Structure and emission properties of dinuclear Copper(I) complexes on pyridyltriazole basis

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Table S1. Crystal data and structure refinements for the complexes 1–5

Parameter	**1**	**2**	**3**	**4**	**5**
Formula	$C_{63}H_{60}Cu_2I_2N_{10}O_3P_2$	$C_{62}H_{50}Cl_6Cu_2I_2N_{10}P_2$	$C_{30}H_{24}CuIN_5P$	$C_{64}H_{58}Cu_2I_2N_8O_2P_2$	$C_{62}H_{50}Cu_2I_2N_8P_2$
Temperature, K	150	150	100	150	100
Crystal system	triclinic	monoclinic	triclinic	monoclinic	triclinic
Space group	$P\bar{1}$	$C2/c$	$P\bar{1}$	$P2_1/n$	$P\bar{1}$
a, Å b, Å c, Å α, deg. β, deg. γ, deg. V, Å^3	11.3677(6) 12.0415(6) 13.6045(7) 65.426(2) 78.953(2) 64.641(2) 1530.17(14)	27.091(4) 8.3928(14) 28.914(5) 90 104.454(5) 90 6365.9(18)	8.71370(10) 12.3406(2) 13.8265(2) 105.3280(10) 101.0740(10) 104.3550(10) 1335.29(3)	9.3493(4) 15.3341(7) 20.8594(10) 90 100.620(2) 90 2939.2(2)	10.8722(10) 12.3493(10) 12.7434(10) 109.563(3) 111.852(3) 100.786(2) 1398.1(2)
Z	1	4	2	4	1
μ_{Mo}. mm^{-1}	1.810	1.989	11.028	1.880	1.970
D_{calc}, g cm^{-3}	1.571	1.660	1.681	1.598	1.603
θ_{max}, deg	27.88	26.37	77.15	28.28	26.00
Parameters	373	382	343	366	348
No. unique	7227	6517	5566	7309	5428
No. I > 2σ(I)	5502	4294	5445	6299	5026
R_{int}	0.0752	0.1259	0.0627	0.2667	0.0319
GOF	1.004	1.042	1.108	1.021	1.036
R_1(I > 2σ(I))	0.0475	0.0878	0.0320	0.0664	0.0382
wR_2 (I > 2σ(I))	0.0837	0.1960	0.0877	0.1616	0.1051

Table S2. Selected bond lengths and angles of complexes **1-5**

1	2	3	4	5
Bond's length (Å)				
Cu1…Cu1 2.8926(10) Cu1-N1 2.050(3) Cu1-P1 2.2362(12) Cu1-I1 2.6694(6)	Cu1…Cu1 2.827(2) Cu1-N1 2.069(8) Cu1-P1 2.249(3) Cu1-I1 2.6344(13)	Cu1…Cu1 3.037(9) Cu1-I1 2.6624(4) Cu1-Cu1 3.0374(8) Cu1-P1 2.2342(7)	Cu1…Cu1 2.9904(9) Cu1-I1 2.6750(5) Cu1-I1 2.6603(5) Cu1-P1 2.2292(10)	Cu1…Cu1 2.8627(8) Cu1-I1 2.6900(4) Cu1-I1 2.6546(5) Cu1-P1 2.2316(9)

Cu1-I1 2.6787(6)	Cu1-I1 2.7239(14)	Cu1-N8 2.067(2)	Cu1-N1 2.048(3)	Cu1-N1 2.050(3)
Angles (deg.)				
Cu1-I1-Cu1A 65.48(2) I1-Cu1-I1A 114.52(2) P1-Cu1-I1 107.54(3) P1-Cu1-I1A 114.87(3) N1-Cu1-I1 104.86(9) N1-Cu1-I1A 102.72(9) N1-Cu1-P1 111.88(10)	Cu1-I1-Cu1A 63.66(4) I1-Cu1-I1A 116.34(4) P1-Cu1-I1A 104.30(8) P1-Cu1-I1 113.10(8) N1-Cu1-I1 105.4(2) N1-Cu1-I1A 102.8(2) N1-Cu1-P1 114.8(2)	Cu1-I1-Cu1A 69.915(14) I1-Cu1-I1A 110.085(14) P1-Cu1-I1 110.53(2) P1-Cu1-I1A 114.75(2) N8-Cu1-I1A 104.24(6) N8-Cu1-I1 105.57(7) N8-Cu1-P1 111.12(7)	Cu1-I1-Cu1A 68.178(16) I1-Cu1-I1A 111.822(16) P1-Cu1-I1 104.45(3) P1-Cu1-I1A 107.07(3) N1-Cu1-I1 106.19(9) N1-Cu1-I1A 104.27(9) N1-Cu1-P1 123.07(10)	Cu1-I1-Cu1A 64.770(14) I1-Cu1-I1A 115.231(14) P1-Cu1-I1 110.21(2) P1-Cu1-I1A 107.95(3) N1-Cu1-I1A 102.01(7) N1-Cu1-I1 108.82(8) N1-Cu1-P1 112.46(8)

Table S3. D-H…A interactions in crystals **1-5**.

Interaction	D-H, Å	H…A, Å	D…A, Å	D-H-A, deg.
1				
O1S-H...N5 (1+*x*, *y*, *z*)	0.84	1.96	2.800(6)	177
N2-H...O1S	0.88	1.88	2.748(5)	168
O2S-H...I1	0.84	2.81	3.620(14)	162
2				
N4-H...N5 (*x*, 1+*y*, *z*)	0.94(10)	1.88(10)	2.817(11)	175(10)
C00V-H…I1 (*x*, 1+*y*, *z*)	0.93	3.156	3.876	135.72
3				
N5-H...N6 (1+*x*, *y*, *z*)	0.86	2.15	3.005(4)	173
C012-H...I1 (1-*x*, -*y*, 1-*z*)	0.93	3.02	3.927(3)	167
4				
O1S-H...N4 (2-*x*, 2-*y*, 1-*z*)	0.80(6)	2.04(6)	2.801(5)	158(6)
N3-H...O1S	0.88	1.84	2.710(4)	168
5				
N9-H...I1 (1-*x*, 1-*y*, -*z*)	0.80(4)	2.85(4)	3.598(4)	157(4)

Table S4. Selected parameters of π-π intermolecular interactions in **1**, **4** and **5** (the analysis was done using PLATON software [A.L. Spek, Acta Cryst. 2009, D65, 148-155]).

Aromatic fragment I	Aromatic fragment J [symmetry index]	C_g-C_g, Å[a]	α, deg. [a]	C_g(I)_Perp, Å[a]	C_g(J)_Perp, Å[a]	Slippage
1						
C25-C30 (phenyl ring)	C25-C30 (phenyl ring) (2-*x*, 1-*y*, 1-*z*)	3.641(3)	0	3.392(2)	3.393(2)	1.323
4						
N2-C00J (triazole ring)	C00L-C00Q (phenyl ring) (1-*x*, 2-*y*, 1-*z*)	3.800(2)	4.7(2)	3.3989(16)	3.5093(17)	1.457
5						
N8-C7 (triazole ring)	C12-C17 (phenyl ring) (2-*x*, 1-*y*, -*z*)	3.695(2)	3.5(2)	3.4030(15)	3.4384(16)	1.353

[a] C_g-C_g = distance between ring centroids (Å); α = dihedral angle between planes I and J (deg.); β = angle C_g(I)->C_g(J) or C_g(I)->Me vector and normal to plane I (deg.); γ = angle C_g(I)->C_g(J) vector and normal to plane J (deg.); C_g(I)_Perp = Perpendicular distance of Cg(I) on ring J (Å); C_g(J)_Perp = Perpendicular distance of Cg(J) on ring I (Å).

Table S5. C-X…π interactions in the crystal **1-5** (Cg is centroid of aromatic 5,6-membered ring; X-Perp is perpendicular distance of X on ring; γ is angle X->Cg vector and normal to ring plane).

Interaction	X…Cg, Å	X-Perp, Å	γ, deg.	C-X…Cg, deg.	C…Cg, Å
1					
C17-H…pyridyl ring (N5-C11) (1-*x*, 1-*y*, 1-*z*)	2.72	2.68	9.36	143	3.522(6)
C23-H…phenyl ring (C25-C30) (1-*x*, 1-*y*, 1-*z*)	2.94	-2.87	12.70	157	3.836(7)
2					
C1S-Cl1…triazol ring (N2-C7)	3.649(7)	3.237	27.49	122.5(6)	4.777(17)
C1S-Cl3…pyridyl ring (N5-C10) (*x*, 1+*y*, *z*)	3.628(7)	3.516	14.31	120.4(6)	4.791(17)
3					
C00M-H…phenyl ring (C00F-C00N) (1+*x*, *y*, *z*)	2.61	-2.61	4.38	146	3.426(4)
C00O-H…pyridyl ring	2.59	2.58	4.22	159	3.473(4)

(N6-C00I) (2-*x*, 1-*y*, 1-*z*)					
4					
C00O-H…phenyl ring (C00C-C00N) (3/2-*x*, -1/2+*y*, 1/2-*z*)	2.87	-2.87	2.67	139	3.647(5)
5					
C16-H…phenyl ring (C24-C29) (2-*x*, 1-*y*, 1-*z*)	2.99	-2.74	23.69	150	3.845(5)
C20-H…triazole ring (N8-C7) (1-*x*, 1-*y*, -*z*)	2.95	-2.74	21.36	137	3.695(4)
C21-H…phenyl ring (C24-C29) (1-*x*, 2-*y*, 1-*z*)	2.67	2.58	14.43	153	3.540(5)
C32-H…phenyl ring (C18-C23) (2-*x*, 2-*y*, 1-*z*)	2.90	2.70	21.43	152	3.763(5)

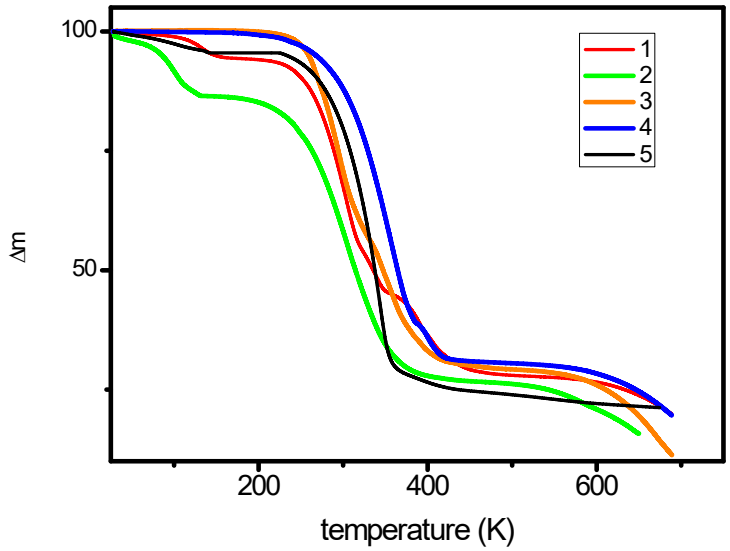
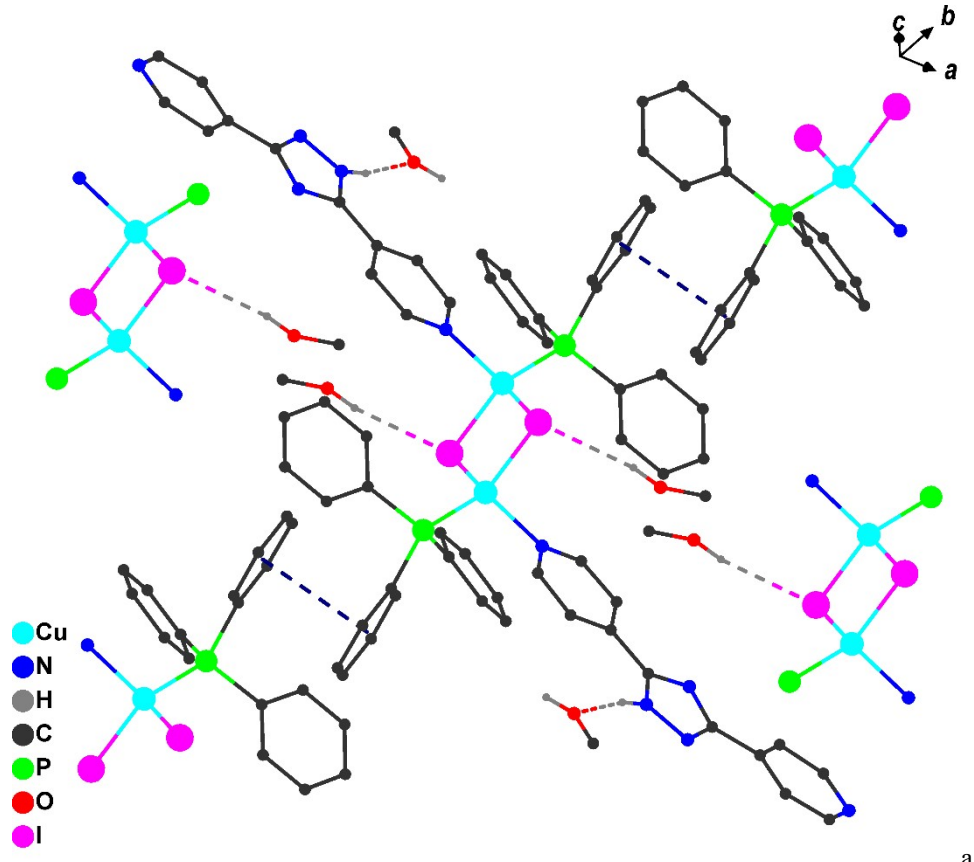


Figure S1. TG curve of 1-5.



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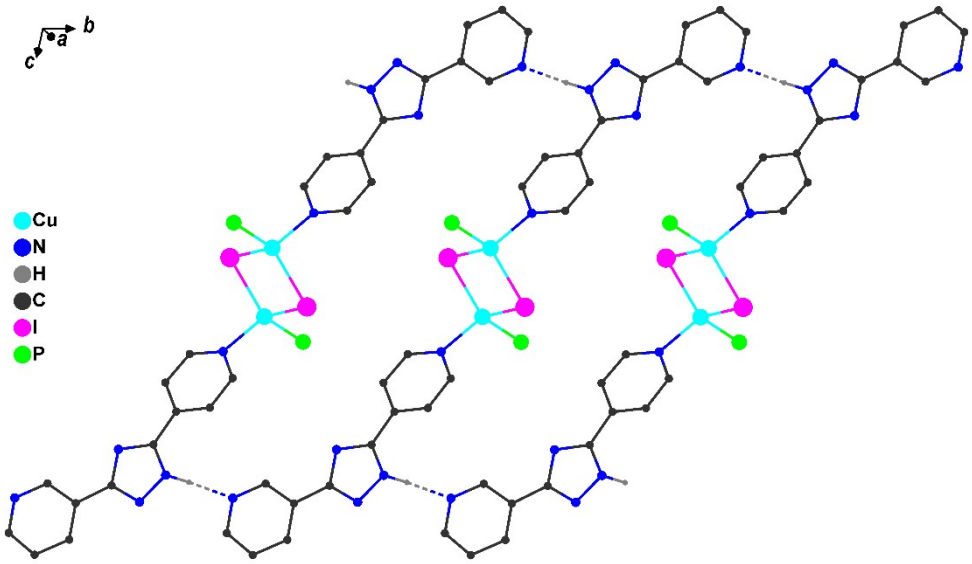

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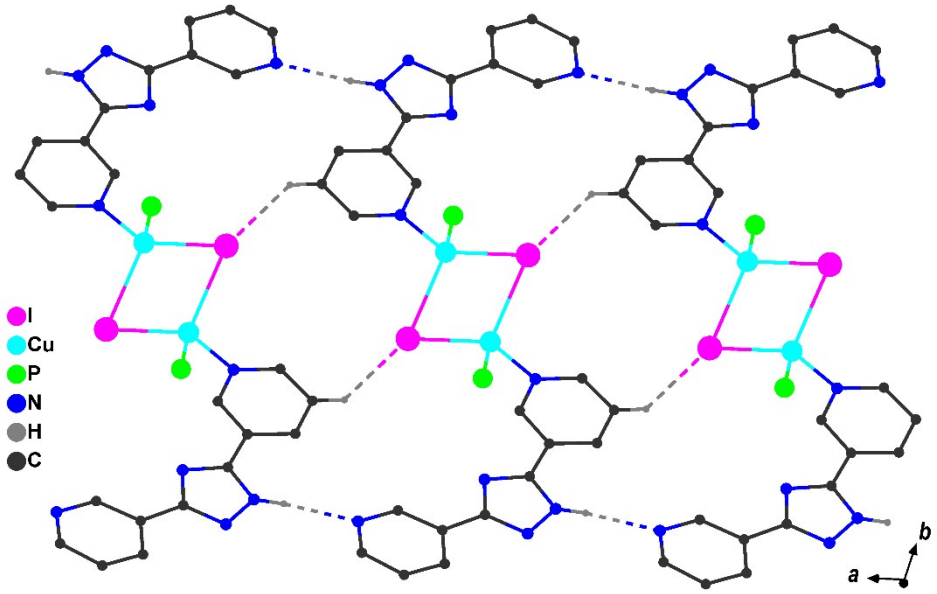

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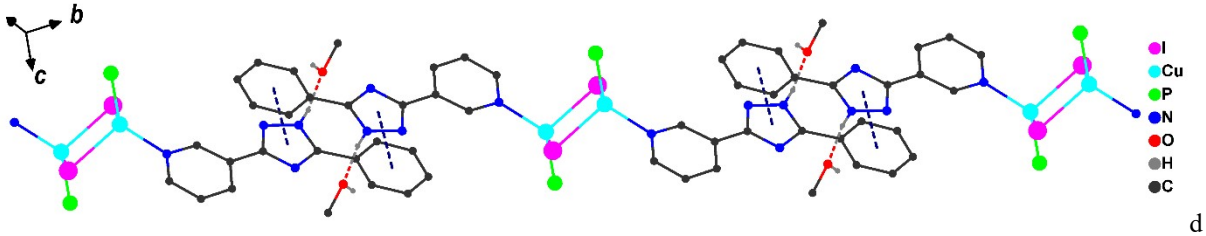


d

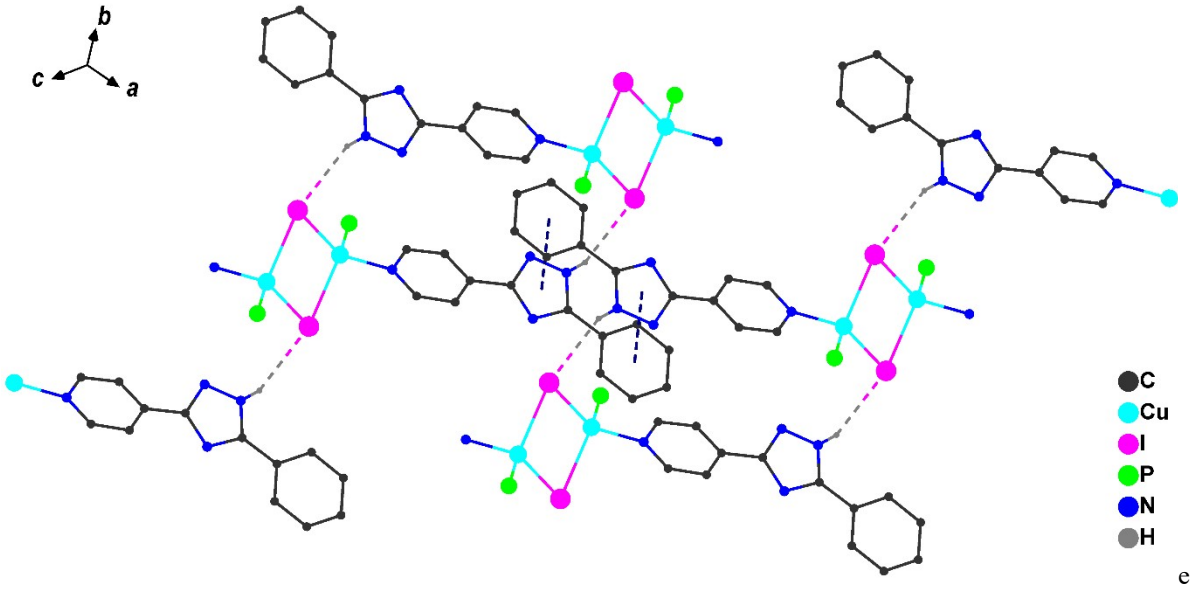


Figure S2. Fragments of crystal packing for **1** (a), **2** (b), **3** (c), **4** (d), and **5** (e) (H atoms at carbon atoms are omitted; Ph rings are omitted (b-e); π···π stacking interactions and H-bond are indicated by dash lines).

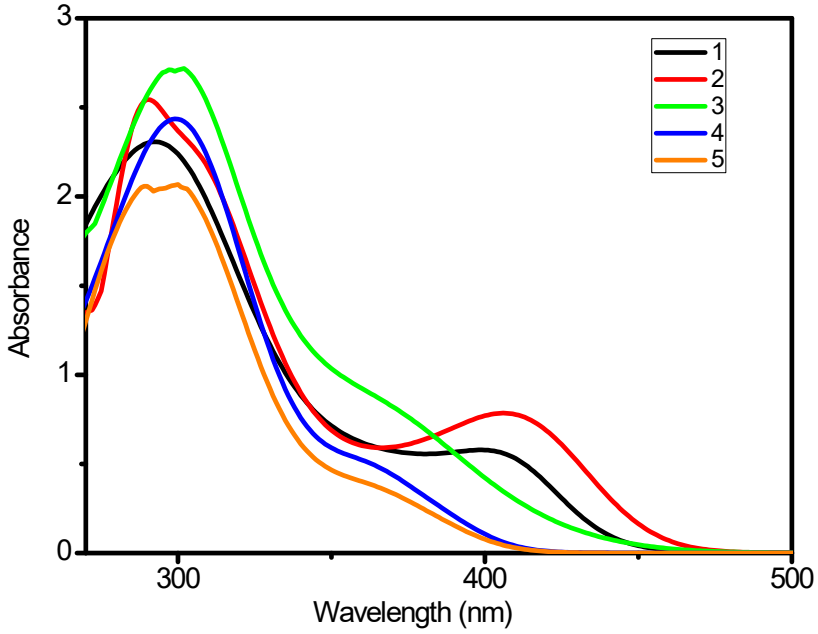


Figure S3. Absorption spectra of 1-5 in THF solution.

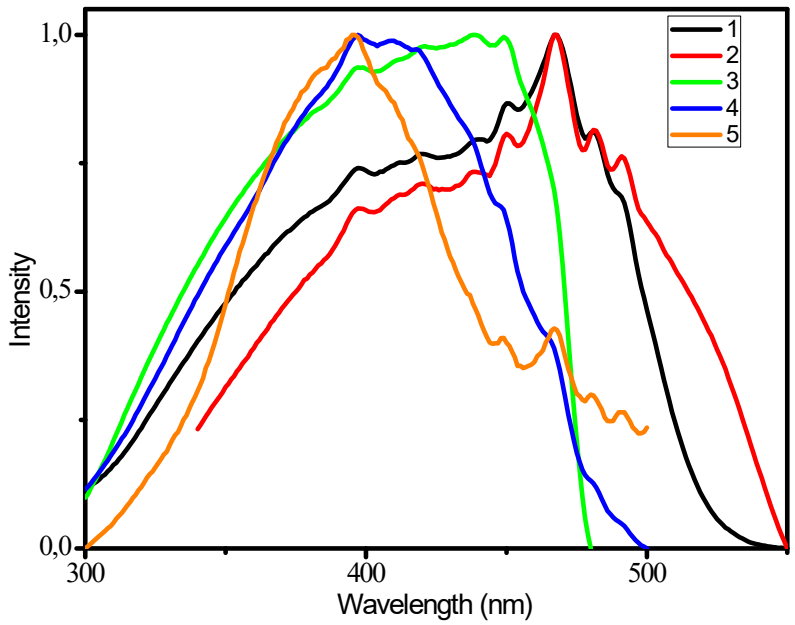


Figure S4. Excitation spectra of solid state samples of 1-5

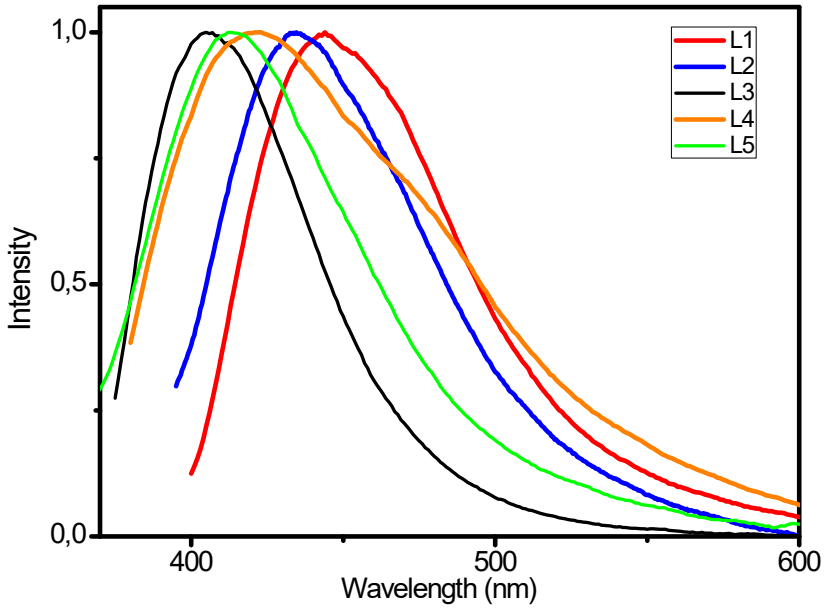


Figure S5. Normalized luminescent spectra of solid L1-L5

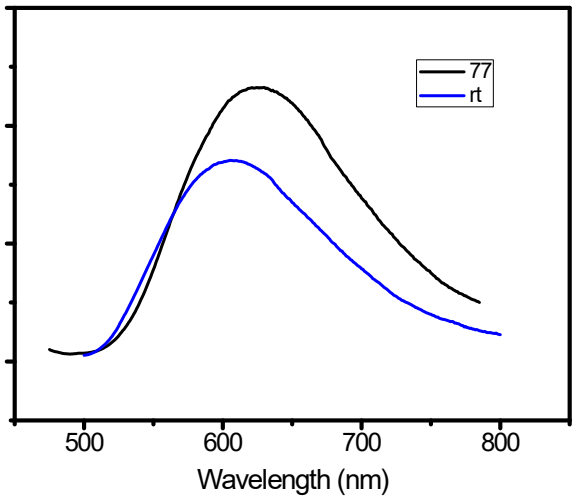


Figure S6. PL spectra of 1 at RT and 77 K.

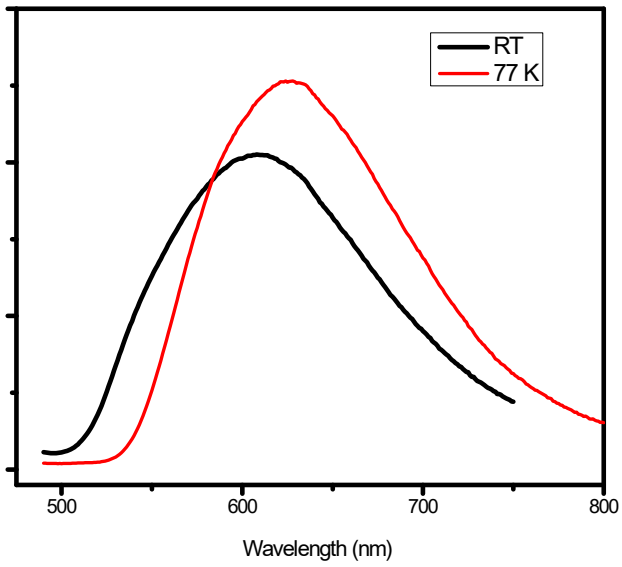


Figure S7. PL spectra of 2 at RT and 77 K.

