Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Recognition of π-Hole Donor Ability of Iodopentafluorobenzene – a Conventional σ-Hole Donor for Crystal Engineering Involving Halogen Bonding

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Table S1. Crystal data and structure refinement for **1** and **1**•2IPFB.

	1	**1**•2IPFB
CCDC No.	1875983	1875984
Empirical formula	$C_{32}H_{72}I_6N_2Pt_2$	$C_{22}H_{36}F_5I_4NPt$
M_W/g	1636.49	1112.21
T/K	100(2)	100(2)
Radiation	Mo$K\alpha$ (λ = 0.71073 Å)	Mo$K\alpha$ (λ = 0.71073 Å)
Crystal color, shape	dark green, prism	brown, prism
Crystal size/mm^3	0.20 × 0.16 × 0.09	0.15 × 0.10 × 0.08
Crystal system	monoclinic	triclinic
Space group	$P2_1/c$	P-1
a/Å	14.5589(3)	9.3533(5)
b/Å	13.8558(3)	12.0866(7)
c/Å	23.7553(4)	14.5096(6)
α/°	90	80.144(4)
β/°	101.602(2)	75.835(4)
γ/°	90	78.965(5)
V/Å^3	4694.13(16)	1547.65(14)
Z	4	2
ρ_c/g·cm^{-3}	2.316	2.387
μ/mm^{-1}	9.922	8.564
F(000)	3008.0	1020.0
2Θ range/°	5.004 to 54.998	5.268 to 57
Reflections collected	33422	15865
Independent reflections	10760 [R_{int} = 0.0290, R_{sigma} = 0.0301]	7859 [R_{int} = 0.0309, R_{sigma} = 0.0441]
Data/restraints/parameters	10760/0/387	7859/0/302
Goodness-of-fit on F^2	1.046	1.047
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0219, wR_2 = 0.0385	R_1 = 0.0321, wR_2 = 0.0729
Final R indexes [all data]	R_1 = 0.0299, wR_2 = 0.0406	R_1 = 0.0424, wR_2 = 0.0792
Largest diff. peak/hole / e·Å^{-3}	0.83/–0.67	2.37/–1.42

Table S2. Bond lengths for the $[Pt_2(\mu\text{-}I_2)I_4]^{2-}$ anion in **1** and **1**•2IPFB.

Atoms	Length, Å	Atoms	Length, Å
1		**1•2IPFB**	
Pt1–I4	2.5879(3)	Pt1–I1	2.5792(4)
Pt1–I3	2.5938(3)	Pt1– I1^{1}	2.6036(4)
Pt1–I2	2.5989(3)	Pt1–I2	2.5972(4)
Pt1–I1	2.6060(3)	Pt1–I3	2.6049(4)
Pt2–I4	2.5896(3)	I1–Pt1^{1}	2.6036(4)
Pt2–I3	2.5924(3)		
Pt2–I6	2.6004(3)		
Pt2–I5	2.6069(3)		

^{1} 2–X,2–Y,1–Z

Table S3. Bond angles for the $[Pt_2(\mu\text{-}I_2)I_4]^{2-}$ anion in **1** and **1**•2IPFB.

Atoms	Angle, °	Atoms	Angle, °
1		**1•2IPFB**	
I3–Pt2–I6	174.696(9)	I1^{1}–Pt1–I3	174.174(12)
I3–Pt2–I5	91.209(8)	I1–Pt1–I3	90.771(12)
I6–Pt2–I5	94.030(9)	I2–Pt1–I3	92.234(12)
I4–Pt2–I3	84.769(8)	I1–Pt1– I1^{1}	84.486(12)
I4–Pt2–I6	89.997(9)	I2–Pt1– I1^{1}	92.683(12)
I4–Pt2–I5	175.962(10)	I1–Pt1– I2	175.776(13)
Pt2–I3–Pt1	95.115(8)	Pt1–I1–Pt1^{1}	95.514(12)
Pt1–I4–Pt2	95.328(8)		
I2–Pt1–I1	93.904(9)		
I4–Pt1–I1	175.471(9)		
I4–Pt1–I3	84.776(8)		
I4–Pt1–I2	90.449(8)		
I3–Pt1–I2	174.978(9)		
I3–Pt1–I1	90.905(8)		

^{1} 2–X,2–Y,1–Z

Table S4. CSD search for noncovalent interactions involving IPFB.

CCDC Code	Fragment of Adduct	Atoms	Distance, *d* (Å)	Angle, °	Type of contact	Refs
NEHCUB	(IPFB)•(fluoranthene)	H2•••F2	2.533	C9–H2•••F2 = 137.03	HB	[1]
		H4•••F5	2.603	C11–H4•••F5 = 131.18		
		H1•••F4	2.636	C8–H1•••F4 = 157.96		
		C3•••C13	3.374(4)		π-stacking	
		C4•••C17	3.353(4)			
		C2•••C21	3.382(4)			
	(IPFB)•(IPFB)	I1•••I1	3.6833(5)	C1–I1•••I1 = 139.14(7)	I type contact	
		F5•••F5	2.775(4)	C6–F5•••F5 = 134.16(17)	contact	
AXURUI	(IPFB)•[1,2,3]triazalo-[3,5-α]quinolone	I1•••N3	3.0661(16)	C11–I1•••N3 = 167.49(6)	XB	[2]
		H5•••I1	3.1724(4)	C7–H5•••I1 = 132.71	HB	
		H1•••F4	2.435	C1–H1•••F4 = 136.74	HB	
		H5•••F1	2.626	C7–H5•••F1 = 160.51		
		H6•••F3	2.479	C8–H6•••F3 = 144.25		
		C16•••C4	3.290(3)		π-stacking	
		C12•••C4	3.314(3)			
		C13•••C6	3.290(3)			
	(IPFB)•(IPFB)	F1•••F2	2.8699(15)	C12–F1•••F2 = 143.00(12) C13–F2•••F1 = 155.83(11)	contact	
		F5•••F5	2.588(2)	C16–F5•••F5 = 163.90(13)		
CUPKII	(IPFB)•(4-(*N*,*N*-dimethylamino)pyridi-ne)	I1•••N1	2.693(3)	C1–I1•••N1 = 178.43(11)	XB	[3]
		H9•••F4	2.539	C13–H9•••F4 = 132.6	HB	
		H2•••F5	2.633	C8–H2•••F5 = 141.6		
		C5•••C11	3.317(5)		π-stacking	

