974	-3.43955277	-1.1039131
O	-6.15107099	-0.99384415	-0.88850457
C	-1.86263232	1.90452328	-2.31208104
H	-2.41612793	0.98974673	-2.49867611
C	1.87075071	0.23549682	-2.21352176
C	-0.68237295	-2.0972081	-0.22046278
C	0.49887185	-2.489944	-0.24069281
C	1.85809352	1.57169877	-2.64166605
H	2.18275238	2.36144157	-1.97135586
C	-2.33961447	1.79599829	1.57522891
C	2.20510708	-4.26265495	-0.38780509
H	1.42605578	-5.01125397	-0.2765513
C	-3.90064606	-0.15902662	-0.41720347
H	-4.25302229	0.85856098	-0.29353796
C	3.52593669	-4.64164771	-0.53295431
H	3.77592537	-5.69994055	-0.53670383
C	1.8283653	-2.88195029	-0.36893525
C	5.95951353	1.80533022	-0.99104539
H	6.69056248	1.94891067	-1.78216234
C	-2.03066716	-1.75873476	-0.3606648
C	-1.25427585	2.10190935	-1.06789046
C	-3.0524447	2.97362382	1.30919419
H	-3.01970836	3.41763269	0.31947741
C	3.86528406	0.84825345	-0.22034996
C	4.81513146	1.04625817	-1.23711476
H	4.65460053	0.61079451	-2.21864468
C	1.43155972	-0.77211414	-3.08359428
H	1.43182425	-1.80622818	-2.75839571

C	1.44484173	1.89138021	-3.93363317
H	1.44782537	2.92746576	-4.25708231
C	-2.52680182	-0.42124185	-0.23718506
C	-4.80441596	-1.16532126	-0.71128811
C	-2.98435013	-2.78853856	-0.64815654
H	-2.6161492	-3.80271456	-0.73694618
C	6.16564178	2.37795446	0.26842697
H	7.05686739	2.97026859	0.45709396
C	-0.51648827	3.27484578	-0.83950795
H	-0.02655139	3.42710222	0.11954165
C	4.07347643	1.43402997	1.03623496
H	3.33745094	1.30087888	1.82231029
C	-4.32560162	-2.50982323	-0.82240545
C	-2.39769991	1.23936431	2.86232334
H	-1.85331626	0.32447304	3.07658974
C	4.21505553	-2.32387863	-0.65490038
H	5.00012269	-1.57909919	-0.74761334
C	1.01064476	0.88430538	-4.80023708
H	0.67953217	1.13610009	-5.80428828
C	-0.4275138	4.2554511	-1.82625959
H	0.13409322	5.16606226	-1.63457531
C	0.99896227	-0.44464583	-4.37070277
H	0.6589911	-1.23200852	-5.03797774
C	4.55369586	-3.68046131	-0.66456531
H	5.59052252	-3.98608839	-0.76055734
C	-6.66168692	0.31825595	-0.74100685
H	-6.47409687	0.70997958	0.268539
H	-7.73743701	0.24134948	-0.90910776
H	-6.22367548	1.00399551	-1.48045581
C	-3.15512593	1.84592305	3.86330024
H	-3.19115138	1.40313427	4.85494865
C	-4.8735914	-4.79572477	-1.21056686
H	-4.43267054	-5.15340586	-0.27088424
H	-4.15165505	-4.93189479	-2.02660726
H	-5.78258084	-5.35910363	-1.42750885
C	2.89131791	-1.90928127	-0.51417942
C	-3.8076128	3.58395606	2.31511043
H	-4.35457038	4.49739619	2.09611025
C	-3.8613216	3.02332308	3.59284606
H	-4.44714959	3.49964943	4.37424116
C	-1.76000601	2.88237104	-3.30540069
H	-2.23232377	2.71851723	-4.27015111
C	-1.05639033	4.06295842	-3.06121534
H	-0.98656906	4.82571472	-3.8322373

C	5.22078304	2.19226791	1.28075281
H	5.37162952	2.6406043	2.25883535

Table S20. Cartesian coordinates of the optimized T_1 geometry for complex **4**.

Atom	x	y	z
I	2.015276	3.880144	2.830256
Cu	-0.467318	4.620325	2.995647
P	-1.921372	2.921929	3.530261
P	-0.965786	6.833009	2.650089
O	1.264572	9.921048	7.315765
O	0.846376	11.132933	5.060659
C	-3.444476	7.68689	3.708792
H	-2.921559	7.781604	4.655778
C	-3.667157	3.406133	3.819495
C	-0.344844	5.728617	5.498774
C	-0.553436	4.507706	5.742687
C	-4.346255	4.061642	2.780572
H	-3.830834	4.272172	1.847571
C	-0.220271	7.694969	1.213929
C	-0.395037	2.701805	7.367824
H	0.053242	3.396985	8.070708
C	-0.022865	9.116508	4.00107
H	-0.174466	9.628464	3.059136
C	-0.563278	1.372949	7.695967
H	-0.251218	1.018618	8.674769
C	-0.782517	3.195676	6.071943
C	-3.229051	-0.393094	1.428881
H	-4.15568	-0.940634	1.277097
C	-0.097342	7.056227	5.34427
C	-2.744225	7.287638	2.562601
C	-0.761019	8.865281	0.656232
H	-1.694508	9.268994	1.037114
C	-2.028805	1.450793	2.449746
C	-3.219128	0.737061	2.250806
H	-4.135348	1.064568	2.732825
C	-4.3309	3.173952	5.031331
H	-3.813774	2.673147	5.843505
C	-5.675991	4.446228	2.938476
H	-6.189803	4.949221	2.125819
C	-0.337621	7.767943	4.086189
C	0.507795	9.825905	5.0848
C	0.451214	7.809689	6.454969
H	0.633658	7.274418	7.377637