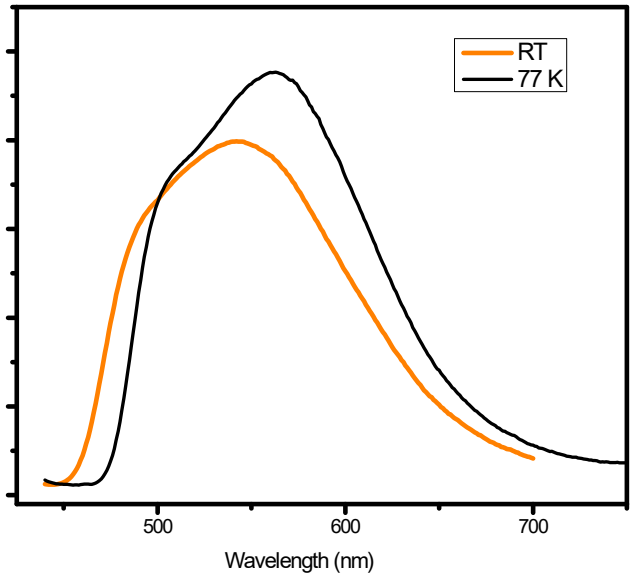


Figure S8. PL spectra of 3 at RT and 77 K.

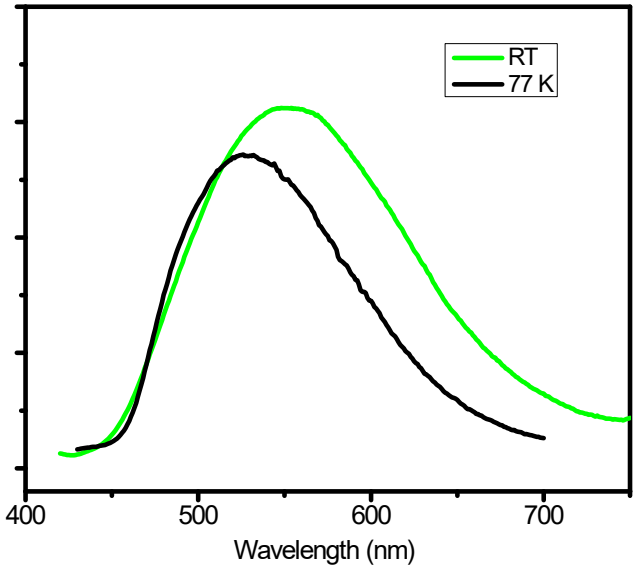


Figure S9. PL spectra of 4 at RT and 77 K.

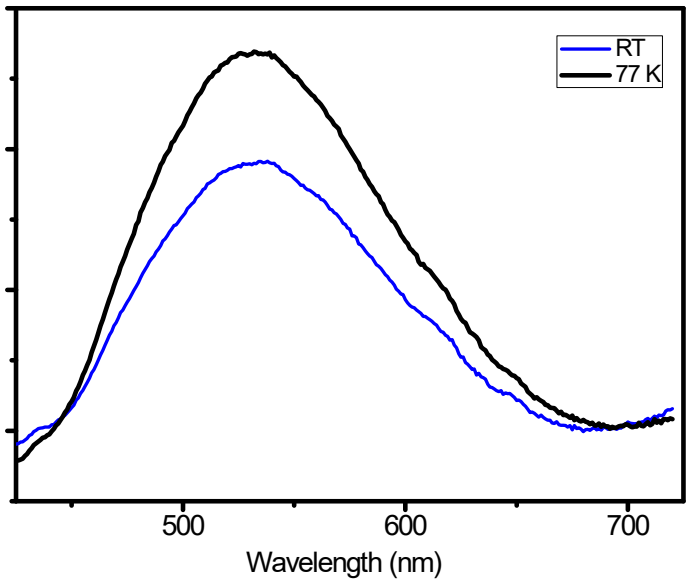


Figure S10. PL spectra of 5 at RT and 77 K.

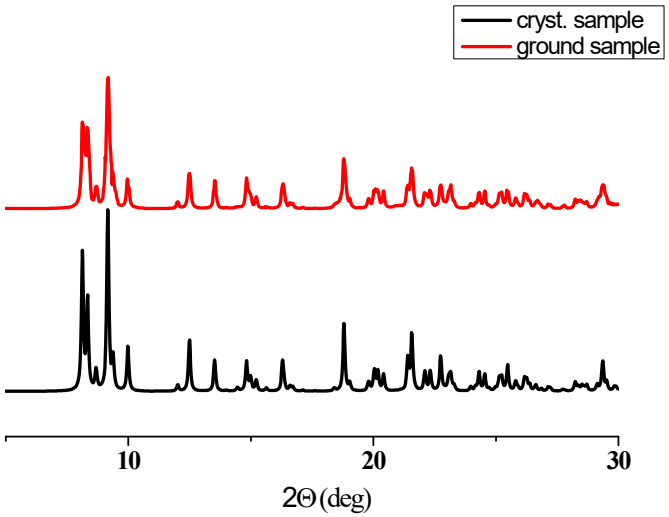
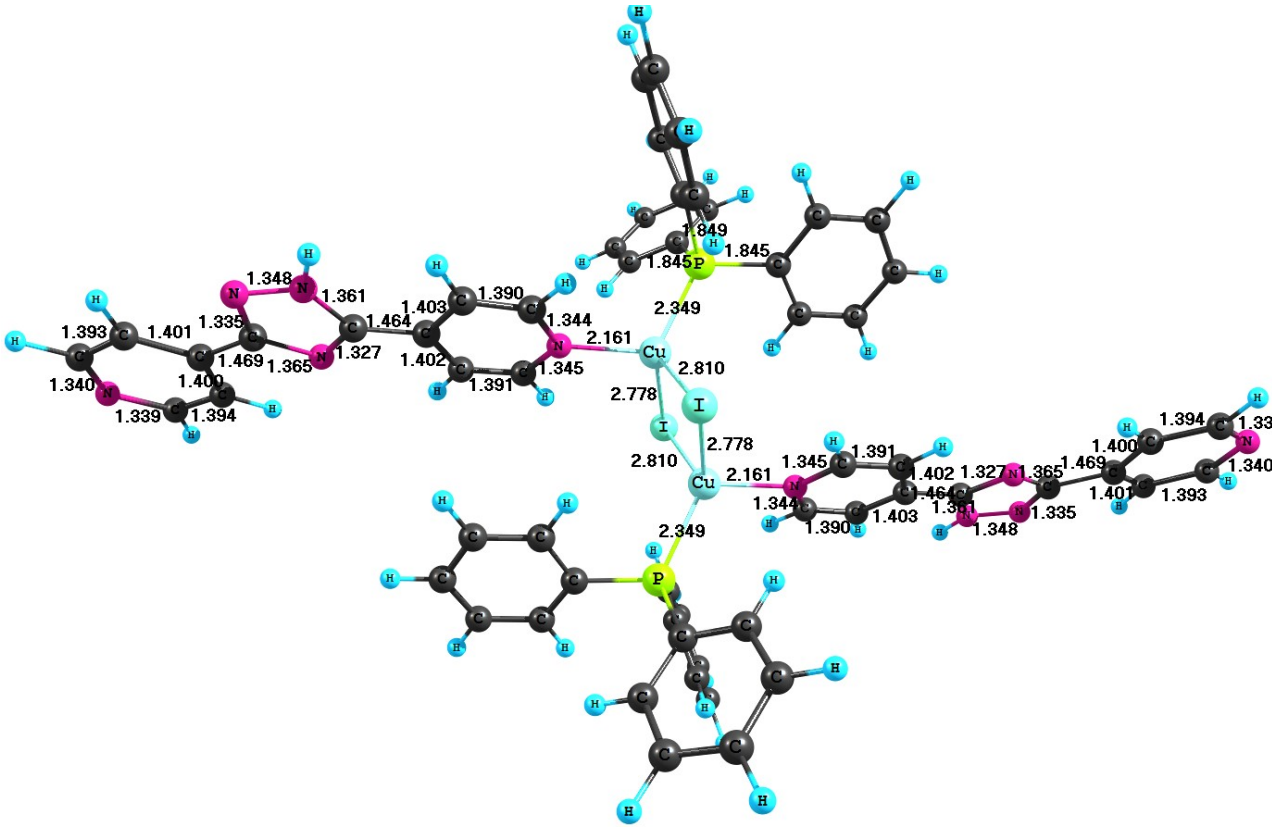
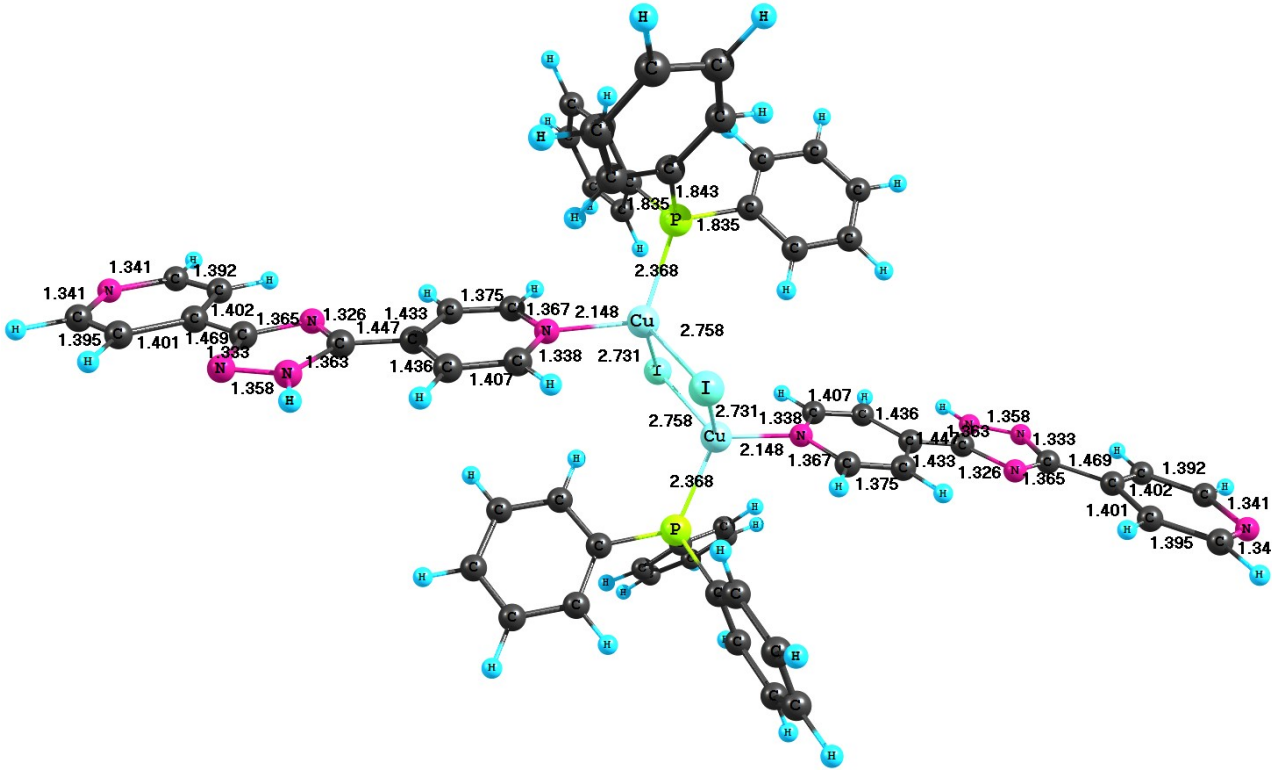


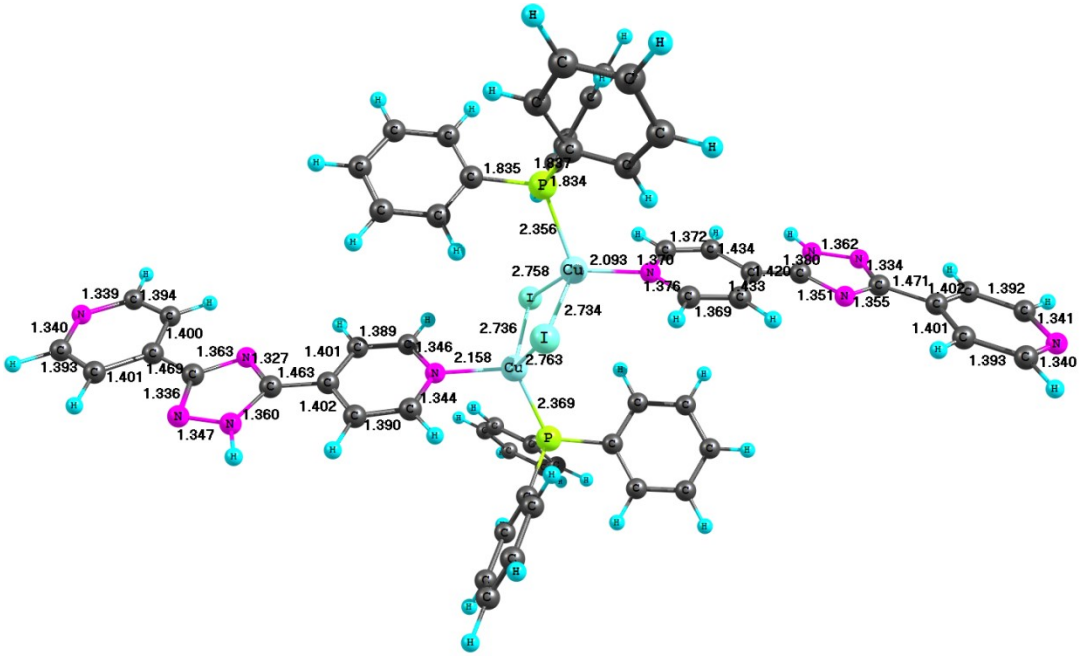
Figure S11. Powder XRD patterns of crystalline and ground samples of 4.



S_0

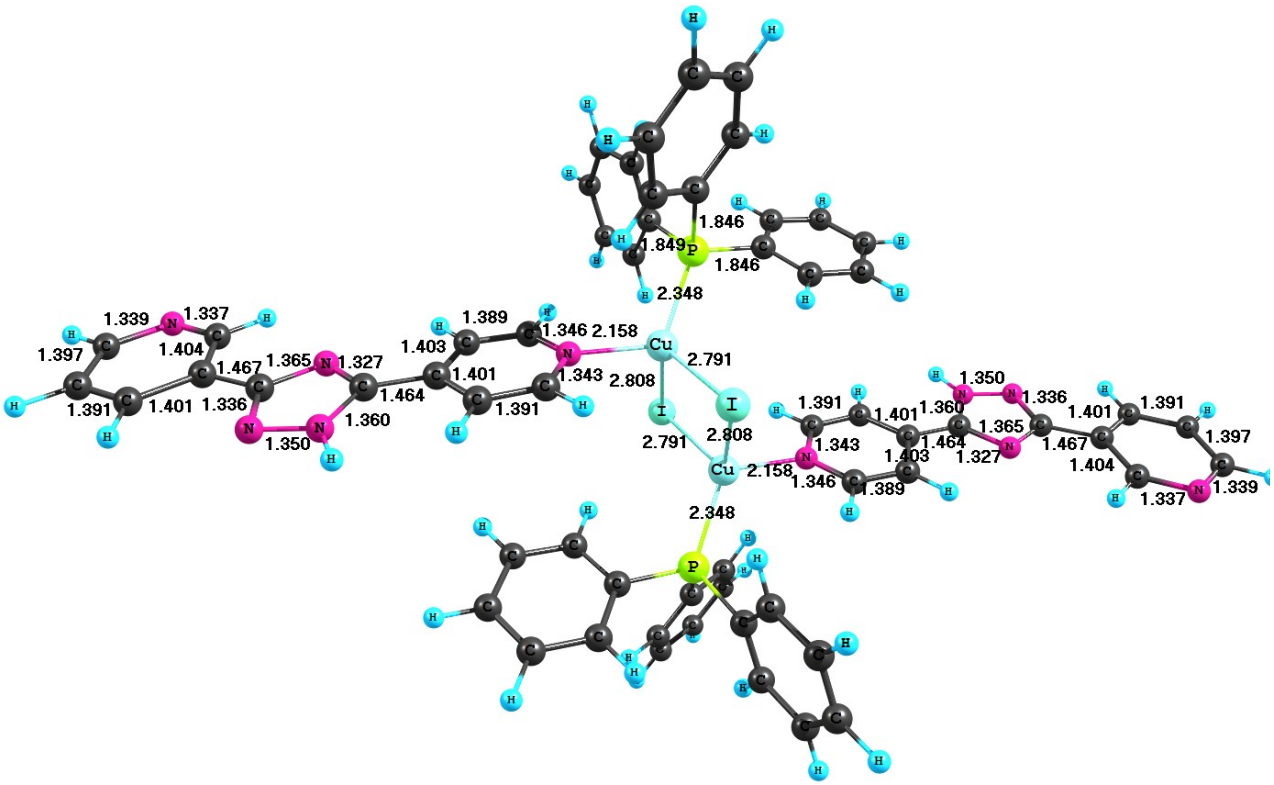


S_1



T_1

Figure S12. The optimized molecular structure and selected bond lengths (Å) of the complex **1** in the S_0, S_1 and T_1 states calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.



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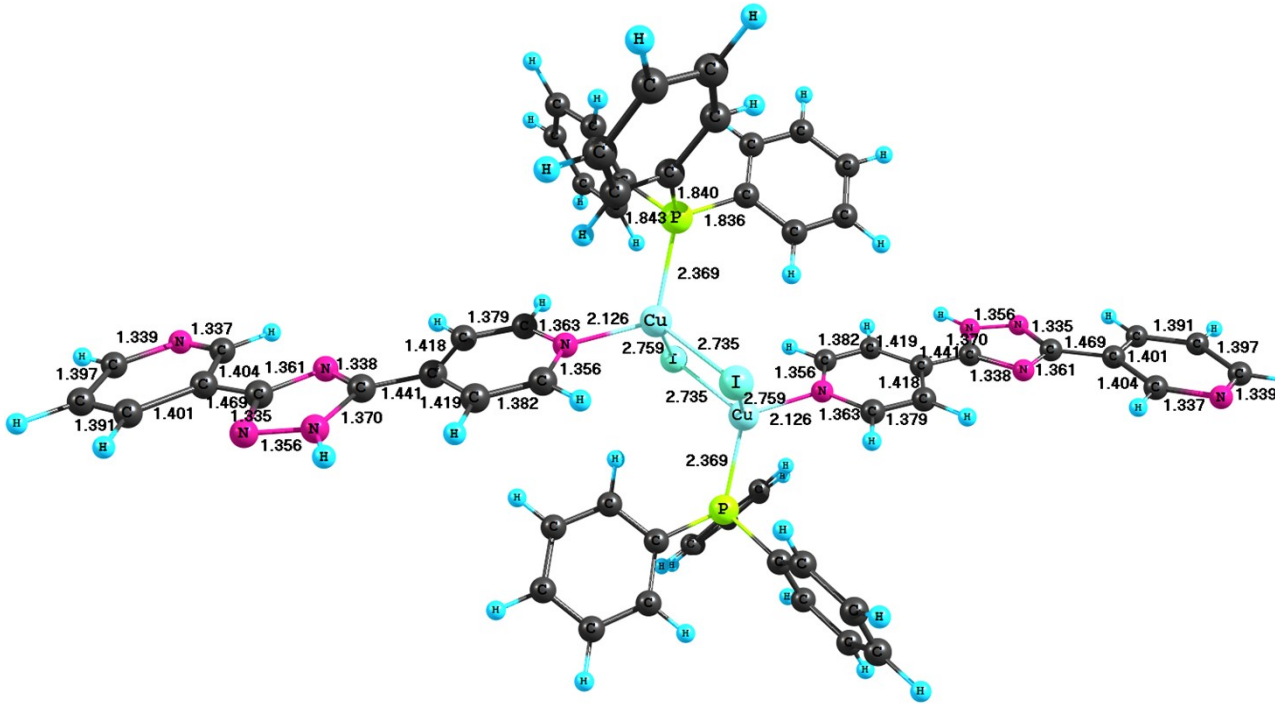
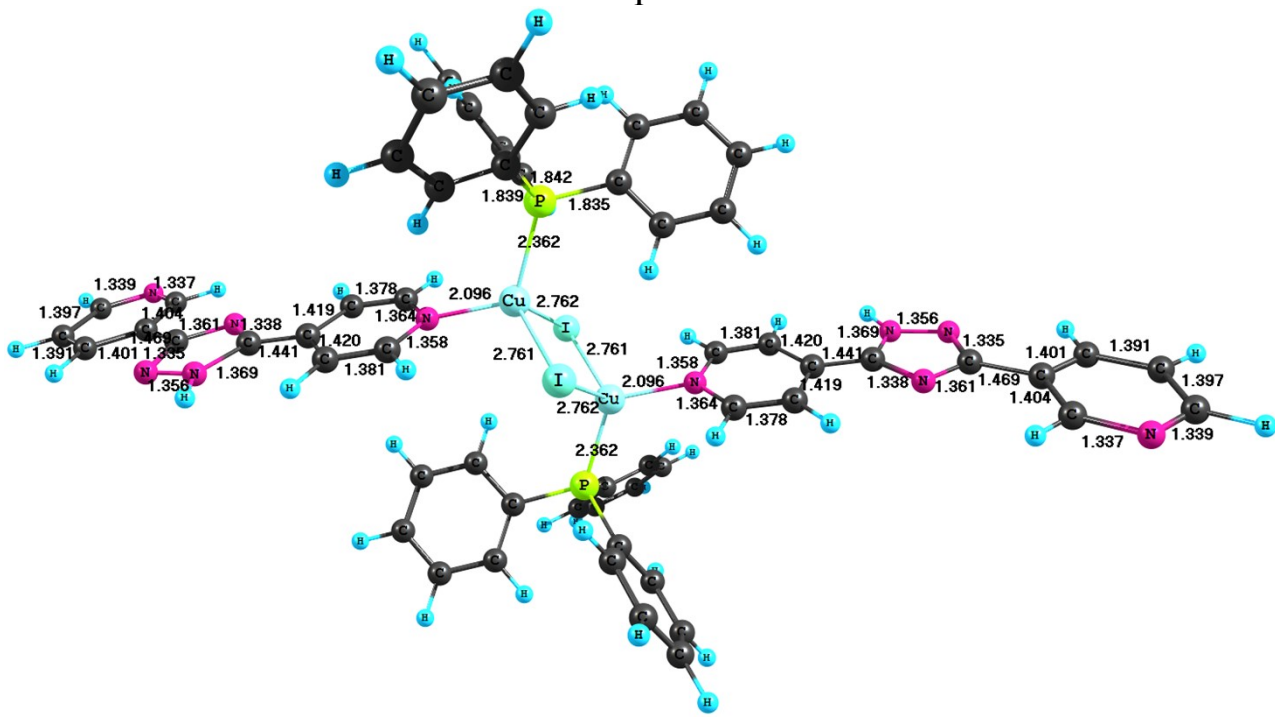
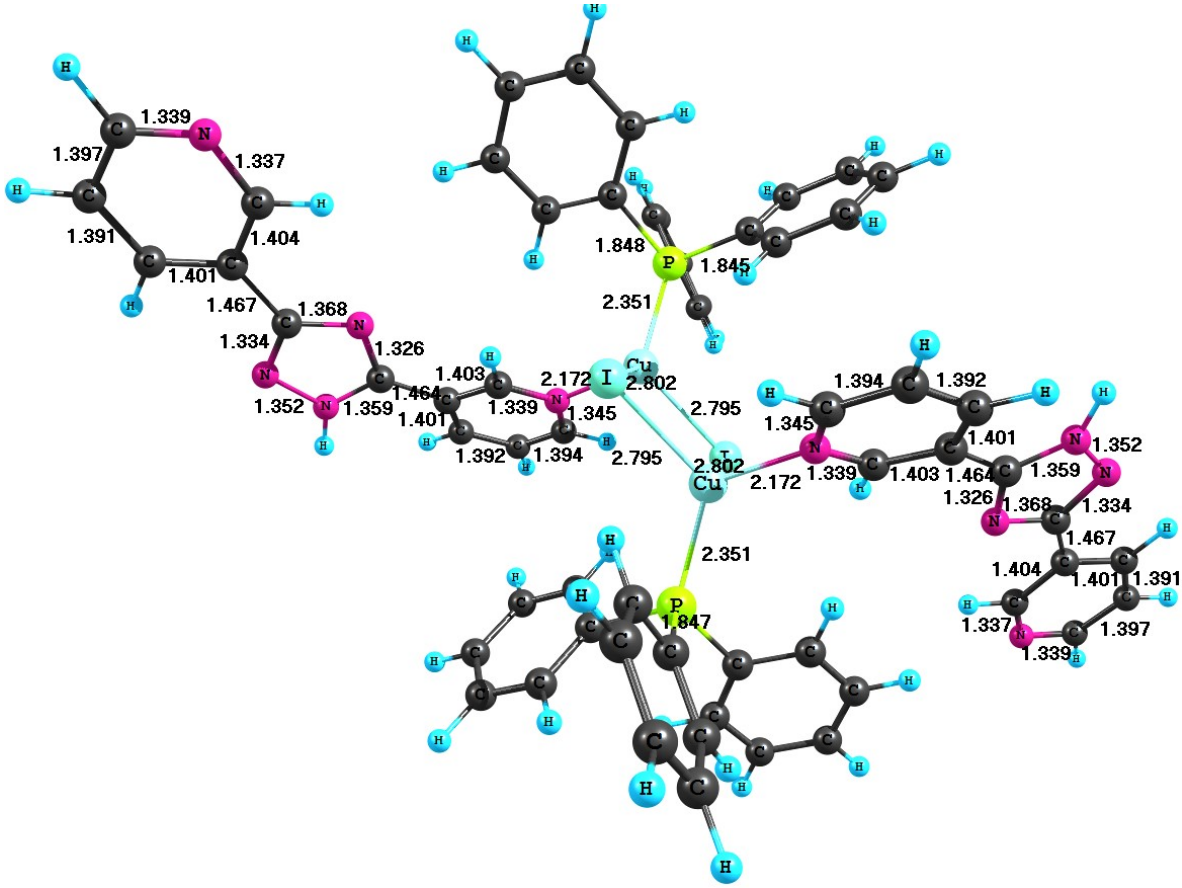