EBIHEF	(IPFB)•(2,4,6-trimethylbenzonitrile)	I1•••N1	3.092(4)	C1–I1•••N1 = 175.97(10)	XB	[4]
		C14•••F3	3.108(7)	C4–F3•••C14 = 168.9(3) C10–C14•••F3 = 175.8(3)	contact	
		H4•••F5	2.583	C13–H4•••F5 = 145.7(3)	HB	
	(IPFB)•(IPFB)	F2•••F2	2.917(6)	C3–F2•••F2 = 140.2(3)	contact	
FUYFAI03	(IPFB)•(1,4-diazabicyclo[2.2.2]oc-tane)	I1•••N1	2.6813(13)	C1–I1•••N1 = 177.96(5)	XB	[5]
		I2•••N2	2.6819(13)	C7–I2•••N2 = 178.64(5)		
		I3•••N3	2.7011(13)	C19–I3•••N3 = 177.19(5)		
		I4•••N4	2.7134(13)	C25–I4•••N4 = 177.04(5)		
		C17•••F16	2.9201(18)	C26–F16•••C17 = 164.97(9)	contact	
		C18•••F16	2.9783(18)	C26–F16•••C18 = 138.12(9)		
		C32•••F15	3.0020(18)	C24–F15•••C32 = 157.97(10)		
		C31•••F15	3.0341(18)	C24–F15•••C31 = 144.91(9)		
		H21•••F10	2.526	C35–H21•••F10 = 134.83	HB	
		H4•••F1	2.585	C14–H4•••F1 = 134.22		
		H6•••F3	2.587	C15–H6•••F3 = 135.32		
		H23•••F14	2.603	C36–H23•••F14 = 148.62		
		H9•••F16	2.625	C17–H9•••F16 = 97.27		
		H7•••F12	2.651	C16–H7•••F12 = 176.96		
	(IPFB)•(IPFB)	C10•••I1	3.6683(17)	C1–I1•••C10 = 76.48(5)	lp(I)–π	
		C4•••I2	3.6618(16)	C7–I2•••C4 = 75.75(5)		
		C28•••I3	3.5606(17)	C19–I3•••C28 = 75.68(5)		
		C22•••I4	3.6436(16)	C25–I4•••C22 = 75.09(5)		
		C26•••F15	3.1350(18)	C24–F15•••C26 = 110.91(9)	lp(F)–π	
		C24•••F16	3.1634(18)	C26–F16•••C24 = 109.34(9)		
		F18•••F20	2.6145(15)	C28–F18•••F20 = 142.39(11) C30–F20•••F18 = 160.48(9)	contact	

		F3•••F11	2.7441(14)	C4–F3•••F11 = 124.51(10) C20–F11•••F3 = 158.94(9)		
		F2•••F7	2.7718(15)	C3–F2•••F7 = 122.40(9) C9–F7•••F2 = 141.92(10)		
		F9•••F12	2.7870(14)	C11–F9•••F12 = 127.59(9) C21–F12•••F9 = 126.25(9)		
		F14•••F19	2.8286(15)	C23–F14•••F19 = 137.51(10) C29–F19•••F14 = 158.92(11)		
		F4•••F17	2.8437(15)	C5–F4•••F17 = 162.60(10) C27–F17•••F4 = 130.81(9)		
		F5•••F13	2.8610(14)	C6–F5•••F13 = 148.55(9) C22–F13•••F5 = 144.04(10)		
		C20•••C26	3.351		π-stacking	
FUYFAI04	(IPFB)•(1,4-diazabicyclo[2.2.2]oc-tane)	I1•••N1	2.690(3)	C1–I1•••N1 = 178.00(9)	XB	[5]
		I2•••N2	2.684(2)	C7–I2•••N2 = 178.79(10)		
		I3•••N3	2.706(2)	C19–I3•••N3 = 177.48(9)		
		I4•••N4	2.716(3)	C25–I4•••N4 = 177.09(9)		
		C17•••F16	2.943(3)	C26–F16•••C17 = 165.33(16)	contact	
		C18•••F16	2.999(3)	C26–F16•••C18 = 138.63(16)		
		C32•••F15	3.009(3)	C24–F15•••C32 = 158.45(18)		
		C31•••F15	3.045(3)	C24–F15•••C31 = 145.10(16)		
		H21•••F10	2.539	C35–H21•••F10 = 135.87	HB	
		H4•••F1	2.618	C14–H4•••F1 = 134.26		
		H6•••F3	2.605	C15–H6•••F3 = 136.81		
		H23•••F14	2.623	C36–H23•••F14 = 148.35		
		H9•••F16	2.646	C17–H9•••F16 = 97.44		
		H7•••F12	2.670	C16–H7•••F12 = 176.72		

