Supporting Information

Designing luminescent diimine-Cu (I)-phosphine complexes by tuning N-ligand counteranions: correlation of weak interactions, luminescence and THz absorption spectra

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Table of Contents

level. All hydrogen atoms and solvent molecules are omitted for clarity.

Fig. S10. Coordination environment of Cu(I) for **3**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity.

Fig. S11. Coordination environment of Cu(I) for **4**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity.

Fig. S12. Coordination environment of Cu(I) for **5**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity.

Fig. S13. Coordination environment of Cu(I) for **6**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity.

Fig. S14. Weak hydrogen bonds in **3**, including C-H···F bonds (C2-H2···F1 [i], 2.44 Å, C19-H19···F4 [ii], 2.41 Å, C20-H20B···F3 [iii], 2.47 Å, C33-H33A···F4 [iii], 2.52 Å, C35-H35···F3 [iii], 2.49 Å, C42-H42···F2, 2.40 Å, Symmetric codes: [i] 1/2-x, 1/2-y, 1/2-z; [ii] 1-x, 1-y, 1-z; [iii] x, -1+y, z).

Fig. S15. Weak hydrogen bonds in **4**, including C-H···O bonds (C9-H9···O4 [i], 2.50 Å, C17-H17···O1 [ii], 2.46 Å, C20-H20A···O2, 2.54 Å, C33-H33B···O1, 2.54 Å, C36-H36···O3 [iii], 2.44 Å, C45-H45···O2, 2.57 Å, Symmetric codes: [i] 1-x, 1/2+y, 1/2-z; [ii] 1-x, 1-y, 1-z; [iii] -1/2+x, 1-y, z).

Fig. S16. Weak hydrogen bonds in **5**, including C-H···F bonds (C1-H1···F1, 2.32 Å, C3-H3···F4 [i], 2.24 Å, C10-H10···F2 [ii], 2.49 Å, C13-H13A···F1, 2.49 Å, C14-H14B···F1, 2.49 Å, C29-H29···F1 [iii], 2.53 Å, C34-H34···F3 [ii], 2.36 Å, Symmetric codes: [i] 2-x, 2-y, 1-z; [ii] -1+x, y, z; [iii] 2-x, 1-y, 1-z).

Fig. S17. Weak hydrogen bonds in **6**, including C-H···O bonds (C2-H2B···O2, 2.55 Å, C18-H18···O1 [i], 2.55 Å, C32-H32···O3 [i], 2.53 Å, C39-H39···O4 [ii], 2.37 Å, C41-H41···O2, 2.37 Å, Symmetric codes: [i] 1+x, y, z; [ii] 1-x, 1-y, -z).

Fig. S18. UV-vis absorption spectra for ligands in CH_2Cl_2 at room temperature.

Fig. S19. Solid-state UV-vis spectra for complexes **1**-**6**.

Table S1. Crystallographic data for **1**-**6**.

Table S2. Selected bond length (Å) and angles (°) for **1**-**6**.

Table S3. Intermolecular π-π interactions for complex **1**

Table S4. Intermolecular C-H···π interactions for complex **2**.

Table S5. Intermolecular π-π interactions for complex **3**

Table S6. Intermolecular C-H···π interactions for complex **3**.

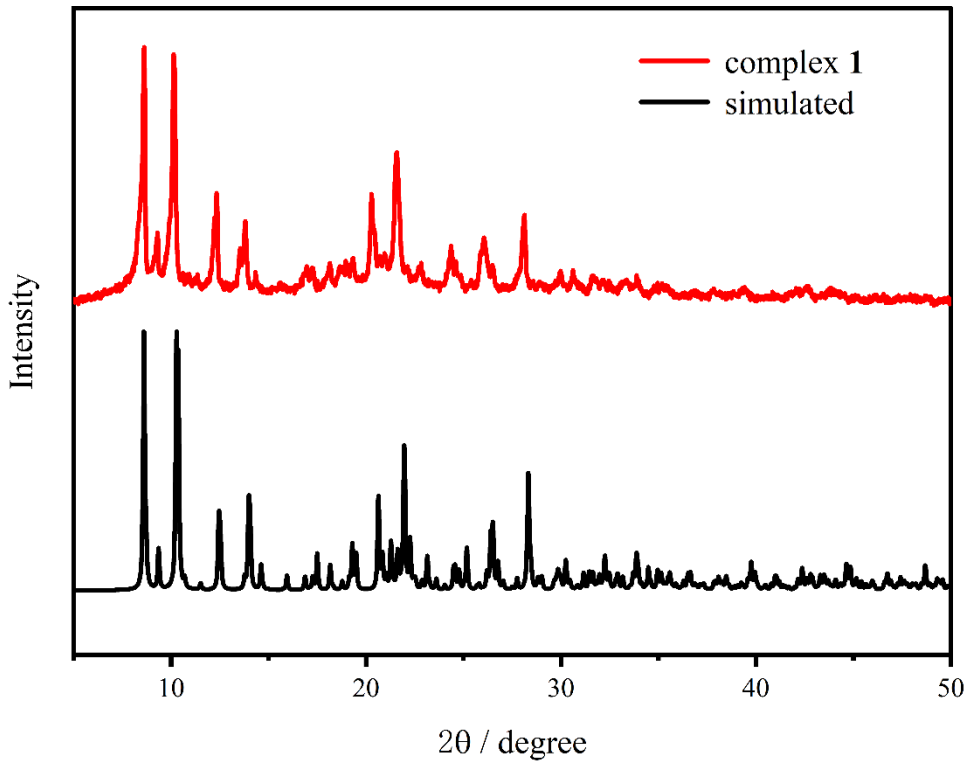


Fig. S1. The PXRD patterns for complex **1**: simulated from single crystal data (Black) and single-phase polycrystalline sample (Red).

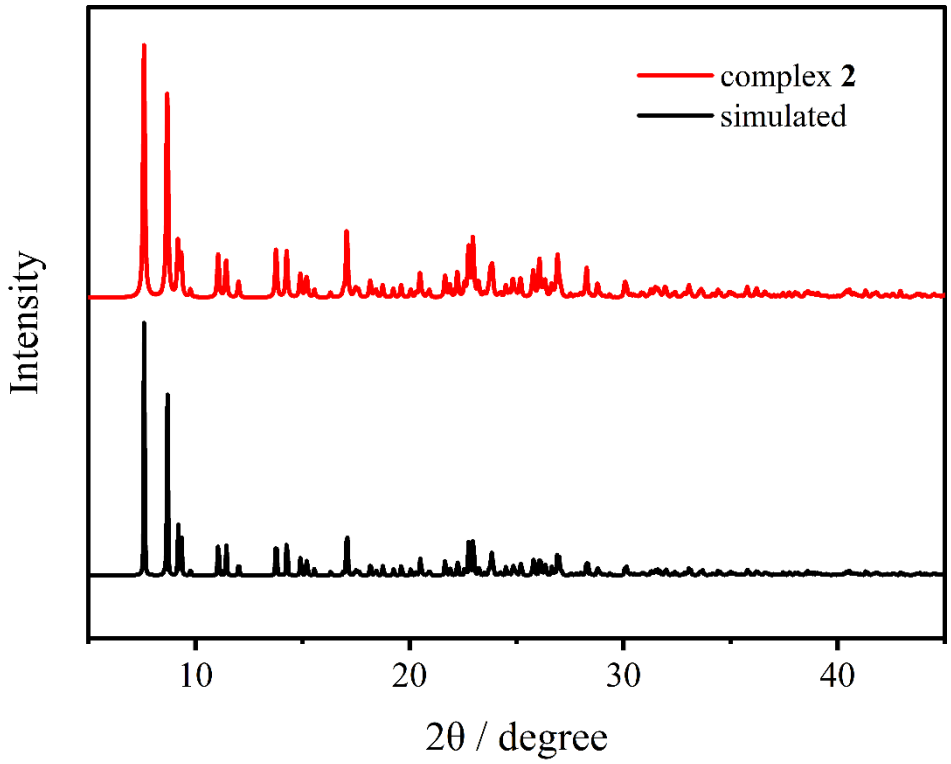


Fig. S2. The PXRD patterns for complex **2**: simulated from single crystal data (Black) and single-phase polycrystalline sample (Red).

