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新型酰胺功能化铱[III]配合物的光电性能

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Photoelectric Properties of Novel Amide-Functionalized Ir(III) Complexes

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Table S1 Selected parameters of complexes optimized at B3LYP/6-31G level

	Bond angle			
	(1)	(2)	(3)	(4)
A(C1,Ir,N1)/(°)	79.19	80.02	79.15	79.08
A(C1,Ir,C2)/(°)	172.24	89.30	172.53	172.47
A(C1,Ir,N2)/(°)	95.20	95.03	95.47	95.48
A(C1,Ir,N3)/(°)	96.60	173.25	96.40	96.40
A(C1,Ir,N4)/(°)	89.47	97.65	89.18	89.37
A(N1,Ir,C2)/(°)	95.27	96.24	95.41	95.38
A(N1,Ir,N2)/(°)	88.27	173.93	88.17	88.21
A(N1,Ir,N3)/(°)	174.32	96.26	174.25	174.02
A(N1,Ir,N4)/(°)	96.01	85.11	96.19	95.94
A(C2,Ir,N2)/(°)	79.10	80.11	79.13	79.13
A(C2,Ir,N3)/(°)	89.28	96.75	89.34	89.45
A(C2,Ir,N4)/(°)	96.57	173.05	96.55	96.33
A(N2,Ir,N3)/(°)	95.95	89.01	95.92	96.16
A(N2,Ir,N4)/(°)	174.20	99.10	174.16	174.15
A(N3,Ir,N4)/(°)	80.05	76.32	80.01	80.00

Table S2 Electronic absorptions of complexes based on TD-DFT calculations at the B3LYP/6-31G level

Complex	Excited state	transition	coeff (contri)	*E*/eV	Osillator strength	assign	λ_{cal}/nm[a]	λ_{abs}/nm[b]
(1)	4	H[c]-1→L[d]	0.43226 (38%)	2.72	0.0926	LLCT[e] /MLCT	456	469
		H→L+1	0.41922 (36%)			LLCT/MLCT		
	11	H→L+2	0.63219(84%)	3.39	0.0188	MLCT	365	380
	24	H-7→L	0.5097 3(60%)	3.90	0.0764	LLCT/MLCT	318	338
	35	H-4→L+3	0.38997(37%)	4.16	0.0677	ILCT[f]	298	288
(2)	4	H-1→L	0.61504(79%)	2.65	0.0046	LLCT	468	471
	13	H-5→L	0.42679(39%)	3.15	0.0459	LLCT/MLCT	394	383
		H-4→L+1	0.38953(32%)			LLCT/MLCT		
	28	H-7→L	0.34476(27%)	3.90	0.0617	ILCT	318	337
		H-7→L+1	0.31571(21%)			ILCT		
		H-6→L+1	0.45780(47%)			ILCT		
	38	H-3→L+4	0.37394(31%)	4.13	0.0432	ILCT/MLCT	300	289
		H - 2 →L+4	0.30725(21%)			ILCT/MLCT		
(3)	4	H-1→L+1	0.60203(75%)	2.84	0.0720	LLCT/MLCT	437	468
	17	H-8→L+1	0.29912(20%)	3.45	0.0213	ILCT	360	379
		H-6→L+1	0.29271(19%)			ILCT		
		H-5→L+1	0.31572(22%)			ILCT		
	43	H-18 → L+1	0.36988(34%)	4.07	0.0463	LLCT/MLCT	305	289
		H-3→	0.43761(48%)			ILCT/MLCT		

		L+3						
(4)	2	H→L	0.63617(83%)	2.69	0.0817	LLCT/MLCT	461	468
	5	H-2→L	0.34229(25%)	2.97	0.0647	LLCT	418	412
		H-1→L+1	0.42896(39%)			LLCT/MLCT		
		H→L+1	0.38685(32%)			LLCT/MLCT		
	15	H-3→L+1	0.56972(71%)	3.46	0.0139	LLCT	358	338
	35	H-7→L+1	0.48156(52%)	4.30	0.1373	LLCT/MLCT	288	290

[a] theoretical calculating value, [b] UV-Vis absorption in CH_2Cl_2, [c] the highest occupied molecular orbital, [d] the lowest unoccupied molecular orbital [e] ligand to ligand charge transfer, [f] intra-ligand charge transfer, coeff: coefficients of the wavefunction for each excitation, contri: contribution percentage, *E*: excitation energy.

Table S3 Frontier molecular orbital compositions for complexes based on TD-DFT calculation at the B3LYP/6-31G level

Complex	Orbital	Energy/eV	Prevailing bond type
(1)	L+3	-4.04	93% π^*(ppy)
	L+2	-4.06	95% π^*(ppy)
	L+1	-4.96	93% π^*(phen)
	L	-4.97	95% π^*(phen)
	H	-8.17	37% *d*(Ir) + 59% π(ppy)
	H-1	-8.19	30% *d*(Ir) + 61% π(ppy)
	H-4	-8.75	90% π(ppy)
	H-7	-9.44	12% *d*(Ir) + 74% π(phen) + 15% π(ppy)
(2)	L+4	-3.86	17% π^*(phen) + 78% π^*(ppy)
	L+1	-5.12	97% π^*(phen)
	L	-5.19	95% π^*(phen)
	H	-7.76	45% *d*(Ir) + 50% π(ppy)
	H-1	-8.38	89% π(ppy)
	H-2	-8.55	30% *d*(Ir) + 68% π(ppy)
	H-3	-8.67	25% *d*(Ir) + 69% π(ppy)
	H-4	-8.81	59% *d*(Ir) + 37% π(ppy)
	H-5	-8.88	54% *d*(Ir) + 36% π(ppy)
	H-6	-9.57	95% π(phen)
	H-7	-9.70	99% π(phen)
(3)	L+3	-3.86	93% π^*(ppy)
	L+1	-4.62	98% π^*(phen)
	L	-4.68	90% π^*(phen)
	H	-7.96	54% *d*(Ir) + 36% π(ppy)
	H-1	-8.00	34% *d*(Ir) + 58% π(ppy)
	H-3	-8.50	79% π(ppy)
	H-5	-8.54	99% π(phen)
	H-6	-8.59	90% π(phen)
	H-8	-8.70	98% π(phen)
	H-18	-9.31	39% *d*(Ir) + 29% π(phen) + 33% π(ppy)
(4)	L+1	-4.50	98% π^*(phen)
	L	-4.73	89% π^*(phen)
	H	-8.00	28% *d*(Ir) + 18% π(phen) + 54% π(ppy)
	H-1	-8.02	40% *d*(Ir) + 56% π(ppy)
	H-2	-8.30	28% π(phen) + 67% π(ppy)
	H-3	-8.46	49% π(phen) + 47% π(ppy)
	H-7	-9.35	42% *d*(Ir) + 21% π(phen) + 37% π(ppy)