	(IPFB)•(IPFB)	C10•••I1	3.681(4)	C1–I1•••C10 = 76.37(11)	lp(I)–π	
		C4•••I2	3.668(3)	C7–I2•••C4 = 75.78(10)		
		C28•••I3	3.579(3)	C19–I3•••C28 = 75.75(8)		
		C22•••I4	3.649(3)	C25–I4•••C22 = 74.99(9)		
		F18•••F20	2.625(3)	C28–F18•••F20 = 142.1(2) C30–F20•••F18 = 161.07(18)	contact	
		F3•••F11	2.754(2)	C4–F3•••F11 = 124.94(16) C20–F11•••F3 = 159.99(17)		
		F2•••F7	2.774(3)	C3–F2•••F7 = 123.01(18) C9–F7•••F2 = 142.5(2)		
		F9•••F12	2.796(3)	C11–F9•••F12 = 127.91(18) C21–F12•••F9 = 127.70(17)		
		F14•••F19	2.835(3)	C23–F14•••F19 = 137.5(2) C29–F19•••F14 = 158.6(2)		
		F4•••F17	2.850(3)	C5–F4•••F17 = 162.46(17) C27–F17•••F4 = 131.12(19)		
		F5•••F13	2.863(3)	C6–F5•••F13 = 149.72(16) C22–F13•••F5 = 144.17(17)		
		C20•••C26	3.374		π-stacking	
FUYFAI05	(IPFB)•(1,4-diazabicyclo[2.2.2]oc-tane)	I1•••N1	2.711(5)	C1–I1•••N1 = 177.95(15)	XB	[5]
		I2•••N2	2.690(5)	C7–I2•••N2 = 178.58(18)		
		I3•••N3	2.723(5)	C19–I3•••N3 = 177.74(19)		
		I4•••N4	2.711(5)	C25–I4•••N4 = 178.03(15)		
		C17•••F16	2.972(6)	C26–F16•••C17 = 165.2(4)	contact	
		C18•••F16	3.017(6)	C26–F16•••C18 = 140.1(4)		
		C32•••F15	2.990(5)	C24–F15•••C32 = 160.0(3)		
		C31•••F15	3.030(5)	C24–F15•••C31 = 144.9(3)		

		H21•••F10	2.630	C35–H21•••F10 = 135.6	HB	
		H4•••F1	2.656	C14–H4•••F1 = 135.5		
		H6•••F3	2.631	C15–H6•••F3 = 140.3		
	(IPFB)•(IPFB)	C4•••I2	3.675(6)	C7–I2•••C4 = 75.32(19)	lp(I)–π	
		C28•••I3	3.616(7)	C19–I3•••C28 = 75.85(18)		
		C22•••I4	3.642(6)	C25–I4•••C22 = 75.18(16)		
		F18•••F20	2.648(6)	C28–F18•••F20 = 141.0(5) C30–F20•••F18 = 163.7(3)	contact	
		F3•••F11	2.766(5)	C4–F3•••F11 = 127.0(3) C20–F11•••F3 = 162.6(3)		
		F2•••F7	2.786(5)	C3–F2•••F7 = 123.6(3) C9–F7•••F2 = 142.5(2)		
		F9•••F12	2.791(5)	C11–F9•••F12 = 128.3(4) C21–F12•••F9 = 131.4(4)		
		F14•••F19	2.828(6)	C23–F14•••F19 = 135.6(4) C29–F19•••F14 = 158.4(5)		
		F4•••F17	2.845(5)	C5–F4•••F17 = 162.1(3) C27–F17•••F4 = 131.2(4)		
		F5•••F13	2.865(6)	C6–F5•••F13 = 152.3(3) C22–F13•••F5 = 144.8(4)		
		C20•••C26	3.400		π-stacking	
FUYFAI06	(IPFB)•(1,4-diazabicyclo[2.2.2]oc-tane)	I4•••N4	2.695(5)	C25–I4•••N4 = 177.92(16)	XB	[5]
	(IPFB)•(IPFB)	F28•••F30	2.669(7)	C46–F28•••F30 = 140.6(5) C48–F30•••F28 = 164.8(4)	contact	
		F4•••F27	2.855(6)	C5–F4•••F27 = 160.9(3)		

				C45–F27•••F4 = 130.4(3)		
GAJRER	(IPFB)•(2,1,3-benzoselenadiazole)	I1•••N2	3.073(3)	C4–I1•••N2 = 171.17(14)	XB	[6]
		I2•••N3	2.961(3)	C9–I2•••N3 = 174.76(11)		
		Se1•••F8	3.289(2)	C11–F8•••Se1 = 129.06(19)	ChB	
		Se2•••F1	3.308(2)	C6–F1•••Se2 = 128.23(19)	contact	
		H5•••F10	2.393	C20–H5•••F10 = 161.67	HB	
		H1•••F9	2.448	C14–H1•••F9 = 136.4		
		H3•••F1	2.491	C17–H3•••F1 = 138.8		
		H6•••F7	2.555	C21–H6•••F7 = 156.9		
		H7•••F4	2.606	C23–H7•••F4 = 130.0		
		C8•••C18	3.341		π-stacking	
		C11•••C16	3.345			
		C10•••C17	3.379			
		C9•••C18	3.392			
	(IPFB)•(IPFB)	I1•••F8	3.450(2)	C4–I1•••F8 = 125.96(13) C11–F8•••I1 = 144.02(19)	contact	
		F3•••F7	2.706(3)	C3–F3•••F7 = 160.1(2) C7–F7•••F3 = 160.2(3)		
		F9•••F9	2.872(5)	C12–F9•••F9 = 109.2(2)		
		F5•••F6	2.902(3)	C1–F5•••F6 = 107.62(18) C10–F6•••F5 = 141.0(2)		
GUQQIU	(IPFB)•pyrene	H7•••I1	3.049	C16–H7•••I1 = 126.5	HB	[7]
		H6•••F5	2.545	C15–H6•••F5 = 134.9	HB	
		H9•••F4	2.578	C19–H9•••F4 = 152.2		
		H2•••F2	2.615	C8–H2•••F2 = 141.9		
		C4•••C18	3.242		π-stacking	
		C4•••C14	3.291			

