Electronic Supplementary Material (ESI) for RSC Advances.

Modification of the emission colour and quantum efficiency for oxazoline- and thiazoline-containing iridium complexes via different N^O ligands

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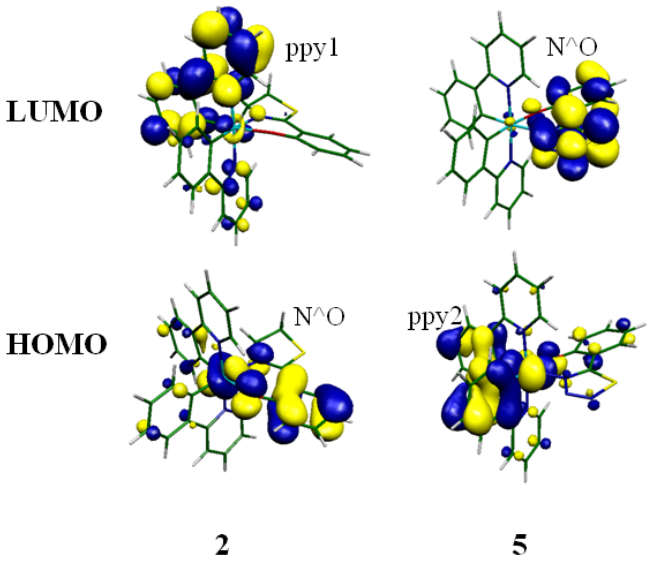

Fig. S1. Contour plots of the HOMO and LUMO for complexes **2** and **5**.

Table S1 Calculated phosphorescent emission wavelength (nm) of the complexes **1** and **2** in CH_2Cl_2 media with the TDDFT method at the PBE0, M062X, M052X, B3LYP and Cam-B3LYP level, respectively, together with the experimental values

	λ_{cal} (PBE0)	λ_{cal} (M062X)	λ_{cal} (M052X)	λ_{cal} (B3LYP)	λ_{cal} (Cam-B3LYP)	Exp.[19]
1	572	476	498	577	551	527
2	675	595	595	677	645	542

Table S2 Selected optimized parameters for complex **2** in the ground state from different density functionals

		PBE0		B3LYP		M052x	
	Exp.[a]	Calc.[b]	δ[c]	Calc.[b]	δ[c]	Calc.[b]	δ[c]
Ir-N1	2.141	2.169	1.31	2.218	3.60	2.194	2.48
Ir-N2	2.048	2.050	0.10	2.075	1.32	2.065	0.83
Ir-N3	2.033	2.036	0.15	2.060	1.31	2.049	0.79
Ir-O1	2.131	2.144	0.61	2.167	1.69	2.162	1.45
Ir-C1	2.017	2.001	0.79	2.018	0.05	1.996	-1.04
Ir-C2	1.999	1.995	0.20	2.016	0.85	1.992	-0.35

[a] Crystal data from (ref. 19). [b]Calculated. [c] (%)= $\frac{calc-\exp}{\exp}\times 100$

Table S3 Calculated absorption wavelength (nm) with the largest oscillator strengths for complexes **1** and **2** in CH_2Cl_2 media with the TDDFT method at the PBE0, B3LYP, M052X M062X and Cam-B3LYP level, respectively, together with the experimental data.

	λ_{cal} (PBE0)	λ_{cal} (B3LYP)	λ_{cal} (M052X)	λ_{cal} (M062X)	λ_{cal} (Cam-B3LYP)	Exp.[19]
1	250	266	203	221	208	249
2	248	263	213	216	214	243

Table S4 Calculated absorption wavelength (nm) and oscillator strength (*f*) of the complexes **1** and **2** with the TDDFT method at the PBE0 level in gas phase and CH_2Cl_2 media, together with the experimental data.

	gas-phase			CH_2Cl_2 media			Exp.[19]
	state	λ_{cal}	*f*	state	λ_{cal}	*f*	
1	S_1	436	0.0115	S_1	412	0.0370	
	S_{30}	260	0.1957	S_{33}	250	0.2973	249
	T_1	483	0.0000	T_1	467	0.0000	
2	S_1	435	0.0136	S_1	412	0.0402	
	S_{34}	259	0.1434	S_{39}	248	0.1534	243
	T_1	509	0.0000	T_1	498	0.0000	

Table S5 Calculated absorption wavelength (nm) and oscillator strength (*f*) of the complexes **1** and **2** with the TDDFT method at the PBE0 level using the PBE0, B3LYP and M052X optimized the ground state geometries, together with the experimental data.