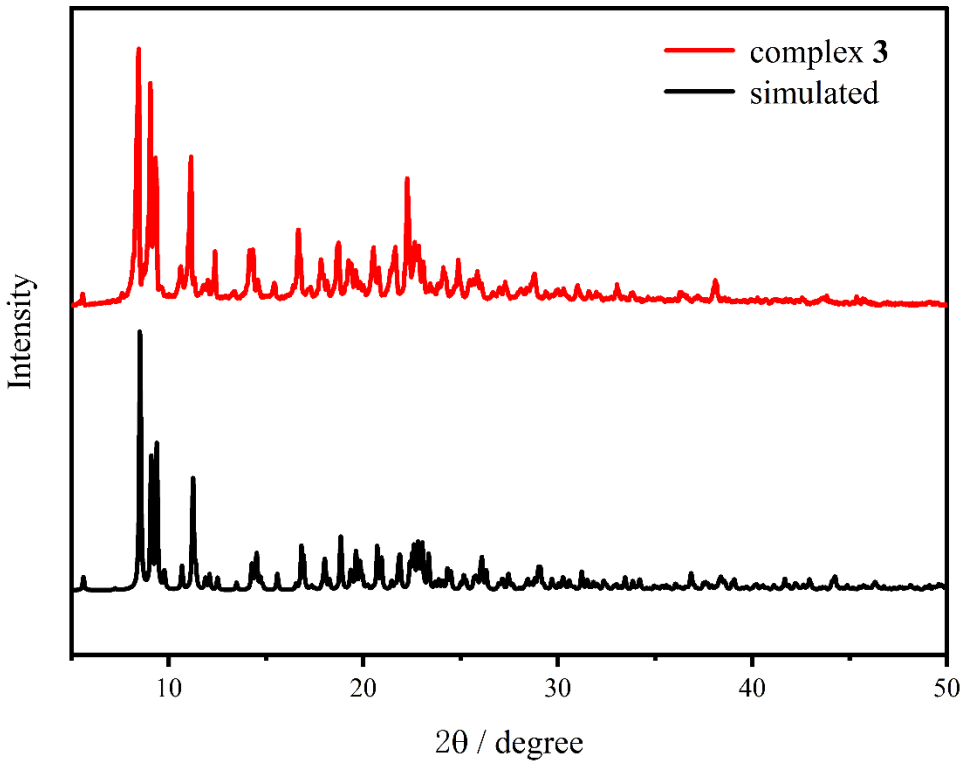


Fig. S3. The PXRD patterns for complex **3**: simulated from single crystal data (Black) and single-phase polycrystalline sample (Red).

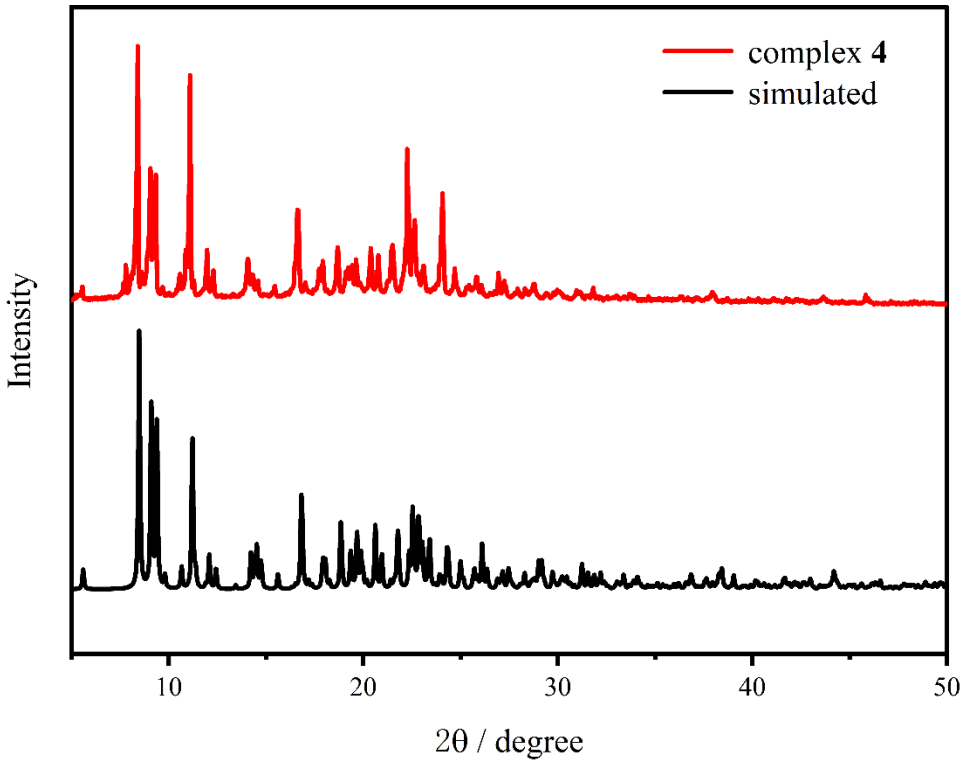


Fig. S4. The PXRD patterns for complex **4**: simulated from single crystal data (Black) and single-phase polycrystalline sample (Red).