C	-2.051708	-0.818752	0.807433
H	-2.061198	-1.698194	0.168867
C	-3.439364	7.156297	1.349402
H	-2.912442	6.835317	0.454524
C	-0.848407	1.025382	1.818073
H	0.074046	1.582264	1.965213
C	0.744444	9.141064	6.339121
C	0.976295	7.174057	0.697243
H	1.398839	6.266743	1.121622
C	-1.525985	0.92898	5.5037
H	-1.958472	0.229585	4.794063
C	-6.335322	4.209783	4.14901
H	-7.368678	4.521534	4.27608
C	-4.798195	7.462911	1.276633
H	-5.318655	7.376863	0.326115
C	-5.658417	3.580677	5.195921
H	-6.162735	3.399121	6.141551
C	-1.123297	0.468088	6.76864
H	-1.242647	-0.57948	7.027394
C	0.678379	11.853102	3.84241
H	1.277628	11.409137	3.038505
H	1.028058	12.864699	4.050562
H	-0.377314	11.879124	3.545317
C	1.625564	7.822725	-0.355634
H	2.551083	7.409827	-0.747359
C	1.556096	9.310532	8.567198
H	2.293828	8.507198	8.448234
H	0.645201	8.908913	9.02921
H	1.968948	10.102858	9.192588
C	-1.382374	2.259753	5.140517
C	-0.110183	9.507823	-0.398849
H	-0.538958	10.410509	-0.826814
C	1.085886	8.988791	-0.905382
H	1.590231	9.48849	-1.728267
C	-4.810029	7.972727	3.638212
H	-5.341614	8.277007	4.535783
C	-5.487996	7.873458	2.421628
H	-6.547874	8.106727	2.366384
C	-0.86284	-0.108395	1.004584
H	0.054527	-0.432108	0.520479

Table S21. Cartesian coordinates of the optimized S_0 geometry for complex **5**.

Atom	x	y	z

Br	-0.98967115	-1.08256598	-3.31045293
Cu	-0.62699376	-0.58822268	-1.00037998
P	1.38352354	-0.92540421	0.0367332
P	-2.48484572	0.1941601	0.12049341
O	6.11402339	1.3294491	0.03354115
O	5.16651972	3.71627025	-0.38306556
C	-0.5493418	2.36173741	-0.72550707
C	1.99214362	1.80068147	-0.35488415
C	-1.90774251	2.70190449	-0.95944775
C	2.88414325	2.89331102	-0.44328298
H	2.47025142	3.87225016	-0.63446988
C	-2.22910248	3.94426022	-1.53046353
H	-1.42737451	4.62564704	-1.78633232
C	2.39295125	-2.31037452	-0.61766168
C	2.50687926	0.51690796	-0.11107554
C	1.34506541	-1.25179449	1.84222081
C	3.89240293	0.35149426	0.01909892
H	4.28387946	-0.64130883	0.18109236
C	-2.32608689	0.57992143	1.90530669
C	4.76814221	1.42205859	-0.07455023
C	4.25076309	2.72297909	-0.3050343
C	0.60872358	2.06027007	-0.53658621
C	-2.02383331	-0.47698791	2.77299165
H	-1.90673558	-1.48046264	2.38152538
C	-2.94907931	1.80394537	-0.62468136
C	-4.01554298	-0.80023892	0.00976311
C	1.74837921	-0.30029079	2.78126857
H	2.13231485	0.65614826	2.44929319
C	-2.44653876	1.87276707	2.42003778
H	-2.67832467	2.69924949	1.76056834
C	-4.99202511	-0.80851081	1.01149908
H	-4.84718795	-0.22598272	1.91319652
C	2.24219563	-2.62275942	-1.97354048
H	1.50110143	-2.0999933	-2.57002082
C	-3.55202122	4.28435675	-1.78023978
H	-3.7845999	5.24192855	-2.23094499
C	-4.27048522	2.1596262	-0.88926273
H	-5.06638309	1.46643835	-0.6486656
C	3.31603937	-3.02139011	0.15922724
H	3.42072255	-2.80131893	1.2148766
C	-1.99383609	1.04492646	4.64435684
H	-1.86566712	1.22496549	5.70550819
C	0.83402408	-2.47820193	2.28799241
H	0.50601249	-3.21999133	1.5678767

C	-1.87288649	-0.24774162	4.13460593
H	-1.64268511	-1.07455332	4.79408316
C	-6.14782274	-1.56894109	0.85107675
H	-6.90125737	-1.57452282	1.63055683
C	4.09133493	-4.02289855	-0.41898136
H	4.80125318	-4.57299978	0.18846136
C	1.18721729	-1.81141137	4.58057059
H	1.1334717	-2.03027853	5.64079674
C	-4.57459123	3.39156972	-1.46354694
H	-5.60708159	3.6509967	-1.66553263
C	-4.20048536	-1.56231153	-1.15078416
H	-3.43721717	-1.56288243	-1.92307495
C	3.95017064	-4.32111979	-1.77427707
H	4.55246992	-5.10321765	-2.22234083
C	6.67867383	0.03691735	0.22533184
H	6.42775761	-0.63173967	-0.60399808
H	6.33994038	-0.4069272	1.16726446
H	7.75529219	0.1892991	0.26070101
C	-2.27463654	2.10303524	3.78449525
H	-2.36782514	3.1106485	4.17353493
C	0.76750244	-2.76022213	3.64769859
H	0.38563614	-3.71893893	3.97992618
C	3.02453274	-3.62274195	-2.54681024
H	2.89837161	-3.86127467	-3.59638839
C	1.66582541	-0.57963278	4.14423233
H	1.97904319	0.16787837	4.86379613
C	-6.33536866	-2.31931851	-0.30909278
H	-7.2358373	-2.91031414	-0.43195214
C	-5.36231034	-2.31365144	-1.30743362
H	-5.50158286	-2.89997435	-2.20822275
C	4.70354466	5.03564577	-0.64304022
H	4.18772626	5.0910694	-1.60708997
H	5.59432037	5.65972382	-0.67002577
H	4.0354851	5.38495441	0.15112804

Table S22. Cartesian coordinates of the optimized S_1 geometry for complex **5**.