	PBE0			B3LYP			M052X			Exp.[19]
	state	λ_{cal}	*f*	state	λ_{cal}	*f*	state	λ_{cal}	*f*	
1	S_1	412	0.0370	S_1	413	0.0410	S_1	414	0.0410	
	S_{33}	250	0.2973	S_{34}	253	0.1898	S_{34}	251	0.2769	249
	T_1	467	0.0000	T_1	470	0.0000	T_1	464	0.0000	
2	S_1	412	0.0402	S_1	411	0.0425	S_1	417	0.0440	
	S_{39}	248	0.1534	S_{38}	253	0.1036	S_{38}	249	0.1176	243
	T_1	498	0.0000	T_1	500	0.0000	T_1	488	0.0000	

Table S6 Optimized S_0 structure for the complex **1**

C	-0.55591000	-2.25177100	2.04859300	C	3.36931300	-0.00666000	2.95079500
H	0.04672300	-1.74211500	2.80525900	H	3.66842200	0.54422500	3.84017800
H	0.08704500	-2.99760700	1.56324300	C	2.23873200	0.38878500	2.24260300
C	-1.84820700	-2.85260200	2.60225500	H	1.67117700	1.24903300	2.58973100
H	-1.83619700	-3.93991100	2.70064600	C	1.81957100	-0.29216600	1.09004500
H	-2.14390800	-2.40804800	3.56024100	C	-1.28431800	1.74612400	1.94849400
C	-2.30114500	-1.54259600	0.83535800	H	-1.59309900	0.76680700	2.29479600
C	-3.18260300	-0.91967900	-0.11729900	C	-1.73736700	2.91173200	2.54027200
C	-2.69264700	-0.07425100	-1.16856400	H	-2.42222400	2.86076300	3.37973300
C	-3.67176700	0.44307800	-2.06656300	C	-1.29645100	4.12936200	2.02412900
H	-3.30345400	1.08169200	-2.86425400	H	-1.63054200	5.06799700	2.45723400
C	-5.01164700	0.16251300	-1.93403600	C	-0.42485500	4.12873900	0.94913200
H	-5.71836200	0.59012900	-2.64229800	H	-0.06857000	5.06411200	0.53245700
C	-5.47891200	-0.66506400	-0.89678700	C	0.00603500	2.92056900	0.38916300
H	-6.53738500	-0.88341400	-0.79442100	C	0.93382000	2.77479500	-0.72277000
C	-4.56598600	-1.19476500	-0.01374200	C	1.51727900	3.86093100	-1.38814600
H	-4.89907400	-1.84218400	0.79132800	H	1.27920000	4.88246100	-1.10043900
C	0.45022200	-2.04193900	-2.16100300	C	2.40814700	3.63992000	-2.42656300
H	-0.44878300	-1.53175300	-2.49303700	H	2.86228200	4.47918100	-2.94597000
C	1.00763300	-3.11974500	-2.82873900	C	2.71664900	2.32822900	-2.79383900
H	0.53627600	-3.49841300	-3.72918900	H	3.41894100	2.14856900	-3.60520900
C	2.17453100	-3.68689600	-2.31804800	C	2.13596000	1.24971500	-2.13360500
H	2.64164100	-4.53164300	-2.81670800	H	2.39850900	0.24215500	-2.44627800
C	2.73968400	-3.15909300	-1.16800600	C	1.22368200	1.43674600	-1.08694200
H	3.65151900	-3.58217700	-0.76059000	Ir	0.21810100	0.05415500	-0.04534700
C	2.14008900	-2.06864300	-0.52981300	N	-1.04393400	-1.30179000	1.05541100
C	2.61198300	-1.39595500	0.67477600	N	0.99768700	-1.53800900	-1.04594000
C	3.75034400	-1.79214800	1.38908000	N	-0.43962900	1.74237300	0.90746400
H	4.34473500	-2.64087400	1.05756900	O	-1.45679600	0.22920600	-1.39166500
C	4.13019900	-1.10051800	2.52922200	O	-2.83612400	-2.50465700	1.62393500
H	5.01345700	-1.40386300	3.08430600				