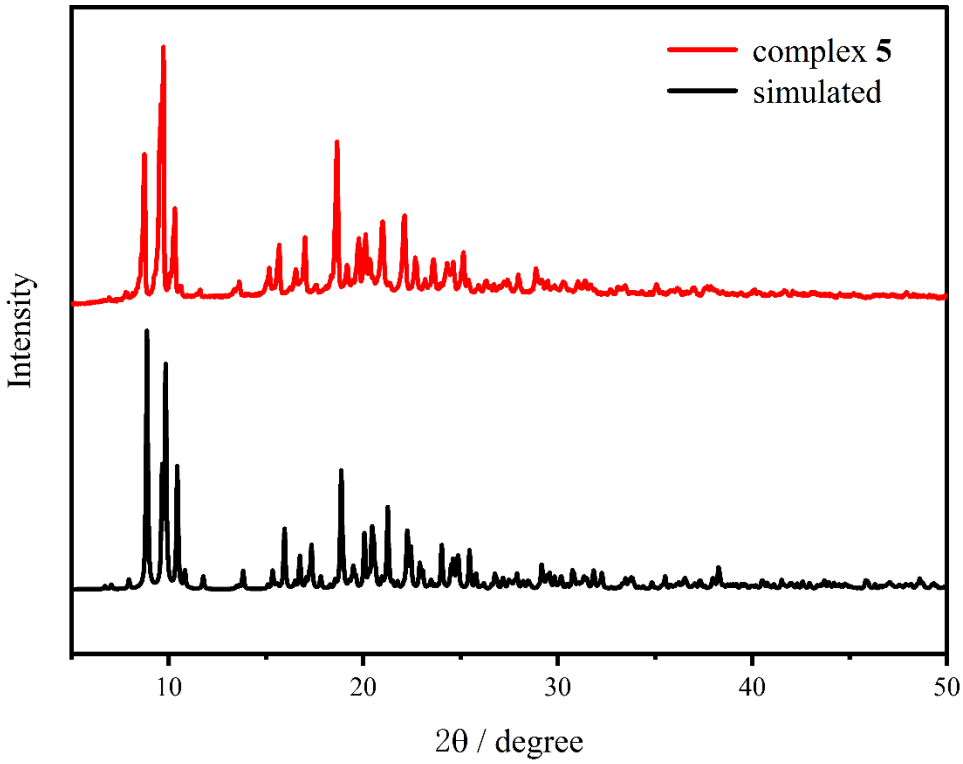


Fig. S5. The PXRD patterns for complex **5**: simulated from single crystal data (Black) and single-phase polycrystalline sample (Red).

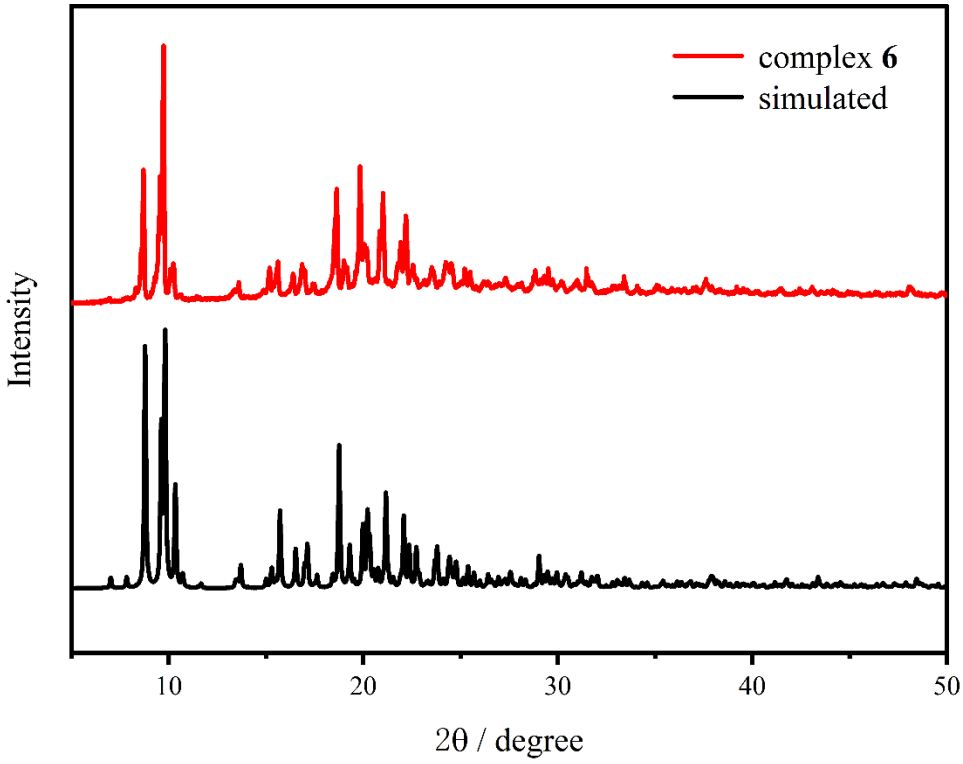


Fig. S6. The PXRD patterns for complex **6**: simulated from single crystal data (Black) and single-phase polycrystalline sample (Red).

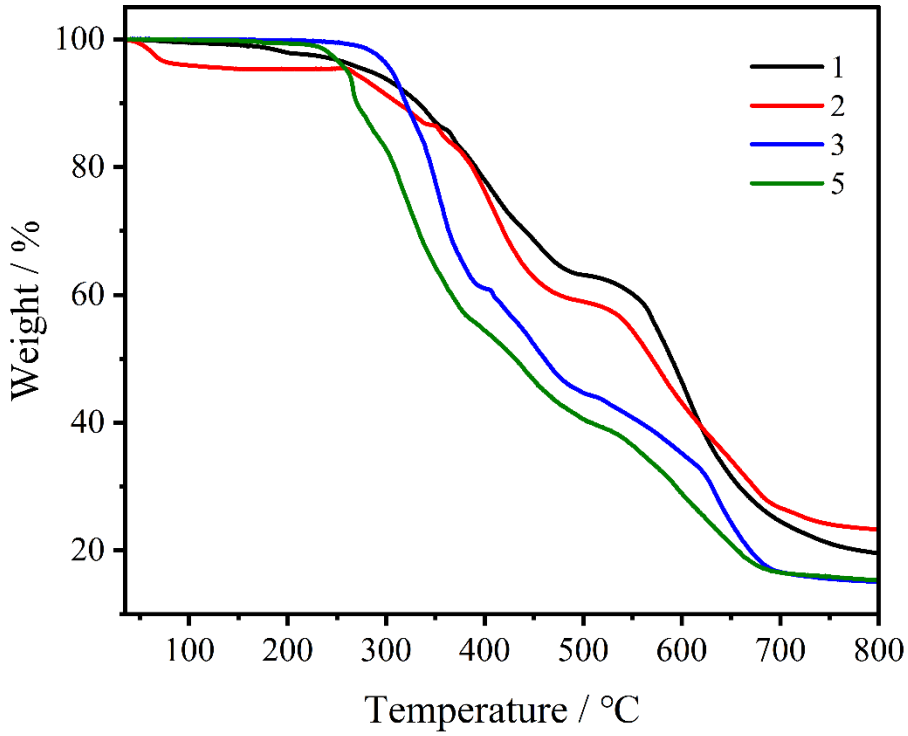


Fig. S7. Thermal stability curves for complexes **1**, **2**, **3**, **5**.

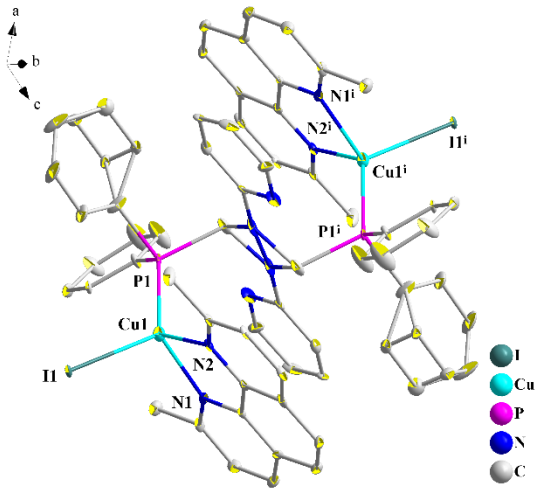


Fig. S8. Coordination environment of Cu(I) for **1**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity Symmetric codes: [i] 2-x, 1-y, 1-z.