S_1

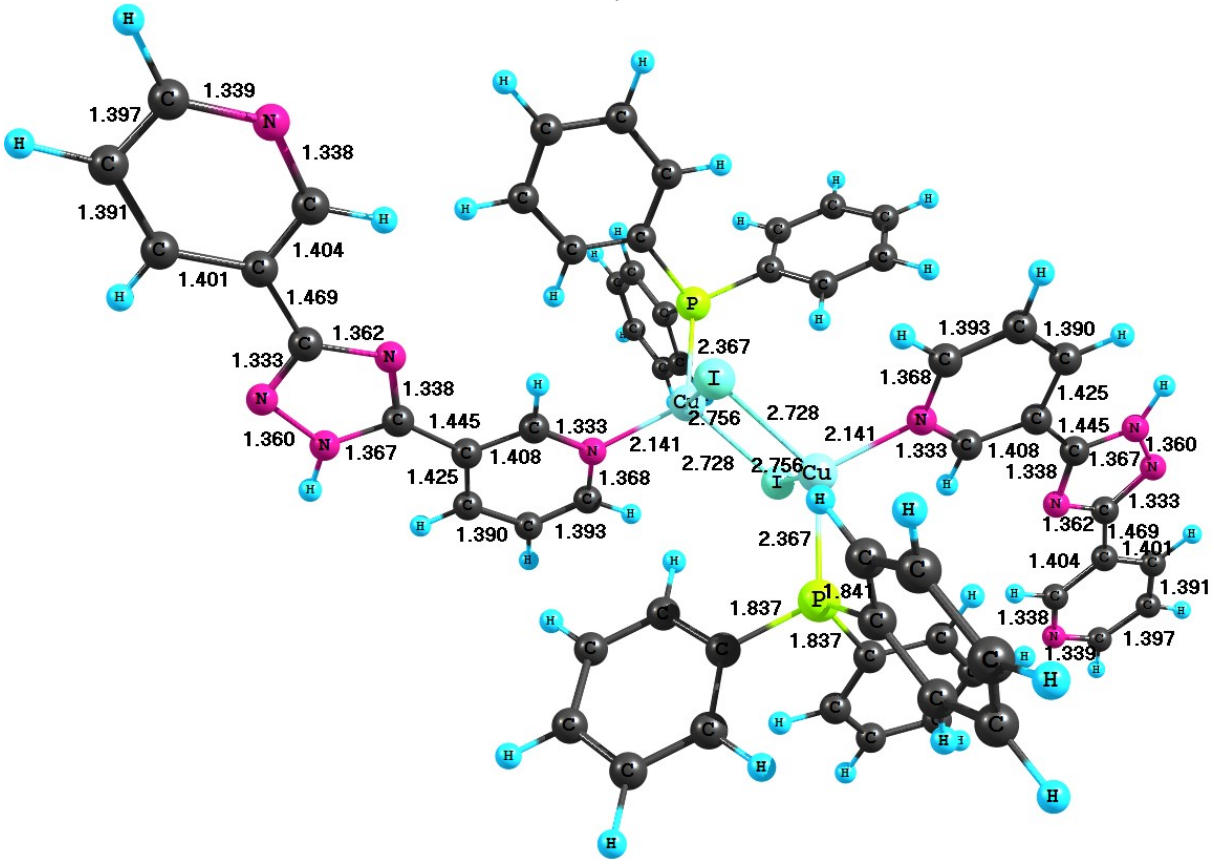


T_1

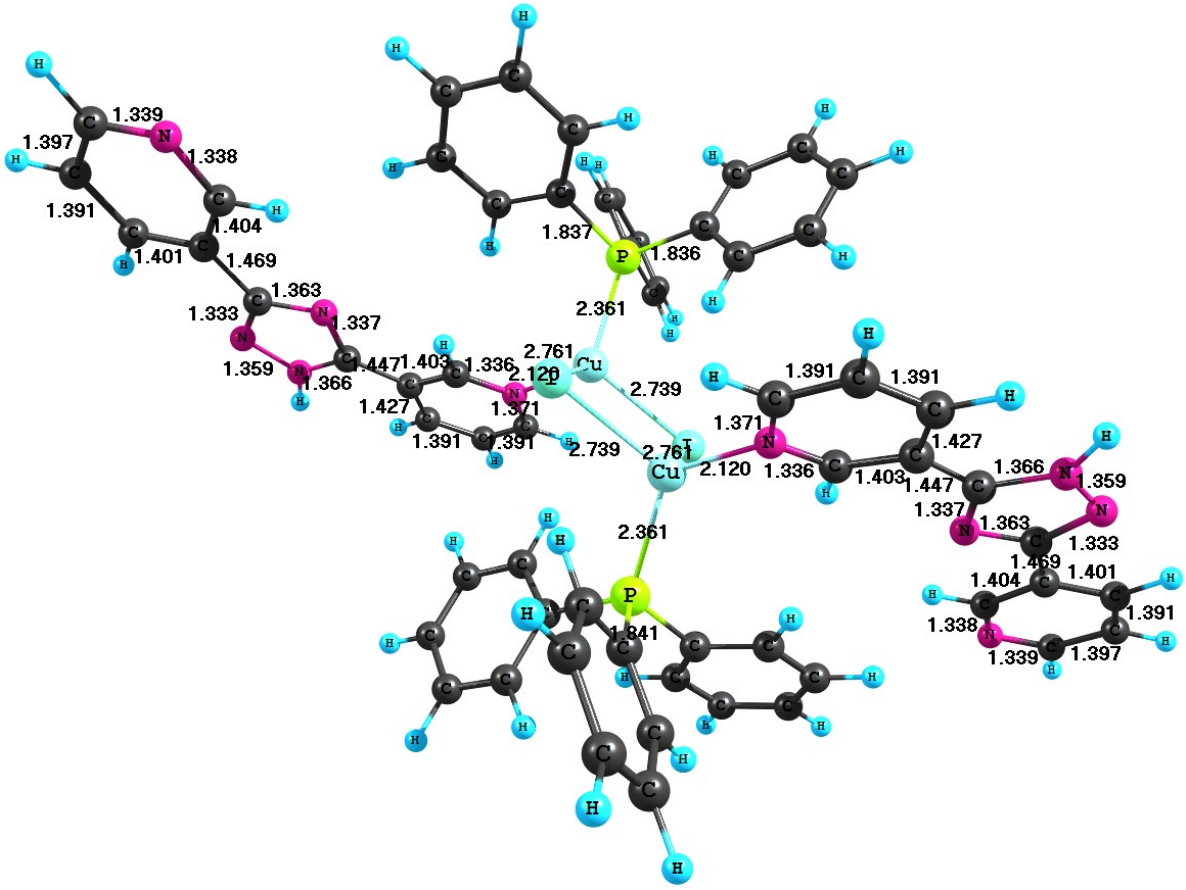
Figure S13. The optimized molecular structure and selected bond lengths (Å) of the complex **2** in the S_0, S_1 and T_1 states calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.



S_0

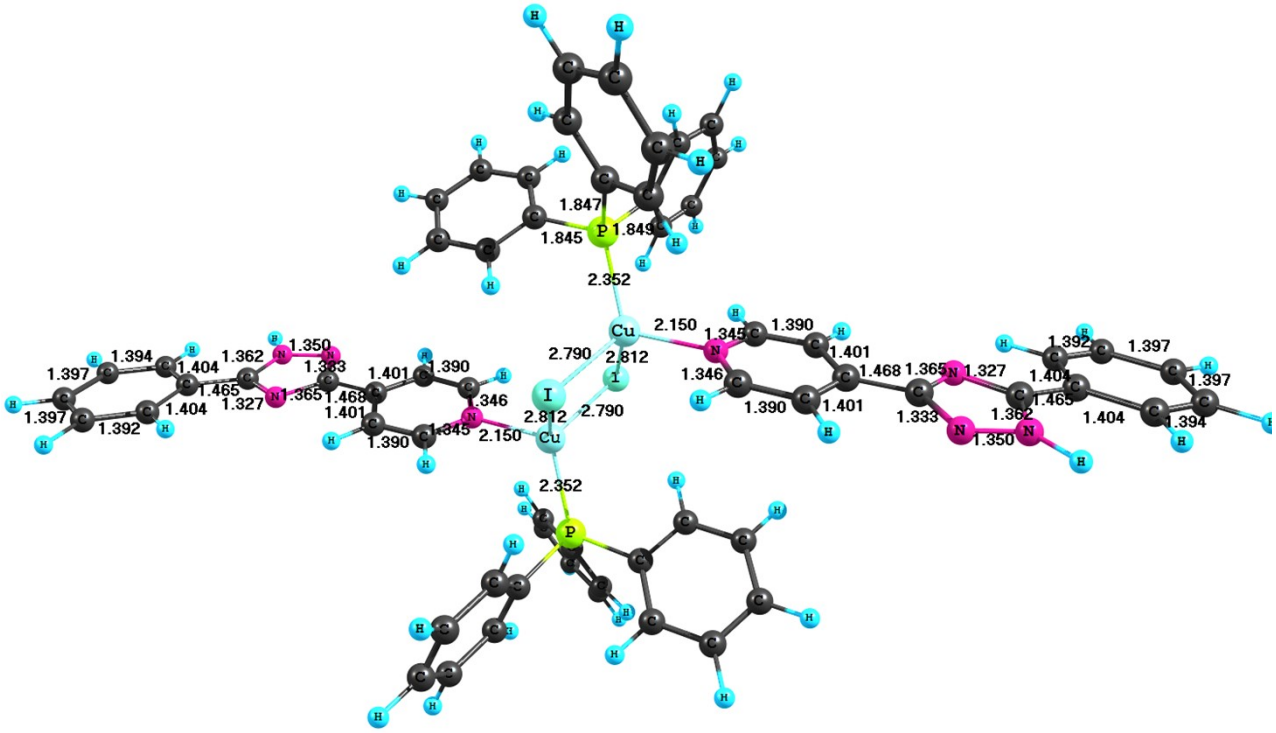


S_1

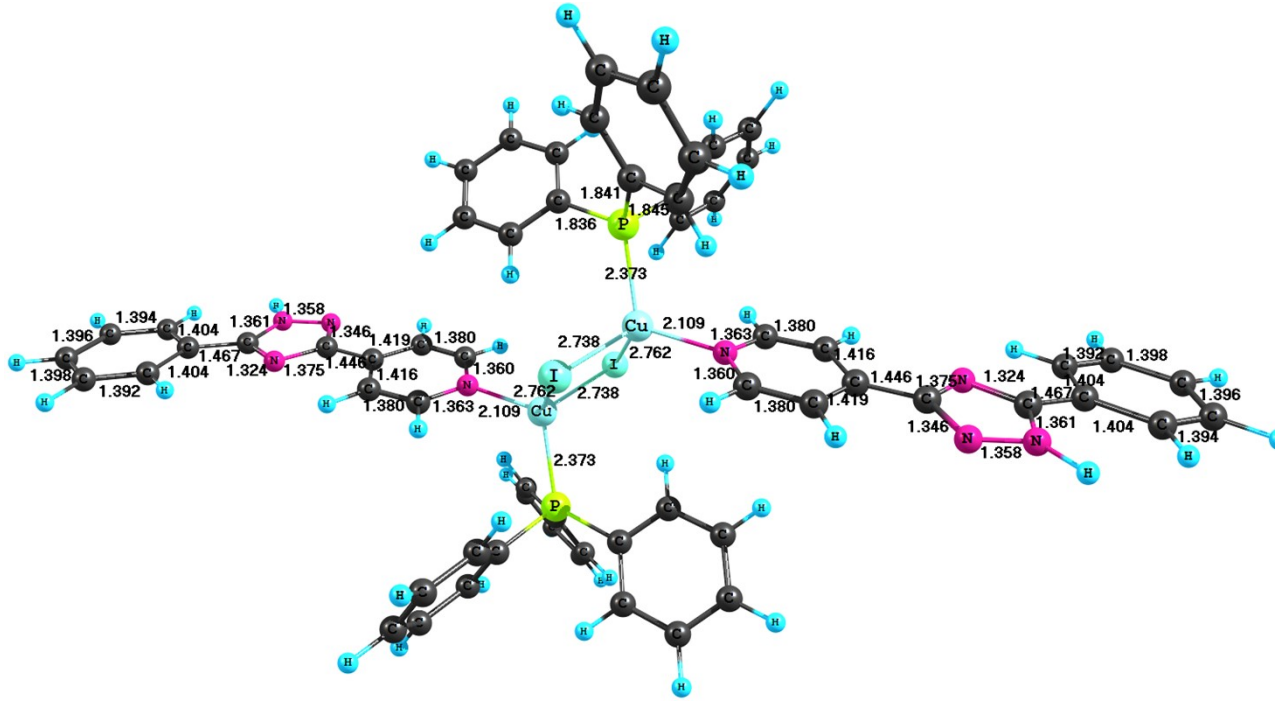


T_1

Figure S14. The optimized molecular structure and selected bond lengths (Å) of the complex **3** in the S_0, S_1 and T_1 states calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.



S_0



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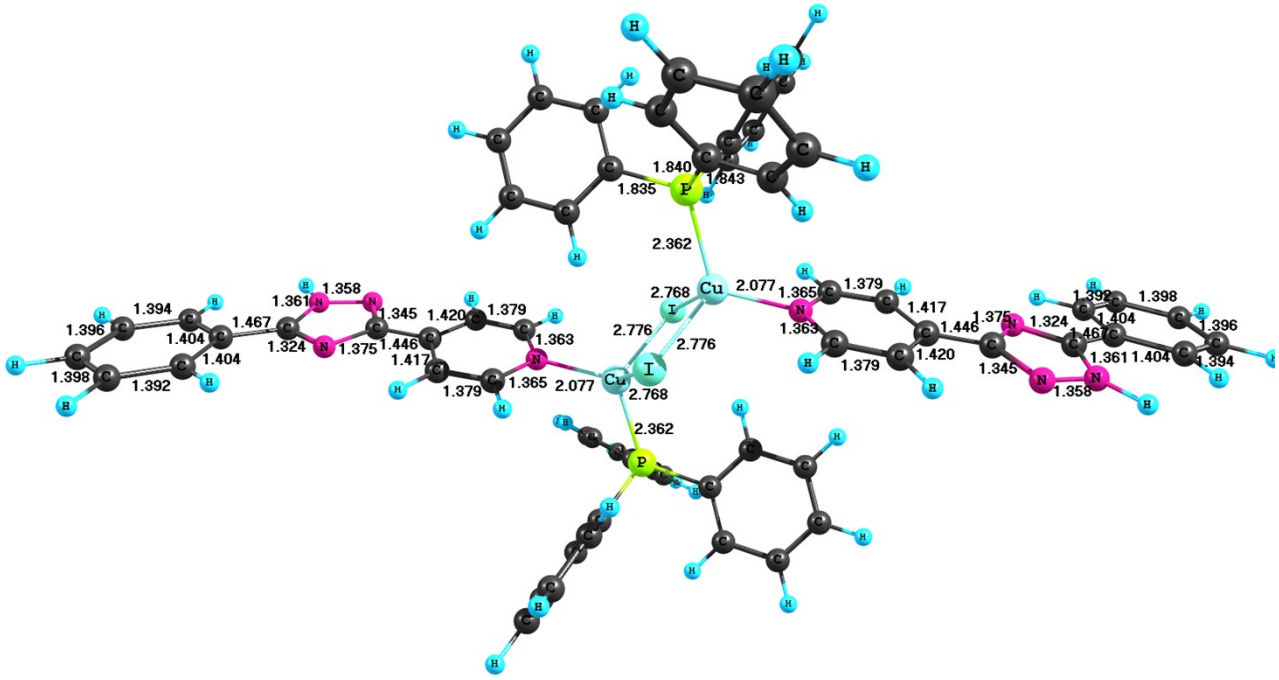
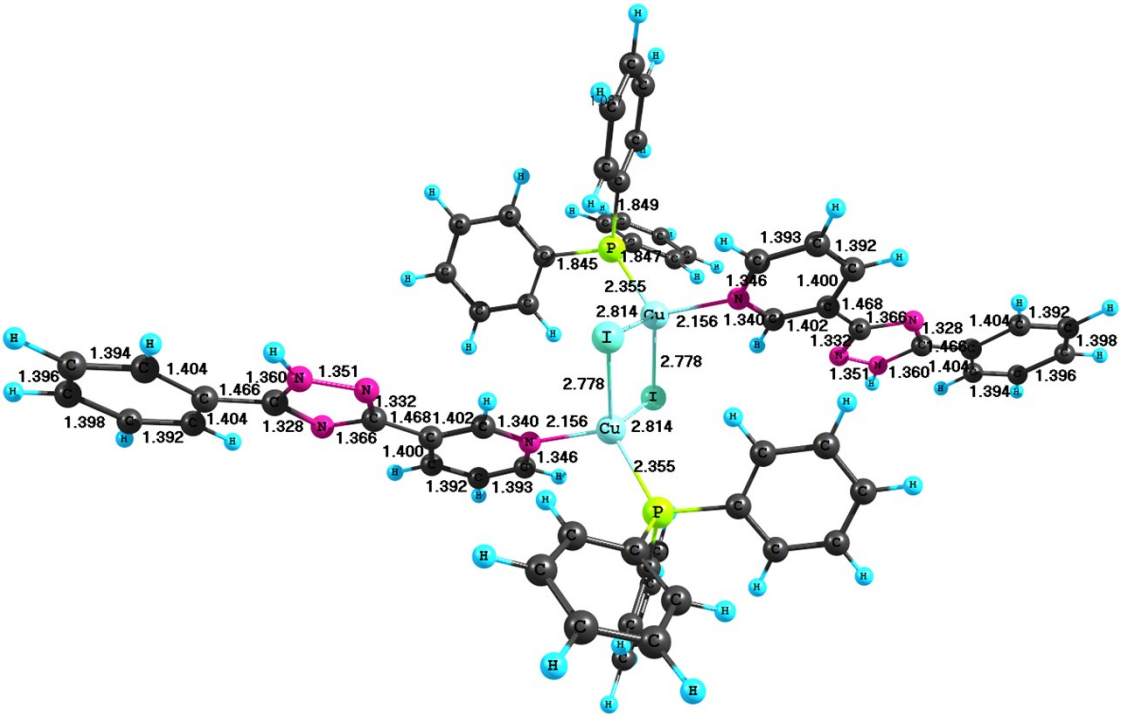
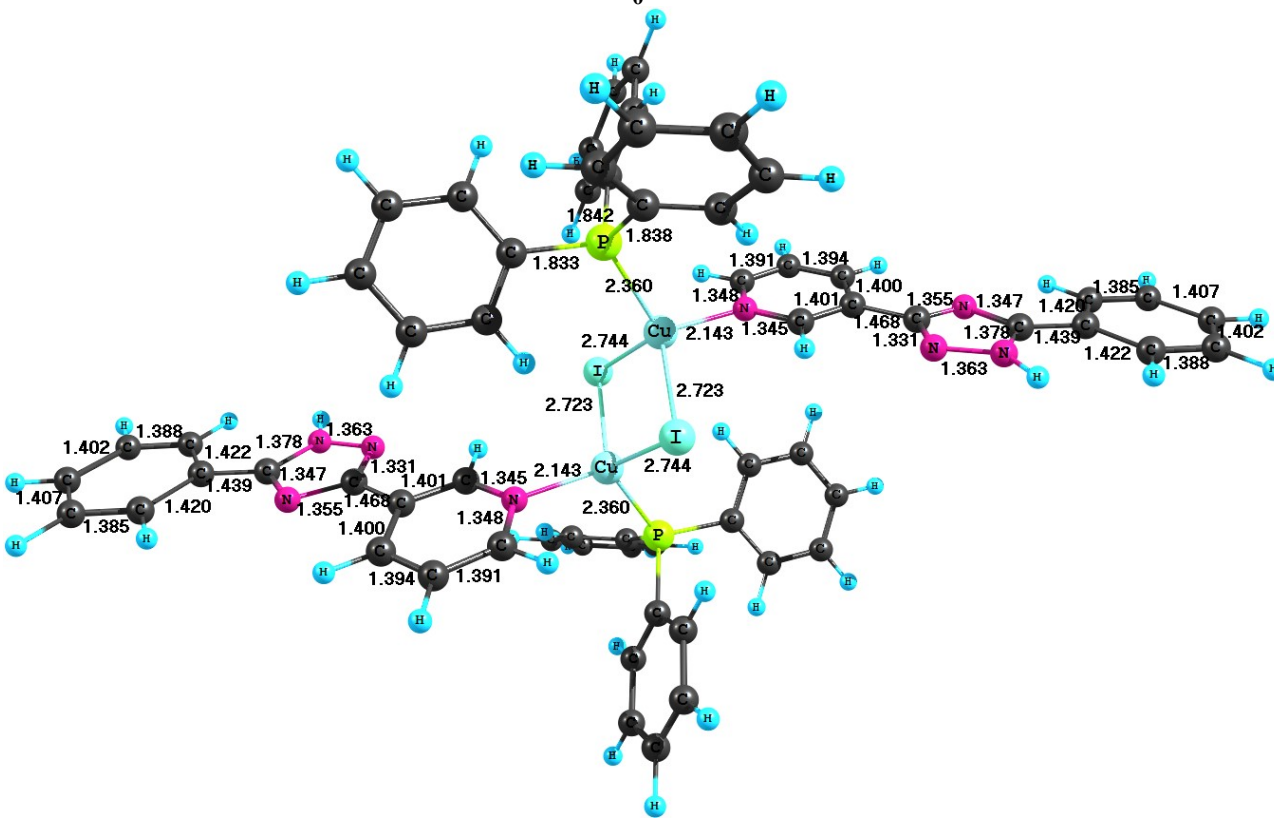


T_1

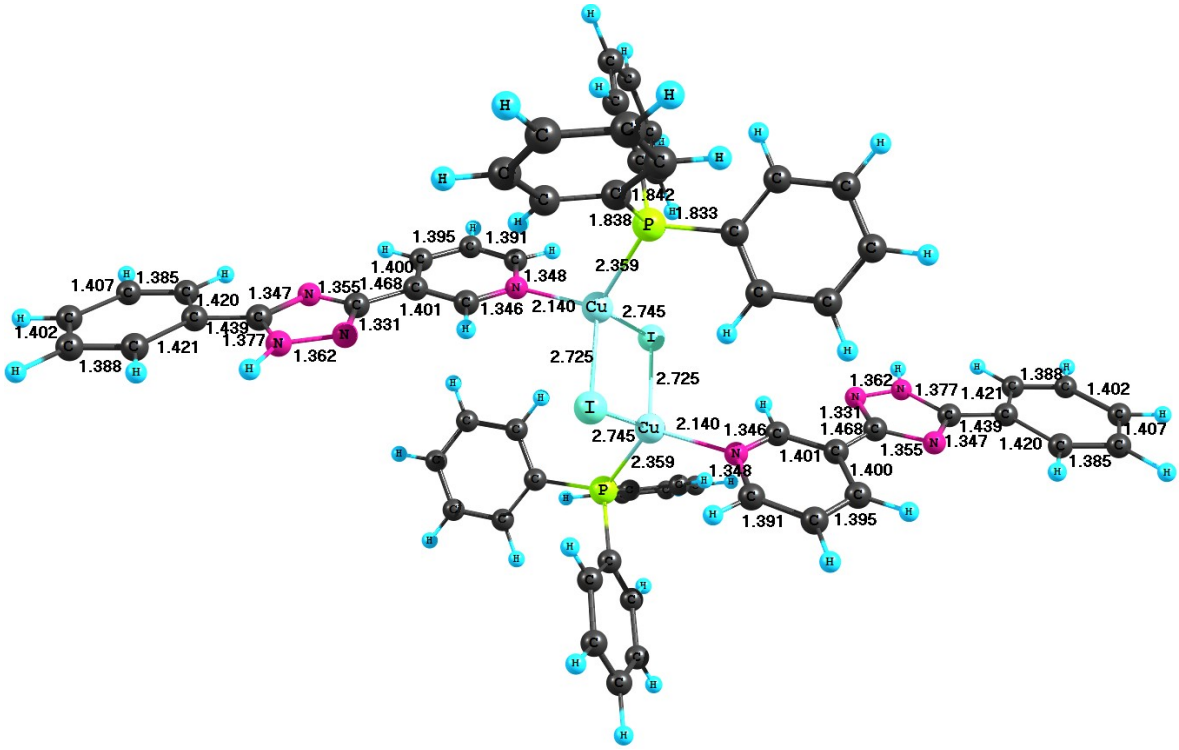
Figure S15. The optimized molecular structure and selected bond lengths (Å) of the complex **4** in the S_0, S_1 and T_1 states calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.



S_0



S_1



T_1

Figure S16. The optimized molecular structure and selected bond lengths (Å) of the complex **5** in the S_0, S_1 and T_1 states calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

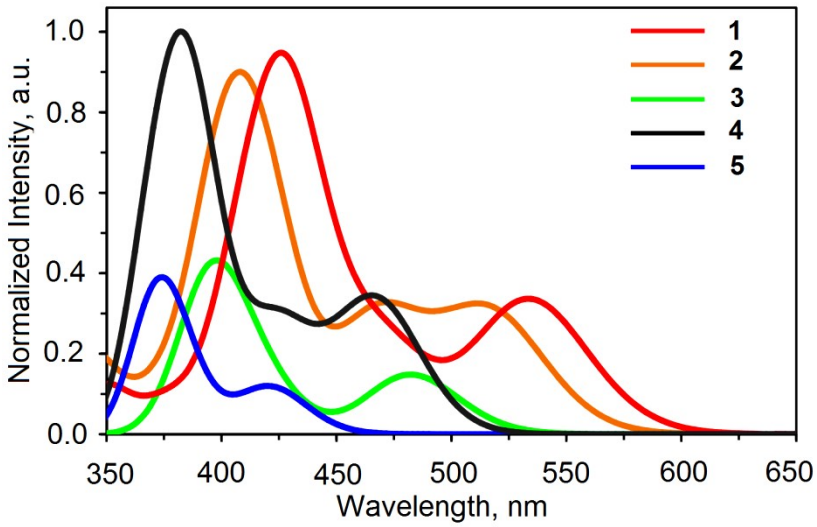


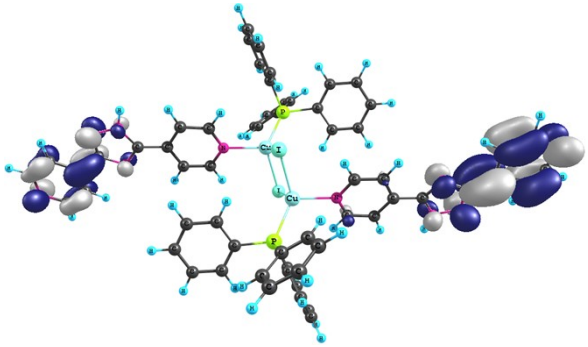
Figure S17. TDDFT simulated absorption spectra of the complexes **1**–**5** calculated at the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Table S3. Wavelengths (λ), oscillator strengths (*f*) and orbital assignment of the selected electronic transitions in the simulated absorption spectra of the **1**–**5** complexes calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

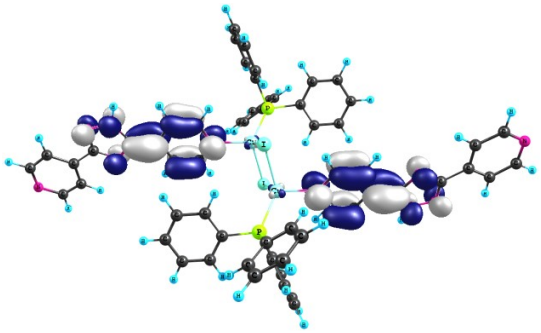
Complex	Transition	λ_{vac}	f_{vac}	Assignment
1	$S_0 \rightarrow S_1$	534	0.0277	HOMO → LUMO (+98%)
	$S_0 \rightarrow S_2$	533	0.0001	HOMO → LUMO+1 (+98%)
	$S_0 \rightarrow S_3$	477	0.0012	HOMO-1→LUMO+1 (+70%) HOMO-1→ LUMO (+17%) HOMO-2 → LUMO+1 (+7%)
	$S_0 \rightarrow S_4$	476	0.0057	HOMO-1→ LUMO (+71%) HOMO-1→ LUMO+1 (17%) HOMO-2→ LUMO (+6%)
	$S_0 \rightarrow S_5$	467	0.0133	HOMO-2→ LUMO (+79%) HOMO-1→LUMO (10%) HOMO-5→ LUMO+1 (+6%)
	$S_0 \rightarrow S_8$	435	0.0092	HOMO-3→ LUMO+1 (+59%) HOMO-4→ LUMO+1 (39%)
	$S_0 \rightarrow S_{10}$	430	0.0556	HOMO-4→ LUMO+1 (+59%) HOMO-3→ LUMO+1 (+35%)
	$S_0 \rightarrow S_{11}$	409	0.0312	HOMO-5→ LUMO+1 (+87%) HOMO-2→ LUMO (8%)
	$S_0 \rightarrow S_{12}$	408	0.0002	HOMO-5→ LUMO (+86%) HOMO-2→ LUMO+1 (8%)
	$S_0 \rightarrow S_{14}$	378	0.0068	HOMO-6→ LUMO +1 (+98%)
	$S_0 \rightarrow S_{16}$	374	0.0007	HOMO → LUMO+3 (+91%) HOMO → LUMO+4 (+6%)
	$S_0 \rightarrow S_{17}$	350	0.0010	HOMO → LUMO+5 (+69%) HOMO → LUMO+4 (22%) HOMO → LUMO+2 (7%)
	$S_0 \rightarrow S_{18}$	350	0.0080	HOMO → LUMO+4 (+69%) HOMO → LUMO+5 (+22%) HOMO → LUMO+3 (7%)
	$S_0 \rightarrow S_{19}$	345	0.0012	HOMO-7→ LUMO (+80%) HOMO-8→ LUMO (14%)
2	$S_0 \rightarrow S_1$	517	0.0248	HOMO →LUMO (+98%)
	$S_0 \rightarrow S_2$	516	0	HOMO →LUMO+1 (+98%)
	$S_0 \rightarrow S_3$	471	0.0195	HOMO-1→LUMO (+91%)
	$S_0 \rightarrow S_5$	460	0.0065	HOMO-2→LUMO (+83%) HOMO-1→LUMO (+7%) HOMO-5→LUMO+1 (5%)
	$S_0 \rightarrow S_8$	425	0.0020	HOMO-3→LUMO+1 (+85%) HOMO-4→LUMO+1 (+13%)
	$S_0 \rightarrow S_{10}$	419	0.0433	HOMO-4→LUMO+1 (+81%) HOMO-3→LUMO+1 (11%) HOMO-2→LUMO (+5%)
	$S_0 \rightarrow S_{11}$	400	0.0482	HOMO-5→LUMO+1 (+88%) HOMO-2→LUMO (+6%)