		C5•••C17	3.338			
		C5•••C16	3.340			
IKIXOR	(IPFB1)•complex Pt^{IV}	I2•••I1	3.5716(9)	C19–I2•••I1 = 173.5(2)	XB	[8]
	(IPFB2)•complex Pt^{IV}	I3•••N3	2.849(6)	C25–I3•••N3 = 176.5(3)	XB	
		F9•••Cl1	3.179(6)	C11–Cl1•••F9 = 124.0(2) C27–F9•••Cl1 = 173.2(7)	contact	
		H17•••F8	2.543	C16–H17•••F8 = 154.4	HB	
		H12•••F6	2.606	C6–H12•••F6 = 133.8		
	(IPFB1)•(IPFB2)	F2•••F7	2.851(12)	C21–F2•••F7 = 140.4(6) C29–F7•••F2 = 158.1(5)	contact	
IKIYAE	(IPFB1)•complex Pt^{IV}	I3•••I2	3.4954(8)	C51–I3•••I2 = 170.95(18)	XB	[8]
		H7•••F2	2.412(5)	C13–H7•••F2 = 153.1	HB	
		H5•••F3	2.410	C9–H5•••F3 = 143.9		
	(IPFB2)•complex Pt^{IV}	I4•••N3	2.886(8)	C57–I4•••N3 = 176.4(2)	XB	
		H29•••I4	3.090	C30–H29•••I4 = 142.2	HB	
	(IPFB1)•(IPFB2)	F4•••F7	2.804(9)	C55–4•••F7 = 162.6(5) C58–F7•••F4 = 150.5(6)	contact	
		C29•••I3	3.679(9)	C51–I3•••C60 = 80.2(3)	lp(I)–π	
IKIYEI	(IPFB1)•complex Pt^{IV}	I2•••N3	2.784(9)	C26–I2•••N3 = 175.4(4)	XB	[8]
	(IPFB2)•complex Pt^{IV}	I3•••I1	3.4179(10)	C32–I3•••I1 = 168.6(3)	XB	
		H21•••F6	2.597	C21–H21•••F6 = 135.2	HB	
		H17•••F10	2.653	C16–H17•••F10 = 128.1		
		H25•••F7	2.668	C25–H25•••F7 = 114.0		
	(IPFB1)•(IPFB1)	F2•••F2	2.649(16)	C28–F2•••F2 = 175.6(10)	contact	
	(IPFB2)•(IPFB2)	F8•••F8	2.849(17)	C35–F8•••F8 = 112.3(8)	contact	
		F8•••F9	2.901(11)	C35–F8•••F9 = 148.1(9) C36–F9•••F8 = 112.0(7)		

	(IPFB2)•(IPFB1)	F9•••F2	2.931(13)	C36–F9•••F2 = 89.1(7) C28–F2•••F9 = 90.2(7)	contact	
		C33•••C28	3.396		π-stacking	
IQEWIK	(IPFB)•(4'-Octyloxy-4-stilbazole)	I1•••N1	2.811(3)	C6–I1•••N1 = 168.40(10)	XB	[9]
		H12•••F2	2.524	C20–H12•••F2 = 119.19	HB	
		H2•••F5	2.550	C8–H2•••F5 = 167.50		
		H6•••F5	2.617	C13–H6•••F5 = 171.55		
	(IPFB)•(IPFB)	F3•••F4	2.821(3)	C3–F3•••F4 = 169.17(18) C4–F4•••F3 = 125.19(17)	contact	
KAGKEI	(IPFB)•(tris(dialky1-amino)sulfonium perfluoro-2-methyl-2-pentyl carbanion)	I1•••F1	2.455(4)	C7–I1•••F1 = 175.6(3)	XB	[10]
		I2•••F1	2.509(4)	C13–I2•••F1 = 176.8(3)		
		H5•••F9	2.478	C2–H5•••F9 = 144.7	HB	
		F10•••F8	2.817(8)	C17–F10•••F8 = 87.3(4) C15–F8•••F10 = 141.0(7)	contact	
		F8•••F2	2.824(8)	C15–F8•••F2 = 83.0(4) C8–F2•••F8 = 145.3(5)		
	(IPFB)•(IPFB)	C17•••F8	3.066(10)	C15–F8•••C17 = 137.4(7)	lp(F)–π	
LEZPIQ	(IPFB)•(2,4,6-trimethylpyridine)	I1•••N1	2.863(3)	C1–I1•••N1 = 180.00	XB	[11]
		H4•••F1	2.636	C8–H4•••F1 = 153.29	HB	
		H1•••F1	2.658	C6–H1•••F1 = 145.28		
	(IPFB)•(IPFB)	C2•••F1	3.139(2)	C2–F1•••C2 = 115.21(10)	lp(F)–π	
		F1•••F1	2.840(2)	C2–F1•••F1 = 89.77(12)	contact	
LEZPOW	(IPFB)•(2,6-dimethylpyridine)	I1•••N1	2.961(2)	C1–I1•••N1 = 180.00	XB	[11]
		H5•••F1	2.485	C8–H5•••F1 = 153.03	HB	
		H2•••F3	2.526	C7–H2•••F3 = 180.00		
	(IPFB)•(IPFB)	F1•••F1	2.777(3)	C2–F1•••F1 = 98.09(13)	contact	
LEZPUC	(IPFB)•(3,5-	I1•••N1	2.831(3)	C1–I1•••N1 = 180.00	XB	[11]