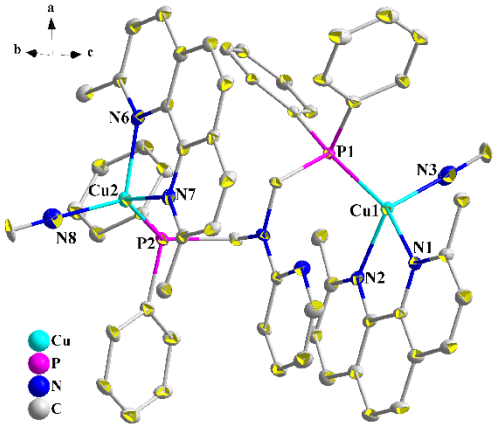


Fig. S9. Coordination environment of Cu(I) for **2**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms and solvent molecules are omitted for clarity.

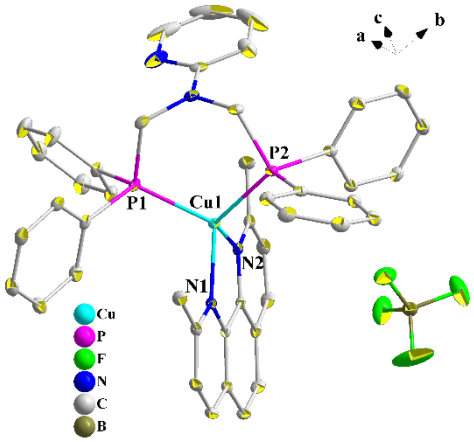


Fig. S10. Coordination environment of Cu(I) for **3**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity.

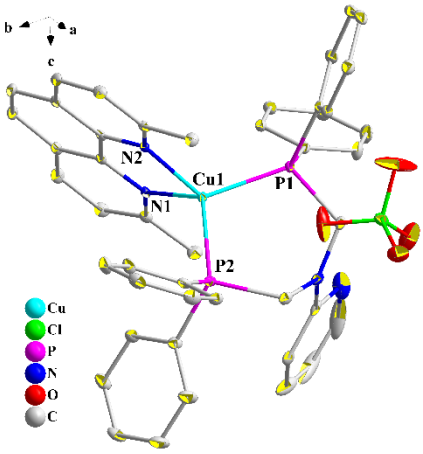


Fig. S11. Coordination environment of Cu(I) for **4**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity.

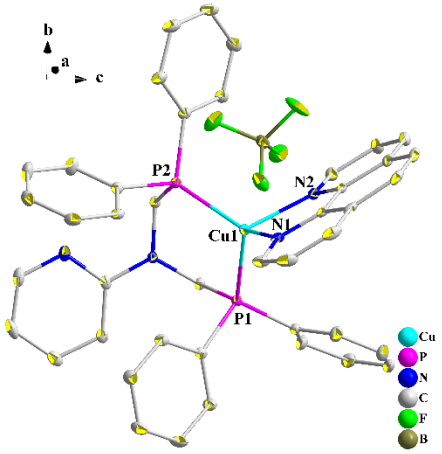


Fig. S12. Coordination environment of Cu(I) for **5**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity.

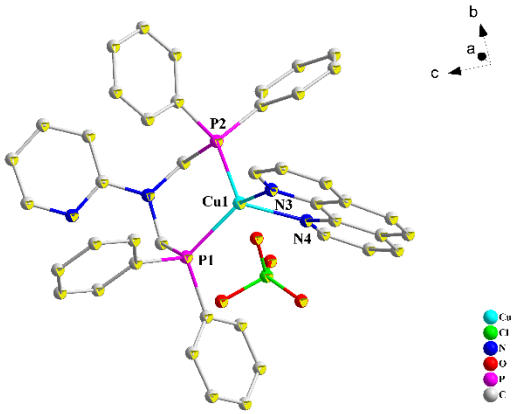
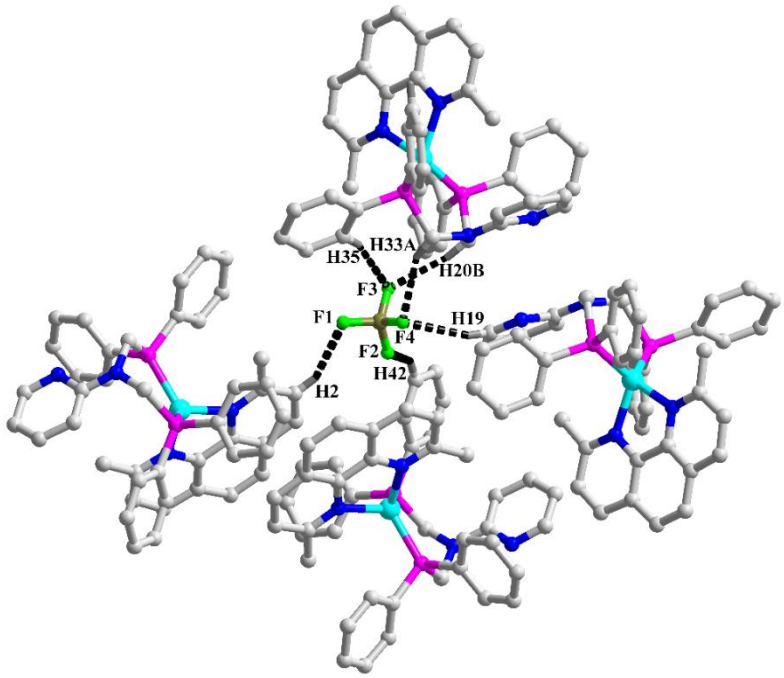


Fig. S13. Coordination environment of Cu(I) for **6**. Thermal ellipsoids drawn at the 30% probability level. All hydrogen atoms are omitted for clarity.



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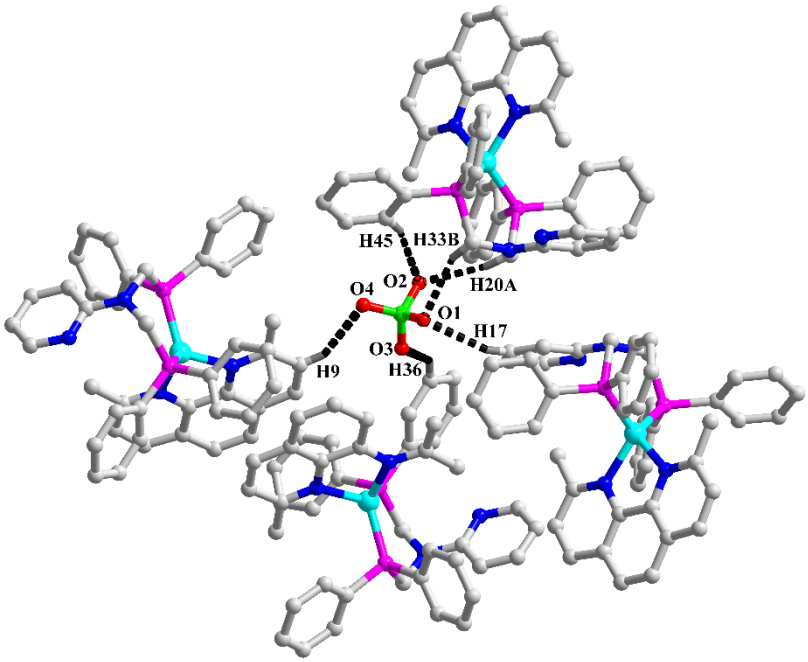