Atom	x	y	z
Br	-1.61233571	0.48942633	-3.239803
Cu	-0.60371903	0.1084968	-1.16385135
P	1.33197973	-0.87332273	-0.31083172
P	-2.42093326	0.245127	0.27715971
O	6.11599336	1.01727177	0.67089114
O	5.29267077	3.48825079	0.61773634

C	-0.51127	2.54475856	-0.1003456
C	2.0119715	1.80197295	0.0608967
C	-1.84192992	2.94152033	-0.00792497
C	2.98593627	2.83805873	0.23514724
H	2.63730692	3.86275403	0.21547863
C	-2.22211209	4.31844643	-0.07576298
H	-1.44507047	5.06070677	-0.23244102
C	2.15607553	-1.90977038	-1.58107789
C	2.48212941	0.44851947	0.07471219
C	1.24148193	-1.99183993	1.1338388
C	3.8506195	0.18098616	0.28562774
H	4.18556133	-0.84931511	0.2737336
C	-1.91074026	-0.09722751	1.99384107
C	4.77344687	1.19491301	0.4729586
C	4.32162794	2.55351955	0.43770771
C	0.66795132	2.14852815	-0.09446605
C	-1.88776559	-1.4168669	2.47399603
H	-2.19325256	-2.23616558	1.8308024
C	-2.90467139	1.98063067	0.18447783
C	-3.88940237	-0.79374714	-0.00073514
C	1.80475795	-1.64070657	2.36548991
H	2.28354957	-0.67338384	2.47921821
C	-1.48922761	0.95087217	2.82557766
H	-1.49465406	1.97007528	2.45642515
C	-4.80089013	-1.02820497	1.04413536
H	-4.6153524	-0.61407283	2.03011328
C	1.90772644	-1.6361719	-2.93477638
H	1.18763398	-0.87146701	-3.21150151
C	-3.5448499	4.7018445	0.04312113
H	-3.79715696	5.75760648	-0.02086172
C	-4.23041469	2.39595381	0.30233522
H	-5.0129875	1.65413833	0.43344394
C	3.07087123	-2.91946351	-1.24194284
H	3.25635985	-3.15734311	-0.19873877
C	-1.08546692	-0.63024913	4.6147004
H	-0.76920198	-0.8374046	5.6334905
C	0.60693217	-3.23712601	0.99439422
H	0.16310642	-3.51495514	0.04141885
C	-1.49557927	-1.6778223	3.78452865
H	-1.49281396	-2.69917644	4.15086207
C	-5.94534174	-1.79269001	0.81658165
H	-6.64744163	-1.96384925	1.62807021
C	3.73617594	-3.63150743	-2.2413439
H	4.44205727	-4.41132636	-1.96734805

C	1.15486081	-3.78537275	3.28591857
H	1.13070381	-4.48415885	4.1179368
C	-4.57078165	3.74981131	0.23292645
H	-5.6084058	4.05861623	0.30652014
C	-4.13633437	-1.33902449	-1.26910849
H	-3.43905163	-1.15795837	-2.0801347
C	3.49340446	-3.34557634	-3.58830323
H	4.01047964	-3.90227577	-4.36510203
C	6.60239488	-0.31210626	0.66130107
H	6.40679711	-0.80281072	-0.30250416
H	6.15260481	-0.90897406	1.46784081
H	7.67947707	-0.23789853	0.82162312
C	-1.07482893	0.68019941	4.13112844
H	-0.75132176	1.49655068	4.77089695
C	0.57114773	-4.13224232	2.06224904
H	0.09086676	-5.09957111	1.94035396
C	2.57684754	-2.34783973	-3.93192921
H	2.3741748	-2.12711472	-4.97627466
C	1.75998099	-2.53650438	3.43713891
H	2.20121416	-2.2556099	4.38953871
C	-6.18736942	-2.3339964	-0.44994279
H	-7.07732654	-2.93270366	-0.62393588
C	-5.28214662	-2.10583908	-1.48961834
H	-5.46439821	-2.52484136	-2.47521848
C	4.91678924	4.85637437	0.57198079
H	4.48116374	5.11529496	-0.40181885
H	5.83790918	5.42108473	0.72443917
H	4.20001966	5.09789094	1.36792655

Table S23. Cartesian coordinates of the optimized T_1 geometry for complex **5**.