Table S7 Optimized S_0 structure for the complex **2**

Ir	-0.29532800	0.07362200	-0.08194900	C	2.49875900	0.39825000	-1.37872900
S	3.37216300	-2.48773800	1.46519800	C	-3.19476700	2.39677700	-2.34797300
C	-1.78369700	-0.49282900	1.12028200	H	-3.94997900	2.24183600	-3.11570200
C	-1.49244600	1.46756300	-0.87479000	C	-2.17232700	-3.55867500	-2.58483400
O	1.22261200	0.51926200	-1.52947300	H	-2.61968300	-4.38283700	-3.13353300
N	0.32042400	1.70532200	0.99512500	C	1.67073900	2.81194200	2.63036500
N	1.17118000	-1.29332200	0.74744500	H	2.43472800	2.73469700	3.39616900
C	3.16444200	-0.43965700	-0.41812400	C	1.25810800	1.67774000	1.95374000
C	-1.99717700	3.87378600	-0.88198900	H	1.68312100	0.70384500	2.16535600
H	-1.81417700	4.87690700	-0.50378100	C	-2.16045300	0.04070300	2.36182600
C	-3.95066000	-1.57717500	2.60194600	H	-1.61459900	0.89060700	2.76571700
H	-4.77892700	-1.98561100	3.17408200	C	4.57972300	-0.47336500	-0.40277300
C	3.33117300	1.13349200	-2.27321600	H	5.08158700	-1.10929900	0.32309000
H	2.81744400	1.75598500	-3.00002700	C	-2.68989500	-3.17933300	-1.35653200
C	1.08830100	4.03231300	2.29265900	H	-3.54424300	-3.69901400	-0.93672700
H	1.38695100	4.94721100	2.79657400	C	-3.22028300	-0.49010100	3.09016800
N	-1.04413600	-1.46534500	-1.18385500	H	-3.48747900	-0.05195700	4.04960800
C	5.34969800	0.27097100	-1.26557300	C	-1.07820200	-2.87037800	-3.10802400
H	6.43303200	0.22538600	-1.21644400	H	-0.64612100	-3.13198800	-4.06782000
C	-2.95711800	3.68492400	-1.86373000	C	-0.54284700	-1.82546900	-2.37361600
H	-3.51906800	4.53097000	-2.24939900	H	0.29964900	-1.22792600	-2.70848700
C	-2.11531400	-2.11573300	-0.65287000	C	-3.61141700	-2.12598600	1.37496300
C	-2.54392100	-1.59310800	0.63959300	H	-4.18202400	-2.96924200	0.99199800
C	4.70298200	1.07990600	-2.21707700	C	2.44665100	-1.29320900	0.50193600
H	5.29193600	1.67076100	-2.91527900	C	0.76241200	-2.21977300	1.79556900
C	-1.27437400	2.77934100	-0.38929900	H	-0.21281000	-2.64819000	1.55175900
C	0.12212700	4.06508000	1.30242100	H	0.63499000	-1.65085400	2.72814300
H	-0.34434800	5.00300300	1.02293400	C	1.82600700	-3.30142700	1.94591800
C	-0.26247500	2.88771200	0.65118200	H	1.64322100	-4.14667400	1.27481800
C	-2.47636600	1.30996100	-1.85908600	H	1.90153800	-3.67001100	2.97129100
H	-2.68658900	0.32116300	-2.25867600				