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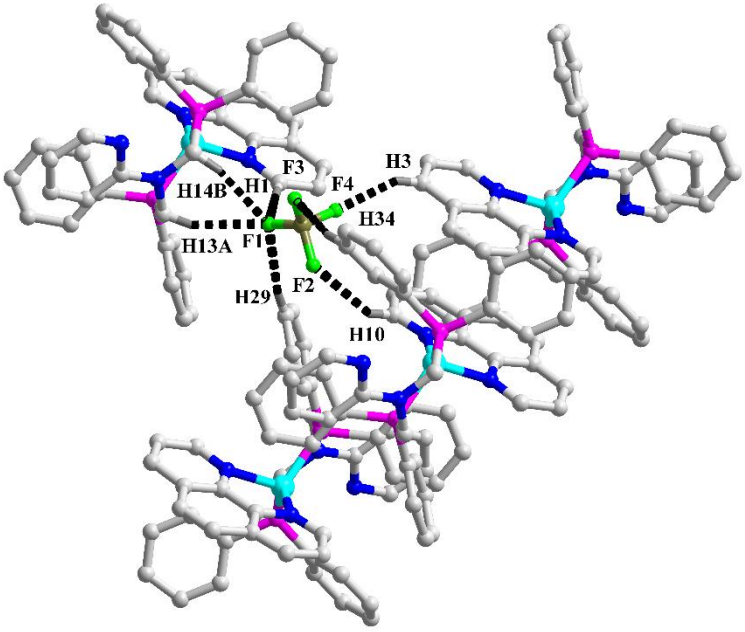

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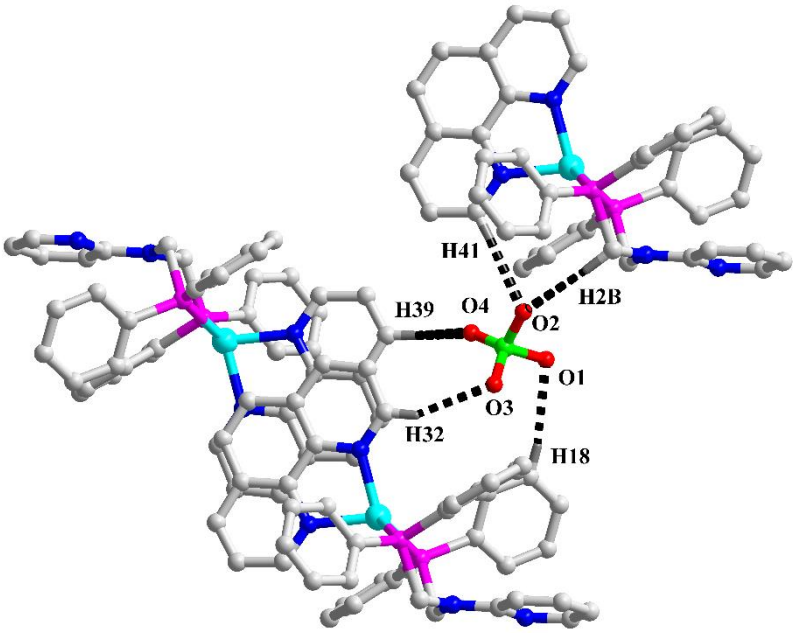

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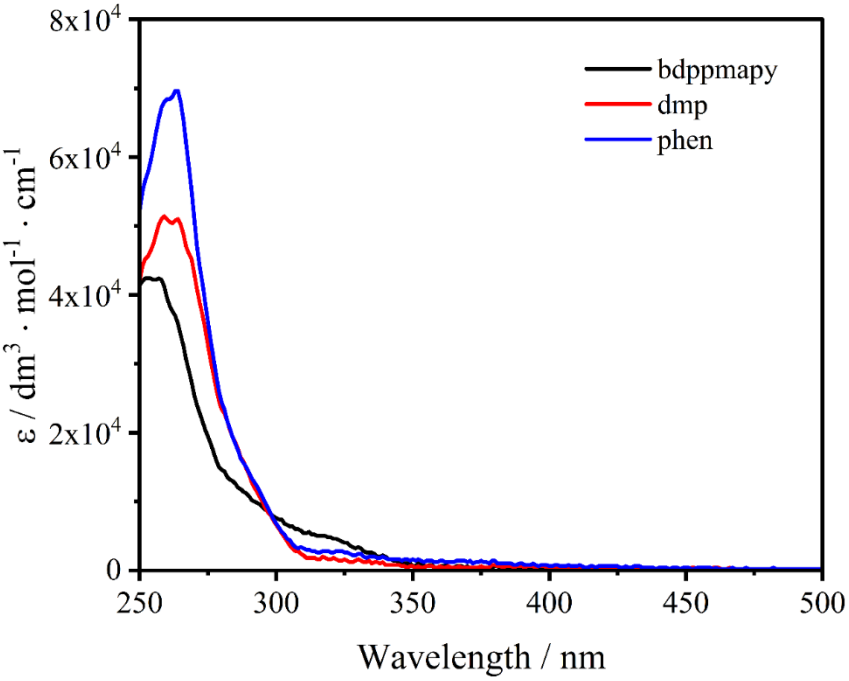

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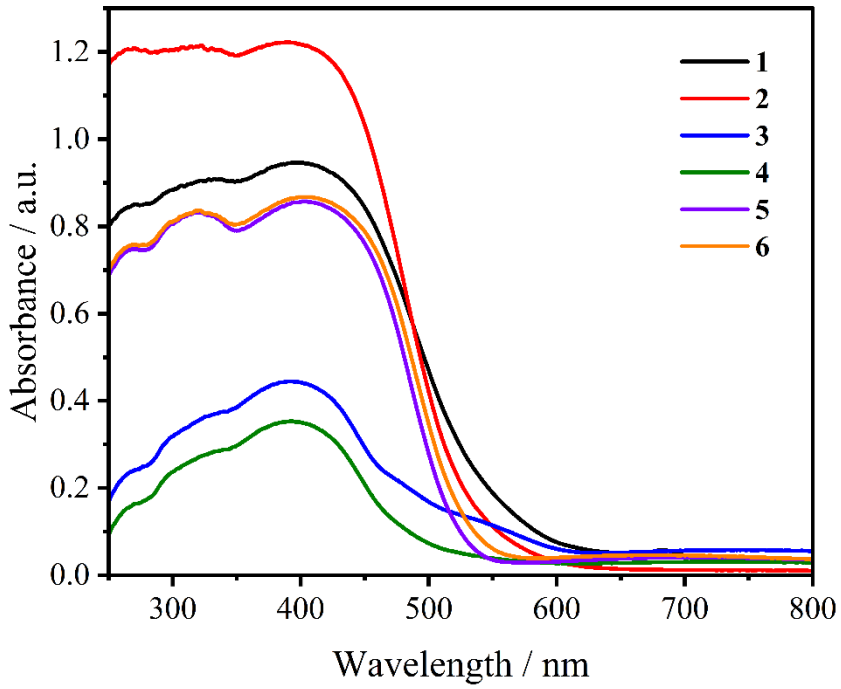

Fig. S19. Solid-state UV-vis spectra for complexes **1**-**6**.

Table S1. Crystallographic data for **1**-**6**.