Atom	x	y	z
Br	1.745093	1.811201	4.276363
Cu	-0.488972	2.038191	5.119222
P	-0.943842	1.355092	7.25365
P	-1.954505	2.933698	3.596374
O	0.876039	2.948192	11.910389
O	1.165042	5.418501	11.174191
C	-0.638108	4.860874	5.561715
C	-0.160125	3.996585	7.983692
C	-0.825146	5.39533	4.312649
C	0.350824	4.960485	8.94188
H	0.479637	5.979346	8.600569
C	-0.438843	6.757719	4.050135

H	-0.031782	7.34383	4.868125
C	-0.130682	-0.188963	7.815384
C	-0.337748	2.608637	8.435007
C	-2.704872	1.116802	7.719188
C	0.007634	2.273277	9.734799
H	-0.097245	1.243192	10.051581
C	-3.694255	3.18248	4.123227
C	0.508587	3.217011	10.640536
C	0.675131	4.595591	10.218507
C	-0.430762	4.401735	6.717041
C	-4.37774	2.07929	4.657413
H	-3.868888	1.124567	4.753392
C	-1.381057	4.623269	3.217398
C	-2.07951	2.121496	1.963477
C	-3.421243	2.104481	8.407321
H	-2.918744	3.012251	8.727602
C	-4.350494	4.417668	4.037323
H	-3.830355	5.279382	3.631087
C	-3.263078	2.102169	1.212012
H	-4.162441	2.567603	1.604395
C	1.076458	-0.543467	7.192009
H	1.46233	0.062005	6.374489
C	-0.551962	7.291931	2.783745
H	-0.238068	8.316549	2.603319
C	-1.470228	5.192897	1.95627
H	-1.869952	4.604215	1.135864
C	-0.634598	-0.98758	8.854896
H	-1.577408	-0.732029	9.329901
C	-6.353028	3.436462	4.984577
H	-7.382102	3.535118	5.319987
C	-3.373389	-0.046237	7.302423
H	-2.832139	-0.81639	6.758416
C	-5.702052	2.201826	5.073757
H	-6.216844	1.340142	5.486204
C	-3.288147	1.48034	-0.038986
H	-4.209253	1.466361	-0.615962
C	0.065562	-2.12091	9.273481
H	-0.334162	-2.736229	10.075681
C	-5.429534	0.754131	8.298522
H	-6.482152	0.61196	8.527999
C	-1.058238	6.515727	1.719562
H	-1.134647	6.936512	0.721669
C	-0.92062	1.509305	1.457173
H	-0.005611	1.513728	2.045993

C	1.273427	-2.465083	8.657638
H	1.816302	-3.349058	8.98201
C	0.777112	1.603584	12.375009
H	1.398615	0.933426	11.7695
H	-0.264204	1.259614	12.357099
H	1.142308	1.622465	13.402142
C	-5.673247	4.543716	4.471872
H	-6.171617	5.507379	4.404538
C	-4.722617	-0.232172	7.602539
H	-5.222561	-1.14541	7.289997
C	1.774169	-1.676148	7.618202
H	2.706313	-1.943699	7.128229
C	-4.778	1.925263	8.689793
H	-5.323034	2.701709	9.219863
C	-2.131834	0.880312	-0.545957
H	-2.152512	0.397121	-1.519363
C	-0.950674	0.896874	0.20323
H	-0.051109	0.426193	-0.184093
C	1.382211	6.781443	10.827982
H	2.108232	6.865807	10.00979
H	1.779964	7.254034	11.726676
H	0.44149	7.26628	10.537675

Table S24. Cartesian coordinates of the optimized S_0 geometry for complex **6**.

Atom	x	y	z
Cu	0.64111174	-0.4949141	-1.23934074
P	2.53008701	0.14899772	-0.09678354
P	-1.34496364	-0.93752769	-0.20376234
Cl	0.92386575	-0.79529679	-3.47338625
O	-6.074472	1.29821727	0.12626994
O	-5.1287593	3.71876367	0.00173035
C	2.98047357	1.84809944	-0.61865721
C	4.04159472	-0.82858899	-0.41487734
C	1.93510383	2.78630926	-0.79235342
C	-2.84853841	2.90983687	-0.18986184
H	-2.43553041	3.90505212	-0.26176732
C	-1.95710471	1.81474708	-0.24990512
C	0.58043165	2.41799842	-0.57973503
C	-2.4705703	0.51033858	-0.16163711
C	2.24847935	4.09865666	-1.18367845
H	1.4439537	4.81122838	-1.31613638
C	2.44547825	0.27374615	1.72964868
C	-4.21358583	2.72349638	-0.05709271

C	-0.57561799	2.09540246	-0.41498956
C	4.29641218	2.23717364	-0.86383067
H	5.09466121	1.51515944	-0.74792302
C	3.5661843	4.47025777	-1.41503372
H	3.79191419	5.48342123	-1.72607664
C	4.59210805	3.53934141	-1.25970472
H	5.62036849	3.82421467	-1.4485765
C	-2.35594933	-2.24233135	-1.00236246
C	-1.27552041	-1.46903687	1.55137438
C	5.06900099	-0.97188254	0.52373044
H	4.97786767	-0.51168086	1.50026033
C	-3.85453226	0.33006119	-0.03689784
H	-4.24576455	-0.67500649	0.00417626
C	2.61240704	1.47562733	2.42133072
H	2.83628657	2.38582314	1.87981981
C	-4.72989998	1.40390531	0.01432376
C	6.20567107	-1.71037908	0.20390315
H	6.99920712	-1.82146888	0.93415237
C	-0.79061603	-2.75035777	1.84615366
H	-0.50665054	-3.41869495	1.04060461
C	-2.18892084	-2.41945252	-2.38075471
H	-1.43668214	-1.84528705	-2.91319181
C	2.49648945	1.50689854	3.81060587
H	2.62536112	2.44533706	4.33792258
C	-3.29038687	-3.02290674	-0.31004633
H	-3.40469303	-2.91009217	0.76152732
C	4.15379112	-1.43572143	-1.67229213
H	3.34805549	-1.33620311	-2.39376913
C	-0.69497682	-3.18000992	3.16496506
H	-0.33419306	-4.17955269	3.37976952
C	2.22535255	0.3391325	4.51807522
H	2.14023752	0.36438389	5.59835154
C	-1.62295804	-0.61446267	2.59983118
H	-1.98710841	0.38242876	2.38494684
C	-4.06291934	-3.95764792	-0.9936141
H	-4.78183401	-4.56233328	-0.45220179
C	6.32203254	-2.30471724	-1.05224196
H	7.20758564	-2.87930942	-1.29903953
C	2.1534609	-0.89377256	2.44594361
H	2.00035693	-1.82732987	1.91758928
C	2.05783566	-0.8632722	3.83126093
H	1.83404001	-1.7735584	4.37243131
C	-2.96884368	-3.35390223	-3.0590708
H	-2.83095865	-3.4882834	-4.12553789