	$S_0 \rightarrow S_{14}$	377	0.0099	HOMO-6→LUMO+1 (+97%)
	$S_0 \rightarrow S_{15}$	356	0.0063	HOMO→LUMO+2 (+75%) HOMO→LUMO+5 (+23%)
	$S_0 \rightarrow S_{18}$	340	0.0144	HOMO→LUMO+5 (+71%) HOMO→LUMO+2 (22%)
	$S_0 \rightarrow S_{19}$	340	0.0008	HOMO-7→LUMO (+83%) HOMO-8→LUMO (+7%)
3	$S_0 \rightarrow S_1$	483	0.0123	HOMO→LUMO (+98%)
	$S_0 \rightarrow S_2$	482	0.0000	HOMO→LUMO+1 (+98%)
	$S_0 \rightarrow S_3$	439	0.0009	HOMO-1→LUMO (+98%)
	$S_0 \rightarrow S_5$	424	0.0031	HOMO-2→LUMO (+86%) HOMO-5→LUMO+1 (+10%)
	$S_0 \rightarrow S_8$	414	0.0073	HOMO→LUMO+3 (+97%)
	$S_0 \rightarrow S_9$	402	0.0099	HOMO-3→LUMO (+97%)
	$S_0 \rightarrow S_{11}$	394	0.0217	HOMO-4→LUMO (+95%)
	$S_0 \rightarrow S_{14}$	381	0.0017	HOMO-1→LUMO+3 (+96%)
	$S_0 \rightarrow S_{15}$	378	0.0020	HOMO-5→LUMO (+75%) HOMO-2→LUMO+1 (12%) HOMO-2→LUMO+3 (6%)
4	$S_0 \rightarrow S_1$	468	0.0276	HOMO→LUMO (+50%) HOMO→LUMO+2 (48%)
	$S_0 \rightarrow S_2$	467	0.0000	HOMO→LUMO+1 (+50%) HOMO→LUMO+3 (48%)
	$S_0 \rightarrow S_3$	429	0.0031	HOMO→LUMO+2 (+50%) HOMO→LUMO (+49%)
	$S_0 \rightarrow S_6$	428	0.0050	HOMO-1→LUMO +2 (+38%) HOMO-1→LUMO (37%) HOMO-2→LUMO+2 (10%) HOMO-2→LUMO (+8%)
	$S_0 \rightarrow S_7$	423	0.0153	HOMO-2→LUMO +2 (+37%) HOMO-2→LUMO (31%) HOMO-1→LUMO (12%) HOMO-1→LUMO+2 (+11%)
	$S_0 \rightarrow S_9$	392	0.0003	HOMO-1→LUMO (+50%) HOMO-1→LUMO+2 (+47%)
	$S_0 \rightarrow S_{12}$	391	0.0008	HOMO-4→LUMO+1 (+35%) HOMO-4→LUMO+3 (34%) HOMO-3→LUMO+1 (+14%) HOMO-3→LUMO+3 (14%)
	$S_0 \rightarrow S_{14}$	388	0.0562	HOMO-3→LUMO+1 (+31%) HOMO-3→LUMO+3 (29%) HOMO-4→LUMO+1 (14%) HOMO-4→LUMO+3 (+13%) HOMO-2→LUMO (9%)
	$S_0 \rightarrow S_{15}$	383	0.0048	HOMO-2→LUMO (+50%) HOMO-2→LUMO+2 (+41%)
	$S_0 \rightarrow S_{17}$	372	0.0354	HOMO-5→LUMO+3 (+44%) HOMO-5→LUMO+1 (41%) HOMO-2→LUMO+2 (10%)
	$S_0 \rightarrow S_{20}$	364	0.0066	HOMO-3→LUMO+3 (+43%)

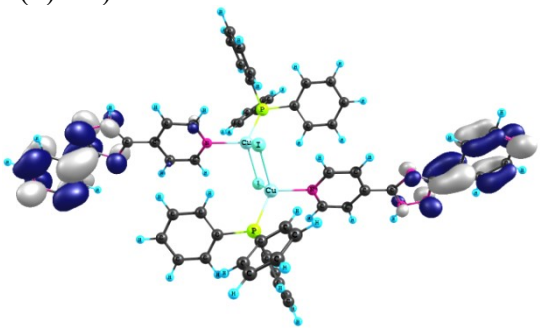
				HOMO-3→LUMO+1 (+41%) HOMO-4→LUMO+1 (+8%) HOMO-4→LUMO+3 (+7%)
5	$S_0 \rightarrow S_1$	425	0.0038	HOMO→LUMO (+96%)
	$S_0 \rightarrow S_2$	424	0.0000	HOMO →LUMO+1 (+96%)
	$S_0 \rightarrow S_3$	419	0.0000	HOMO →LUMO+2 (+96%)
	$S_0 \rightarrow S_4$	418	0.0062	HOMO →LUMO+3 (+96%)
	$S_0 \rightarrow S_5$	386	0.0010	HOMO-1→LUMO (+80%) HOMO-1→LUMO+3 (11%)
	$S_0 \rightarrow S_8$	383	0.0025	HOMO-1→LUMO+3 (+58%) HOMO-2→LUMO+3 (18%) HOMO-1→LUMO (+16%)
	$S_0 \rightarrow S_{10}$	379	0.0079	HOMO-2→LUMO+3 (+39%) HOMO-2→LUMO (26%) HOMO-1→LUMO +3 (+24%)
	$S_0 \rightarrow S_{12}$	376	0.0007	HOMO-2→LUMO (+64%) HOMO-2→LUMO+3 (+25%)
	$S_0 \rightarrow S_{13}$	371	0.0227	HOMO→LUMO+4 (+90%)



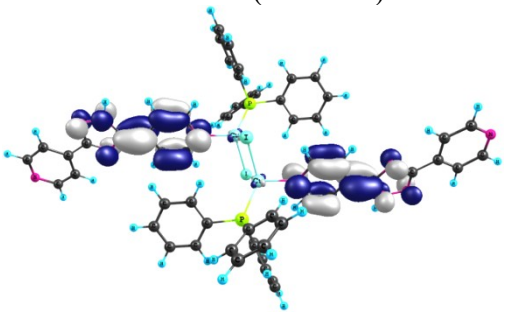
LUMO+3 (-1.34(6) eV)



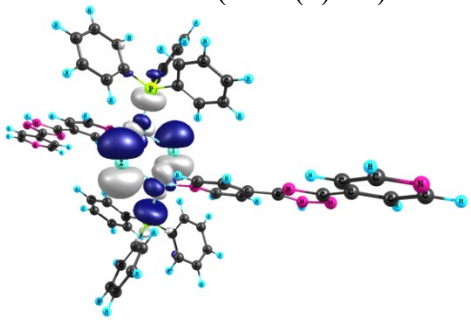
LUMO+1 (-2.11 eV)



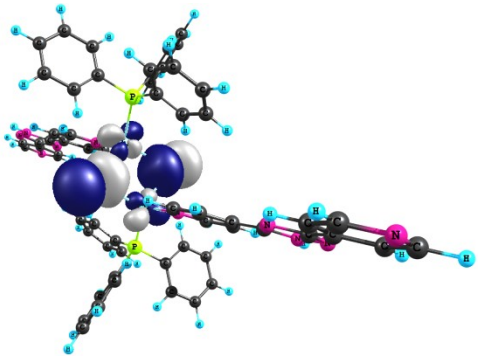
LUMO+2 (-1.34(7) eV)



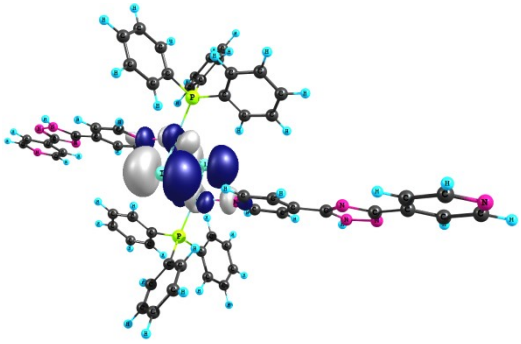
LUMO (-2.12 eV)



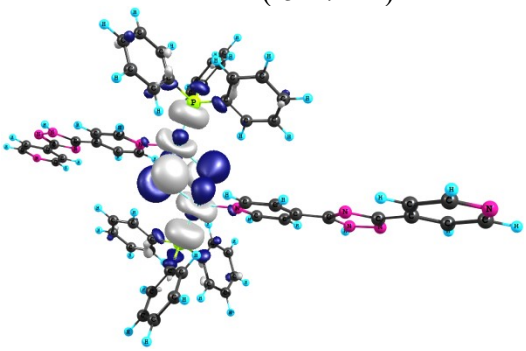
HOMO (-4.96 eV)



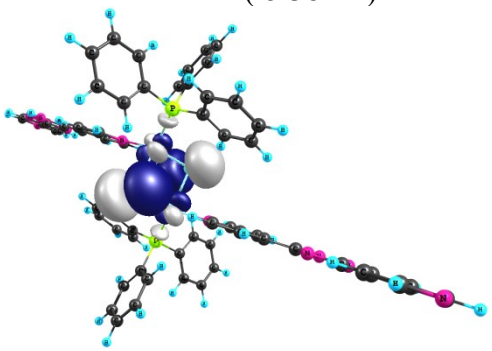
HOMO-1 (-5.27 eV)



HOMO-2 (-5.38 eV)

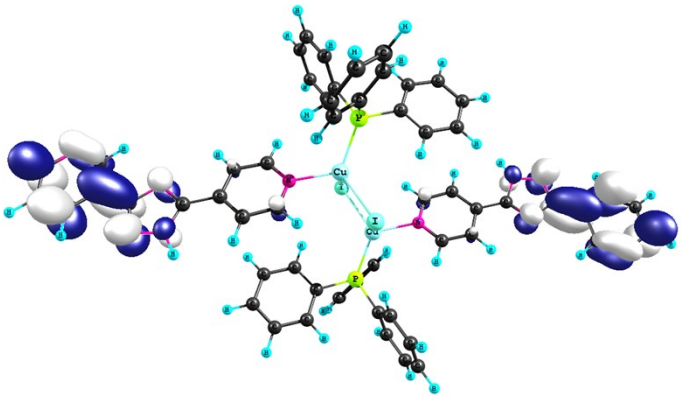


HOMO-3 (-5.49 eV)

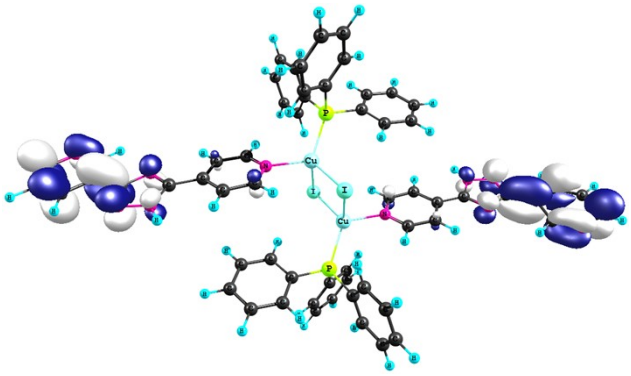


HOMO-4 (-5.51 eV)

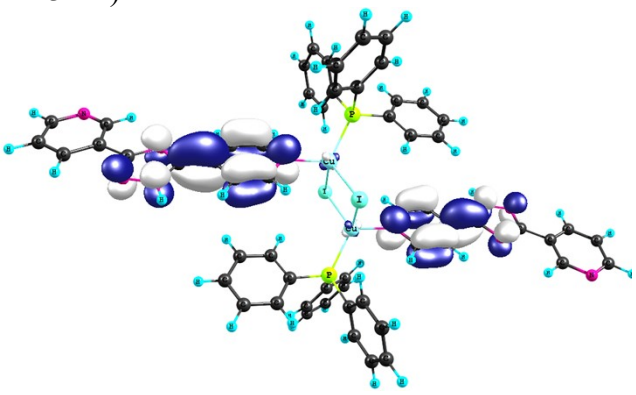
Figure S18. Selected molecular orbitals of the complex **1** calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.



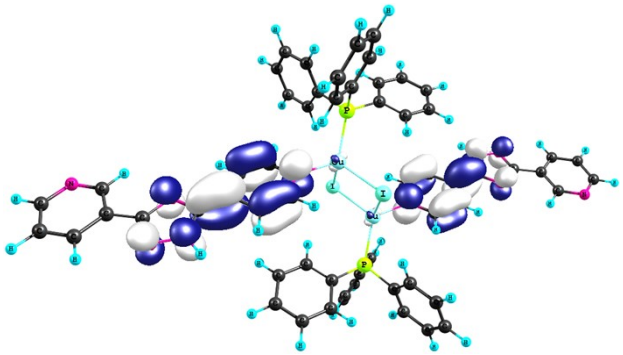
LUMO+3 (-1.13 eV)



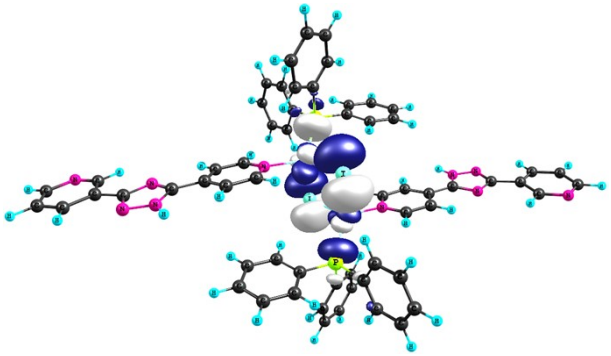
LUMO+2 (-1.14 eV)



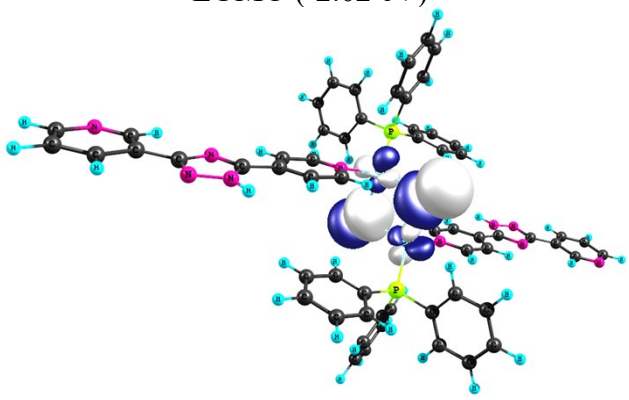
LUMO+1 (-2.01 eV)



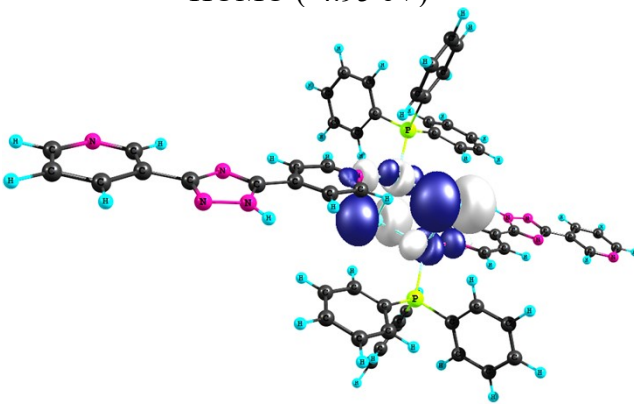
LUMO (-2.02 eV)



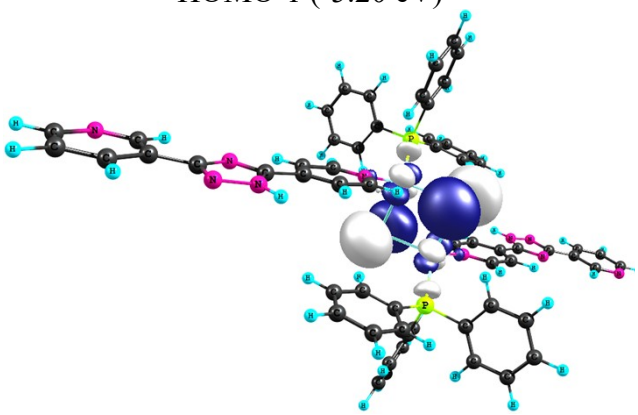
HOMO (-4.95 eV)



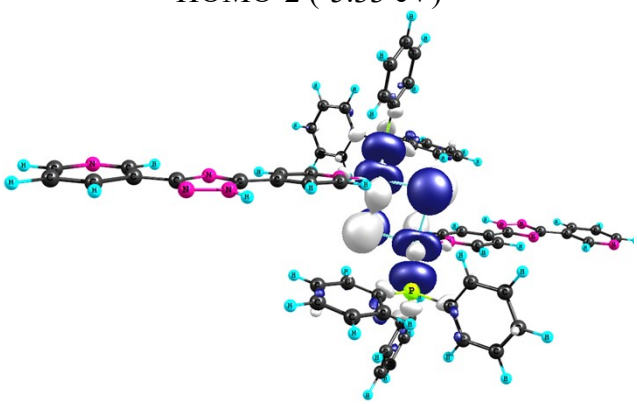
HOMO-1 (-5.20 eV)



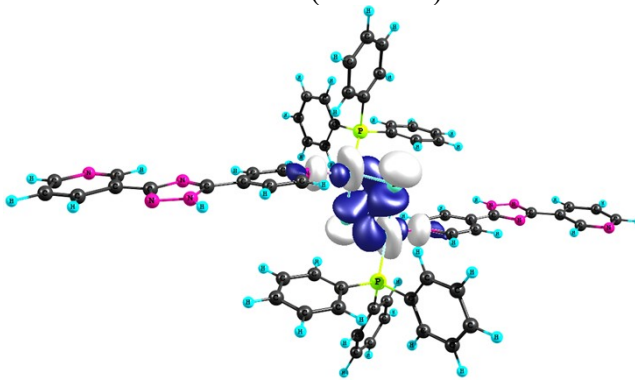
HOMO-2 (-5.33 eV)



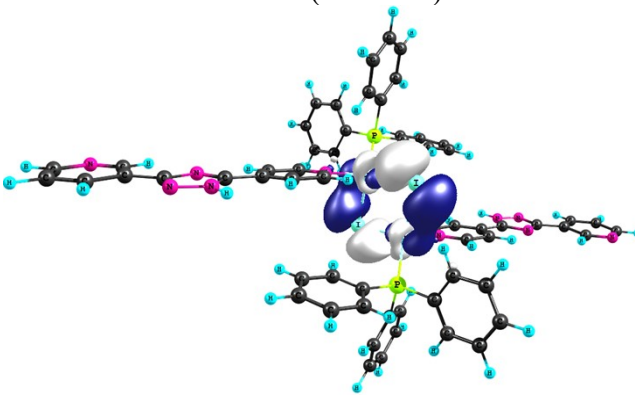
HOMO-3 (-5.47 eV)



HOMO-4 (-5.50 eV)

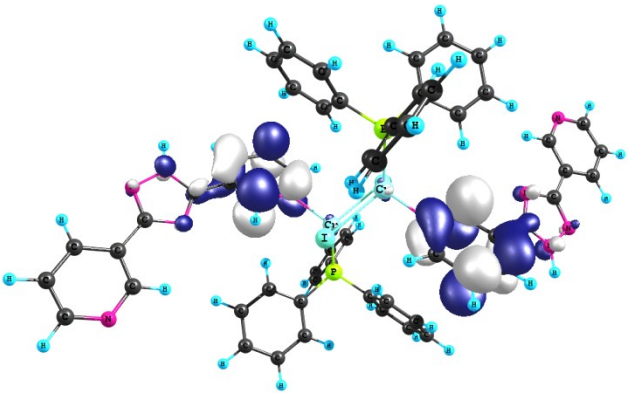


HOMO-5 (-5.69 eV)

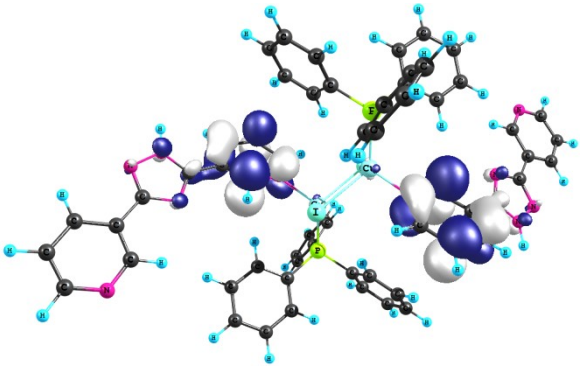


HOMO-6 (-5.85 eV)

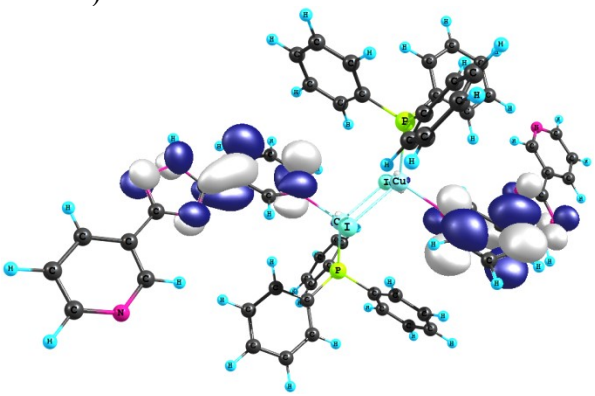
Figure S19. Selected molecular orbitals of the complex **2** calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.



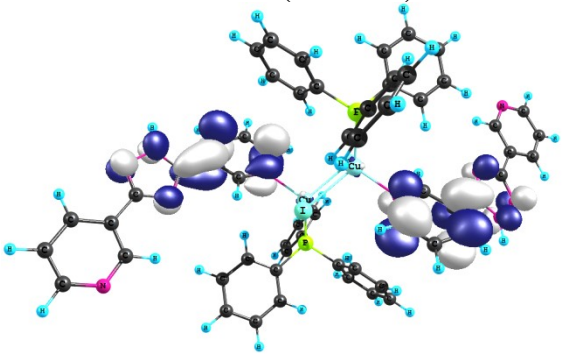
LUMO+3 (-1.21 eV)



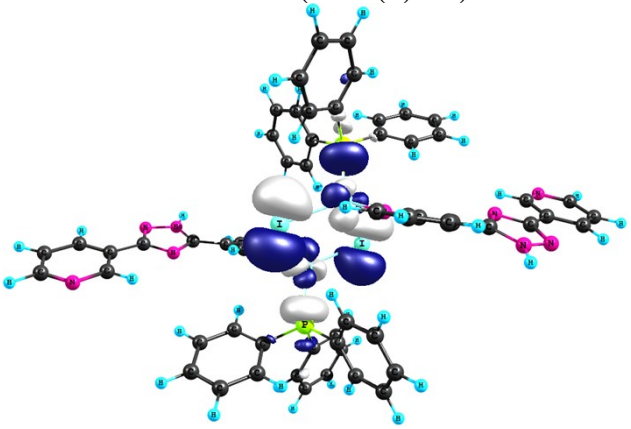
LUMO+2 (-1.22 eV)



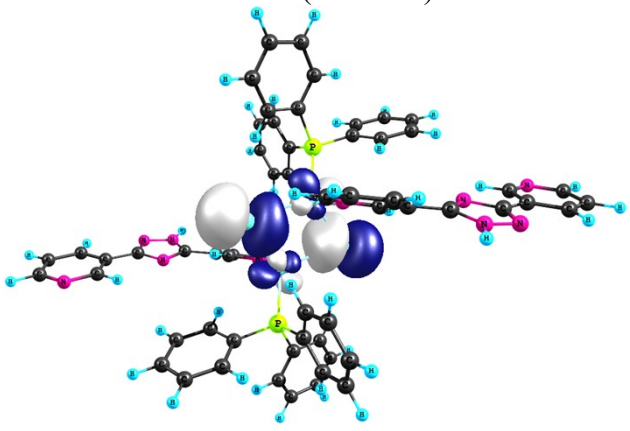
LUMO+1 (-1.69(9) eV)



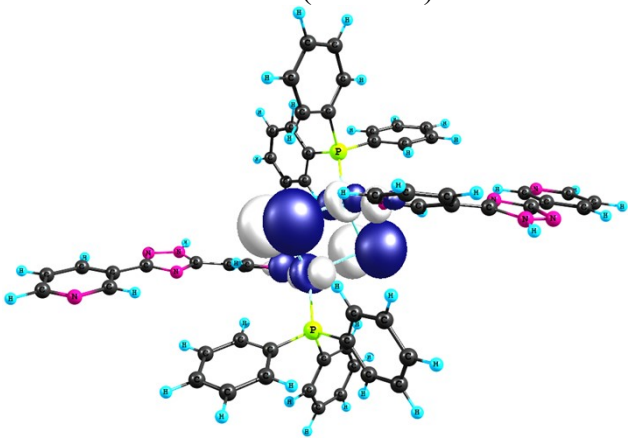
LUMO (-1.70 eV)



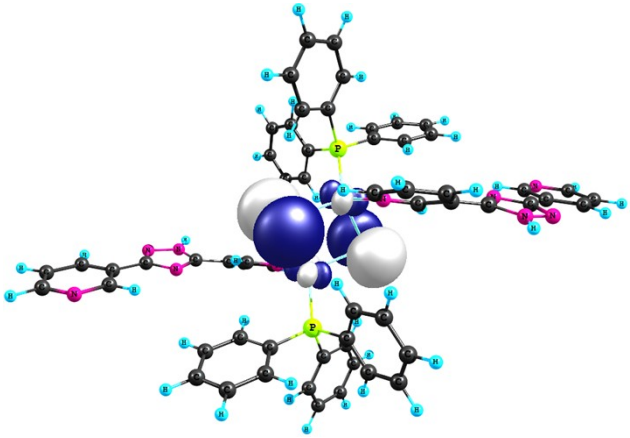
HOMO (-4.81 eV)



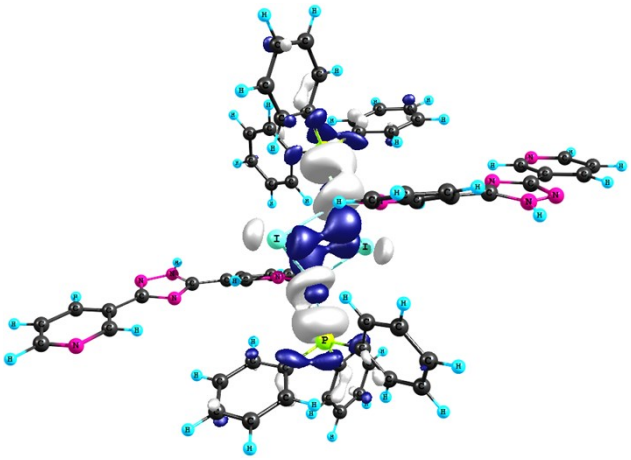
HOMO-1 (-5.09 eV)



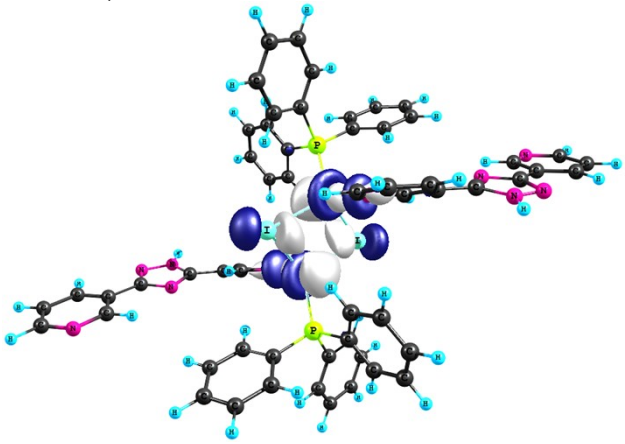
HOMO-2 (-5.26 eV)



HOMO-3 (-5.34 eV)

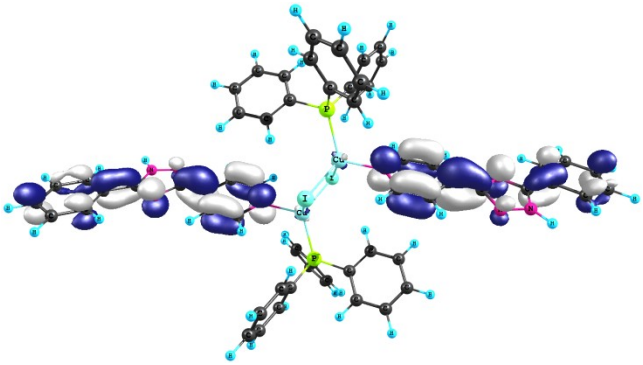


HOMO-4 (-5.36 eV)

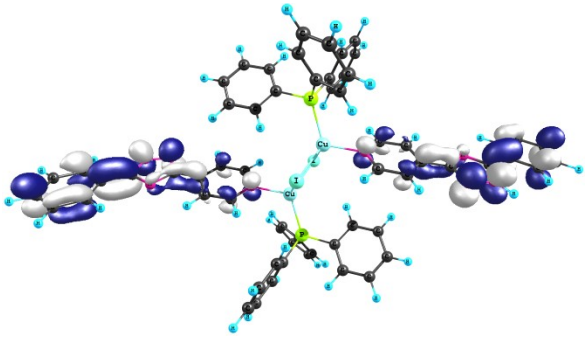


HOMO-5 (-5.59 eV)

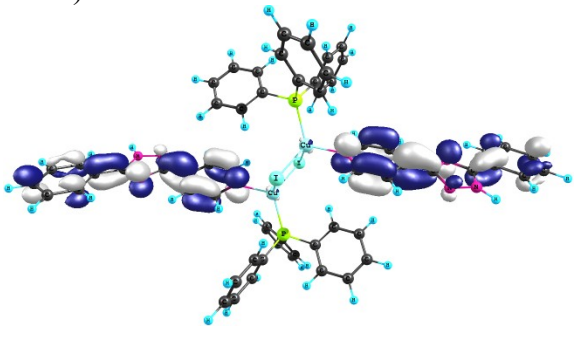
Figure S20. Selected molecular orbitals of the complex **3** calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.