	dimethylpyridine)	H2•••F3	2.422	C7–H2•••F3 = 180.0	HB	
LEZPUC01	(IPFB)•(3,5-dimethylpyridine)	I1•••N1	2.841(9)	C8–I1•••N1 = 178.7(4)	XB	[11]
		H2•••F3	2.476	C3–H2•••F3 = 172.2	HB	
		C13•••C3	3.395		π-stacking	
	(IPFB)•(IPFB)	F4•••F4	2.825	C12–F4•••F4 = 95.3(9)	contact	
LEZQAJ	(IPFB)•(4-methylpyridine)	I1•••N1	2.841(9)	C1–I1•••N1 = 173.89(9)	XB	[11]
		H7•••I1	3.140	C12–H7•••I1 = 149.9	HB	
		H3•••F5	2.469	C10–H3•••F5 = 146.05		
	(IPFB)•(IPFB)	F2•••F3	2.902(3)	C3–F2•••F3 = 120.00(16) C4–F3•••F2 = 150.81(19)	contact	
LINTUZ	(IPFB1)•(pyridyl macrocycle)	I1•••O1	2.719(2)	C29–I1•••O1 = 173.72(7)	XB	[12]
		C6•••F4	3.098(3)	C33–F4•••C6 = 156.8(2)	contact	
		C7•••F4	3.140(3)	C33–F4•••C7 = 131.36(19)		
		C37•••F1	3.153(4)	C30–F1•••C37 = 118.47(15)		
		H17•••F5	2.487	C14–H17•••F5 = 140.54	HB	
		H24•••F2	2.529	C22–H24•••F2 = 137.00		
		H7•••F4	2.569	C6–H7•••F4 = 115.4		
		H8•••F4	2.664	C7–H8•••F4 = 111.6		
	(IPFB2)•(pyridyl macrocycle)	I2•••O2	2.745(2)	C35–I2•••O2 = 177.13(8)	XB	
		C3•••F6	3.154(3)	C36–F6•••C3 = 127.4(2)	contact	
		H14•••F7	2.601	C13–H14•••F7 = 120.11	HB	
		H3•••F6	2.622	C3–H3•••F6 = 113.84		
	(IPFB3)•(pyridyl macrocycle)	I3•••N6	3.001(3)	C41–I3•••N6 = 169.32(10)	XB	
		H26•••F11	2.650	C23–H26•••F11 = 140.5	HB	
		C46•••C7	3.380		π-stacking	
		C43•••C8	3.381			
	(IPFB)•(IPFB)	F1•••F8	2.915	C30–F1•••F8 = 128.31(19)	contact	

				C38–F8•••F1 = 89.98(17)		
		F1•••F7	2.797(3)	C30–F1•••F7 = 93.48(14) C37–F7•••F1 = 92.28(18)		
		F5•••F5	2.797(4)	C34–F5•••F5 = 110.99(16)		
		F1•••F2	2.879(3)	C30–F1•••F2 = 152.98(18) C31–F2•••F1 = 120.48(16)		
		F12•••F12	2.769(3)	C43–F12•••F12 = 118.63(17)		
		F14•••F14	2.767(4)	C45–F14•••F14 = 117.75(18)		
NAFXEA	(IPFB)•(pyridine)	I1•••N1	2.783(2)	C1–I1•••N1 = 178.96(6)	XB	[13]
		H3•••F3	2.622	C9–H3•••F3 = 153.0	HB	
	(IPFB)•(IPFB)	C6•••F2	3.091(4)	C3–F2•••C6 = 148.8(2)	lp(F)–π	
		F2•••F4	2.972(3)	C3–F2•••F4 = 139.01(18) C6–F4•••F2 = 82.18(15)	contact	
NAFXIE	(IPFB)•(3-methylpyridine)	I1•••N1	2.7279(17)	C1–I1•••N1 = 179.53(7)	XB	[13]
		H6•••F3	2.531	C12–H6•••F3 = 156.0	HB	
		H3•••F4	2.629	C10–H3•••F4 = 137.0		
		H7•••F1	2.664	C12–H7•••F1 = 152.0		
NAFXUQ	(IPFB)•(*N,N,N′,N′*-tetramethylethane-1,2-diamine)	I1•••N1	2.765(2)	C1–I1•••N1 = 178.61(18)	XB	[13]
		H3•••F3	2.635	C8–H3•••F3 = 149.0	HB	
		C7•••F3	3.112(4)	C4–F3•••C7 = 161.69(16)	contact	
	(IPFB)•(IPFB)	C2•••F2	2.934(3)	C3–F2•••C2 = 141.17(15)	lp(F)–π	
		C3•••F2	3.129(3)	C3–F2•••C3 = 154.56(15)		
NUQTIE	(IPFB)•(complex Pt^{II})	I1•••Cl1	3.3330(5)	C32–I1•••Cl1 = 161.47(4)	XB	[14]
		C21•••F3	3.126(2)	C35–F3•••C21 = 154.56(11)	contact	
		C22•••F3	3.125(3)	C35–F3•••C22 = 141.87(12)		
		C11•••F5	3.1280(16)	C37–F5•••C11 = 154.56(11)		
		H7•••F3	2.406	C12–H7•••F3 = 172.04	HB	

		H9•••F2	2.492	C15–H9•••F2 = 160.45		
		H15•••F3	2.547	C22–H15•••F3 = 119.45		
		H14•••F3	2.555	C21–H14•••F3 = 118.79		
		H2•••F5	2.588	C6–H2•••F5 = 151.87		
		H8•••F4	2.651	C13–H8•••F4 = 135.46		
		C36•••C13	3.207		π-stacking	
		C34•••C18	3.364			
		C36•••C12	3.392			
	(IPFB)•(IPFB)	F5•••F5	2.793(2)	C37–F5•••F5 = 121.09(8)	contact	
OQIJEF	(IPFB1)•(thiourea)	I1•••S1	3.1770(14)	C18–I•••S1 = 171.22(13)	XB	15
		H4•••F4	2.538	N2–H4•••F4 = 114.0	HB	
	(IPFB2)•(thiourea)	I2•••S1	3.3205(16)	C24–I2•••S1 = 174.33(13)	XB	
	(IPFB1)•(benzo-18-crown-6)	C22•••C5	3.354		π-stacking	
		C17•••F1	3.001(8)	C19–F•••C17 = 160.5(4)	contact	
		H10•••F5	2.649	C8–H10•••F5 = 154.4	HB	
	(IPFB2)•(benzo-18-crown-6)	C8•••F6	3.120(9)	C25–F6•••C8 = 168.9(4)	contact	
		C14•••F10	3.144(7)	C29–F10•••C14 = 142.7(3)		
		H9•••F6	2.536	C8–H9•••F6 = 117.5	HB	
		H21•••F10	2.566	C14–H21•••F10 = 117.2		
OQITAL	(IPFB1)•(thiourea)	I1•••S1	3.1977(14)	C20–I•••S1 = 178.41(18)	XB	15
	(IPFB2)•(thiourea)	I2•••S1	3.2708(13)	C26–I2•••S1 = 170.0(2)	XB	
	(IPFB2)•(18-crown-6)	H40•••F8	2.625	C19–H40•••F8 = 141.7	HB	
OQITAL01	(IPFB1)•(thiourea)	I1•••S1	3.1724(8)	C16–I1•••S1 = 177.73(8)	XB	15
	(IPFB2)•(thiourea)	I2•••S1	3.2272(8)	C22–I2•••S1 = 168.85(9)	XB	
	(IPFB1)•(18-crown-6)	H8•••F1	2.616	C3–H8•••F1 = 127.5	HB	
		H7•••F3	2.657	C3–H7•••F3 = 125.88		
	(IPFB2)•(18-crown-6)	H32•••I2	3.159	C13–H32•••I2 = 133.52	HB	