C	-3.90673076	-4.12006923	-2.37040536
H	-4.50694375	-4.85064046	-2.90075594
C	5.29712544	-2.16585142	-1.98699537
H	5.38092785	-2.63262807	-2.9615182
C	-6.63825961	-0.00827769	0.16456609
H	-6.39892607	-0.56962541	-0.74398529
H	-7.71414617	0.13823366	0.23234456
H	-6.28796332	-0.56462816	1.04021715
C	-1.05795388	-2.32678307	4.20736611
H	-0.98082492	-2.66076117	5.23564579
C	-4.66666299	5.06033819	-0.09401583
H	-4.16239942	5.2378711	-1.04939817
H	-3.98842736	5.30569985	0.72990483
H	-5.55658517	5.68301027	-0.03058092
C	-1.51053374	-1.04215034	3.92141497
H	-1.78025613	-0.36888381	4.72678761

Table S25. Cartesian coordinates of the optimized S_1 geometry for complex **6**.

Atom	x	y	z
Cu	0.63642291	0.06722993	-1.39112731
P	2.47187467	0.30708038	0.02283717
P	-1.23697041	-0.87014536	-0.362832
Cl	1.53328095	0.27868879	-3.39993768
O	-6.01604009	0.96885272	0.7100319
O	-5.26687507	3.44798843	0.43483115
C	2.9375245	2.03688329	-0.19635712
C	3.93144946	-0.73820172	-0.26963981
C	1.86699433	2.9798063	-0.423975
C	-2.96059945	2.83012262	0.00079268
H	-2.64264642	3.85894324	-0.11049985
C	-1.96501824	1.80896566	-0.13709122
C	0.53604328	2.57315913	-0.45742941
C	-2.39651475	0.44813847	-0.00531232
C	2.23855294	4.35069523	-0.5856044
H	1.45446323	5.07901032	-0.76972503
C	2.03492389	0.06426719	1.77487135
C	-4.27754372	2.52784069	0.28280778
C	-0.63772368	2.17320753	-0.3669979
C	4.26398764	2.46252132	-0.13619507
H	5.05288325	1.73283368	0.02168599
C	3.56212939	4.7451084	-0.52202916
H	3.80783579	5.79571142	-0.65702731
C	4.59619363	3.8105351	-0.2971967

H	5.63389405	4.12642828	-0.26828173
C	-2.07589218	-1.98441747	-1.55434458
C	-1.06504257	-1.91192468	1.12928574
C	4.89390747	-0.91928513	0.73951565
H	4.75308141	-0.4630062	1.7142533
C	-3.74716299	0.16256988	0.2855969
H	-4.05357563	-0.87391545	0.36197132
C	1.60127211	1.15412209	2.54511484
H	1.55429572	2.14351225	2.10455823
C	-4.68876183	1.16414335	0.43959495
C	6.03325428	-1.68450982	0.48960926
H	6.7751893	-1.81522341	1.27268399
C	-0.41483581	-3.15275353	1.02619616
H	-0.00559401	-3.47201776	0.07079862
C	-1.87830168	-1.77102737	-2.92746453
H	-1.18489415	-1.00668006	-3.26751044
C	1.24197266	0.96380417	3.8805751
H	0.9092101	1.81207117	4.47219813
C	-2.95548033	-2.99598213	-1.13615434
H	-3.10182462	-3.18658723	-0.07714429
C	4.12144499	-1.33527205	-1.52486357
H	3.38629702	-1.18897261	-2.30940703
C	-0.31954783	-3.9911128	2.13564757
H	0.17291923	-4.95551714	2.04319507
C	1.31983514	-0.30710041	4.45524485
H	1.04721196	-0.45106404	5.49726233
C	-1.58445279	-1.50688919	2.36376942
H	-2.07426941	-0.54213597	2.44831836
C	-3.6352954	-3.77058886	-2.07740815
H	-4.31324975	-4.5514971	-1.74276585
C	6.21937978	-2.27774988	-0.76305837
H	7.1063644	-2.87560443	-0.95437694
C	2.07841591	-1.21741239	2.34767983
H	2.39262665	-2.06962148	1.75365133
C	1.74047257	-1.39665175	3.68686756
H	1.78907928	-2.38841181	4.12457132
C	-2.5617047	-2.54608238	-3.86593243
H	-2.39740596	-2.37249753	-4.92573712
C	-3.44236482	-3.54608487	-3.44398546
H	-3.97026802	-4.15203997	-4.17527573
C	5.26396197	-2.10046824	-1.76724897
H	5.40415741	-2.55807919	-2.74248303
C	-6.46565591	-0.36910079	0.8170841
H	-6.29840727	-0.92316092	-0.11730006

H	-7.53643263	-0.309801	1.02009641
H	-5.96514318	-0.89494714	1.64296716
C	-0.86056835	-3.59163901	3.36284472
H	-0.79076451	-4.24667397	4.22722912
C	-4.93346247	4.81798321	0.26959205
H	-4.54697466	5.01281367	-0.73923482
H	-4.1912204	5.13812847	1.01268452
H	-5.86349384	5.36852431	0.41964769
C	-1.48178503	-2.34659457	3.47585001
H	-1.88963586	-2.02480154	4.43013496

Table S26. Cartesian coordinates of the optimized T_1 geometry for complex **6**.