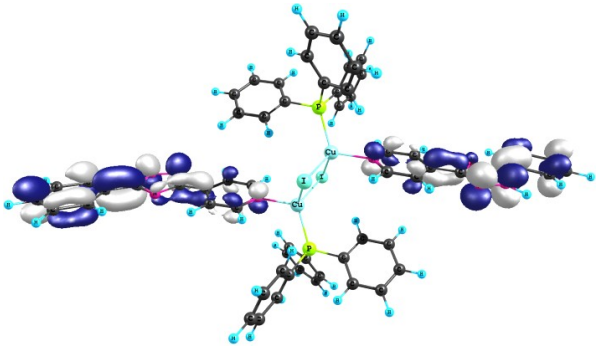
LUMO+3 (-1.29 eV)



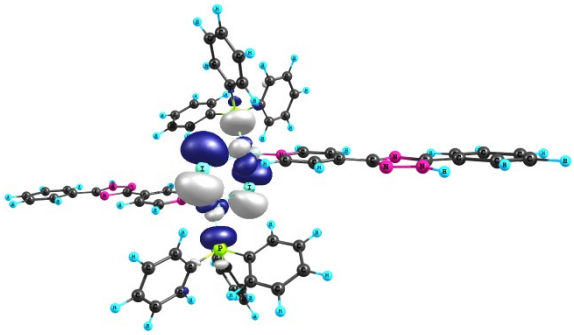
LUMO+1 (-1.41 eV)



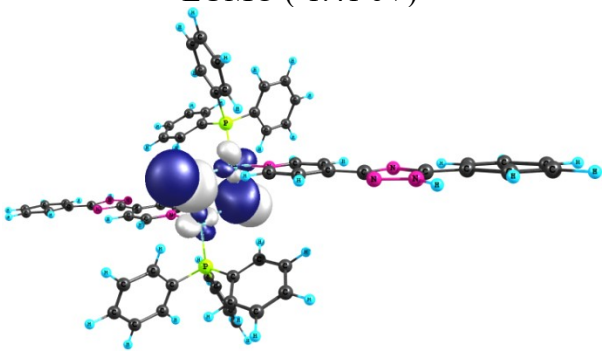
LUMO+2 (-1.30 eV)



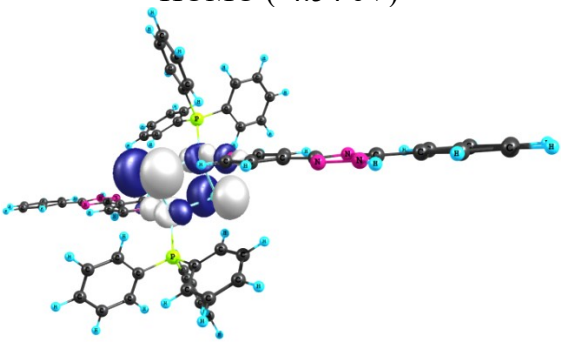
LUMO (-1.41 eV)



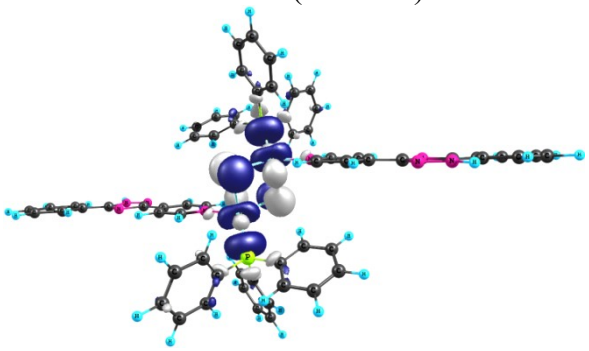
HOMO (-4.54 eV)



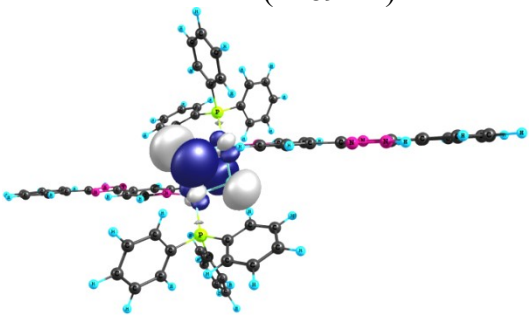
HOMO-1 (-4.81 eV)



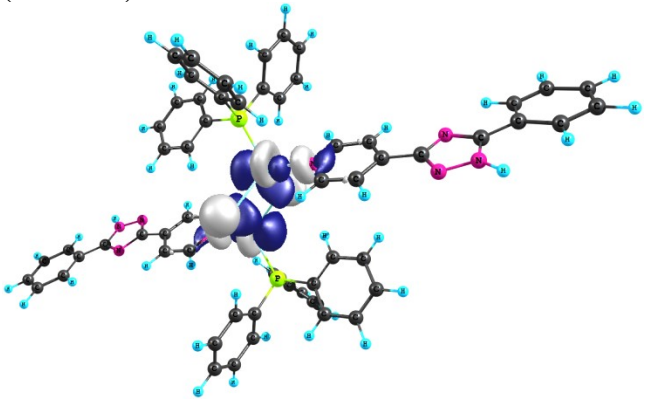
HOMO-2 (-4.89 eV)



HOMO-3 (-5.05 eV)

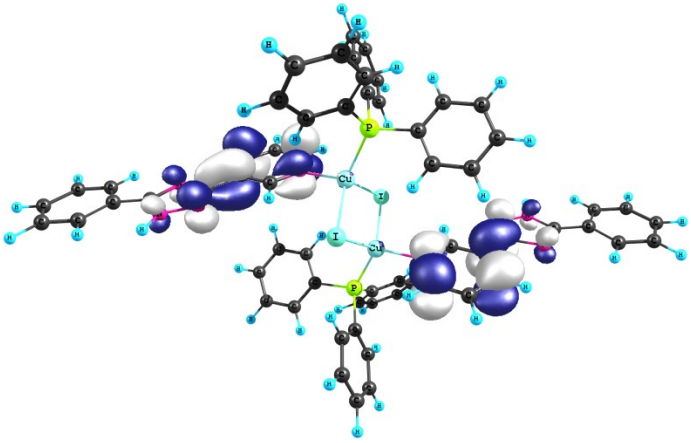


HOMO-4 (-5.06 eV)

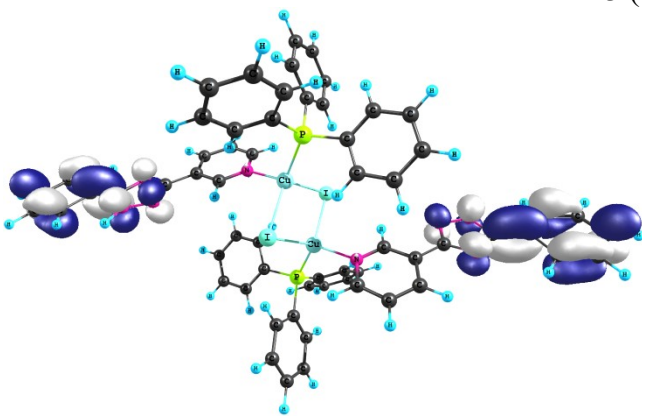


HOMO-5 (-5.26 eV)

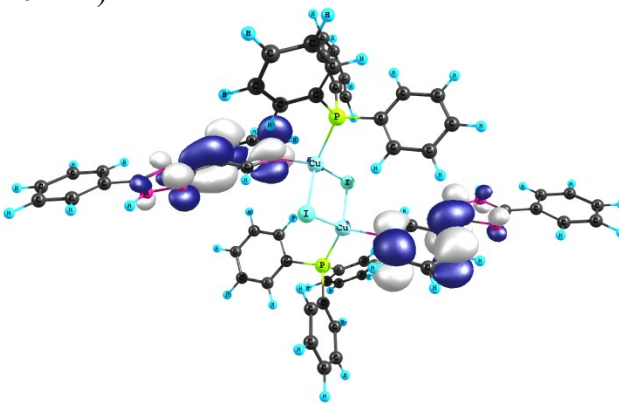
Figure S21. Selected molecular orbitals of the complex **4** calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.



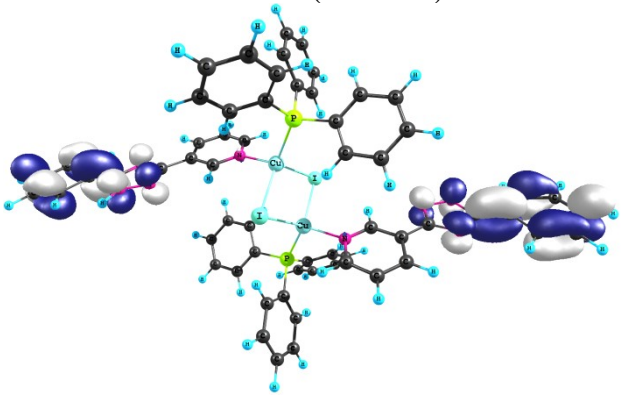
LUMO+3 (-1.02 eV)



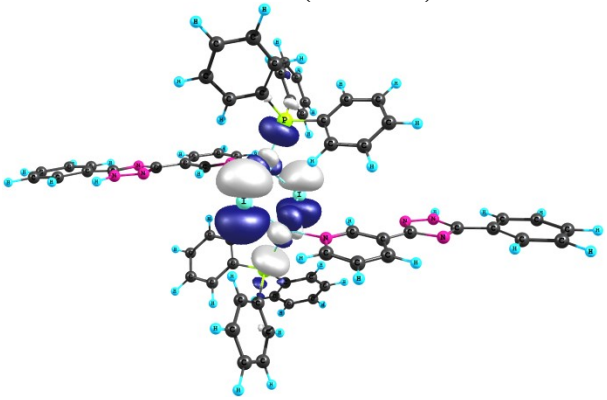
LUMO+1 (-1.03 eV)



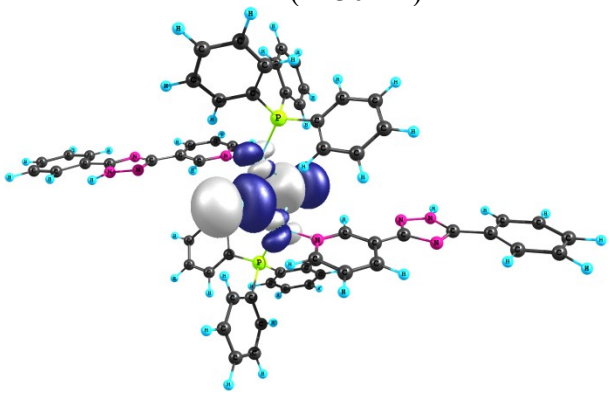
LUMO+2 (-1.29 eV)



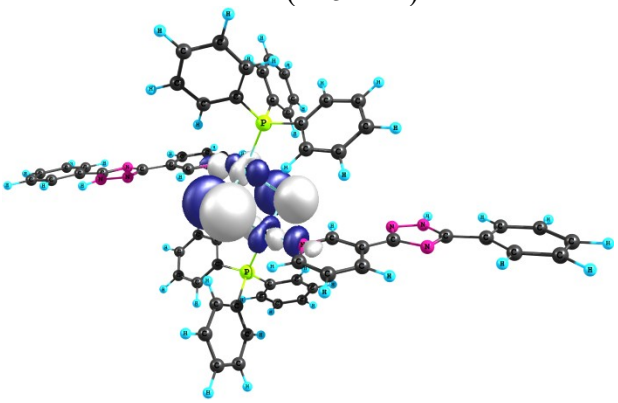
LUMO (-1.30 eV)



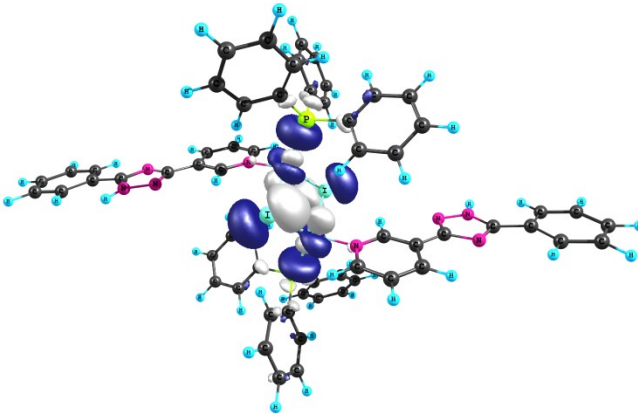
HOMO (-4.54 eV)



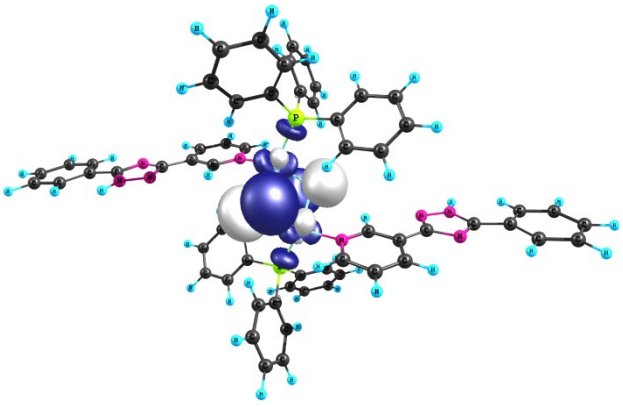
HOMO-1 (-4.84 eV)



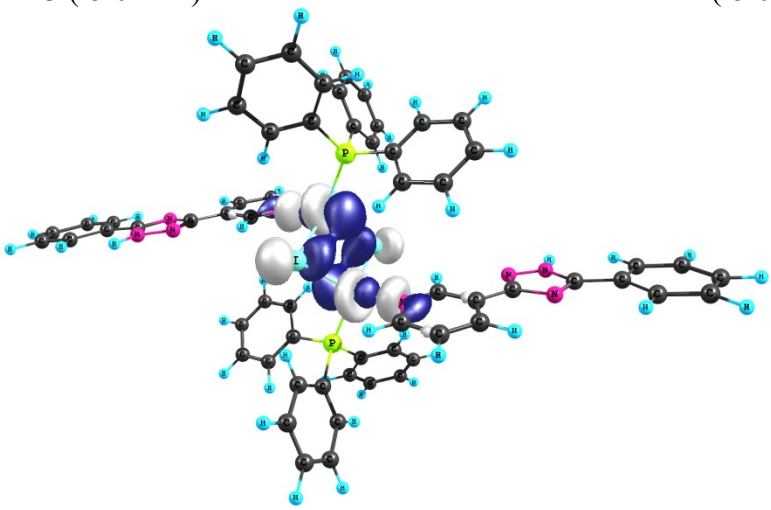
HOMO-2 (-4.93 eV)



HOMO-3 (-5.04 eV)



HOMO-4 (-5.07 eV)



HOMO-5 (-5.28 eV)

Figure S22. Selected molecular orbitals of the complex **5** calculated using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Table S4. Spectroscopic data of the S_1–S_0 electronic transition in the emission spectra of the **1**–**5** complexes calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Complex	Transition	$\lambda_{em.}$, nm	E, eV	f
1	S_1–S_0	693	1.79	0.0143
2	S_1–S_0	638	1.94	0.0348
3	S_1–S_0	601	2.06	0.0123
4	S_1–S_0	555	2.23	0.0344
5	S_1–S_0	502	2.47	0.0024

λ – the emission wavelength; f – calculated oscillator strength.

Table S5. Spectroscopic data of the T_1–S_0 electronic transition of the **1**–**5** complexes calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Complex	Transition	$\lambda_{em.}$, nm	*E*, eV	*f*
1	T_1–S_0	738	1.68	0
2	T_1–S_0	675	1.83	0
3	T_1–S_0	617	2.01	0
4	T_1–S_0	584	2.12	0
5	T_1–S_0	523	2.37	0

Table S6. The optimized Cartesian coordinates of the complex **1** in the ground singlet state (S_0) calculated at the DFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	29	-0.751064	-1.389570	0.038971
2	7	-2.887972	-1.176765	-0.199110
3	7	-7.836415	-1.286522	-1.785542
4	1	-7.536204	-1.803000	-2.600007
5	7	-9.144331	-0.996291	-1.636679
6	7	-7.930925	-0.192965	0.100594
7	7	-12.752762	1.231095	1.255366
8	6	-3.662802	-0.552587	0.705845
9	1	-3.143007	-0.148374	1.570024
10	6	-5.038625	-0.413554	0.557472
11	1	-5.629311	0.098924	1.307858
12	6	-5.659988	-0.942602	-0.581995
13	6	-4.847987	-1.585132	-1.528138
14	1	-5.252681	-2.014380	-2.439952
15	6	-3.480042	-1.675560	-1.297660
16	1	-2.826610	-2.160516	-2.015811
17	6	-7.108718	-0.804380	-0.741998
18	6	-9.158739	-0.331625	-0.478892
19	6	-10.393846	0.201231	0.111112
20	6	-10.363613	0.893562	1.327453
21	1	-9.423877	1.042801	1.847826
22	6	-11.561213	1.381854	1.847996
23	1	-11.563033	1.923509	2.792622
24	6	-12.768553	0.566373	0.091651
25	1	-13.743810	0.451341	-0.378765
26	6	-11.634343	0.036409	-0.519183
27	1	-11.706020	-0.493165	-1.463177
28	6	1.805955	-3.878639	0.100145
29	6	2.617423	-2.987709	0.822693
30	1	2.161613	-2.166647	1.370912
31	6	4.003030	-3.149828	0.834322
32	1	4.620084	-2.457603	1.400826
33	6	4.596920	-4.189179	0.113497
34	1	5.677206	-4.308251	0.117556
35	6	3.797817	-5.070355	-0.616290
36	1	4.253124	-5.878725	-1.182640
37	6	2.408922	-4.919397	-0.621539
38	1	1.796761	-5.611051	-1.192399
39	6	-0.509125	-4.500433	1.719689
40	6	0.171871	-5.628152	2.206203
41	1	1.039399	-6.008845	1.674931
42	6	-0.251762	-6.258599	3.376860
43	1	0.285499	-7.128750	3.745058
44	6	-1.357947	-5.770245	4.076800
45	1	-1.683036	-6.259901	4.990983

46	6	-2.036261	-4.644977	3.605869
47	1	-2.887665	-4.250756	4.154143
48	6	-1.610847	-4.010463	2.437455
49	1	-2.121696	-3.118285	2.087415
50	6	-0.678253	-4.680576	-1.185546
51	6	-0.555081	-4.202611	-2.503681
52	1	-0.067949	-3.248701	-2.689651
53	6	-1.059786	-4.940397	-3.574682
54	1	-0.949922	-4.559696	-4.586813
55	6	-1.708176	-6.157601	-3.347278
56	1	-2.105429	-6.729459	-4.181867
57	6	-1.844345	-6.633916	-2.042927
58	1	-2.347923	-7.579163	-1.856940
59	6	-1.330618	-5.903140	-0.967749
60	1	-1.438899	-6.288612	0.040823
61	15	-0.018417	-3.617389	0.175503
62	53	-0.142745	0.109017	2.297626
63	29	0.750709	1.389298	-0.039065
64	7	2.887595	1.175812	0.198605
65	7	7.836820	1.285009	1.782533
66	1	7.536988	1.801181	2.597331
67	7	9.144718	0.995173	1.632748
68	7	7.930528	0.192781	-0.104414
69	7	12.752016	-1.229709	-1.262613
70	6	3.662289	0.554018	-0.708112
71	1	3.142289	0.151653	-1.573031
72	6	5.038200	0.415032	-0.560582
73	1	5.628769	-0.095463	-1.312411
74	6	5.659815	0.941536	0.579924
75	6	4.847949	1.581461	1.527947
76	1	5.252817	2.008417	2.440760
77	6	3.479889	1.672060	1.298178
78	1	2.826542	2.154940	2.017804
79	6	7.108655	0.803445	0.739045
80	6	9.158627	0.331284	0.474509
81	6	10.393517	-0.200972	-0.116489
82	6	10.362741	-0.892732	-1.333141
83	1	9.422735	-1.041967	-1.853027
84	6	11.560157	-1.380485	-1.854615
85	1	11.561556	-1.921698	-2.799494
86	6	12.768326	-0.565529	-0.098595
87	1	13.743832	-0.450475	0.371301
88	6	11.634343	-0.036139	0.513156
89	1	11.706440	0.493005	1.457359
90	6	-1.805374	3.879330	-0.096462
91	6	-2.617818	2.988960	-0.818589
92	1	-2.162807	2.167851	-1.367411
93	6	-4.003369	3.151691	-0.829054
94	1	-4.621193	2.459895	-1.395236
95	6	-4.596212	4.191107	-0.107473
96	1	-5.676447	4.310673	-0.110651
97	6	-3.796132	5.071723	0.621926
98	1	-4.250625	5.880136	1.188870
99	6	-2.407306	4.920147	0.626010
100	1	-1.794380	5.611339	1.196612
101	6	0.508332	4.501980	-1.717460
102	6	-0.171683	5.631551	-2.201045
103	1	-1.037607	6.012884	-1.667614
104	6	0.250842	6.263044	-3.371525
105	1	-0.285638	7.134639	-3.737441
106	6	1.354922	5.773874	-4.074230
107	1	1.679140	6.264337	-4.988290
108	6	2.032246	4.646804	-3.606207
109	1	2.882004	4.252007	-4.156614
110	6	1.607955	4.011280	-2.437921
111	1	2.118040	3.117825	-2.090038
112	6	0.680270	4.679063	1.187846
113	6	0.555783	4.200981	2.505823
114	1	0.066608	3.248052	2.691419
115	6	1.061819	4.937375	3.577145
116	1	0.950893	4.556622	4.589140
117	6	1.712888	6.153245	3.350243
118	1	2.111157	6.724021	4.185090
119	6	1.850414	6.629614	2.046059
120	1	2.356077	7.573823	1.860452
121	6	1.335346	5.900262	0.970551
122	1	1.444663	6.285807	-0.037876
123	15	0.018838	3.617507	-0.173697
124	53	0.141772	-0.108944	-2.297644

Table S7. The optimized Cartesian coordinates of the complex **1** in the exited singlet state (S_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-3.209070	-3.798435	-0.063083
2	6	-3.402112	-4.981113	0.653987
3	6	-2.303152	-5.651219	1.195946
4	6	-1.014438	-5.146643	1.013969
5	6	-0.812156	-3.958900	0.292353
6	6	-1.923344	-3.282885	-0.235422
7	1	-1.778497	-2.359735	-0.789071
8	1	-4.059333	-3.275404	-0.492525
9	1	-4.403733	-5.381354	0.788219
10	1	-2.446651	-6.571524	1.755793
11	1	-0.165220	-5.676908	1.433696
12	6	1.935989	-3.556806	2.540000
13	6	2.723876	-4.135760	3.534044
14	6	3.531244	-5.236410	3.236598
15	6	3.541642	-5.759452	1.942902
16	6	2.748373	-5.187394	0.945980
17	6	1.936205	-4.080723	1.236362
18	1	2.717689	-3.717454	4.536775
19	1	4.155578	-5.678498	4.008100
20	1	4.171295	-6.612107	1.703967
21	1	2.767048	-5.599945	-0.057432
22	7	-13.095562	-1.289421	-1.353507
23	6	-12.888799	-1.851664	-0.155912
24	6	-11.660735	-1.862185	0.502611
25	6	-10.564379	-1.250347	-0.117767
26	6	-10.762733	-0.657952	-1.371206
27	6	-12.037903	-0.706775	-1.935062
28	1	-13.755857	-2.323756	0.303963
29	1	-11.554931	-2.332240	1.474248
30	6	-9.241350	-1.225529	0.520227
31	1	-9.938147	-0.177233	-1.885353
32	7	-9.006842	-1.776263	1.714915
33	7	-7.697319	-1.524149	1.900257
34	6	-7.181507	-0.842349	0.842816
35	7	-8.144802	-0.642657	-0.045867
36	1	-7.253277	-1.834466	2.753214
37	6	-5.790599	-0.403913	0.705640
38	6	-4.807821	-0.667744	1.668851
39	6	-3.510244	-0.211890	1.458691
40	7	-3.149045	0.478979	0.364768
41	6	-4.089178	0.725208	-0.567437
42	6	-5.408326	0.309227	-0.440149
43	1	-6.139006	0.528760	-1.209751
44	1	-5.022702	-1.225004	2.575458
45	1	-3.762867	1.280618	-1.440983
46	1	-2.720749	-0.407770	2.178204
47	29	-1.139962	1.228029	0.105446
48	6	-3.134679	5.293384	-0.827917
49	6	-2.217651	4.284040	-1.158581
50	6	-2.213350	3.767033	-2.466146
51	6	-3.100831	4.258308	-3.423333
52	6	-4.011839	5.262832	-3.085556
53	6	-4.026438	5.777552	-1.788473
54	1	-3.153210	5.704538	0.176209
55	1	-4.730601	6.560401	-1.519988
56	1	-4.706844	5.641111	-3.830098
57	1	-1.511605	2.982351	-2.737539
58	1	-3.081714	3.853533	-4.431473
59	6	-2.997269	4.240624	3.598451
60	6	-2.578688	3.724163	2.373130
61	6	-1.510166	4.313005	1.676661
62	6	-0.858196	5.418713	2.241685
63	6	-1.273478	5.927725	3.474332
64	6	-2.342959	5.343215	4.153333
65	1	-3.826344	3.776133	4.125448
66	1	-2.661602	5.739795	5.113330
67	1	-0.755880	6.781109	3.903492
68	1	-0.024107	5.880717	1.724553