Complex	**1**	**2**	**3**	**4**	**5**	**6**
Formula	$C_{59}H_{52}Cu_2I_2N_6P_2$	$C_{64}H_{64}Cu_2N_8O_3P_2$	$C_{45}H_{40}BCuF_4N_4P_2$	$C_{45}H_{40}ClCuN_4O_4P_2$	$C_{43}H_{36}BCuF_4N_4P_2$	$C_{43}H_{36}CuN_4P_2ClO_4$
Formula weight	1287.88	1182.23	849.10	861.74	821.05	833.85
T / K	100(2)	100(2)	99.99(10)	99.97(10)	106.7	298(2)
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/c$	C_C	$I2/a$	$I2/a$	$P\dot{1}$	$P\dot{1}$
a / Å	12.647(3)	11.7324(2)	24.6200(2)	24.6439(3)	11.5699(5)	11.7400(11)
b / Å	17.053(3)	20.7132(3)	10.20780(9)	10.20305(13)	12.5429(3)	12.5965(13)
c / Å	17.208(3)	23.3587(4)	31.7453(3)	31.8756(4)	13.6715(4)	13.7194(14)
α / (°)	90	90	90	90	88.298(2)	88.186(2)
β / (°)	131.69(3)	95.466(2)	98.0520(9)	98.5114(11)	73.809(3)	73.7570(10)
γ / (°)	90	90	90	90	87.479(3)	87.479(2)
V / Å^3	2771.2(14)	5650.71(16)	7899.46(13)	7926.63(16)	1903.17(12)	1945.6(3)
Z	2	4	8	8	2	2
D_{calc} / g·cm^{-3}	1.543	1.387	1.428	1.444	1.433	1.423
F(000)	1284	2456	3504	3568	844	860
Goodness-of-fit on F^2	1.153	1.059	1.058	1.024	1.038	1.051
R_{int}	0.1453	0.0475	0.0547	0.0371	0.0178	0.0392
$R_1[I > 2\sigma(I)]$ [a]	0.0788	0.0827	0.0432	0.0389	0.0290	0.0632
$wR_2[I > 2\sigma(I)]$ [b]	0.2015	0.2124	0.1082	0.0947	0.0669	0.1504
R_1 (all data) [a]	0.0802	0.0832	0.0440	0.0407	0.0339	0.0870
wR_2 (all data) [b]	0.2023	0.2129	0.1088	0.0958	0.0698	0.1597
CCDC	2075018	2075019	2075020	2075021	2075022	2075023

[a] $R = \sum(||F_o| - |F_c||)/\sum|F_o|$.
[b] $wR = [\sum w(|F_o|^2 - |F_c|^2)^2/\sum w(F_o^2)]^{1/2}$.

Table S2. Selected bond length (Å) and angles (°) for **1**-**6**.

1			
Cu(1)-I(1)	2.642(2)	P(1)-Cu(1)-I(1)	118.73(8)
Cu(1)-P(1)	2.199(3)	N(1)-Cu(1)-I(1)	107.7(2)
Cu(1)-N(1)	2.091(7)	N(1)-Cu(1)-P(1)	120.0(2)
Cu(1)-N(2)	2.101(7)	N(1)-Cu(1)-N(2)	80.4(3)
		N(2)-Cu(1)-I(1)	101.0(2)
		N(2)-Cu(1)-P(1)	121.9(2)
			Dihedral Angle
		I1-Cu1-P1/N1-Cu1-N2	94.370

2			
Cu(1)-P(1)	2.2411(18)	N(1)-Cu(1)-P(1)	112.57(18)
Cu(1)-N(2)	2.123(6)	N(2)-Cu(1)-P(1)	117.37(17)
Cu(1)-N(1)	2.095(6)	N(2)-Cu(1)-N(1)	80.3(2)
Cu(1)-N(3)	1.941(9)	N(3)-Cu(1)-P(1)	115.0(3)
Cu(2)-P(2)	2.2372(19)	N(3)-Cu(1)-N(1)	107.9(3)
Cu(2)-N(7)	2.095(6)	N(3)-Cu(1)-N(2)	117.9(3)
Cu(2)-N(6)	2.123(7)	N(7)-Cu(2)-P(2)	116.62(17)
Cu(2)-N(8)	1.943(8)	N(7)-Cu(2)-N(6)	79.5(2)
		N(6)-Cu(2)-P(2)	116.29(17)
		N(8)-Cu(2)-P(2)	115.1(2)
		N(8)-Cu(2)-N(7)	112.0(3)
		N(8)-Cu(2)-N(6)	112.5(3)
			Dihedral Angle
		P1-Cu1-N3/N1-Cu1-N2	87.516
		P2-Cu2-N8/N6-Cu2-N7	90.423
3			
Cu(1)-P(1)	2.2505(6)	P(1)-Cu(1)-P(2)	107.55(2)
Cu(1)-P(2)	2.2563(6)	N(1)-Cu(1)-P(2)	121.45(5)
Cu(1)-N(1)	2.0689(18)	N(1)-Cu(1)-P(1)	112.39(5)
Cu(1)-N(2)	2.0673(18)	N(2)-Cu(1)-P(2)	116.32(5)
		N(2)-Cu(1)-P(1)	115.92(5)
		N(1)-Cu(1)-N(2)	81.81(7)
			Dihedral Angle
		P1-Cu1-P2/N1-Cu1-N2	86.407
4			
Cu(1)-P(1)	2.2537(6)	P(2)-Cu(1)-P(1)	107.77(2)
Cu(1)-P(2)	2.2518(6)	N(1)-Cu(1)-P(2)	115.96(5)
Cu(1)-N(1)	2.0664(17)	N(1)-Cu(1)-P(1)	116.61(5)
Cu(1)-N(2)	2.0672(17)	N(2)-Cu(1)-N(1)	81.87(7)
		N(2)-Cu(1)-P(2)	112.01(5)
		N(2)-Cu(1)-P(1)	121.15(5)
			Dihedral Angle
		P1-Cu1-P2/N1-Cu1-N2	86.441
5			
Cu(1)-P(1)	2.2304(5)	P(1)-Cu(1)-P(2)	104.855(19)
Cu(1)-P(2)	2.2417(5)	N(2)-Cu(1)-P(1)	110.65(4)
Cu(1)-N(1)	2.0606(16)	N(2)-Cu(1)-P(2)	114.28(5)

Cu(1)-N(2)	2.0710(15)	N(1)-Cu(1)-P(1)	116.30(4)
		N(1)-Cu(1)-P(2)	127.07(5)
		N(2)-Cu(1)-N(1)	81.48(6)
			Dihedral Angle
		P1-Cu1-P2/N1-Cu1-N2	91.822
6			
Cu(1)-N(3)	2.054(4)	N(3)-Cu(1)-N(4)	80.70(15)
Cu(1)-N(4)	2.061(3)	N(3)-Cu(1)-P(1)	127.51(11)
Cu(1)-P(1)	2.2327(12)	N(3)-Cu(1)-P(2)	116.18(10)
Cu(1)-P(2)	2.2239(14)	N(4)-Cu(1)-P(1)	115.06(10)
		N(4)-Cu(1)-P(2)	110.46(12)
		P(2)-Cu(1)-P(1)	104.67(5)
			Dihedral Angle
		P1-Cu1-P2/N3-Cu1-N4	91.551

Table S3 Intermolecular π-π interactions for complex **1**.