Table S8 Optimized S_0 structure for the complex **3**

C	-0.25297900	-2.43966200	1.91504700	C	3.23794300	0.41821700	3.06510700
H	-0.15061000	-1.90434200	2.86896200	H	3.40833500	0.97503500	3.98431200
H	0.74916000	-2.75400700	1.61310500	C	2.07566000	0.63746400	2.33313400
C	-1.25250300	-3.59888800	2.01316800	H	1.35461300	1.36724300	2.69390700
H	-0.94690300	-4.44406200	1.37886400	C	1.81575000	-0.05663700	1.14142600
H	-1.38719200	-3.96351000	3.03559200	C	-1.61215200	1.39095400	1.94018900
C	-2.08322900	-1.88633300	0.72878500	H	-1.74889200	0.36357800	2.25599200
C	-3.03866700	-1.23691100	-0.14750100	C	-2.28418300	2.43951000	2.54295600
C	-2.61991600	-0.37826200	-1.21688600	H	-2.97172800	2.24229100	3.35819500
C	-3.64515500	0.09151800	-2.08749800	C	-2.05732200	3.73029100	2.06808300
H	-3.32503600	0.72386300	-2.91071000	H	-2.56932100	4.58083400	2.50936700
C	-4.97394600	-0.21028700	-1.89159200	C	-1.16747200	3.91699600	1.02456800
H	-5.71928300	0.18993100	-2.57568700	H	-0.97335000	4.91266500	0.64184800
C	-5.37827200	-1.01292400	-0.81172400	C	-0.50783100	2.82262900	0.45381000
H	-6.42833900	-1.22881700	-0.64027800	C	0.47273000	2.87927600	-0.62072200
C	-4.41116400	-1.51604900	0.03220800	C	0.87963400	4.07283700	-1.23142600
H	-4.71491100	-2.11575000	0.88757600	H	0.45053400	5.02603500	-0.93085800
C	0.87089800	-1.89598100	-2.20966900	C	1.83976200	4.04756200	-2.23066000
H	-0.09582000	-1.53921000	-2.55277300	H	2.15805600	4.97063600	-2.70723500
C	1.62695000	-2.83528500	-2.89090200	C	2.39454000	2.82431400	-2.61370700
H	1.25499000	-3.25786200	-3.81808400	H	3.15246800	2.79908700	-3.39399900
C	2.86150300	-3.20749900	-2.35975800	C	1.98840200	1.63899000	-2.00855600
H	3.48359600	-3.93888200	-2.86834200	H	2.44069600	0.70479200	-2.33252800
C	3.29356600	-2.63143100	-1.17563900	C	1.01274300	1.62631800	-1.00283300
H	4.25338000	-2.90387200	-0.75050500	Ir	0.21990800	0.05367400	-0.04701900
C	2.49448400	-1.68530900	-0.52471600	N	-0.84031000	-1.54315700	0.92294400
C	2.80400100	-0.98605800	0.71628400	N	1.29241800	-1.34309600	-1.06372500
C	3.97436700	-1.20497800	1.45537300	N	-0.75263300	1.56848100	0.92642900
H	4.71925800	-1.92131300	1.11523200	O	-1.40089800	-0.03142800	-1.47486900
C	4.19351400	-0.50531800	2.63159000	N	-2.46591800	-2.96997800	1.50392400
H	5.10054200	-0.67037800	3.20636600	H	-3.16478500	-3.57555800	1.09646500