69	1	-3.081989	2.856676	1.956263
70	15	-1.014606	3.589525	0.055157
71	53	0.287704	0.296761	2.210535
72	53	-0.290756	0.064839	-2.214653
73	29	1.217299	-0.926264	-0.129150
74	15	0.868664	-3.278989	-0.033153
75	6	0.589912	4.372182	-0.359303
76	6	0.658057	5.629571	-0.983598
77	6	1.774979	3.709411	-0.006658
78	6	3.012162	4.306371	-0.257148
79	6	3.073995	5.559409	-0.868591
80	6	1.897377	6.218564	-1.234481
81	1	1.943229	7.189810	-1.719572
82	1	4.038412	6.018621	-1.067421
83	1	3.922413	3.781607	0.014252
84	1	1.738119	2.725934	0.452208
85	1	-0.251903	6.145173	-1.275147
86	1	1.326287	-2.689379	2.776754
87	6	1.380195	-4.044305	-1.625721
88	6	0.690714	-5.112410	-2.218515
89	6	1.133852	-5.648230	-3.429669
90	6	2.267343	-5.127131	-4.055719
91	6	2.958941	-4.064140	-3.469663
92	6	2.516954	-3.518697	-2.264624
93	1	-0.190819	-5.526754	-1.739646
94	1	0.590862	-6.473657	-3.882375
95	1	2.609620	-5.546134	-4.998140
96	1	3.840492	-3.651808	-3.952147
97	1	3.051451	-2.683509	-1.822050
98	7	3.250252	-0.420716	-0.387856
99	6	4.169343	-0.684434	0.602394
100	6	5.515726	-0.462041	0.486128
101	6	6.063375	0.076685	-0.724046
102	6	5.099600	0.349357	-1.753482
103	6	3.766338	0.098103	-1.542685
104	1	3.763035	-1.093527	1.522024
105	1	6.182288	-0.691615	1.309874
106	6	7.456970	0.308439	-0.858537
107	1	5.400132	0.767504	-2.710799
108	1	3.044332	0.317792	-2.323141
109	7	8.412977	0.093893	0.071655
110	6	9.561377	0.470072	-0.545227
111	7	9.430916	0.910730	-1.796749
112	7	8.084170	0.806640	-1.984163
113	1	7.690419	1.057602	-2.876188
114	6	10.874051	0.400658	0.114195
115	6	10.990402	-0.067459	1.429420
116	6	12.255644	-0.116737	2.014055
117	7	13.388591	0.257626	1.402176
118	6	13.260276	0.703523	0.143835
119	6	12.050350	0.794895	-0.538291
120	1	12.009610	1.162742	-1.557866
121	1	14.184751	1.008044	-0.346837
122	1	10.102611	-0.379539	1.967739
123	1	-12.215685	-0.257699	-2.909083
124	1	12.367080	-0.473833	3.037420

Table S8. The optimized Cartesian coordinates of the complex **1** in the exited triplet state (T_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	29	-0.892923	-1.268647	0.020453
2	7	-2.968991	-1.027792	-0.202660
3	7	-7.963895	-1.134481	-1.831935
4	1	-7.652391	-1.630065	-2.648152
5	7	-9.297924	-0.848051	-1.691190
6	7	-8.101965	-0.073583	0.099151
7	7	-12.942770	1.293056	1.206663
8	6	-3.812111	-0.427661	0.732501
9	1	-3.337551	-0.034551	1.621561
10	6	-5.156530	-0.302513	0.593803
11	1	-5.737925	0.182344	1.369111

12	6	-5.838114	-0.801098	-0.590414
13	6	-4.953305	-1.433618	-1.558430
14	1	-5.337907	-1.848347	-2.486884
15	6	-3.614134	-1.517562	-1.328384
16	1	-2.983873	-1.994659	-2.072255
17	6	-7.220728	-0.669906	-0.749199
18	6	-9.303286	-0.217238	-0.518550
19	6	-10.551015	0.294046	0.063511
20	6	-10.549810	0.955568	1.298096
21	1	-9.613910	1.088104	1.829658
22	6	-11.755413	1.426937	1.814323
23	1	-11.770283	1.943387	2.774540
24	6	-12.931871	0.657043	0.025320
25	1	-13.900117	0.550286	-0.464295
26	6	-11.787222	0.146699	-0.581636
27	1	-11.838005	-0.359312	-1.539706
28	6	1.629966	-3.789951	0.162106
29	6	2.460777	-2.908657	0.873893
30	1	2.034878	-2.055469	1.393674
31	6	3.838029	-3.122780	0.915217
32	1	4.472214	-2.436677	1.467892
33	6	4.399581	-4.207345	0.236765
34	1	5.473559	-4.367434	0.263290
35	6	3.579783	-5.080362	-0.480185
36	1	4.011998	-5.923480	-1.011401
37	6	2.199494	-4.875765	-0.520346
38	1	1.570350	-5.559453	-1.081348
39	6	-0.810296	-4.215844	1.747147
40	6	-0.160538	-5.287900	2.378337
41	1	0.754968	-5.698474	1.962965
42	6	-0.688966	-5.819828	3.553985
43	1	-0.182300	-6.647107	4.042600
44	6	-1.858919	-5.288312	4.103382
45	1	-2.264381	-5.706420	5.020266
46	6	-2.507023	-4.221870	3.476745
47	1	-3.417741	-3.807828	3.897888
48	6	-1.985404	-3.680563	2.301736
49	1	-2.499814	-2.856598	1.814191
50	6	-0.869122	-4.528632	-1.171288
51	6	-0.658458	-4.129043	-2.501652
52	1	-0.107153	-3.219874	-2.721286
53	6	-1.153506	-4.896678	-3.552772
54	1	-0.984855	-4.578793	-4.577294
55	6	-1.878203	-6.060876	-3.285437
56	1	-2.277200	-6.652045	-4.104325
57	6	-2.099452	-6.456643	-1.966143
58	1	-2.667838	-7.356872	-1.753000
59	6	-1.600173	-5.694691	-0.909013
60	1	-1.780103	-6.010251	0.112895
61	15	-0.183148	-3.503864	0.185834
62	53	-0.098666	0.092083	2.237906
63	29	0.876156	1.300166	-0.027233
64	7	2.993822	1.040285	0.206916
65	7	7.974888	1.140902	1.777013
66	1	7.693213	1.683076	2.580180
67	7	9.280716	0.823109	1.619551
68	7	8.042752	-0.005339	-0.091762
69	7	12.831528	-1.529760	-1.242677
70	6	3.784774	0.391643	-0.689804
71	1	3.276967	-0.028549	-1.550596
72	6	5.149193	0.248360	-0.543659
73	1	5.731470	-0.281384	-1.288610
74	6	5.799107	0.792892	0.590610
75	6	4.973230	1.466741	1.524190
76	1	5.379121	1.914952	2.426048
77	6	3.614299	1.562115	1.295156
78	1	2.977756	2.079918	2.005458
79	6	7.225628	0.642843	0.744739
80	6	9.271542	0.130751	0.477579
81	6	10.495206	-0.434996	-0.107435
82	6	10.447920	-1.154168	-1.308050
83	1	9.502249	-1.298265	-1.819073
84	6	11.633644	-1.673583	-1.824649
85	1	11.620736	-2.235935	-2.757262
86	6	12.864629	-0.838976	-0.094177
87	1	13.844413	-0.729101	0.368159
88	6	11.742979	-0.276924	0.510717
89	1	11.828689	0.272771	1.441987
90	6	-1.617084	3.854697	-0.089105
91	6	-2.490357	2.940914	-0.701757
92	1	-2.108793	2.044602	-1.179263

93	6	-3.866471	3.159941	-0.670819
94	1	-4.534348	2.434621	-1.119594
95	6	-4.378397	4.287907	-0.026457
96	1	-5.451820	4.445463	0.010407
97	6	-3.515312	5.196237	0.589989
98	1	-3.912664	6.068883	1.100830
99	6	-2.136940	4.982839	0.564930
100	1	-1.474252	5.691300	1.052885
101	6	0.748587	4.299510	-1.765872
102	6	0.084735	5.398388	-2.332404
103	1	-0.798754	5.807763	-1.852177
104	6	0.548557	5.954615	-3.524836
105	1	0.025342	6.800717	-3.960709
106	6	1.672221	5.421513	-4.161039
107	1	2.025331	5.855038	-5.092338
108	6	2.335236	4.326454	-3.604305
109	1	3.204926	3.903604	-4.099099
110	6	1.873739	3.764329	-2.413426
111	1	2.388293	2.906773	-1.989248
112	6	0.930966	4.579326	1.142362
113	6	0.764674	4.179530	2.479886
114	1	0.194569	3.285617	2.715495
115	6	1.311338	4.934050	3.516601
116	1	1.164883	4.619594	4.545995
117	6	2.045027	6.088587	3.230022
118	1	2.475668	6.674224	4.037161
119	6	2.221954	6.486858	1.904862
120	1	2.789605	7.384142	1.675496
121	6	1.668547	5.738198	0.863250
122	1	1.808014	6.061705	-0.162760
123	15	0.185366	3.549293	-0.188593
124	53	0.183523	-0.120368	-2.233162

Table S9. The optimized Cartesian coordinates of the complex **2** in the ground singlet state (S_0) calculated at the DFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	29	1.203976	-0.064035	1.090936
2	7	0.629431	-1.217712	2.821280
3	7	0.014526	-4.839897	6.428329
4	7	-1.923233	-4.673017	7.592610
5	7	-1.821659	-3.686189	6.677414
6	1	-2.573137	-3.017661	6.585956
7	7	1.146737	-8.303871	8.653129
8	6	1.328281	-2.314526	3.169950
9	1	2.227043	-2.510475	2.593485
10	6	0.942222	-3.167022	4.196478
11	1	1.532383	-4.040878	4.447294
12	6	-0.234547	-2.888140	4.906922
13	6	-0.960164	-1.746221	4.542678
14	1	-1.880395	-1.462493	5.044388
15	6	-0.495440	-0.946696	3.503434
16	1	-1.037986	-0.059936	3.188469
17	6	-0.659280	-3.788867	5.979666
18	6	-0.786788	-5.350153	7.408926
19	6	-0.440770	-6.538270	8.197127
20	6	0.768042	-7.216053	7.975147
21	1	1.452067	-6.853285	7.212042
22	6	0.314746	-8.763070	9.596386
23	1	0.644955	-9.650173	10.134707
24	6	-0.911718	-8.166887	9.900229
25	1	-1.547420	-8.582790	10.676277
26	6	-1.296696	-7.035382	9.189104
27	1	-2.240178	-6.536653	9.388008
28	6	4.689925	-0.507054	1.399128
29	6	4.546538	-1.725639	0.711089
30	1	3.697774	-1.874534	0.048187
31	6	5.480995	-2.748417	0.880043
32	1	5.357013	-3.682753	0.338919
33	6	6.562279	-2.576054	1.747718
34	1	7.284833	-3.376107	1.885610
35	6	6.707112	-1.373750	2.441859

36	1	7.543580	-1.233857	3.121756
37	6	5.779492	-0.343547	2.268111
38	1	5.904233	0.586028	2.814153
39	6	3.699680	2.015093	2.471393
40	6	2.901007	1.946521	3.623239
41	1	2.115062	1.199236	3.684542
42	6	3.097658	2.839926	4.677360
43	1	2.468779	2.777594	5.561453
44	6	4.087034	3.820730	4.587929
45	1	4.234692	4.522399	5.404614
46	6	4.879375	3.905319	3.440777
47	1	5.645354	4.672493	3.362662
48	6	4.687730	3.009082	2.388022
49	1	5.303638	3.087260	1.496919
50	6	3.952621	1.678002	-0.384520
51	6	5.189652	1.450773	-1.004453
52	1	5.870394	0.707238	-0.601672
53	6	5.555567	2.179430	-2.139551
54	1	6.518222	1.994389	-2.609430
55	6	4.694695	3.146314	-2.660826
56	1	4.987390	3.721943	-3.535667
57	6	3.458186	3.375551	-2.050409
58	1	2.781351	4.126356	-2.449771
59	6	3.083185	2.640934	-0.925409
60	1	2.113330	2.813047	-0.465268
61	53	0.721805	-1.949785	-0.932786
62	15	3.393417	0.783683	1.130822
63	29	-1.203976	0.064035	-1.090936
64	7	-0.629431	1.217712	-2.821280
65	7	-0.014526	4.839897	-6.428329
66	7	1.923233	4.673017	-7.592610
67	7	1.821659	3.686189	-6.677414
68	1	2.573137	3.017661	-6.585956
69	7	-1.146737	8.303871	-8.653129
70	6	-1.328281	2.314526	-3.169950
71	1	-2.227043	2.510475	-2.593485
72	6	-0.942222	3.167022	-4.196478
73	1	-1.532383	4.040878	-4.447294
74	6	0.234547	2.888140	-4.906922
75	6	0.960164	1.746221	-4.542678
76	1	1.880395	1.462493	-5.044388
77	6	0.495440	0.946696	-3.503434
78	1	1.037986	0.059936	-3.188469
79	6	0.659280	3.788867	-5.979666
80	6	0.786788	5.350153	-7.408926
81	6	0.440770	6.538270	-8.197127
82	6	-0.768042	7.216053	-7.975147
83	1	-1.452067	6.853285	-7.212042
84	6	-0.314746	8.763070	-9.596386
85	1	-0.644955	9.650173	-10.134707
86	6	0.911718	8.166887	-9.900229
87	1	1.547420	8.582790	-10.676277
88	6	1.296696	7.035382	-9.189104
89	1	2.240178	6.536653	-9.388008
90	6	-4.689925	0.507054	-1.399128
91	6	-4.546538	1.725639	-0.711089
92	1	-3.697774	1.874534	-0.048187
93	6	-5.480995	2.748417	-0.880043
94	1	-5.357013	3.682753	-0.338919
95	6	-6.562279	2.576054	-1.747718
96	1	-7.284833	3.376107	-1.885610
97	6	-6.707112	1.373750	-2.441859
98	1	-7.543580	1.233857	-3.121756
99	6	-5.779492	0.343547	-2.268111
100	1	-5.904233	-0.586028	-2.814153
101	6	-3.699680	-2.015093	-2.471393
102	6	-2.901007	-1.946521	-3.623239
103	1	-2.115062	-1.199236	-3.684542
104	6	-3.097658	-2.839926	-4.677360
105	1	-2.468779	-2.777594	-5.561453
106	6	-4.087034	-3.820730	-4.587929
107	1	-4.234692	-4.522399	-5.404614
108	6	-4.879375	-3.905319	-3.440777
109	1	-5.645354	-4.672493	-3.362662
110	6	-4.687730	-3.009082	-2.388022
111	1	-5.303638	-3.087260	-1.496919
112	6	-3.952621	-1.678002	0.384520
113	6	-5.189652	-1.450773	1.004453
114	1	-5.870394	-0.707238	0.601672
115	6	-5.555567	-2.179430	2.139551
116	1	-6.518222	-1.994389	2.609430

117	6	-4.694695	-3.146314	2.660826
118	1	-4.987390	-3.721943	3.535667
119	6	-3.458186	-3.375551	2.050409
120	1	-2.781351	-4.126356	2.449771
121	6	-3.083185	-2.640934	0.925409
122	1	-2.113330	-2.813047	0.465268
123	53	-0.721805	1.949785	0.932786
124	15	-3.393417	-0.783683	-1.130822

Table S10. The optimized Cartesian coordinates of the complex **2** in the exited singlet state (S_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	29	1.045319	-0.256558	1.170368
2	7	0.489243	-1.432689	2.851917
3	7	0.140900	-4.984824	6.595278
4	7	-1.359506	-4.482110	8.225455
5	7	-1.327616	-3.509322	7.280777
6	1	-1.917491	-2.698584	7.389053
7	7	1.154142	-8.639965	8.547560
8	6	1.113984	-2.616615	3.106322
9	1	1.859420	-2.924958	2.379998
10	6	0.842013	-3.404496	4.204615
11	1	1.368745	-4.339419	4.357893
12	6	-0.135913	-2.991726	5.145137
13	6	-0.786947	-1.760603	4.873860
14	1	-1.557603	-1.365831	5.530024
15	6	-0.451387	-1.037715	3.745138
16	1	-0.951556	-0.100659	3.521612
17	6	-0.422479	-3.807940	6.297290
18	6	-0.455597	-5.349142	7.762805
19	6	-0.139944	-6.596780	8.470240
20	6	0.815901	-7.487992	7.958403
21	1	1.323358	-7.246105	7.028018
22	6	0.535681	-8.949879	9.694094
23	1	0.827109	-9.892385	10.155733
24	6	-0.430709	-8.138055	10.292527
25	1	-0.900827	-8.439466	11.224215
26	6	-0.774302	-6.941824	9.670858
27	1	-1.519088	-6.276173	10.095903
28	6	4.490788	-0.745419	1.569090
29	6	4.439351	-1.916365	0.793654
30	1	3.681106	-2.023573	0.022677
31	6	5.354839	-2.946073	1.008234
32	1	5.304055	-3.845629	0.401023
33	6	6.324684	-2.825545	2.006977
34	1	7.031329	-3.632400	2.180436
35	6	6.378690	-1.668449	2.785193
36	1	7.129608	-1.569335	3.564309
37	6	5.468184	-0.631425	2.569018
38	1	5.519297	0.264668	3.178772
39	6	3.453449	1.766479	2.625477
40	6	2.799780	1.469029	3.833513
41	1	2.195006	0.570187	3.914595
42	6	2.916216	2.325892	4.927162
43	1	2.407931	2.084047	5.856459
44	6	3.672322	3.496256	4.823431
45	1	3.754940	4.168288	5.673239
46	6	4.315457	3.803403	3.623595
47	1	4.900225	4.715000	3.535575
48	6	4.209803	2.943514	2.528077
49	1	4.712419	3.193741	1.599323
50	6	3.910253	1.454192	-0.250116
51	6	5.279237	1.463697	-0.565131
52	1	5.984561	0.918309	0.054696
53	6	5.738318	2.170871	-1.676815
54	1	6.799080	2.172868	-1.912856
55	6	4.838206	2.872310	-2.482759
56	1	5.198634	3.423109	-3.347438
57	6	3.475283	2.859642	-2.180497
58	1	2.768648	3.392812	-2.809295

59	6	3.009933	2.148970	-1.072720
60	1	1.947044	2.129787	-0.852642
61	53	0.668304	-1.871278	-1.035006
62	15	3.259502	0.583266	1.229963
63	29	-1.045319	0.256558	-1.170368
64	7	-0.489243	1.432689	-2.851917
65	7	-0.140900	4.984824	-6.595278
66	7	1.359506	4.482110	-8.225455
67	7	1.327616	3.509322	-7.280777
68	1	1.917491	2.698584	-7.389053
69	7	-1.154142	8.639965	-8.547560
70	6	-1.113984	2.616615	-3.106322
71	1	-1.859420	2.924958	-2.379998
72	6	-0.842013	3.404496	-4.204615
73	1	-1.368745	4.339419	-4.357893
74	6	0.135913	2.991726	-5.145137
75	6	0.786947	1.760603	-4.873860
76	1	1.557603	1.365831	-5.530024
77	6	0.451387	1.037715	-3.745138
78	1	0.951556	0.100659	-3.521612
79	6	0.422479	3.807940	-6.297290
80	6	0.455597	5.349142	-7.762805
81	6	0.139944	6.596780	-8.470240
82	6	-0.815901	7.487992	-7.958403
83	1	-1.323358	7.246105	-7.028018
84	6	-0.535681	8.949879	-9.694094
85	1	-0.827109	9.892385	-10.155733
86	6	0.430709	8.138055	-10.292527
87	1	0.900827	8.439466	-11.224215
88	6	0.774302	6.941824	-9.670858
89	1	1.519088	6.276173	-10.095903
90	6	-4.490788	0.745419	-1.569090
91	6	-4.439351	1.916365	-0.793654
92	1	-3.681106	2.023573	-0.022677
93	6	-5.354839	2.946073	-1.008234
94	1	-5.304055	3.845629	-0.401023
95	6	-6.324684	2.825545	-2.006977
96	1	-7.031329	3.632400	-2.180436
97	6	-6.378690	1.668449	-2.785193
98	1	-7.129608	1.569335	-3.564309
99	6	-5.468184	0.631425	-2.569018
100	1	-5.519297	-0.264668	-3.178772
101	6	-3.453449	-1.766479	-2.625477
102	6	-2.799780	-1.469029	-3.833513
103	1	-2.195006	-0.570187	-3.914595
104	6	-2.916216	-2.325892	-4.927162
105	1	-2.407931	-2.084047	-5.856459
106	6	-3.672322	-3.496256	-4.823431
107	1	-3.754940	-4.168288	-5.673239
108	6	-4.315457	-3.803403	-3.623595
109	1	-4.900225	-4.715000	-3.535575
110	6	-4.209803	-2.943514	-2.528077
111	1	-4.712419	-3.193741	-1.599323
112	6	-3.910253	-1.454192	0.250116
113	6	-5.279237	-1.463697	0.565131
114	1	-5.984561	-0.918309	-0.054696
115	6	-5.738318	-2.170871	1.676815
116	1	-6.799080	-2.172868	1.912856
117	6	-4.838206	-2.872310	2.482759
118	1	-5.198634	-3.423109	3.347438
119	6	-3.475283	-2.859642	2.180497
120	1	-2.768648	-3.392812	2.809295
121	6	-3.009933	-2.148970	1.072720
122	1	-1.947044	-2.129787	0.852642
123	53	-0.668304	1.871278	1.035006
124	15	-3.259502	-0.583266	-1.229963

Table S11. The optimized Cartesian coordinates of the complex **2** in the exited triplet state (T_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	29	1.046376	-0.257755	1.248235
2	7	0.486669	-1.409198	2.907983
3	7	0.078845	-5.002469	6.605759
4	7	-1.267613	-4.414540	8.338430
5	7	-1.213442	-3.426479	7.411104
6	1	-1.731503	-2.575582	7.567899
7	7	0.911680	-8.768070	8.429398
8	6	1.013713	-2.653380	3.094907
9	1	1.672433	-3.009672	2.309390
10	6	0.745145	-3.439683	4.194297
11	1	1.190979	-4.422902	4.292028
12	6	-0.121459	-2.961816	5.211121
13	6	-0.671387	-1.668607	5.010226
14	1	-1.353670	-1.221527	5.727843
15	6	-0.349644	-0.951431	3.875350
16	1	-0.774941	0.032603	3.704905
17	6	-0.401686	-3.776805	6.365406
18	6	-0.470595	-5.342670	7.803339
19	6	-0.216292	-6.627685	8.467198
20	6	0.635108	-7.578843	7.883777
21	1	1.108150	-7.355093	6.930987
22	6	0.335000	-9.056001	9.603089
23	1	0.574573	-10.029811	10.028113
24	6	-0.527466	-8.184764	10.272556
25	1	-0.967301	-8.470535	11.223748
26	6	-0.807893	-6.950260	9.695628
27	1	-1.471640	-6.238190	10.176093
28	6	4.492541	-0.690471	1.554446
29	6	4.539690	-1.790582	0.680327
30	1	3.851011	-1.848908	-0.158171
31	6	5.467029	-2.811537	0.881895
32	1	5.494059	-3.655092	0.197651
33	6	6.349626	-2.755381	1.964218
34	1	7.065826	-3.556368	2.125333
35	6	6.303855	-1.670364	2.840011
36	1	6.986450	-1.620634	3.683960
37	6	5.381697	-0.640533	2.637931
38	1	5.358044	0.200310	3.323119
39	6	3.440991	1.821424	2.616175
40	6	2.794061	1.543999	3.832503
41	1	2.187086	0.648347	3.930990
42	6	2.920998	2.416058	4.913221
43	1	2.418315	2.189332	5.849352
44	6	3.680098	3.582075	4.787457
45	1	3.770617	4.266071	5.626833
46	6	4.316016	3.869797	3.578802
47	1	4.903007	4.778109	3.473638
48	6	4.200442	2.994623	2.496916
49	1	4.697154	3.229815	1.561167
50	6	3.838677	1.482677	-0.267813
51	6	5.202493	1.525214	-0.602662
52	1	5.931593	1.010472	0.015965
53	6	5.624916	2.224690	-1.733471
54	1	6.681672	2.252792	-1.985279
55	6	4.693214	2.884560	-2.538839
56	1	5.025199	3.428748	-3.418938
57	6	3.335688	2.838763	-2.216432
58	1	2.605020	3.339870	-2.844205
59	6	2.906957	2.136544	-1.088590
60	1	1.848533	2.091047	-0.852624
61	53	0.748858	-1.825562	-1.006525
62	15	3.238273	0.621306	1.236918
63	29	-1.046376	0.257755	-1.248235
64	7	-0.486669	1.409198	-2.907983
65	7	-0.078845	5.002469	-6.605759
66	7	1.267613	4.414540	-8.338430
67	7	1.213442	3.426479	-7.411104
68	1	1.731503	2.575582	-7.567899
69	7	-0.911680	8.768070	-8.429398
70	6	-1.013713	2.653380	-3.094907
71	1	-1.672433	3.009672	-2.309390
72	6	-0.745145	3.439683	-4.194297
73	1	-1.190979	4.422902	-4.292028
74	6	0.121459	2.961816	-5.211121
75	6	0.671387	1.668607	-5.010226
76	1	1.353670	1.221527	-5.727843

77	6	0.349644	0.951431	-3.875350
78	1	0.774941	-0.032603	-3.704905
79	6	0.401686	3.776805	-6.365406
80	6	0.470595	5.342670	-7.803339
81	6	0.216292	6.627685	-8.467198
82	6	-0.635108	7.578843	-7.883777
83	1	-1.108150	7.355093	-6.930987
84	6	-0.335000	9.056001	-9.603089
85	1	-0.574573	10.029811	-10.028113
86	6	0.527466	8.184764	-10.272556
87	1	0.967301	8.470535	-11.223748
88	6	0.807893	6.950260	-9.695628
89	1	1.471640	6.238190	-10.176093
90	6	-4.492541	0.690471	-1.554446
91	6	-4.539690	1.790582	-0.680327
92	1	-3.851011	1.848908	0.158171
93	6	-5.467029	2.811537	-0.881895
94	1	-5.494059	3.655092	-0.197651
95	6	-6.349626	2.755381	-1.964218
96	1	-7.065826	3.556368	-2.125333
97	6	-6.303855	1.670364	-2.840011
98	1	-6.986450	1.620634	-3.683960
99	6	-5.381697	0.640533	-2.637931
100	1	-5.358044	-0.200310	-3.323119
101	6	-3.440991	-1.821424	-2.616175
102	6	-2.794061	-1.543999	-3.832503
103	1	-2.187086	-0.648347	-3.930990
104	6	-2.920998	-2.416058	-4.913221
105	1	-2.418315	-2.189332	-5.849352
106	6	-3.680098	-3.582075	-4.787457
107	1	-3.770617	-4.266071	-5.626833
108	6	-4.316016	-3.869797	-3.578802
109	1	-4.903007	-4.778109	-3.473638
110	6	-4.200442	-2.994623	-2.496916
111	1	-4.697154	-3.229815	-1.561167
112	6	-3.838677	-1.482677	0.267813
113	6	-5.202493	-1.525214	0.602662
114	1	-5.931593	-1.010472	-0.015965
115	6	-5.624916	-2.224690	1.733471
116	1	-6.681672	-2.252792	1.985279
117	6	-4.693214	-2.884560	2.538839
118	1	-5.025199	-3.428748	3.418938
119	6	-3.335688	-2.838763	2.216432
120	1	-2.605020	-3.339870	2.844205
121	6	-2.906957	-2.136544	1.088590
122	1	-1.848533	-2.091047	0.852624
123	53	-0.748858	1.825562	1.006525
124	15	-3.238273	-0.621306	-1.236918

Table S12. The optimized Cartesian coordinates of the complex **3** in the ground singlet state (S_0) calculated at the DFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.892748	0.955601	0.851548
2	29	0.686961	1.457208	-0.119601
3	15	0.713930	3.107142	-1.794622
4	7	0.157662	4.898562	4.406648
5	7	1.476514	4.240875	6.017992
6	1	2.139753	3.730945	6.583784
7	7	-2.980331	7.776678	4.721679
8	7	0.660849	5.146071	6.604772
9	7	1.749265	1.961382	1.707149
10	6	1.166255	4.091128	4.702903
11	6	-0.120408	5.522538	5.591322
12	6	-1.175917	6.530863	5.740412
13	6	1.857222	3.195807	3.773359
14	6	1.177681	2.741181	2.633294
15	1	0.138897	3.010284	2.471530
16	6	-3.163830	8.403028	5.890673
17	1	-3.961135	9.144364	5.916218
18	6	-0.135076	4.678612	-1.325319
19	6	-0.088488	2.632660	-3.386807
20	6	0.062624	5.159856	-0.020942