Atom	x	y	z
Cu	11.053566	7.294756	2.694388
P	11.403178	9.416986	1.88875
P	9.684749	6.777384	4.460264
Cl	12.265713	5.633748	1.720877
O	5.40385	3.762103	4.849726
O	4.41292	4.529941	2.579072
C	10.689647	9.571992	0.214793
C	13.148486	9.922746	1.684187
C	9.420147	8.916953	-0.033138
C	6.285368	5.996534	2.135982
H	5.908975	6.318031	1.173623
C	7.562937	6.537603	2.566119
C	8.806732	8.132442	0.911182
C	8.0813	6.11889	3.879827
C	8.809046	9.093775	-1.324573
H	7.8533	8.6141	-1.51138
C	10.63581	10.812191	2.801478
C	5.597313	5.097569	2.900985
C	8.235793	7.379962	1.742864
C	11.291717	10.298704	-0.801867
H	12.249881	10.774911	-0.617441
C	9.436332	9.830097	-2.308249
H	8.964996	9.937737	-3.281488
C	10.687617	10.433175	-2.063817
H	11.183787	11.002968	-2.843471
C	10.29523	5.471819	5.592726
C	9.209706	8.152863	5.583541
C	13.572649	11.255374	1.792037
H	12.855202	12.035427	2.029511
C	7.360262	5.198672	4.62284

H	7.760443	4.868161	5.572697
C	9.744192	11.715328	2.208312
H	9.48912	11.614058	1.158332
C	6.141036	4.669931	4.178126
C	14.917733	11.579377	1.600392
H	15.241392	12.613395	1.687708
C	10.09142	8.560421	6.597641
H	11.029088	8.0313	6.745948
C	11.210685	4.545856	5.067296
H	11.568892	4.657476	4.045729
C	9.185868	12.752029	2.962413
H	8.492582	13.444994	2.492551
C	9.85692	5.336516	6.920626
H	9.163312	6.059082	7.340869
C	14.081242	8.914246	1.390794
H	13.755848	7.877762	1.32657
C	9.760095	9.624532	7.436747
H	10.443225	9.915792	8.230644
C	9.52433	12.902659	4.308562
H	9.094273	13.711922	4.892782
C	8.013459	8.858842	5.397335
H	7.327466	8.5645	4.608774
C	10.319662	4.281838	7.709644
H	9.979081	4.187252	8.737754
C	15.84337	10.576103	1.296962
H	16.889858	10.829695	1.148565
C	10.952055	10.955645	4.161452
H	11.622578	10.245239	4.63725
C	10.412439	12.002295	4.905667
H	10.668928	12.103159	5.95529
C	11.666495	3.489901	5.861053
H	12.376663	2.779636	5.446679
C	11.223112	3.354378	7.179324
H	11.585263	2.535452	7.795441
C	15.42297	9.246532	1.192141
H	16.140169	8.462518	0.964834
C	5.899817	3.270375	6.093498
H	6.872689	2.78262	5.961583
H	5.162179	2.543432	6.434243
H	5.988773	4.081372	6.826334
C	8.558791	10.315779	7.253875
H	8.303565	11.148871	7.903186
C	3.827196	4.879073	1.330008
H	4.486271	4.600619	0.498343

H	3.611678	5.954137	1.285969
H	2.897336	4.312402	1.271942
C	7.693912	9.937461	6.22501
H	6.765722	10.479484	6.065457

Table S27. Cartesian coordinates of the optimized S_0 geometry for complex 7.

Atom	x	y	z
Cu	0.08324416	-0.63702659	-0.93743403
P	1.91203521	-0.80518393	0.46128496
P	-2.06849958	-0.77841056	-0.17463957
O	4.86872187	4.37381815	-0.12780458
O	6.22987765	2.16079039	-0.02693827
O	-4.57358869	4.55427075	0.96023964
C	4.14199608	3.2392998	0.01812662
C	2.75947099	3.19175214	0.10337291
H	2.17392143	4.09744563	0.046589
C	2.82275265	0.77286465	0.30447507
C	-3.93313498	3.38830011	0.7089187
C	4.88556494	2.03362107	0.07371784
C	-4.18410512	1.03796082	0.19513772
H	-4.81385309	0.18483394	-0.0077465
C	-3.30101469	-1.54697607	-1.29613077
C	2.08078512	1.96389979	0.23655326
C	-2.79240579	0.87072754	0.1639722
C	-0.54682898	1.91553744	0.34864563
C	-1.96362971	1.98096695	0.39507059
C	1.94336068	0.03949271	3.17675321
H	2.42009454	0.94804542	2.8316232
C	0.66391539	1.94720947	0.30018118
C	-2.55821258	3.23293147	0.67230363
H	-1.90673172	4.07658196	0.84558809
C	1.62017279	-0.96726119	2.26424007
C	4.0035707	-2.62189611	1.09928098
H	3.86959038	-2.32864211	2.13337091
C	-4.76630677	2.26741809	0.45947548
C	3.18597175	-2.07129252	0.10617553
C	4.16897425	5.60455006	-0.25053373
H	4.93452683	6.36695408	-0.37977334
H	3.58581426	5.82207181	0.65086543
H	3.50696703	5.5981358	-1.1225569
C	1.65674427	-0.12389868	4.53146262
H	1.90979315	0.66429332	5.23156224
C	4.21676334	0.82511615	0.21968237