	Cg→Cg	Distance / Å	Slippage / Å
1	Cg(20)→Cg(20)^{i}	3.698(7)	1.442

Cg(20) = N1-C2-C3-C4-C5-C6

Symmetric codes: ^{i} 1-x, 1-y, 1-z

Table S4 Intermolecular C-H···π interactions for complex **2**.

	C-H→Cg	H···Cg / Å	C-H···Cg / °	C···Cg / Å	C-H···π / °
2	C9-H9→Cg(10)^{i}	2.89	146	3.7188	68

Cg(10) = C23-C24-C25-C26-C27-C28

Symmetric codes: ^{i} -1+x, y, z

Table S5 Intermolecular π-π interactions for complex **3**.

	Cg→Cg	Distance / Å	Slippage / Å
3	Cg(3)→Cg(3)^{i}	3.6114	1.442

Cg(3) = N1-C1-C2-C3-C4-C5

Symmetric codes: ^{i} 1/2-x, 1/2-y, 1/2-z

Table S6 Intermolecular C-H···π interactions for complex **3**.

	C-H→Cg	H···Cg / Å	C-H···Cg / °	C···Cg / Å	C-H···π / °
3	C11-H11→Cg(9)^{i}	2.70	155	3.569(2)	72
	C20-H20A→Cg(5)^{ii}	2.97	139	3.758(3)	34
	C31-H31→Cg(9)^{iii}	2.97	161	3.859(3)	86

Cg(5) = N4-C15-C16-C19-C18-C17

Cg(9) = C34-C35-C36-C37-C38-C39

Symmetric codes: ^{i} 1/2-x, 1/2-y, 1/2-z; ^{ii} 1-x, 1-y, 1-z; ^{iii} x, -1+y, z

Table S7 Typical hydrogen bonds in asymmetric units for complexes **3**.

	Hydrogen bonds	D-H / Å	H···A / Å	D···A / Å	D-H···A / °
3	C2-H2···F1 [i]	0.93	2.44	3.267(3)	149
	C19-H19···F4 [ii]	0.93	2.40	3.271(4)	155
	C20-H20B···F3 [iii]	0.97	2.47	3.426(3)	168
	C33-H33A···F4 [iii]	0.97	2.52	3.423(3)	156
	C35-H35···F3 [iii]	0.93	2.49	3.378(3)	159
	C42-H42···F2	0.93	2.40	3.168(3)	140

Symmetric codes: [i] 1/2-x, 1/2-y, 1/2-z; [ii] 1/2-x, y, 1-z; [iii] 1/2+x, 1-y, z

Table S8 Intermolecular π-π interactions for complex **4**.

	Cg→Cg	Distance / Å	Slippage / Å
4	Cg(4)→Cg(4)[i]	3.5841	1.404

Cg(4) = N2-C6-C7-C8-C9-C10

Symmetric codes: [i] 1/2-x, 3/2-y, 1/2-z

Table S9 Intermolecular C-H···π interactions for complex **4**.

	C-H→Cg	H···Cg / Å	C-H···Cg / °	C···Cg / Å	C-H···π / °
4	C12-H12→Cg(10)[i]	2.64	156	3.514(2)	70
	C20-H20B→Cg(5)[ii]	2.97	140	3.761(3)	35

Cg(10) = C40-C41-C42-C43-C44-C45

Cg(5) = N4-C15-C16-C17-C18-C19

Symmetric codes: [i] 1/2-x, 3/2-y, 1/2-z; [ii] 1-x, 1-y, 1-z

Table S10 Typical hydrogen bonds in asymmetric units for complexes **4**.

	Hydrogen bonds	D-H / Å	H···A / Å	D···A / Å	D-H···A / °
4	C9-H9···O4 [i]	0.93	2.50	3.319(3)	147
	C17-H17···O1 [ii]	0.93	2.46	3.316(4)	154
	C20-H20A···O2	0.97	2.54	3.496(4)	168
	C33-H33B···O1	0.97	2.54	3.443(3)	155
	C36-H36···O3 [iii]	0.93	2.44	3.182(3)	137
	C45-H45···O2	0.93	2.57	3.456(3)	159

Symmetric codes: [i] 1-x, 1/2+y, 1/2-z; [ii] 1-x, 1-y, 1-z; [iii] -1/2+x, 1-y, z

Table S11 Intermolecular π-π interactions for complex **5**.

	Cg→Cg	Distance / Å	Slippage / Å
5	Cg(6)→Cg(6)[i]	3.7476	1.722

Cg(4) = C4-C5-C6-C7-C12-C11

Symmetric codes: [i] 1-x, 2-y, 1-z

Table S12 Intermolecular C-H···π interactions for complex **5**.

C-H→Cg	H···Cg / Å	C-H···Cg angle / °	C···Cg distance / Å	C-H···π / °

5	C8-H8→Cg(10)[i]	2.94	153	3.813(2)	72
	C13-H13B→Cg(5)[ii]	2.99	114	3.514(2)	25

Cg(10) = 38-C39-C40-C41-C42-C43

Cg(5) = N4-C15-C16-C17-C18-C19

Symmetric codes: [i] 1-x, 2-y, 1-z; [ii] 2-x, 1-y, -z

Table S13 Typical hydrogen bonds in asymmetric units for complexes **5**.

	Hydrogen bonds	D-H / Å	H···A / Å	D···A / Å	D-H···A / °
5	C1-H1···F1	0.95	2.32	3.264(2)	173
	C3-H3···F4 [i]	0.95	2.24	3.075(4)	147
	C10-H10···F2 [ii]	0.95	2.49	3.297(3)	143
	C13-H13A···F1	0.99	2.49	3.432(2)	158
	C14-H14B···F1	0.99	2.49	3.422(2)	157
	C29-H29···F1 [iii]	0.95	2.53	3.466(3)	168
	C34-H34···F3 [ii]	0.95	2.36	3.287(3)	166

Symmetric codes: [i] 2-x, 2-y, 1-z; [ii] -1+x, y, z; [iii] 2-x, 1-y, 1-z

Table S14 Intermolecular π-π interactions for complex **6**.

	Cg→Cg	Distance / Å	Slippage / Å
6	Cg(10)→Cg(10)[i]	3.749(3)	1.652

Cg(4) = C35-C36-C37-C38-C43-C42

Symmetric codes: [i] 2-x, 1-y, -z

Table S15 Typical hydrogen bonds in asymmetric units for complexes **6**.

	Hydrogen bonds	D-H / Å	H···A / Å	D···A / Å	D-H···A / °
6	C2-H2B···O2	0.97	2.55	3.486(6)	162
	C18-H18···O1 [i]	0.93	2.55	3.453(9)	163
	C32-H32···O3 [i]	0.93	2.53	3.324(7)	143
	C39-H39···O4 [ii]	0.93	2.37	3.176(10)	145
	C41-H41···O2	0.93	2.37	3.303(7)	175

Symmetric codes: [i] 1+x, y, z; [ii] 1-x, 1-y, -z

Table S16. Energy, oscillator strength and major contribution of the calculated transitions for **1**-**6**.