		H36•••F8	2.520	C15–H36•••F8 = 144.39		
	(IPFB2)•(IPFB1)	C20•••F9	3.166(4)	C26–F9•••C20 = 105.93(19)	lp(F)–π	
	(IPFB1)•(IPFB1)	C20•••C20	3.310		π-stacking	
OQIVER	(IPFB1)•(thiourea)	I2•••S1	3.1632(8)	C35–I2•••S1 = 179.37(11)	XB	[15]
	(IPFB2)•(thiourea)	I4•••S2	3.1592(8)	C47–I4•••S2 = 177.15(12)	XB	
	(IPFB1)•(18-crown-6)	H40•••F8	2.511	C18–H40•••F8 = 132.6	HB	
		H50•••F6	2.588	C23–H50•••F6 = 155.4		
		H60•••F8	2.664	C28–H60•••F8 = 131.2		
	(IPFB2)•(18-crown-6)	H16•••F18	2.620	C6–H16•••F18 = 133.2	HB	
OQIVER01	(IPFB1)•(thiourea)	I2•••S1	3.1311(5)	C35–I2•••S1 = 178.75(7)	XB	[15]
	(IPFB2)•(thiourea)	I4•••S2	3.1301(5)	C47–I4•••S2 = 176.75(8)	XB	
	(IPFB1)•(18-crown-6)	C18•••F8	3.167(3)	C38–F8•••C18 = 140.64(17)	contact	
		H40•••F8	2.417	C18–H40•••F8 = 132.04	HB	
		H50•••F6	2.547	C23–H50•••F6 = 160.10		
		H60•••F8	2.599	C28–H60•••F8 = 128.72		
	(IPFB2)•(18-crown-6)	H16•••F18	2.620	C6–H16•••F18 = 133.2	HB	
	(IPFB1)•(IPFB2)	C37•••F7	3.162(4)	C37–F7•••C37 = 105.51(18)	lp(F)–π	
		C39•••C51	3.342		π-stacking	
OYOMAS	(IPFB)•(4-(2-(4-(decyloxy)phenyl)vinyl)pyridine)	I1•••N1	2.7886(19)	C6–I1•••N1 = 177.86(8)	XB	[16]
		H10•••F5	2.602	C19–H10•••F5 = 140.0	HB	
		H4•••F4	2.666	C11–H4•••F4 = 141.5		
		H5•••F2	2.682	C12–H5•••F2 = 149.6		
TUWHOK	(IPFB)•(4-(2-thienyl)pyridine)	I1•••N1	2.7670(16)	C1–I1•••N1 = 178.75(6)	XB	[17]
		C15•••F5	3.012	C6–F5•••C15 = 153.32(11)	contact	
		H2•••F3	2.512	C8–H2•••F3 = 135.59	HB	
		H4•••F2	2.563	C12–H4•••F2 = 155.78		
XOHWIB	(IPFB)•(Phenazine)	I1•••N1	2.9149(16)	C1–I1•••N1 = 178.10(7)	XB	[18]

		H7•••F5	2.644	C17–H7•••F5 = 122.17	HB	
		H5•••F2	2.667	C15–H5•••F2 = 176.39		
		H6•••F5	2.679	C16–H6•••F5 = 120.49		
		C5•••C18	3.383		π-stacking	
	(IPFB)•(IPFB)	F5•••F5	2.924(3)	C6–F5•••F5 = 93.21(12)	contact	
XOHWOH	(IPFB)•(Acridine)	I1•••N1	2.8995(16)	C1–I1•••N1 = 179.07(6)	XB	[18]
		H2•••F2	2.538	C10–H2•••F2 = 130.54	HB	
		H6•••F5	2.656	C16–H6•••F5 = 120.43		
		H7•••F5	2.658	C17–H7•••F5 = 120.70		
	(IPFB)•(IPFB)	F5•••F5	2.872(2)	C6–F5•••F5 = 92.08(10)	contact	
YABJAM	(IPFB)•(carbene)	I1•••C3	2.754(3)	C1–I1•••C3 = 178.91(14)	XB	[19]
		H12•••I1	3.00	C41–H12•••I1 = 152	HB	
		H4•••I1	3.01	C30–H4•••I1 = 147		
		H30•••I1	3.07	C40–H30•••I1 = 145		
		H22•••I1	3.08	C31–H22•••I1 = 143		
		H13•••F3	2.451	C34–H13•••F3 = 131		
	(IPFB)•(IPFB)	C13•••I1	3.626(4)	C1–I1•••C13 = 83.99(11)	lp(I)–π	
ZAHGAQ	(IPFB)•(IPFB)	I1•••F5	3.445(4)	C1–I1•••F5 = 156.79(11)	XB	[20]
		F2•••F3	2.848(5)	C3–F2•••F3 = 160.0(3) C4–F3•••F2 = 160.8(3)	contact	
		F1•••F4	2.880(4)	C2–F1•••F4 = 90.0(2) C5–F4•••F1 = 88.6(2)		
		F3•••F4	2.902(4)	C4–F3•••F4 = 134.9(3) C5–F4•••F3 = 163.3(3)		
		C5•••F1	3.146(5)	C2–F1•••C5 = 115.2(2)	lp(F)–π	
		C4•••C4	3.306		π-stacking	
ZEQKUE	(IPFB)•(complex Cu^{II})	I1•••O2	3.038(7)	C39–I1•••O2 = 167.9(3)	XB	[21]