Table S9 Optimized S_0 structure for the complex **4**

C	2.42622700	-1.26707800	-1.04834800	C	-1.85894100	-0.39798100	-1.02942100
C	3.29365500	-0.71034800	-0.06899900	C	0.89937700	2.01355600	-1.98121800
C	2.78102200	0.06595700	1.02952900	H	1.25094000	1.10268100	-2.45128300
C	3.75610500	0.55372600	1.95392600	C	1.17969700	3.25936500	-2.51370100
H	3.37831200	1.14211300	2.78474000	H	1.77042400	3.33859500	-3.41967700
C	5.09669400	0.30186100	1.80394700	C	0.68672500	4.38520900	-1.85593600
H	5.79800100	0.70083900	2.53350600	H	0.88789700	5.38195600	-2.23811900
C	5.58183400	-0.46330200	0.72114800	C	-0.06980000	4.21775200	-0.70920100
H	6.64424400	-0.65571000	0.61200500	H	-0.46982700	5.07896300	-0.18604800
C	4.68553600	-0.95830200	-0.19146800	C	-0.32984600	2.93433100	-0.21614100
H	5.03344400	-1.55085400	-1.03283400	C	-1.14018600	2.61381400	0.95005800
C	-0.07477700	-2.21761700	1.97851700	C	-1.76714200	3.58051100	1.74692600
H	0.76619300	-1.62210700	2.31910200	H	-1.64873700	4.64004200	1.53238100
C	-0.44228000	-3.41555300	2.56655600	C	-2.54992200	3.19000700	2.82210300
H	0.12603200	-3.80258700	3.40523300	H	-3.03792100	3.93636200	3.44258400
C	-1.54799500	-4.09376900	2.05350300	C	-2.70846900	1.82958300	3.09457600
H	-1.86530100	-5.03817700	2.48678800	H	-3.32776700	1.51784500	3.93287600
C	-2.24423500	-3.55060200	0.98651700	C	-2.08339500	0.86894900	2.30519800
H	-3.10976900	-4.06102900	0.57911000	H	-2.22694300	-0.18168000	2.54357900
C	-1.83568100	-2.33423300	0.42843600	C	-1.27596100	1.23069200	1.22026100
C	-2.47354200	-1.62500000	-0.67176100	Ir	-0.22039600	0.04055400	0.01640500
C	-3.61465300	-2.09241500	-1.33614300	N	1.11788500	-1.11305800	-1.22705200
H	-4.07136200	-3.03839900	-1.05456600	N	-0.74608700	-1.69992600	0.94021300
C	-4.17378300	-1.34656700	-2.36170200	N	0.17475400	1.84824500	-0.86517400
H	-5.05916900	-1.70504700	-2.87899300	O	1.54609800	0.32902400	1.25926800
C	-3.59003600	-0.12870300	-2.71845100	O	2.88989100	-2.07736600	-2.00023700
H	-4.02961400	0.46364200	-3.51805800	N	1.78058400	-2.43053500	-2.79126200
C	-2.45483700	0.33651700	-2.06214800	N	0.78580000	-1.85542500	-2.30605500
H	-2.02539500	1.28935700	-2.36179800				