Excited state	Energy / eV (/ nm)	Oscillator strength	Major contribution (%)
1 absorption	4.8393 (256.20)	0.0987	HOMO-26→LUMO+2 (2.73) HOMO-25 → LUMO (3.36) HOMO-16 → LUMO+2 (2.56) HOMO-14 → LUMO+6 (8.36) HOMO-14 → LUMO+7 (3.83) HOMO-13 → LUMO+4 (2.51) **HOMO-13 → LUMO+5 (30.78)**

			HOMO-13 → LUMO+8 (12.08)
			HOMO-10 → LUMO+13 (2.48)
1 emission	2.0756 (597.34)	0.0251	HOMO-9 → LUMO+1 (2.07)
			HOMO-7 → LUMO (5.04)
			HOMO-7 → LUMO+1 (3.63)
			HOMO-6 → LUMO (39.15)
			HOMO-5 → LUMO (3.18)
			HOMO-4 → LUMO (40.71)
			HOMO-2 → LUMO (3.31)
2 absorption	4.7933 (258.66)	0.1715	HOMO-28 → LUMO+1 (3.56)
			HOMO-27 → LUMO+1 (12.19)
			HOMO-26 → LUMO+1 (5.35)
			HOMO-24 → LUMO+2 (6.92)
			HOMO-24 → LUMO+3 (2.98)
			HOMO-23 → LUMO+1 (12.93)
			HOMO-22 → LUMO+1 (7.11)
			HOMO-21 → LUMO+1 (4.41)
			HOMO-20 → LUMO+1 (3.61)
			HOMO-19 → LUMO+1 (8.75)
			HOMO-19 → LUMO+3 (2.37)
			HOMO-13 → LUMO+3 (6.97)
			HOMO-6 → LUMO+12 (2.90)
2 emission	3.3366 (530.61)	0.0270	HOMO-8 → LUMO (3.18)
			HOMO-8 → LUMO+1 (7.00)
			HOMO-7 → LUMO (33.23)
			HOMO-6 → LUMO (39.30)
			HOMO-5 → LUMO (9.50)
			HOMO-4 → LUMO (3.78)
3 **4** absorption	4.8558 (255.33)	0.1706	**HOMO-16 → LUMO (17.51)**
			HOMO-14 → LUMO+1 (2.91)
			HOMO-11 → LUMO+1 (2.54)
			HOMO-9 → LUMO+2 (2.30)
			HOMO-3 → LUMO+3 (12.02)
			HOMO-2 → LUMO+5 (17.06)
			HOMO-1 → LUMO+10 (15.45)
			HOMO-1 → LUMO+11 (9.06)
3 **4** emission	2.3920 (518.32)	0.1144	**HOMO-1 → LUMO (98.00)**
5 **6** absorption	4.6879 (264.48)	0.1386	**HOMO-15 → LUMO (21.55)**
			HOMO-15 → LUMO+1 (2.80)
			HOMO-12 → LUMO+1 (4.50)
			HOMO-5 → LUMO+1 (4.15)
			HOMO-4 → LUMO+1 (6.30)
			HOMO-3 → LUMO+2 (10.06)

				HOMO-2 → LUMO+5	(20.45)
				HOMO → LUMO+11	(10.66)
5	**6**	2.5319	0.0198	HOMO-3 → LUMO	(8.03)
emission		(489.69)		HOMO-2 → LUMO	(28.55)
				HOMO-1 → LUMO	**(59.20)**

Table S17. Calculated molecular frontier orbital energy / eV for **1**-**6**.

Frontier orbital	**1**	**2**	**3** and **4**	**5** and **6**
HOMO-29	-7.473	-7.532	-11.858	-11.849
HOMO-28	-7.411	-7.524	-11.810	-11.807
HOMO-27	-7.329	-7.495	-11.758	-11.761
HOMO-26	-7.305	-7.493	-11.626	-11.665
HOMO-25	-7.267	-7.390	-11.549	-11.520
HOMO-24	-7.234	-7.332	-11.462	-11.331
HOMO-23	-7.197	-7.308	-11.341	-11.256
HOMO-22	-7.155	-7.267	-11.307	-11.125
HOMO-21	-7.087	-7.220	-11.254	-10.983
HOMO-20	-7.051	-7.187	-11.174	-10.965
HOMO-19	-6.974	-7.164	-10.947	-10.933
HOMO-18	-6.951	-7.111	-10.344	-10.418
HOMO-17	-6.847	-7.019	-9.824	-9.909
HOMO-16	-6.797	-7.000	-9.812	-9.731
HOMO-15	-6.737	-6.863	-9.637	-9.576
HOMO-14	-6.436	-6.808	-9.575	-9.542
HOMO-13	-6.399	-6.790	-9.519	-9.516
HOMO-12	-6.328	-6.246	-9.478	-9.457
HOMO-11	-6.276	-6.217	-9.421	-9.426
HOMO-10	-5.930	-6.206	-9.362	-9.389
HOMO-9	-5.870	-6.142	-9.362	-9.351
HOMO-8	-5.792	-6.131	-9.343	-9.300
HOMO-7	-5.687	-6.058	-9.312	-9.288
HOMO-6	-5.588	**-5.785**	-9.263	-9.248
HOMO-5	-5.114	-5.457	-9.247	-9.225
HOMO-4	**-5.029**	-5.427	-9.149	-9.059
HOMO-3	-5.001	-5.417	-8.694	-8.697
HOMO-2	-4.952	-5.329	-8.540	-8.451
HOMO-1	-4.898	-5.149	**-7.922**	**-7.931**
HOMO	-4.825	-5.012	-7.842	-7.857
LUMO	**-2.191**	**-2.220**	**-4.696**	**-4.524**
LUMO+1	-2.154	-2.144	-4.573	-4.304
LUMO+2	-2.047	-2.097	-3.404	-3.381
LUMO+3	-2.011	-2.029	-3.224	-3.174
LUMO+4	-1.154	-1.128	-3.128	-3.157

LUMO+5	-1.050	-1.012	-2.990	-3.075
LUMO+6	-0.901	-0.920	-2.921	-3.011
LUMO+7	-0.874	-0.838	-2.889	-2.956
LUMO+8	-0.805	-0.822	-2.755	-2.827
LUMO+9	-0.804	-0.756	-2.732	-2.682
LUMO+10	-0.691	-0.711	-2.652	-2.628
LUMO+11	-0.675	-0.595	-2.530	-2.469
LUMO+12	-0.550	-0.424	-2.398	-2.418
LUMO+13	-0.447	-0.376	-2.145	-2.198
LUMO+14	-0.322	-0.259	-2.050	-1.939
LUMO+15	-0.217	-0.243	-1.631	-1.648
LUMO+16	-0.193	-0.188	-1.396	-1.426
LUMO+17	-0.137	-0.103	-1.360	-1.151
LUMO+18	0.512	0.528	-1.082	-1.117
LUMO+19	0.548	0.617	-0.963	-1.053
LUMO+20	0.660	0.668	-0.922	-0.940
LUMO+21	0.678	0.766	-0.853	-0.798
LUMO+22	0.834	0.867	-0.742	-0.749
LUMO+23	0.947	0.970	-0.622	-0.710
LUMO+24	1.001	1.048	-0.560	-0.649
LUMO+25	1.105	1.068	-0.438	-0.431
LUMO+26	1.119	1.099	-0.371	-0.363
LUMO+27	1.137	1.131	-0.303	-0.275
LUMO+28	1.222	1.216	-0.196	-0.223
LUMO+29	1.298	1.333	-0.123	-0.188