		H2•••F5	2.557	C4–H2•••F5 = 119.3	HB	
		H25•••F3	2.586	C36–H25•••F3 = 154.5		
		H5•••F1	2.614	C8–H5•••F1 = 140.9		
		H16•••F4	2.662	C23–H16•••F4 = 158.4		
		C4•••F5	3.119(11)	C44–F5•••C4 = 125.8(6)	contact	
		C43•••C9	3.382		π-stacking	
ZEQLAL	(IPFB)•(complex Ni^{II})	I1•••O2	3.0699(19)	C2–I1•••O2 = 168.23(10)	XB	[21]
		H6•••F4	2.528	C13–H6•••F4 = 120.99	HB	
		H4•••F5	2.579	C10–H4•••F5 = 143.2		
		H24•••F2	2.581	C41–H24•••F2 = 157.5		
		H18•••F1	2.617	C31–H18•••F1 = 158.7		
		C1•••C16	3.389		π-stacking	
		C6•••C12	3.393			
[Pt(btpy)(PPh_3)CN]•IPFB (**1c**)	(IPFB)•(complex Pt^{II})	I1•••N1	2.8215(19)	C–I1•••N1 = 172.21(5)	XB	[22]
		H27•••F2	2.5114	C27–H27•••F2 = 163.66	HB	
		H21•••F3	2.5324	C21–H21•••F3 = 119.78		
		H22•••F3	2.5227	C22–H22•••F3 = 120.15		
		H12•••F3	2.4450	C12–H12•••F3 = 175.13		
[Pt(bfpy)(PPh_3)CN]•IPFB (**2c**)	(IPFB1)•(complex Pt^{II})	I1•••N1C	2.863(2)	C32–I•••N = 175.02(5)	XB	[22]
		H8•••F1	2.6533	C8–H8•••F1 = 120.28	HB	
		H16•••F3	2.666	C16–H16•••F3 = 129.05		
		C34•••C9	3.288		π-stacking	
		C32•••C13	3.362			
	(IPFB2)•(complex Pt^{II})	I1A•••N1C	2.815(5)	C34A–I1A•••N1C = 167.7(7)	XB	
		H7•••F1A	2.58	C7–H7•••F1A = 128.2	HB	
		H30•••F5A	2.37	C30–H30•••F5A = 123.3		
		H12•••F5A	2.60	C12–H12•••F5A = 154.4		

		C32A•••C13	3.191		π-stacking	
		C35A•••C6	3.362			

Table S5. Cartesian atomic coordinates for model structures.

Atom	*x*	*y*	*z*
1•2IPFB			
Pt	12.609686	14.272423	6.098421
I	13.385599	13.656391	8.479738
I	11.742573	14.721891	3.691858
I	11.921367	16.653135	6.900702
Pt	14.274591	11.291816	7.849435
I	13.498678	11.907848	5.468117
I	15.141704	10.842348	10.255998
I	14.962910	8.911104	7.047154
I	11.492068	11.596098	2.057169
F	9.232302	10.120549	0.324985
F	11.453083	6.264678	–1.145119
F	9.211741	7.784830	–1.015404
F	13.724804	9.352307	1.544028
F	13.711054	7.059779	0.135294
C	11.467605	9.799578	0.986113
C	10.348043	9.376815	0.316616
C	12.609972	7.811684	0.196665
C	10.329441	8.184920	–0.391935
C	11.461991	7.409188	–0.463069
C	12.610147	8.995192	0.913585
I	15.042787	13.434089	16.005025
F	12.783021	11.958540	14.272841
F	15.003802	8.102669	12.802737
F	12.762460	9.622820	12.932452
F	17.275523	11.190297	15.491883
F	17.261773	8.897770	14.083150
C	15.018324	11.637569	14.933969
C	13.898762	11.214805	14.264472
C	16.160691	9.649675	14.144520
C	13.880160	10.022910	13.555921
C	15.012709	9.247179	13.484787
C	16.160866	10.833182	14.861440
I	15.392209	13.968141	11.890686
F	17.651975	15.443690	13.622871
F	15.431194	19.299560	15.092975
F	17.672536	17.779409	14.963260
F	13.159473	16.211932	12.403828

F	13.173223	18.504460	13.812562
C	15.416672	15.764660	12.961742
C	16.536234	16.187424	13.631239
C	14.274305	17.752555	13.751191
C	16.554836	17.379319	14.339790
C	15.422287	18.155051	14.410925
C	14.274130	16.569047	13.034271
I	11.841490	12.130150	–2.057169
F	14.101256	13.605699	–0.324985
F	11.880476	17.461570	1.145119
F	14.121817	15.941419	1.015404
F	9.608754	14.373941	–1.544028
F	9.622504	16.666469	–0.135294
C	11.865954	13.926670	–0.986113
C	12.985515	14.349433	–0.316616
C	10.723586	15.914564	–0.196665
C	13.004117	15.541329	0.391935
C	11.871568	16.317060	0.463069
C	10.723411	14.731057	–0.913585
IKIYAE			
Pt	–2.009820	18.528433	5.023030
I	–3.074587	19.237154	7.448281
N	–2.008972	20.603016	4.486537
N	0.083668	19.221650	5.459487
C	1.133214	18.489672	5.924037
C	1.647952	20.806658	4.576980
H	1.793994	21.622418	4.112430
C	–0.808030	21.208873	4.393353
C	0.911327	17.322980	6.809285
C	–1.833307	23.241416	3.695843
H	–1.773043	24.144835	3.409439
C	–3.120758	21.321279	4.223429
H	–3.968334	20.903857	4.324835
C	0.359238	20.382081	4.830495
N	1.633906	16.226653	6.522882
C	4.513084	21.777460	4.630424
H	3.847195	22.451297	4.708534
C	–3.073124	22.624229	3.817804
H	–3.872872	23.098300	3.623214
C	6.798176	21.118531	4.305650
C	–0.687770	22.519874	3.998691
H	0.169124	22.928350	3.935655