21	1	0.703057	4.611549	0.663136
22	6	-2.008061	6.861276	4.659244
23	1	-1.875186	6.354766	3.706371
24	6	3.022790	1.571116	1.892016
25	1	3.433099	0.922753	1.123373
26	6	2.404512	3.654552	-2.300818
27	6	2.738293	4.994971	-2.548382
28	1	1.983970	5.769091	-2.446314
29	6	5.017770	4.356919	-3.059043
30	1	6.028701	4.629369	-3.351045
31	6	-0.976949	5.395048	-2.188425
32	1	-1.149691	5.038263	-3.198996
33	6	4.038586	5.342383	-2.922939
34	1	4.283950	6.384916	-3.109005
35	6	-1.235039	1.823946	-3.326640
36	1	-1.602990	1.483883	-2.362226
37	6	-1.386521	7.196971	6.955179
38	1	-0.762076	6.965772	7.812542
39	6	-0.556456	6.331988	0.410613
40	1	-0.393525	6.681255	1.426472
41	6	0.387948	3.048014	-4.639359
42	1	1.277988	3.666403	-4.703856
43	6	3.185793	2.788905	3.953514
44	1	3.763820	3.137264	4.805943
45	6	-1.899468	1.455272	-4.496974
46	1	-2.787710	0.831918	-4.434623
47	6	3.770738	1.955566	3.003929
48	1	4.798375	1.622315	3.107714
49	6	-1.420079	1.874293	-5.740209
50	1	-1.935039	1.581985	-6.651965
51	6	-2.398633	8.147735	7.031363
52	1	-2.592805	8.685160	7.954905
53	6	-1.603651	6.565547	-1.753132
54	1	-2.258595	7.107122	-2.430851
55	6	-1.395781	7.036693	-0.455849
56	1	-1.890794	7.943072	-0.117879
57	6	-0.273825	2.667940	-5.809036
58	1	0.107681	2.993878	-6.773271
59	6	4.694278	3.020011	-2.814263
60	1	5.451468	2.246854	-2.915462
61	6	3.399289	2.669551	-2.430846
62	1	3.158731	1.628457	-2.229863
63	53	1.892748	-0.955601	-0.851548
64	29	-0.686961	-1.457208	0.119601
65	15	-0.713930	-3.107142	1.794622
66	7	-0.157662	-4.898562	-4.406648
67	7	-1.476514	-4.240875	-6.017992
68	1	-2.139753	-3.730945	-6.583784
69	7	2.980331	-7.776678	-4.721679
70	7	-0.660849	-5.146071	-6.604772
71	7	-1.749265	-1.961382	-1.707149
72	6	-1.166255	-4.091128	-4.702903
73	6	0.120408	-5.522538	-5.591322
74	6	1.175917	-6.530863	-5.740412
75	6	-1.857222	-3.195807	-3.773359
76	6	-1.177681	-2.741181	-2.633294
77	1	-0.138897	-3.010284	-2.471530
78	6	3.163830	-8.403028	-5.890673
79	1	3.961135	-9.144364	-5.916218
80	6	0.135076	-4.678612	1.325319
81	6	0.088488	-2.632660	3.386807
82	6	-0.062624	-5.159856	0.020942
83	1	-0.703057	-4.611549	-0.663136
84	6	2.008061	-6.861276	-4.659244
85	1	1.875186	-6.354766	-3.706371
86	6	-3.022790	-1.571116	-1.892016
87	1	-3.433099	-0.922753	-1.123373
88	6	-2.404512	-3.654552	2.300818
89	6	-2.738293	-4.994971	2.548382
90	1	-1.983970	-5.769091	2.446314
91	6	-5.017770	-4.356919	3.059043
92	1	-6.028701	-4.629369	3.351045
93	6	0.976949	-5.395048	2.188425
94	1	1.149691	-5.038263	3.198996
95	6	-4.038586	-5.342383	2.922939
96	1	-4.283950	-6.384916	3.109005
97	6	1.235039	-1.823946	3.326640
98	1	1.602990	-1.483883	2.362226
99	6	1.386521	-7.196971	-6.955179
100	1	0.762076	-6.965772	-7.812542
101	6	0.556456	-6.331988	-0.410613

102	1	0.393525	-6.681255	-1.426472
103	6	-0.387948	-3.048014	4.639359
104	1	-1.277988	-3.666403	4.703856
105	6	-3.185793	-2.788905	-3.953514
106	1	-3.763820	-3.137264	-4.805943
107	6	1.899468	-1.455272	4.496974
108	1	2.787710	-0.831918	4.434623
109	6	-3.770738	-1.955566	-3.003929
110	1	-4.798375	-1.622315	-3.107714
111	6	1.420079	-1.874293	5.740209
112	1	1.935039	-1.581985	6.651965
113	6	2.398633	-8.147735	-7.031363
114	1	2.592805	-8.685160	-7.954905
115	6	1.603651	-6.565547	1.753132
116	1	2.258595	-7.107122	2.430851
117	6	1.395781	-7.036693	0.455849
118	1	1.890794	-7.943072	0.117879
119	6	0.273825	-2.667940	5.809036
120	1	-0.107681	-2.993878	6.773271
121	6	-4.694278	-3.020011	2.814263
122	1	-5.451468	-2.246854	2.915462
123	6	-3.399289	-2.669551	2.430846
124	1	-3.158731	-1.628457	2.229863

Table S13. The optimized Cartesian coordinates of the complex **3** in the exited singlet state (S_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.808996	0.931163	0.882317
2	29	0.796137	1.397444	0.114502
3	15	0.748718	3.087843	-1.541338
4	7	0.354796	5.034898	4.362931
5	7	1.961154	4.828364	5.836788
6	1	2.757217	4.517887	6.372328
7	7	-2.927022	7.749427	4.548967
8	7	1.168094	5.812977	6.336761
9	7	1.871382	1.908297	1.894012
10	6	1.469698	4.354419	4.652038
11	6	0.215813	5.898134	5.407533
12	6	-0.885291	6.865615	5.502888
13	6	2.079383	3.318853	3.850439
14	6	1.384869	2.826351	2.729563
15	1	0.390212	3.205011	2.519542
16	6	-2.972630	8.636407	5.551313
17	1	-3.812597	9.329706	5.539706
18	6	-0.240045	4.526449	-0.967880
19	6	0.072821	2.638698	-3.189179
20	6	0.150922	5.173096	0.217723
21	1	1.057399	4.868464	0.732603
22	6	-1.905189	6.886189	4.538625
23	1	-1.883074	6.164332	3.726186
24	6	3.113433	1.392256	2.144867
25	1	3.470869	0.641452	1.450555
26	6	2.424640	3.766205	-1.890433
27	6	2.658849	5.134602	-2.099814
28	1	1.840374	5.843682	-2.024820
29	6	5.006514	4.689697	-2.489180
30	1	6.006337	5.048087	-2.718612
31	6	-1.419242	4.931355	-1.609137
32	1	-1.741108	4.438265	-2.520641
33	6	3.944378	5.591036	-2.397163
34	1	4.114022	6.652608	-2.555872
35	6	-0.748578	1.507719	-3.300434
36	1	-0.954364	0.898392	-2.426790
37	6	-0.955702	7.800610	6.544022
38	1	-0.184883	7.812232	7.308285
39	6	-0.620015	6.205446	0.748589
40	1	-0.311386	6.679654	1.674887
41	6	0.354096	3.402125	-4.334637
42	1	1.000743	4.271781	-4.264674
43	6	3.366736	2.765294	4.110935
44	1	3.966009	3.104456	4.951087

45	6	-1.292696	1.152794	-4.536768
46	1	-1.926485	0.273890	-4.608661
47	6	3.864584	1.798447	3.245733
48	1	4.844600	1.360570	3.412782
49	6	-1.012625	1.917936	-5.669360
50	1	-1.429718	1.637171	-6.632836
51	6	-2.018175	8.698643	6.569307
52	1	-2.106673	9.437929	7.360240
53	6	-2.189758	5.965968	-1.072867
54	1	-3.103442	6.269308	-1.576875
55	6	-1.795726	6.602120	0.105134
56	1	-2.404097	7.396438	0.528453
57	6	-0.187708	3.041686	-5.567567
58	1	0.037291	3.635724	-6.449288
59	6	4.781985	3.327270	-2.279325
60	1	5.604896	2.620865	-2.344680
61	6	3.500537	2.867446	-1.975608
62	1	3.335486	1.807270	-1.803832
63	53	1.808996	-0.931163	-0.882317
64	29	-0.796137	-1.397444	-0.114502
65	15	-0.748718	-3.087843	1.541338
66	7	-0.354796	-5.034898	-4.362931
67	7	-1.961154	-4.828364	-5.836788
68	1	-2.757217	-4.517887	-6.372328
69	7	2.927022	-7.749427	-4.548967
70	7	-1.168094	-5.812977	-6.336761
71	7	-1.871382	-1.908297	-1.894012
72	6	-1.469698	-4.354419	-4.652038
73	6	-0.215813	-5.898134	-5.407533
74	6	0.885291	-6.865615	-5.502888
75	6	-2.079383	-3.318853	-3.850439
76	6	-1.384869	-2.826351	-2.729563
77	1	-0.390212	-3.205011	-2.519542
78	6	2.972630	-8.636407	-5.551313
79	1	3.812597	-9.329706	-5.539706
80	6	0.240045	-4.526449	0.967880
81	6	-0.072821	-2.638698	3.189179
82	6	-0.150922	-5.173096	-0.217723
83	1	-1.057399	-4.868464	-0.732603
84	6	1.905189	-6.886189	-4.538625
85	1	1.883074	-6.164332	-3.726186
86	6	-3.113433	-1.392256	-2.144867
87	1	-3.470869	-0.641452	-1.450555
88	6	-2.424640	-3.766205	1.890433
89	6	-2.658849	-5.134602	2.099814
90	1	-1.840374	-5.843682	2.024820
91	6	-5.006514	-4.689697	2.489180
92	1	-6.006337	-5.048087	2.718612
93	6	1.419242	-4.931355	1.609137
94	1	1.741108	-4.438265	2.520641
95	6	-3.944378	-5.591036	2.397163
96	1	-4.114022	-6.652608	2.555872
97	6	0.748578	-1.507719	3.300434
98	1	0.954364	-0.898392	2.426790
99	6	0.955702	-7.800610	-6.544022
100	1	0.184883	-7.812232	-7.308285
101	6	0.620015	-6.205446	-0.748589
102	1	0.311386	-6.679654	-1.674887
103	6	-0.354096	-3.402125	4.334637
104	1	-1.000743	-4.271781	4.264674
105	6	-3.366736	-2.765294	-4.110935
106	1	-3.966009	-3.104456	-4.951087
107	6	1.292696	-1.152794	4.536768
108	1	1.926485	-0.273890	4.608661
109	6	-3.864584	-1.798447	-3.245733
110	1	-4.844600	-1.360570	-3.412782
111	6	1.012625	-1.917936	5.669360
112	1	1.429718	-1.637171	6.632836
113	6	2.018175	-8.698643	-6.569307
114	1	2.106673	-9.437929	-7.360240
115	6	2.189758	-5.965968	1.072867
116	1	3.103442	-6.269308	1.576875
117	6	1.795726	-6.602120	-0.105134
118	1	2.404097	-7.396438	-0.528453
119	6	0.187708	-3.041686	5.567567
120	1	-0.037291	-3.635724	6.449288
121	6	-4.781985	-3.327270	2.279325
122	1	-5.604896	-2.620865	2.344680
123	6	-3.500537	-2.867446	1.975608
124	1	-3.335486	-1.807270	1.803832

Table S14. The optimized Cartesian coordinates of the complex **3** in the exited triplet state (T_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	-1.792360	0.942043	0.867505
2	29	0.820774	1.422783	0.115387
3	15	0.758952	3.070332	-1.575192
4	7	0.341407	5.004701	4.383168
5	7	1.944260	4.785172	5.857322
6	1	2.741025	4.469465	6.389002
7	7	-2.975422	7.675095	4.621988
8	7	1.137519	5.747180	6.377275
9	7	1.896671	1.928259	1.870530
10	6	1.462809	4.332572	4.661569
11	6	0.186982	5.842007	5.447220
12	6	-0.927295	6.791985	5.562108
13	6	2.091217	3.320888	3.840610
14	6	1.397043	2.824482	2.726426
15	1	0.389520	3.177956	2.533811
16	6	-3.039911	8.530698	5.650136
17	1	-3.890101	9.211513	5.654182
18	6	-0.217129	4.525998	-1.023687
19	6	0.076294	2.592155	-3.211115
20	6	0.137539	5.138242	0.191164
21	1	1.003082	4.788437	0.746018
22	6	-1.941049	6.827532	4.591851
23	1	-1.903533	6.131289	3.757791
24	6	3.157167	1.442960	2.104157
25	1	3.526502	0.709550	1.397539
26	6	2.438758	3.728191	-1.943164
27	6	2.692296	5.096915	-2.123849
28	1	1.886994	5.817200	-2.019655
29	6	5.025254	4.622510	-2.563883
30	1	6.027065	4.969474	-2.802046
31	6	-1.344244	4.987989	-1.717549
32	1	-1.638191	4.522387	-2.652587
33	6	3.980477	5.538856	-2.432348
34	1	4.165298	6.600944	-2.569117
35	6	-0.780774	1.485177	-3.292301
36	1	-1.009509	0.909180	-2.401996
37	6	-1.017084	7.694579	6.630072
38	1	-0.251333	7.694034	7.399497
39	6	-0.617729	6.192989	0.699834
40	1	-0.338152	6.640356	1.648661
41	6	0.386525	3.311551	-4.377433
42	1	1.060576	4.161734	-4.330365
43	6	3.397764	2.801418	4.082920
44	1	3.998673	3.151474	4.917041
45	6	-1.331453	1.111309	-4.519910
46	1	-1.992332	0.250942	-4.568640
47	6	3.909446	1.856455	3.199241
48	1	4.902803	1.442805	3.348493
49	6	-1.023113	1.833166	-5.673541
50	1	-1.445736	1.537355	-6.630082
51	6	-2.092202	8.576513	6.675293
52	1	-2.195905	9.290580	7.487255
53	6	-2.099601	6.044978	-1.203524
54	1	-2.973508	6.392516	-1.747918
55	6	-1.741680	6.646736	0.003587
56	1	-2.338904	7.459194	0.407894
57	6	-0.162687	2.932140	-5.601583
58	1	0.084497	3.492085	-6.499518
59	6	4.781026	3.259132	-2.382629
60	1	5.590576	2.540949	-2.479141
61	6	3.497505	2.813376	-2.067901
62	1	3.317290	1.752107	-1.918972
63	53	1.792360	-0.942043	-0.867505
64	29	-0.820774	-1.422783	-0.115387
65	15	-0.758952	-3.070332	1.575192
66	7	-0.341407	-5.004701	-4.383168
67	7	-1.944260	-4.785172	-5.857322

68	1	-2.741025	-4.469465	-6.389002
69	7	2.975422	-7.675095	-4.621988
70	7	-1.137519	-5.747180	-6.377275
71	7	-1.896671	-1.928259	-1.870530
72	6	-1.462809	-4.332572	-4.661569
73	6	-0.186982	-5.842007	-5.447220
74	6	0.927295	-6.791985	-5.562108
75	6	-2.091217	-3.320888	-3.840610
76	6	-1.397043	-2.824482	-2.726426
77	1	-0.389520	-3.177956	-2.533811
78	6	3.039911	-8.530698	-5.650136
79	1	3.890101	-9.211513	-5.654182
80	6	0.217129	-4.525998	1.023687
81	6	-0.076294	-2.592155	3.211115
82	6	-0.137539	-5.138242	-0.191164
83	1	-1.003082	-4.788437	-0.746018
84	6	1.941049	-6.827532	-4.591851
85	1	1.903533	-6.131289	-3.757791
86	6	-3.157167	-1.442960	-2.104157
87	1	-3.526502	-0.709550	-1.397539
88	6	-2.438758	-3.728191	1.943164
89	6	-2.692296	-5.096915	2.123849
90	1	-1.886994	-5.817200	2.019655
91	6	-5.025254	-4.622510	2.563883
92	1	-6.027065	-4.969474	2.802046
93	6	1.344244	-4.987989	1.717549
94	1	1.638191	-4.522387	2.652587
95	6	-3.980477	-5.538856	2.432348
96	1	-4.165298	-6.600944	2.569117
97	6	0.780774	-1.485177	3.292301
98	1	1.009509	-0.909180	2.401996
99	6	1.017084	-7.694579	-6.630072
100	1	0.251333	-7.694034	-7.399497
101	6	0.617729	-6.192989	-0.699834
102	1	0.338152	-6.640356	-1.648661
103	6	-0.386525	-3.311551	4.377433
104	1	-1.060576	-4.161734	4.330365
105	6	-3.397764	-2.801418	-4.082920
106	1	-3.998673	-3.151474	-4.917041
107	6	1.331453	-1.111309	4.519910
108	1	1.992332	-0.250942	4.568640
109	6	-3.909446	-1.856455	-3.199241
110	1	-4.902803	-1.442805	-3.348493
111	6	1.023113	-1.833166	5.673541
112	1	1.445736	-1.537355	6.630082
113	6	2.092202	-8.576513	-6.675293
114	1	2.195905	-9.290580	-7.487255
115	6	2.099601	-6.044978	1.203524
116	1	2.973508	-6.392516	1.747918
117	6	1.741680	-6.646736	-0.003587
118	1	2.338904	-7.459194	-0.407894
119	6	0.162687	-2.932140	5.601583
120	1	-0.084497	-3.492085	6.499518
121	6	-4.781026	-3.259132	2.382629
122	1	-5.590576	-2.540949	2.479141
123	6	-3.497505	-2.813376	2.067901
124	1	-3.317290	-1.752107	1.918972

Table S15. The optimized Cartesian coordinates of the complex **4** in the ground singlet state (S_0) calculated at the DFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	29	0.973097	1.273119	-0.162606
2	53	-1.577106	1.067423	-1.274260
3	15	1.226266	3.217123	1.136908
4	7	2.331756	1.140487	-1.823489

5	7	4.742854	0.847833	-6.331038
6	7	5.925905	0.743196	-6.973635
7	7	6.466275	0.742579	-4.861029
8	6	1.910830	1.139259	-3.101692
9	1	0.835832	1.207647	-3.242154
10	6	2.778208	1.044344	-4.184230
11	1	2.391843	1.043776	-5.197376
12	6	4.155822	0.943715	-3.947838
13	6	4.593462	0.936649	-2.616945
14	1	5.650422	0.855822	-2.390170
15	6	3.653744	1.034101	-1.597045
16	1	3.958132	1.023793	-0.555160
17	6	5.118333	0.844438	-5.051861
18	6	6.960854	0.679745	-6.091169
19	6	8.376872	0.561117	-6.449602
20	6	8.813480	0.572417	-7.783961
21	1	8.102977	0.678157	-8.600243
22	6	10.169565	0.455814	-8.082874
23	1	10.494194	0.466911	-9.119478
24	6	11.105920	0.328104	-7.054680
25	1	12.162769	0.237670	-7.289351
26	6	10.678179	0.318279	-5.724314
27	1	11.402018	0.219747	-4.920247
28	6	9.324286	0.433617	-5.420789
29	1	8.978143	0.426816	-4.392877
30	6	0.797177	4.778180	0.248274
31	6	0.953835	4.800937	-1.146538
32	1	1.293076	3.906200	-1.660399
33	6	0.660343	5.953865	-1.875868
34	1	0.783238	5.954346	-2.955709
35	6	0.192618	7.095329	-1.221919
36	1	-0.045930	7.990571	-1.790306
37	6	0.020423	7.079153	0.163852
38	1	-0.352189	7.961913	0.677253
39	6	0.320618	5.928751	0.895694
40	1	0.176186	5.924254	1.972036
41	6	0.223513	3.309231	2.682284
42	6	-1.083005	2.795096	2.637924
43	1	-1.452290	2.342416	1.721239
44	6	-1.902367	2.855488	3.765753
45	1	-2.911296	2.454953	3.717473
46	6	-1.423795	3.414250	4.953366
47	1	-2.060404	3.452368	5.833681
48	6	-0.122802	3.917364	5.008315
49	1	0.257285	4.349134	5.930823
50	6	0.697404	3.868095	3.878690
51	1	1.708528	4.260603	3.931197
52	6	2.957423	3.502520	1.721584
53	6	3.625334	4.730336	1.602588
54	1	3.116342	5.585138	1.168548
55	6	4.946463	4.862896	2.038904
56	1	5.451766	5.820118	1.937416
57	6	5.613635	3.775160	2.603695
58	1	6.640956	3.881087	2.942714
59	6	4.956222	2.548047	2.726564
60	1	5.468878	1.693810	3.161145
61	6	3.641036	2.408512	2.282943
62	1	3.142912	1.445445	2.365022
63	1	5.935921	0.711987	-7.982664
64	29	-0.973097	-1.273119	0.162606
65	53	1.577106	-1.067423	1.274260
66	15	-1.226266	-3.217123	-1.136908
67	7	-2.331756	-1.140487	1.823489
68	7	-4.742854	-0.847833	6.331038
69	7	-5.925905	-0.743196	6.973635
70	7	-6.466275	-0.742579	4.861029
71	6	-1.910830	-1.139259	3.101692
72	1	-0.835832	-1.207647	3.242154
73	6	-2.778208	-1.044344	4.184230
74	1	-2.391843	-1.043776	5.197376
75	6	-4.155822	-0.943715	3.947838
76	6	-4.593462	-0.936649	2.616945
77	1	-5.650422	-0.855822	2.390170
78	6	-3.653744	-1.034101	1.597045
79	1	-3.958132	-1.023793	0.555160
80	6	-5.118333	-0.844438	5.051861
81	6	-6.960854	-0.679745	6.091169
82	6	-8.376872	-0.561117	6.449602
83	6	-8.813480	-0.572417	7.783961
84	1	-8.102977	-0.678157	8.600243
85	6	-10.169565	-0.455814	8.082874

86	1	-10.494194	-0.466911	9.119478
87	6	-11.105920	-0.328104	7.054680
88	1	-12.162769	-0.237670	7.289351
89	6	-10.678179	-0.318279	5.724314
90	1	-11.402018	-0.219747	4.920247
91	6	-9.324286	-0.433617	5.420789
92	1	-8.978143	-0.426816	4.392877
93	6	-0.797177	-4.778180	-0.248274
94	6	-0.953835	-4.800937	1.146538
95	1	-1.293076	-3.906200	1.660399
96	6	-0.660343	-5.953865	1.875868
97	1	-0.783238	-5.954346	2.955709
98	6	-0.192618	-7.095329	1.221919
99	1	0.045930	-7.990571	1.790306
100	6	-0.020423	-7.079153	-0.163852
101	1	0.352189	-7.961913	-0.677253
102	6	-0.320618	-5.928751	-0.895694
103	1	-0.176186	-5.924254	-1.972036
104	6	-0.223513	-3.309231	-2.682284
105	6	1.083005	-2.795096	-2.637924
106	1	1.452290	-2.342416	-1.721239
107	6	1.902367	-2.855488	-3.765753
108	1	2.911296	-2.454953	-3.717473
109	6	1.423795	-3.414250	-4.953366
110	1	2.060404	-3.452368	-5.833681
111	6	0.122802	-3.917364	-5.008315
112	1	-0.257285	-4.349134	-5.930823
113	6	-0.697404	-3.868095	-3.878690
114	1	-1.708528	-4.260603	-3.931197
115	6	-2.957423	-3.502520	-1.721584
116	6	-3.625334	-4.730336	-1.602588
117	1	-3.116342	-5.585138	-1.168548
118	6	-4.946463	-4.862896	-2.038904
119	1	-5.451766	-5.820118	-1.937416
120	6	-5.613635	-3.775160	-2.603695
121	1	-6.640956	-3.881087	-2.942714
122	6	-4.956222	-2.548047	-2.726564
123	1	-5.468878	-1.693810	-3.161145
124	6	-3.641036	-2.408512	-2.282943
125	1	-3.142912	-1.445445	-2.365022
126	1	-5.935921	-0.711987	7.982664

Table S16. The optimized Cartesian coordinates of the complex **4** in the exited singlet state (S_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	29	1.095699	1.125494	-0.314552
2	53	-1.469775	1.105797	-1.269884
3	15	1.360527	3.064215	1.028559
4	7	2.442706	0.984603	-1.930888
5	7	4.961949	0.997834	-6.419254
6	7	6.172493	0.958383	-7.034301
7	7	6.664068	0.860564	-4.908707
8	6	2.060047	1.049348	-3.234407
9	1	0.989707	1.104795	-3.407648
10	6	2.945395	1.036976	-4.293386
11	1	2.576117	1.089714	-5.311791
12	6	4.339634	0.951629	-4.046039
13	6	4.736434	0.880108	-2.688985
14	1	5.788850	0.809742	-2.437598
15	6	3.782132	0.898870	-1.692680
16	1	4.074733	0.842046	-0.648907
17	6	5.307967	0.936974	-5.120367
18	6	7.182943	0.875799	-6.126221
19	6	8.611182	0.813284	-6.454293
20	6	9.080588	0.883903	-7.775495
21	1	8.385974	0.994423	-8.604643
22	6	10.446802	0.818938	-8.045294
23	1	10.794688	0.875461	-9.073091
24	6	11.362900	0.683920	-7.000356
25	1	12.427472	0.633667	-7.211763
26	6	10.903049	0.614708	-5.682247
27	1	11.610373	0.510052	-4.863999

28	6	9.539318	0.678500	-5.408828
29	1	9.167277	0.625488	-4.391321
30	6	0.929904	4.574000	0.067950
31	6	1.211933	4.579134	-1.308482
32	1	1.652174	3.701805	-1.774190
33	6	0.921677	5.702220	-2.083014
34	1	1.144784	5.693603	-3.146278
35	6	0.334663	6.825563	-1.495973
36	1	0.100206	7.696780	-2.101713
37	6	0.042258	6.823625	-0.130978
38	1	-0.420821	7.692399	0.329234
39	6	0.338715	5.704901	0.650229
40	1	0.103981	5.711716	1.709933
41	6	0.429316	3.192694	2.605694
42	6	-0.794206	2.515110	2.722321
43	1	-1.157094	1.901634	1.903357
44	6	-1.543311	2.613797	3.896456
45	1	-2.482686	2.075938	3.978034
46	6	-1.073958	3.380847	4.964101
47	1	-1.654916	3.450329	5.879826
48	6	0.148598	4.049020	4.859616
49	1	0.521094	4.640324	5.692003
50	6	0.899924	3.955575	3.687833
51	1	1.853574	4.470384	3.616864
52	6	3.121009	3.311609	1.521274
53	6	3.828033	4.489841	1.241123
54	1	3.338049	5.306838	0.721850
55	6	5.164095	4.619193	1.628867
56	1	5.701116	5.536765	1.403907
57	6	5.805733	3.578053	2.300196
58	1	6.845770	3.680088	2.597944
59	6	5.107707	2.400823	2.583318
60	1	5.601191	1.583706	3.102428
61	6	3.776673	2.264567	2.191917
62	1	3.246028	1.340929	2.406938
63	1	6.212219	0.981231	-8.041712
64	29	-1.095699	-1.125494	0.314552
65	53	1.469775	-1.105797	1.269884
66	15	-1.360527	-3.064215	-1.028559
67	7	-2.442706	-0.984603	1.930888
68	7	-4.961949	-0.997834	6.419254
69	7	-6.172493	-0.958383	7.034301
70	7	-6.664068	-0.860564	4.908707
71	6	-2.060047	-1.049348	3.234407
72	1	-0.989707	-1.104795	3.407648
73	6	-2.945395	-1.036976	4.293386
74	1	-2.576117	-1.089714	5.311791
75	6	-4.339634	-0.951629	4.046039
76	6	-4.736434	-0.880108	2.688985
77	1	-5.788850	-0.809742	2.437598
78	6	-3.782132	-0.898870	1.692680
79	1	-4.074733	-0.842046	0.648907
80	6	-5.307967	-0.936974	5.120367
81	6	-7.182943	-0.875799	6.126221
82	6	-8.611182	-0.813284	6.454293
83	6	-9.080588	-0.883903	7.775495
84	1	-8.385974	-0.994423	8.604643
85	6	-10.446802	-0.818938	8.045294
86	1	-10.794688	-0.875461	9.073091
87	6	-11.362900	-0.683920	7.000356
88	1	-12.427472	-0.633667	7.211763
89	6	-10.903049	-0.614708	5.682247
90	1	-11.610373	-0.510052	4.863999
91	6	-9.539318	-0.678500	5.408828
92	1	-9.167277	-0.625488	4.391321
93	6	-0.929904	-4.574000	-0.067950
94	6	-1.211933	-4.579134	1.308482
95	1	-1.652174	-3.701805	1.774190
96	6	-0.921677	-5.702220	2.083014
97	1	-1.144784	-5.693603	3.146278
98	6	-0.334663	-6.825563	1.495973
99	1	-0.100206	-7.696780	2.101713
100	6	-0.042258	-6.823625	0.130978
101	1	0.420821	-7.692399	-0.329234
102	6	-0.338715	-5.704901	-0.650229
103	1	-0.103981	-5.711716	-1.709933
104	6	-0.429316	-3.192694	-2.605694
105	6	0.794206	-2.515110	-2.722321
106	1	1.157094	-1.901634	-1.903357
107	6	1.543311	-2.613797	-3.896456
108	1	2.482686	-2.075938	-3.978034