H	4.77650461	-0.09736879	0.25692743
C	-4.4249736	-2.24486203	-0.83787321
H	-4.57129609	-2.40121889	0.22398587
C	1.05586908	-1.29500227	4.98499484
H	0.83780561	-1.42223603	6.03912846
C	4.98666345	-3.54865087	0.75993411
H	5.61514831	-3.97452455	1.53393052
C	-5.35223962	-2.75021555	-1.74571007
H	-6.21848335	-3.29306018	-1.38443834
C	-3.78573944	5.71552863	1.18857752
H	-3.16535488	5.95048005	0.31758218
H	-3.14834995	5.59517743	2.07086426
H	-4.49467388	6.5230482	1.35930252
C	-5.16426527	-2.56275212	-3.11478671
H	-5.88547306	-2.95948079	-3.82021744
C	-2.31321025	-1.6888098	1.39998496
C	3.35741926	-2.46008636	-1.22811518
H	2.7231957	-2.03494356	-1.99912726
C	0.9975928	-2.13420972	2.72405677
H	0.72217663	-2.91204824	2.0218701
C	-3.10922646	-1.37181024	-2.67120819
H	-2.22445091	-0.85877576	-3.03266386
C	7.0118806	0.97176717	-0.03612559
H	8.0427101	1.29953532	-0.15344351
H	6.73402466	0.32228528	-0.87207398
H	6.90731004	0.42048622	0.90411755
C	-4.04185021	-1.87631057	-3.5740099
H	-3.88181619	-1.73969602	-4.63711052
C	-6.97083216	1.40990314	0.21049877
H	-6.79273571	1.01367243	-0.79417133
H	-7.97851524	1.81561418	0.27122238
H	-6.85436787	0.6061659	0.94509555
C	-2.12413529	-3.0774204	1.40235332
H	-1.86879566	-3.588746	0.48043103
C	0.73006941	-2.30224929	4.07680175
H	0.25116124	-3.21072387	4.41892859
C	-2.28494395	-3.80757999	2.57435272
H	-2.15228438	-4.88348211	2.56032758
C	5.16141311	-3.92715136	-0.57062938
H	5.92674397	-4.64880419	-0.83279616
C	4.3465805	-3.38158449	-1.56168372
H	4.47477818	-3.67597825	-2.59685551
C	-2.62382204	-1.04174016	2.59760132
H	-2.75868766	0.03249766	2.6102786

C	-2.61140753	-3.15695256	3.76468441
H	-2.73447924	-3.72562911	4.67921115
C	-2.76828824	-1.77421922	3.77463233
H	-3.00605056	-1.26065558	4.69897333
I	0.6890112	-0.24244243	-3.40989896
O	-6.10030172	2.4986623	0.49656291

Table S28. Cartesian coordinates of the optimized S_1 geometry for complex **7**.

Atom	x	y	z
Cu	0.08298537	-0.35535743	-0.99704346
P	1.86548534	-0.74165597	0.43387915
P	-2.0663692	-0.70390783	-0.20626707
O	5.04177924	4.30229394	0.05584848
O	6.32927238	2.06487647	0.41362326
O	-4.52234845	4.61977734	0.88542175
C	4.25899683	3.19081316	0.13240407
C	2.88092383	3.1941861	0.01674066
H	2.34273472	4.11872571	-0.14957508
C	2.84440296	0.76591239	0.31530938
C	-3.87397329	3.44097874	0.67326556
C	4.96429479	1.96554458	0.33762771
C	-4.13606556	1.03888325	0.47421269
H	-4.7631836	0.15514484	0.44614365
C	-3.25630338	-1.40437466	-1.41862645
C	2.12045485	1.98557295	0.10204293
C	-2.7512125	0.88739547	0.24635089
C	-0.51526589	1.97913259	0.06784902
C	-1.8960791	2.04306455	0.24409716
C	1.16474473	0.25925051	2.96308741
H	1.42060311	1.23106855	2.55622722
C	0.72812677	2.00292958	0.0061665
C	-2.51873349	3.31979794	0.45008432
H	-1.8819188	4.19540607	0.43876278
C	1.30730864	-0.8891894	2.17168985
C	3.88083713	-2.54824591	1.21769108
H	3.86832443	-2.03319164	2.17345954
C	-4.71154261	2.27668083	0.69478401
C	2.9944114	-2.15503133	0.19967404
C	4.40577022	5.550354	-0.16723135
H	5.20772018	6.28989677	-0.19772261
H	3.71086792	5.79401329	0.64757395
H	3.86320935	5.55503346	-1.12180669
C	0.69753158	0.15018248	4.27466685