C	2.745928	20.039199	4.997678
C	2.440356	18.876383	5.695188
H	3.148341	18.333735	6.024073
C	0.105908	17.421372	7.945308
H	–0.397424	18.208509	8.116603
C	5.835103	22.135250	4.418019
H	6.084322	23.047613	4.349501
C	–1.950813	16.520935	5.481413
H	–1.017545	16.225758	5.537598
H	–2.412833	16.011085	4.782533
H	–2.393687	16.368874	6.343365
C	0.781403	15.200095	8.518116
H	0.753494	14.439792	9.088183
C	4.155693	20.426805	4.730460
C	0.054155	16.342040	8.823705
H	–0.467104	16.386764	9.615769
C	5.128310	19.445865	4.641387
H	4.886860	18.533501	4.729089
C	8.171941	21.500173	4.111060
C	–1.275458	18.023651	3.131257
H	–1.809524	17.290182	2.759892
H	–0.341530	17.740401	3.209367
H	–1.333720	18.801843	2.539265
C	–3.869264	18.077320	4.278243
H	–4.556614	18.393367	4.901754
H	–3.951858	17.108306	4.168615
H	–3.988978	18.515612	3.410809
N	9.278948	21.786405	3.957580
C	6.452773	19.794710	4.426241
H	7.118880	19.117891	4.361835
C	1.545512	15.185187	7.375241
H	2.039523	14.401031	7.175170
I	3.532353	15.470524	4.484755
F	3.401238	13.426055	1.995234
F	6.632549	16.172090	4.058986
F	8.472684	15.289542	2.321378
F	7.813078	13.506557	0.415217
F	5.248931	12.597175	0.234330
C	4.970351	14.821434	3.072332
C	6.258758	15.286561	3.150442
C	7.219812	14.848268	2.248750
C	6.852702	13.938887	1.271688

C	5.584954	13.485686	1.182615
C	4.634117	13.912052	2.081567
I	7.998841	11.154389	3.385184
F	5.149558	10.128427	2.328230
F	6.786210	12.668733	5.933630
F	2.643748	10.384843	3.309403
F	4.309481	12.805886	6.973728
F	2.142764	11.601328	5.586930
C	6.049955	11.374728	4.115171
C	4.961364	10.784375	3.473846
C	5.789792	12.063473	5.290934
C	3.461283	11.586420	5.164862
C	4.537658	12.161865	5.810298
C	3.684361	10.918546	3.964432
Pt	12.249456	11.058978	–0.019322
I	11.261991	10.316267	2.453755
N	12.164797	8.977537	–0.567326
N	14.345184	10.302850	0.341218
C	15.435622	11.010975	0.708473
C	12.223840	6.312005	–1.290873
H	12.248563	5.402623	–1.563573
C	15.821954	8.601858	–0.520734
H	15.921118	7.752108	–0.931840
C	14.677506	12.245349	2.733855
H	14.212342	11.476101	3.036703
C	12.976034	11.595365	–1.874643
H	13.164068	10.787356	–2.396748
H	13.800235	12.114160	–1.765015
H	12.306732	12.138012	–2.341934
C	13.410028	6.991805	–1.012691
H	14.247376	6.547550	–1.072987
C	18.548676	7.447987	–0.313811
H	17.825009	6.863597	–0.115110
C	14.562115	9.105745	–0.269960
C	16.741888	10.572683	0.434402
H	17.483435	11.118312	0.664621
C	11.027462	8.300719	–0.804397
H	10.200989	8.759882	–0.715324
C	13.347745	8.327553	–0.648177
C	15.309930	12.260257	1.503278
N	15.971923	13.300828	1.025024
C	18.320820	8.816532	–0.406995

C	11.002679	6.976897	–1.168911
H	10.182268	6.526679	–1.333354
C	10.388443	11.538715	–0.708473
H	10.192753	11.016938	–1.514240
H	10.355182	12.495802	–0.922248
H	9.721287	11.335967	–0.017815
C	20.868451	7.772979	–0.774250
C	16.950821	9.341290	–0.171294
C	12.355100	13.068265	0.456328
H	11.691587	13.563207	–0.067147
H	13.252455	13.408165	0.249404
H	12.174285	13.190510	1.411464
C	19.823382	6.914284	–0.509771
H	19.969070	5.975086	–0.460439
N	23.242167	6.747316	–1.118208
C	19.394766	9.663301	–0.683806
H	19.256186	10.602498	–0.735880
C	20.665697	9.135561	–0.882508
H	21.391810	9.711006	–1.093542
C	14.743716	13.393257	3.512215
H	14.328384	13.420092	4.365946
C	15.423035	14.493460	3.028481
H	15.504858	15.283579	3.547845
C	22.211339	7.203497	–0.955136
C	15.979950	14.415939	1.771867
H	16.392933	15.191150	1.414205
IPFB			
I	–2.316528	–0.000067	0.000029
F	–0.151122	2.402463	–0.000451
F	3.971512	–0.001368	–0.000084
F	2.586356	2.395165	0.000686
F	–0.152535	–2.401824	0.000414
F	2.587295	–2.394259	–0.000242
C	–0.223275	0.000471	–0.000188
C	0.504179	1.199737	–0.000354
C	1.903859	–1.210542	–0.000111
C	1.904945	1.210494	0.000069
C	2.606562	0.000272	–0.000164
C	0.504140	–1.200107	0.000011

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