109	6	1.073958	-3.380847	-4.964101
110	1	1.654916	-3.450329	-5.879826
111	6	-0.148598	-4.049020	-4.859616
112	1	-0.521094	-4.640324	-5.692003
113	6	-0.899924	-3.955575	-3.687833
114	1	-1.853574	-4.470384	-3.616864
115	6	-3.121009	-3.311609	-1.521274
116	6	-3.828033	-4.489841	-1.241123
117	1	-3.338049	-5.306838	-0.721850
118	6	-5.164095	-4.619193	-1.628867
119	1	-5.701116	-5.536765	-1.403907
120	6	-5.805733	-3.578053	-2.300196
121	1	-6.845770	-3.680088	-2.597944
122	6	-5.107707	-2.400823	-2.583318
123	1	-5.601191	-1.583706	-3.102428
124	6	-3.776673	-2.264567	-2.191917
125	1	-3.246028	-1.340929	-2.406938
126	1	-6.212219	-0.981231	8.041712

Table S17. The optimized Cartesian coordinates of the complex **4** in the exited triplet state (T_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	29	1.130087	1.195120	-0.316994
2	53	-1.466338	1.035635	-1.286240
3	15	1.264110	3.094844	1.080773
4	7	2.442764	1.070928	-1.921414
5	7	4.939652	1.316641	-6.416761
6	7	6.130881	1.185196	-7.054405
7	7	6.603174	0.737598	-4.969669
8	6	2.070725	1.349202	-3.202869
9	1	1.016229	1.562074	-3.348917
10	6	2.945390	1.352274	-4.268839
11	1	2.585462	1.579714	-5.266343
12	6	4.316127	1.048525	-4.059181
13	6	4.701059	0.754810	-2.727690
14	1	5.734439	0.512431	-2.505969
15	6	3.760520	0.778011	-1.719473
16	1	4.042165	0.551161	-0.696070
17	6	5.272504	1.036234	-5.143740
18	6	7.118551	0.837659	-6.184709
19	6	8.521223	0.609770	-6.547756
20	6	9.005532	0.839681	-7.845283
21	1	8.344938	1.211797	-8.624602
22	6	10.345085	0.605405	-8.152000
23	1	10.705466	0.788836	-9.160477
24	6	11.219520	0.141053	-7.167462
25	1	12.263476	-0.040816	-7.407484
26	6	10.745387	-0.086157	-5.872423
27	1	11.420722	-0.446379	-5.101121
28	6	9.407835	0.145423	-5.562436
29	1	9.025138	-0.026846	-4.562206
30	6	0.799745	4.594938	0.122245
31	6	1.283988	4.710504	-1.192562
32	1	1.909950	3.927549	-1.612034
33	6	0.960146	5.823333	-1.967450
34	1	1.342390	5.901280	-2.981485
35	6	0.136840	6.824986	-1.446486
36	1	-0.122921	7.687380	-2.054480
37	6	-0.357323	6.710785	-0.146559
38	1	-1.003169	7.483508	0.261751
39	6	-0.027779	5.602644	0.637286
40	1	-0.418785	5.522845	1.646286
41	6	0.269077	3.148615	2.622081
42	6	-0.886254	2.358102	2.708799
43	1	-1.159907	1.703701	1.887746
44	6	-1.679099	2.396892	3.857725
45	1	-2.567164	1.775365	3.916223
46	6	-1.319220	3.216280	4.928643
47	1	-1.933480	3.239445	5.824808
48	6	-0.163270	3.998041	4.853694
49	1	0.124005	4.630646	5.689458
50	6	0.630355	3.965054	3.707231

51	1	1.532233	4.568303	3.658064
52	6	2.992184	3.411528	1.639069
53	6	3.624684	4.654220	1.484946
54	1	3.097860	5.478188	1.014662
55	6	4.934378	4.838227	1.934720
56	1	5.414133	5.805096	1.808176
57	6	5.623252	3.788167	2.542878
58	1	6.642923	3.933441	2.889257
59	6	4.999692	2.547596	2.699693
60	1	5.530901	1.723833	3.168617
61	6	3.695338	2.356783	2.245957
62	1	3.222078	1.385550	2.362674
63	1	6.171225	1.322356	-8.052780
64	29	-1.130087	-1.195120	0.316994
65	53	1.466338	-1.035635	1.286240
66	15	-1.264110	-3.094844	-1.080773
67	7	-2.442764	-1.070928	1.921414
68	7	-4.939652	-1.316641	6.416761
69	7	-6.130881	-1.185196	7.054405
70	7	-6.603174	-0.737598	4.969669
71	6	-2.070725	-1.349202	3.202869
72	1	-1.016229	-1.562074	3.348917
73	6	-2.945390	-1.352274	4.268839
74	1	-2.585462	-1.579714	5.266343
75	6	-4.316127	-1.048525	4.059181
76	6	-4.701059	-0.754810	2.727690
77	1	-5.734439	-0.512431	2.505969
78	6	-3.760520	-0.778011	1.719473
79	1	-4.042165	-0.551161	0.696070
80	6	-5.272504	-1.036234	5.143740
81	6	-7.118551	-0.837659	6.184709
82	6	-8.521223	-0.609770	6.547756
83	6	-9.005532	-0.839681	7.845283
84	1	-8.344938	-1.211797	8.624602
85	6	-10.345085	-0.605405	8.152000
86	1	-10.705466	-0.788836	9.160477
87	6	-11.219520	-0.141053	7.167462
88	1	-12.263476	0.040816	7.407484
89	6	-10.745387	0.086157	5.872423
90	1	-11.420722	0.446379	5.101121
91	6	-9.407835	-0.145423	5.562436
92	1	-9.025138	0.026846	4.562206
93	6	-0.799745	-4.594938	-0.122245
94	6	-1.283988	-4.710504	1.192562
95	1	-1.909950	-3.927549	1.612034
96	6	-0.960146	-5.823333	1.967450
97	1	-1.342390	-5.901280	2.981485
98	6	-0.136840	-6.824986	1.446486
99	1	0.122921	-7.687380	2.054480
100	6	0.357323	-6.710785	0.146559
101	1	1.003169	-7.483508	-0.261751
102	6	0.027779	-5.602644	-0.637286
103	1	0.418785	-5.522845	-1.646286
104	6	-0.269077	-3.148615	-2.622081
105	6	0.886254	-2.358102	-2.708799
106	1	1.159907	-1.703701	-1.887746
107	6	1.679099	-2.396892	-3.857725
108	1	2.567164	-1.775365	-3.916223
109	6	1.319220	-3.216280	-4.928643
110	1	1.933480	-3.239445	-5.824808
111	6	0.163270	-3.998041	-4.853694
112	1	-0.124005	-4.630646	-5.689458
113	6	-0.630355	-3.965054	-3.707231
114	1	-1.532233	-4.568303	-3.658064
115	6	-2.992184	-3.411528	-1.639069
116	6	-3.624684	-4.654220	-1.484946
117	1	-3.097860	-5.478188	-1.014662
118	6	-4.934378	-4.838227	-1.934720
119	1	-5.414133	-5.805096	-1.808176
120	6	-5.623252	-3.788167	-2.542878
121	1	-6.642923	-3.933441	-2.889257
122	6	-4.999692	-2.547596	-2.699693
123	1	-5.530901	-1.723833	-3.168617
124	6	-3.695338	-2.356783	-2.245957
125	1	-3.222078	-1.385550	-2.362674
126	1	-6.171225	-1.322356	8.052780

Table S18. The optimized Cartesian coordinates of the complex **5** in the ground singlet state (S_0) calculated at the DFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	1.504971	1.739461	-0.224258
2	29	-0.898001	0.662283	-1.109957
3	15	-0.905118	0.341339	-3.443378
4	7	-2.440831	1.984691	-0.389270
5	7	-1.623872	6.008127	0.714318
6	7	-1.795760	7.268991	1.167515
7	1	-0.994774	7.880389	1.227386
8	7	-3.791733	6.394754	1.254585
9	6	-2.183229	3.243488	-0.007416
10	1	-1.139188	3.541636	-0.007883
11	6	-3.185987	4.139176	0.390311
12	6	-2.858821	5.514086	0.786047
13	6	-0.388089	1.810003	-4.436964
14	6	-4.510248	3.685126	0.399762
15	1	-5.302864	4.359976	0.706333
16	6	-0.483152	3.075600	-3.839010
17	1	-0.823337	3.156253	-2.810975
18	6	0.193572	-1.003165	-4.068300
19	6	-2.566830	-0.099647	-4.124840
20	6	-0.151758	-1.854123	-5.128702
21	1	-1.119825	-1.754942	-5.610674
22	6	-3.716786	1.556466	-0.373704
23	1	-3.875171	0.525565	-0.673808
24	6	-3.096183	7.501359	1.491676
25	6	-4.775703	2.373346	0.015500
26	1	-5.788904	1.983833	0.012663
27	6	-3.630546	8.762844	2.012432
28	6	1.443489	-1.157672	-3.446607
29	1	1.711958	-0.516717	-2.610810
30	6	0.096837	1.715112	-5.751411
31	1	0.196381	0.741618	-6.222697
32	6	0.740495	-2.836394	-5.564964
33	1	0.460124	-3.492107	-6.385590
34	6	-5.001496	8.844588	2.306264
35	1	-5.621499	7.970534	2.138770
36	6	-2.818372	9.888267	2.225423
37	1	-1.754078	9.854485	2.005800
38	6	-3.180724	0.585469	-5.183607
39	1	-2.662316	1.402659	-5.674827
40	6	2.335655	-2.133657	-3.891954
41	1	3.300031	-2.242176	-3.402848
42	6	1.985958	-2.975852	-4.950288
43	1	2.678981	-3.741352	-5.289974
44	6	-5.544369	10.026930	2.801957
45	1	-6.606358	10.077945	3.025445
46	6	-3.264197	-1.152292	-3.503381
47	1	-2.811709	-1.681736	-2.668572
48	6	-3.366061	11.069572	2.722059
49	1	-2.725993	11.932623	2.881957
50	6	0.462250	2.863339	-6.455160
51	1	0.838895	2.776040	-7.471138
52	6	-4.730140	11.143176	3.011922
53	1	-5.155513	12.064930	3.398812
54	6	-0.121322	4.224137	-4.545353
55	1	-0.195487	5.196585	-4.065959
56	6	0.350777	4.119945	-5.854617
57	1	0.640690	5.012739	-6.402731
58	6	-4.535700	-1.517182	-3.944972
59	1	-5.057830	-2.336164	-3.456841
60	6	-5.138957	-0.829046	-5.001382
61	1	-6.132878	-1.109853	-5.340248
62	6	-4.459849	0.223421	-5.615764
63	1	-4.921937	0.766187	-6.436622
64	53	-1.504971	-1.739461	0.224258
65	29	0.898001	-0.662283	1.109957
66	15	0.905118	-0.341339	3.443378
67	7	2.440831	-1.984691	0.389270
68	7	1.623872	-6.008127	-0.714318
69	7	1.795760	-7.268991	-1.167515
70	1	0.994774	-7.880389	-1.227386

71	7	3.791733	-6.394754	-1.254585
72	6	2.183229	-3.243488	0.007416
73	1	1.139188	-3.541636	0.007883
74	6	3.185987	-4.139176	-0.390311
75	6	2.858821	-5.514086	-0.786047
76	6	0.388089	-1.810003	4.436964
77	6	4.510248	-3.685126	-0.399762
78	1	5.302864	-4.359976	-0.706333
79	6	0.483152	-3.075600	3.839010
80	1	0.823337	-3.156253	2.810975
81	6	-0.193572	1.003165	4.068300
82	6	2.566830	0.099647	4.124840
83	6	0.151758	1.854123	5.128702
84	1	1.119825	1.754942	5.610674
85	6	3.716786	-1.556466	0.373704
86	1	3.875171	-0.525565	0.673808
87	6	3.096183	-7.501359	-1.491676
88	6	4.775703	-2.373346	-0.015500
89	1	5.788904	-1.983833	-0.012663
90	6	3.630546	-8.762844	-2.012432
91	6	-1.443489	1.157672	3.446607
92	1	-1.711958	0.516717	2.610810
93	6	-0.096837	-1.715112	5.751411
94	1	-0.196381	-0.741618	6.222697
95	6	-0.740495	2.836394	5.564964
96	1	-0.460124	3.492107	6.385590
97	6	5.001496	-8.844588	-2.306264
98	1	5.621499	-7.970534	-2.138770
99	6	2.818372	-9.888267	-2.225423
100	1	1.754078	-9.854485	-2.005800
101	6	3.180724	-0.585469	5.183607
102	1	2.662316	-1.402659	5.674827
103	6	-2.335655	2.133657	3.891954
104	1	-3.300031	2.242176	3.402848
105	6	-1.985958	2.975852	4.950288
106	1	-2.678981	3.741352	5.289974
107	6	5.544369	-10.026930	-2.801957
108	1	6.606358	-10.077945	-3.025445
109	6	3.264197	1.152292	3.503381
110	1	2.811709	1.681736	2.668572
111	6	3.366061	-11.069572	-2.722059
112	1	2.725993	-11.932623	-2.881957
113	6	-0.462250	-2.863339	6.455160
114	1	-0.838895	-2.776040	7.471138
115	6	4.730140	-11.143176	-3.011922
116	1	5.155513	-12.064930	-3.398812
117	6	0.121322	-4.224137	4.545353
118	1	0.195487	-5.196585	4.065959
119	6	-0.350777	-4.119945	5.854617
120	1	-0.640690	-5.012739	6.402731
121	6	4.535700	1.517182	3.944972
122	1	5.057830	2.336164	3.456841
123	6	5.138957	0.829046	5.001382
124	1	6.132878	1.109853	5.340248
125	6	4.459849	-0.223421	5.615764
126	1	4.921937	-0.766187	6.436622

Table S19. The optimized Cartesian coordinates of the complex **5** in the exited singlet state (S_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	53	1.426057	1.668618	-0.220684
2	29	-0.991900	0.726322	-1.046821
3	15	-0.962737	0.391335	-3.382389
4	7	-2.538435	2.043861	-0.365615
5	7	-1.761507	6.113932	0.558179
6	7	-1.948097	7.396605	0.980290
7	1	-1.165189	8.030395	0.993840

8	7	-3.929626	6.468727	1.160652
9	6	-2.292461	3.325525	-0.040417
10	1	-1.259419	3.652996	-0.085216
11	6	-3.296750	4.219455	0.353740
12	6	-2.988091	5.613977	0.692844
13	6	-0.408273	1.900519	-4.272210
14	6	-4.610113	3.739395	0.419185
15	1	-5.399514	4.416604	0.728019
16	6	-0.782998	3.152093	-3.755796
17	1	-1.374112	3.210933	-2.846273
18	6	0.068989	-0.985088	-4.015261
19	6	-2.656198	0.045345	-4.018633
20	6	-0.249518	-1.668440	-5.200572
21	1	-1.144156	-1.405943	-5.757457
22	6	-3.808045	1.596024	-0.304958
23	1	-3.964462	0.556144	-0.572921
24	6	-3.256896	7.620157	1.348016
25	6	-4.866324	2.410190	0.085564
26	1	-5.872952	2.005952	0.124034
27	6	-3.783717	8.863968	1.843013
28	6	1.217710	-1.349146	-3.296757
29	1	1.457371	-0.843090	-2.366777
30	6	0.371183	1.845769	-5.437192
31	1	0.679187	0.887405	-5.842703
32	6	0.577549	-2.693082	-5.661553
33	1	0.322601	-3.219699	-6.577080
34	6	-5.157831	8.958995	2.188949
35	1	-5.782422	8.080228	2.066779
36	6	-2.974986	10.021637	2.006940
37	1	-1.917117	9.995096	1.754025
38	6	-3.277503	0.845652	-4.988219
39	1	-2.753212	1.697053	-5.409638
40	6	2.043282	-2.372257	-3.764864
41	1	2.926495	-2.652287	-3.198734
42	6	1.724280	-3.045101	-4.945621
43	1	2.362123	-3.849113	-5.301492
44	6	-5.686593	10.144984	2.670962
45	1	-6.742082	10.192218	2.928916
46	6	-3.354735	-1.052261	-3.485656
47	1	-2.888768	-1.678680	-2.729618
48	6	-3.518600	11.203593	2.491319
49	1	-2.878393	12.075139	2.607563
50	6	0.761621	3.024144	-6.076083
51	1	1.369394	2.970764	-6.975145
52	6	-4.876834	11.284599	2.829992
53	1	-5.296129	12.212021	3.208329
54	6	-0.397239	4.326493	-4.401359
55	1	-0.692510	5.287310	-3.989804
56	6	0.377556	4.263797	-5.561937
57	1	0.686016	5.178832	-6.059894
58	6	-4.644028	-1.347998	-3.925084
59	1	-5.170638	-2.202599	-3.509358
60	6	-5.257854	-0.544865	-4.890494
61	1	-6.265710	-0.771716	-5.226919
62	6	-4.573402	0.549890	-5.418932
63	1	-5.044469	1.177297	-6.170563
64	53	-1.426057	-1.668618	0.220684
65	29	0.991900	-0.726322	1.046821
66	15	0.962737	-0.391335	3.382389
67	7	2.538435	-2.043861	0.365615
68	7	1.761507	-6.113932	-0.558179
69	7	1.948097	-7.396605	-0.980290
70	1	1.165189	-8.030395	-0.993840
71	7	3.929626	-6.468727	-1.160652
72	6	2.292461	-3.325525	0.040417
73	1	1.259419	-3.652996	0.085216
74	6	3.296750	-4.219455	-0.353740
75	6	2.988091	-5.613977	-0.692844
76	6	0.408273	-1.900519	4.272210
77	6	4.610113	-3.739395	-0.419185
78	1	5.399514	-4.416604	-0.728019
79	6	0.782998	-3.152093	3.755796
80	1	1.374112	-3.210933	2.846273
81	6	-0.068989	0.985088	4.015261
82	6	2.656198	-0.045345	4.018633
83	6	0.249518	1.668440	5.200572
84	1	1.144156	1.405943	5.757457
85	6	3.808045	-1.596024	0.304958
86	1	3.964462	-0.556144	0.572921
87	6	3.256896	-7.620157	-1.348016
88	6	4.866324	-2.410190	-0.085564

89	1	5.872952	-2.005952	-0.124034
90	6	3.783717	-8.863968	-1.843013
91	6	-1.217710	1.349146	3.296757
92	1	-1.457371	0.843090	2.366777
93	6	-0.371183	-1.845769	5.437192
94	1	-0.679187	-0.887405	5.842703
95	6	-0.577549	2.693082	5.661553
96	1	-0.322601	3.219699	6.577080
97	6	5.157831	-8.958995	-2.188949
98	1	5.782422	-8.080228	-2.066779
99	6	2.974986	-10.021637	-2.006940
100	1	1.917117	-9.995096	-1.754025
101	6	3.277503	-0.845652	4.988219
102	1	2.753212	-1.697053	5.409638
103	6	-2.043282	2.372257	3.764864
104	1	-2.926495	2.652287	3.198734
105	6	-1.724280	3.045101	4.945621
106	1	-2.362123	3.849113	5.301492
107	6	5.686593	-10.144984	-2.670962
108	1	6.742082	-10.192218	-2.928916
109	6	3.354735	1.052261	3.485656
110	1	2.888768	1.678680	2.729618
111	6	3.518600	-11.203593	-2.491319
112	1	2.878393	-12.075139	-2.607563
113	6	-0.761621	-3.024144	6.076083
114	1	-1.369394	-2.970764	6.975145
115	6	4.876834	-11.284599	-2.829992
116	1	5.296129	-12.212021	-3.208329
117	6	0.397239	-4.326493	4.401359
118	1	0.692510	-5.287310	3.989804
119	6	-0.377556	-4.263797	5.561937
120	1	-0.686016	-5.178832	6.059894
121	6	4.644028	1.347998	3.925084
122	1	5.170638	2.202599	3.509358
123	6	5.257854	0.544865	4.890494
124	1	6.265710	0.771716	5.226919
125	6	4.573402	-0.549890	5.418932
126	1	5.044469	-1.177297	6.170563

Table S20. The optimized Cartesian coordinates of the complex **5** in the exited triplet state (T_1) calculated at the TDDFT level of theory using the B3LYP functional and 6-31G(d) basis set for the C, H, N and P atoms and the effective core potential Lanl2DZ basis set for the heavy Cu and I atoms.

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	**53**	**1.424943**	**1.668631**	**-0.220419**
2	**29**	**-0.995363**	**0.728383**	**-1.046657**
3	**15**	**-0.963701**	**0.391666**	**-3.381623**
4	**7**	**-2.538703**	**2.044577**	**-0.363641**
5	**7**	**-1.761714**	**6.115052**	**0.559481**
6	**7**	**-1.947580**	**7.397379**	**0.980316**
7	**1**	**-1.164359**	**8.030931**	**0.992534**
8	**7**	**-3.929172**	**6.470556**	**1.162555**
9	**6**	**-2.292674**	**3.327112**	**-0.039615**
10	**1**	**-1.259898**	**3.654978**	**-0.087026**
11	**6**	**-3.296429**	**4.220231**	**0.356563**
12	**6**	**-2.987999**	**5.614942**	**0.694758**
13	**6**	**-0.410614**	**1.901926**	**-4.270567**
14	**6**	**-4.609770**	**3.740357**	**0.425867**
15	**1**	**-5.398586**	**4.417376**	**0.736390**
16	**6**	**-0.791395**	**3.152616**	**-3.756312**
17	**1**	**-1.386381**	**3.210031**	**-2.849217**
18	**6**	**0.069836**	**-0.983252**	**-4.014886**
19	**6**	**-2.656325**	**0.044070**	**-4.019356**
20	**6**	**-0.246242**	**-1.664518**	**-5.202049**
21	**1**	**-1.139925**	**-1.401259**	**-5.760124**
22	**6**	**-3.808646**	**1.596697**	**-0.299370**
23	**1**	**-3.965465**	**0.556570**	**-0.566163**
24	**6**	**-3.255719**	**7.621764**	**1.348452**
25	**6**	**-4.866030**	**2.410390**	**0.093227**
26	**1**	**-5.872329**	**2.005578**	**0.134405**
27	**6**	**-3.781769**	**8.866594**	**1.842636**
28	**6**	**1.217229**	**-1.348358**	**-3.294801**

29	1	1.454894	-0.844097	-2.363355
30	6	0.373751	1.849044	-5.432276
31	1	0.686255	0.891438	-5.836121
32	6	0.582017	-2.688030	-5.663376
33	1	0.328972	-3.213012	-6.580378
34	6	-5.155645	8.962003	2.188595
35	1	-5.780389	8.083267	2.067134
36	6	-2.972692	10.023824	2.005529
37	1	-1.914839	9.996717	1.752590
38	6	-3.275423	0.840001	-4.993953
39	1	-2.750176	1.689564	-5.417904
40	6	2.044003	-2.370377	-3.763225
41	1	2.926175	-2.651178	-3.195858
42	6	1.727503	-3.041016	-4.945904
43	1	2.366322	-3.844106	-5.302140
44	6	-5.684060	10.148611	2.669848
45	1	-6.739480	10.196363	2.927926
46	6	-3.356079	-1.051094	-3.482991
47	1	-2.891837	-1.673929	-2.722947
48	6	-3.515804	11.206386	2.489116
49	1	-2.875351	12.077813	2.604668
50	6	0.763156	3.028339	-6.070175
51	1	1.374759	2.976380	-6.966725
52	6	-4.873973	11.287884	2.827849
53	1	-5.292945	12.215716	3.205571
54	6	-0.406659	4.327850	-4.400903
55	1	-0.706626	5.287965	-3.991096
56	6	0.373131	4.267020	-5.558264
57	1	0.680779	5.182776	-6.055407
58	6	-4.644387	-1.348810	-3.923978
59	1	-5.171995	-2.201450	-3.505495
60	6	-5.256002	-0.550075	-4.894399
61	1	-6.263125	-0.778390	-5.232040
62	6	-4.570340	0.542283	-5.426257
63	1	-5.039746	1.166313	-6.181735
64	53	-1.424943	-1.668631	0.220419
65	29	0.995363	-0.728383	1.046657
66	15	0.963701	-0.391666	3.381623
67	7	2.538703	-2.044577	0.363641
68	7	1.761714	-6.115052	-0.559481
69	7	1.947580	-7.397379	-0.980316
70	1	1.164359	-8.030931	-0.992534
71	7	3.929172	-6.470556	-1.162555
72	6	2.292674	-3.327112	0.039615
73	1	1.259898	-3.654978	0.087026
74	6	3.296429	-4.220231	-0.356563
75	6	2.987999	-5.614942	-0.694758
76	6	0.410614	-1.901926	4.270567
77	6	4.609770	-3.740357	-0.425867
78	1	5.398586	-4.417376	-0.736390
79	6	0.791395	-3.152616	3.756312
80	1	1.386381	-3.210031	2.849217
81	6	-0.069836	0.983252	4.014886
82	6	2.656325	-0.044070	4.019356
83	6	0.246242	1.664518	5.202049
84	1	1.139925	1.401259	5.760124
85	6	3.808646	-1.596697	0.299370
86	1	3.965465	-0.556570	0.566163
87	6	3.255719	-7.621764	-1.348452
88	6	4.866030	-2.410390	-0.093227
89	1	5.872329	-2.005578	-0.134405
90	6	3.781769	-8.866594	-1.842636
91	6	-1.217229	1.348358	3.294801
92	1	-1.454894	0.844097	2.363355
93	6	-0.373751	-1.849044	5.432276
94	1	-0.686255	-0.891438	5.836121
95	6	-0.582017	2.688030	5.663376
96	1	-0.328972	3.213012	6.580378
97	6	5.155645	-8.962003	-2.188595
98	1	5.780389	-8.083267	-2.067134
99	6	2.972692	-10.023824	-2.005529
100	1	1.914839	-9.996717	-1.752590
101	6	3.275423	-0.840001	4.993953
102	1	2.750176	-1.689564	5.417904
103	6	-2.044003	2.370377	3.763225
104	1	-2.926175	2.651178	3.195858
105	6	-1.727503	3.041016	4.945904
106	1	-2.366322	3.844106	5.302140
107	6	5.684060	-10.148611	-2.669848
108	1	6.739480	-10.196363	-2.927926
109	6	3.356079	1.051094	3.482991

110	1	2.891837	1.673929	2.722947
111	6	3.515804	-11.206386	-2.489116
112	1	2.875351	-12.077813	-2.604668
113	6	-0.763156	-3.028339	6.070175
114	1	-1.374759	-2.976380	6.966725
115	6	4.873973	-11.287884	-2.827849
116	1	5.292945	-12.215716	-3.205571
117	6	0.406659	-4.327850	4.400903
118	1	0.706626	-5.287965	3.991096
119	6	-0.373131	-4.267020	5.558264
120	1	-0.680779	-5.182776	6.055407
121	6	4.644387	1.348810	3.923978
122	1	5.171995	2.201450	3.505495
123	6	5.256002	0.550075	4.894399
124	1	6.263125	0.778390	5.232040
125	6	4.570340	-0.542283	5.426257
126	1	5.039746	-1.166313	6.181735