H	0.58823244	1.04539113	4.88081189
C	4.24404632	0.7821665	0.42735124
H	4.76830367	-0.15409998	0.57141313
C	-4.29867964	-2.26710998	-1.04869283
H	-4.38740562	-2.60339943	-0.02050897
C	0.37930678	-1.10171265	4.80618225
H	0.02143956	-1.18504901	5.82896879
C	4.77139055	-3.60120751	1.00652914
H	5.45527709	-3.89487474	1.79845205
C	-5.22661666	-2.70133799	-1.99944386
H	-6.02921163	-3.37036667	-1.69964047
C	-3.75574499	5.81245126	0.86025329
H	-3.27333235	5.95415778	-0.11604847
H	-2.98934606	5.80915448	1.64698106
H	-4.46307939	6.62357409	1.04128834
C	-5.12459707	-2.27863274	-3.32670878
H	-5.84528999	-2.61884887	-4.06533513
C	-2.22041831	-1.84260395	1.22041262
C	3.00419252	-2.84401551	-1.02117612
H	2.31319624	-2.5586649	-1.80742563
C	0.96015552	-2.14146134	2.70095545
H	1.0493479	-3.03488945	2.09082429
C	-3.15949699	-0.98570168	-2.75474043
H	-2.35723069	-0.31674347	-3.0510863
C	7.05635758	0.86783919	0.61410547
H	8.10826093	1.15804626	0.64509884
H	6.89618563	0.15726525	-0.20912865
H	6.78157298	0.3859786	1.56347943
C	-4.08791471	-1.41670088	-3.70144051
H	-3.9996643	-1.08458287	-4.7323252
C	-6.90433803	1.38111211	0.89016859
H	-6.87530001	0.87420685	-0.0847479
H	-7.90895447	1.76793192	1.07120637
H	-6.64234385	0.65987636	1.67792541
C	-1.87037064	-3.19219196	1.05223567
H	-1.49130692	-3.53654504	0.09270751
C	0.5142426	-2.24747597	4.01709587
H	0.2571668	-3.22211421	4.41976965
C	-2.03049887	-4.09804281	2.09962375
H	-1.76999057	-5.14339433	1.9552483
C	4.78278316	-4.27671285	-0.21838693
H	5.47532042	-5.09830921	-0.3798869
C	3.89712496	-3.89765323	-1.23035715
H	3.89543058	-4.4234589	-2.18107382

C	-2.69143659	-1.40492062	2.46269694
H	-2.94401461	-0.35821823	2.59983865
C	-2.52368424	-3.65959028	3.33352544
H	-2.64945161	-4.36465852	4.15102344
C	-2.84040617	-2.31228975	3.51529224
H	-3.20509258	-1.96272022	4.47735829
I	0.99708907	-0.27405612	-3.39334521
O	-6.04498635	2.50490029	0.91322126

Table S29. Cartesian coordinates of the optimized T_1 geometry for complex **7**.

Atom	x	y	z
Cu	1.442113	5.730727	11.200388
P	3.019986	5.407578	9.54859
P	1.778699	6.879882	13.15527
O	0.889314	8.018955	4.576749
O	2.021294	5.692582	4.39219
O	-0.62859	12.38532	12.793801
C	1.318898	7.501467	5.752857
C	1.182237	8.096176	6.979077
H	0.683191	9.050539	7.086083
C	2.347414	6.163889	8.042173
C	-0.0663	11.150474	12.769782
C	1.955106	6.205558	5.641131
C	0.75045	9.300112	14.146991
H	0.909933	8.855753	15.121315
C	0.969755	6.217003	14.663983
C	1.64457	7.441451	8.18476
C	1.08984	8.564381	13.013837
C	1.158763	8.485894	10.536337
C	0.854447	9.133766	11.70286
C	5.142797	7.177366	8.85555
H	4.568714	7.429415	7.96949
C	1.404456	7.990543	9.40456
C	0.260006	10.449084	11.635235
H	0.0763	10.86324	10.652304
C	4.642946	6.236977	9.766019
C	4.722971	3.369198	8.533295
H	5.504037	4.121895	8.483482
C	0.182176	10.572966	14.063501
C	3.453718	3.708744	9.024687
C	0.219946	9.272603	4.608951
H	-0.042791	9.493643	3.573697
H	0.877561	10.059186	5.001195

H	-0.689929	9.215226	5.219628
C	6.379159	7.788775	9.083243
H	6.755927	8.520738	8.373379
C	2.462257	5.583315	6.789279
H	2.964709	4.627966	6.701663
C	1.461428	6.445654	15.959338
H	2.390826	6.989216	16.101096
C	7.130037	7.45584	10.213008
H	8.093068	7.928607	10.387004
C	4.985082	2.063347	8.110334
H	5.972069	1.806576	7.734052
C	0.765874	5.965488	17.071078
H	1.156995	6.144082	18.069614
C	-0.92837	13.0013	11.548895
H	-1.641452	12.397913	10.972669
H	-0.017247	13.158039	10.956818
H	-1.376206	13.96465	11.796456
C	-0.426021	5.254328	16.899328
H	-0.965022	4.878646	17.765151
C	3.515272	7.148143	13.6939
C	2.450337	2.728205	9.093894
H	1.466624	2.988237	9.477757
C	5.392869	5.923447	10.909663
H	5.002189	5.215338	11.634606
C	-0.221908	5.494743	14.49619
H	-0.600012	5.297611	13.496234
C	2.580037	4.392101	4.227144
H	2.491683	4.168925	3.163382
H	2.023762	3.650019	4.812183
H	3.636518	4.377484	4.522129
C	-0.915803	5.020094	15.611361
H	-1.835487	4.459492	15.46823
C	0.003114	10.786602	16.42956
H	-0.565509	9.857219	16.557443
H	-0.369142	11.545487	17.11878
H	1.065988	10.597118	16.626818
C	4.236796	6.070932	14.234734
H	3.751962	5.106316	14.364544
C	6.635058	6.517479	11.124413
H	7.204613	6.263631	12.012396
C	5.563758	6.235635	14.630699
H	6.104273	5.398314	15.064714
C	3.981853	1.091587	8.171959
H	4.187513	0.076036	7.843632

C	2.715776	1.427064	8.663175
H	1.933502	0.674891	8.718945
C	4.158991	8.37963	13.520311
H	3.615093	9.216627	13.093263
C	6.195976	7.473216	14.46809
H	7.230754	7.601773	14.774318
C	5.49398	8.538787	13.901958
H	5.982323	9.49894	13.758497
I	-0.83528	4.659839	10.597415
O	-0.186013	11.327366	15.12659