Table S10 Optimized S_0 structure for the complex **5**

Ir	-0.28780100	0.06942700	-0.07122000	C	-2.38282600	1.22801300	-1.98699000
S	3.14028000	-2.62216400	1.52430100	H	-2.58570800	0.22207600	-2.34492400
C	-1.80787300	-0.44988900	1.10951100	C	2.57914500	0.32654600	-1.29078000
C	-1.44092400	1.42764100	-0.97026500	C	-3.06861700	2.29549500	-2.55849200
O	1.31708600	0.46081400	-1.47465200	H	-3.79238000	2.10880400	-3.34894500
N	0.27916600	1.73914000	0.97335500	C	-2.04985400	-3.71193900	-2.43408000
N	1.14229900	-1.28589000	0.85033900	H	-2.46620900	-4.57642000	-2.94369000
C	3.20677500	-0.50059400	-0.28980100	C	1.52934100	2.90207700	2.64806900
C	-1.92215300	3.83378000	-1.11433800	H	2.23683800	2.85111100	3.46835700
H	-1.74736400	4.85248900	-0.77612600	C	1.14973900	1.74384700	1.99337500
C	-3.99485400	-1.48489300	2.58537700	H	1.53855100	0.77446400	2.28174300
H	-4.83035200	-1.87750600	3.15798800	C	-2.23129100	0.15392300	2.29964700
C	3.45758100	1.02158000	-2.18008600	H	-1.71455900	1.03655600	2.66876000
H	2.97982100	1.63447800	-2.93857200	C	4.62423600	-0.55499200	-0.22064500
C	0.98224000	4.11143400	2.22237000	H	5.08658400	-1.16155200	0.55668500
H	1.25607700	5.04419200	2.70718500	C	-2.59299700	-3.28549500	-1.23369400
N	-0.99628000	-1.52222600	-1.12794000	H	-3.43598400	-3.80877200	-0.79632100
C	5.42871800	0.14777800	-1.08031800	C	-3.30295400	-0.35474100	3.02698100
H	6.50911500	0.09693300	-0.99197400	H	-3.60727000	0.13436300	3.94990300
C	-2.83910400	3.60400800	-2.12792400	C	-0.96920100	-3.02010500	-2.98146100
H	-3.37570100	4.43423400	-2.57848500	H	-0.51885100	-3.31708300	-3.92232900
C	-2.05782500	-2.17149300	-0.57733200	C	-0.47173400	-1.92717900	-2.29313100
C	-2.52874100	-1.58983000	0.67153400	H	0.36059200	-1.32824300	-2.64931900
C	4.82254500	0.94110200	-2.07811100	C	-3.60680900	-2.10008400	1.40549400
H	5.44559300	1.50196800	-2.77102900	H	-4.14597100	-2.97907200	1.05982200
C	-1.23291900	2.75943700	-0.53689000	C	2.45642600	-1.33660700	0.59546100
C	0.07875900	4.10965100	1.17398100	N	0.72552500	-2.21778800	1.72944600
H	-0.36444700	5.03777100	0.83107100	N	1.60854800	-2.98778400	2.19090300
C	-0.27543900	2.90874200	0.54917400				

Table S11 Optimized S_0 structure for the complex **6**

C	-3.07896700	-1.28704000	-0.03304600	C	-1.49259400	1.51317600	1.97669400
C	-2.68293000	-0.43968300	-1.12128900	H	-1.60266700	0.51354600	2.38030300
C	-3.73142900	-0.00285000	-1.98423900	C	-2.13099400	2.60205600	2.54327100
H	-3.43696700	0.62791900	-2.81789300	H	-2.76677800	2.46402300	3.41093000
C	-5.04759600	-0.34124100	-1.77236900	C	-1.93360200	3.85659300	1.96837600
H	-5.81026300	0.03021700	-2.45315800	H	-2.42110600	4.73649800	2.37856600
C	-5.42351400	-1.14812400	-0.68235500	C	-1.10061300	3.96998100	0.86897400
H	-6.46542200	-1.39520400	-0.50572600	H	-0.92533500	4.93734000	0.41182700
C	-4.43971500	-1.61037200	0.16226900	C	-0.47139600	2.83751500	0.33990900
H	-4.72653000	-2.21604300	1.02115800	C	0.46164700	2.82001300	-0.77715100
C	0.78732700	-2.03630900	-2.10041600	C	0.84608300	3.96804500	-1.48222900
H	-0.17051200	-1.66848700	-2.45582600	H	0.42929300	4.94066400	-1.23095000
C	1.49710000	-3.04428200	-2.72989300	C	1.76942300	3.87173700	-2.51140100
H	1.09705300	-3.51016400	-3.62392800	H	2.07086300	4.75935900	-3.06059500
C	2.72231800	-3.43120900	-2.18660200	C	2.31127300	2.62433800	-2.82941100
H	3.30723800	-4.22001100	-2.65154800	H	3.04211800	2.54468200	-3.63138600
C	3.19213200	-2.79847500	-1.04767700	C	1.92724300	1.48340800	-2.13158400
H	4.14395800	-3.08376200	-0.61374000	H	2.36777900	0.52789900	-2.40422600
C	2.43998100	-1.78110300	-0.44964300	C	0.98700600	1.54380300	-1.09539200
C	2.80261000	-1.00696800	0.72879200	Ir	0.22334500	0.04060600	-0.02659300
C	3.99023700	-1.20062600	1.44506000	N	1.24436400	-1.43064200	-0.99556300
H	4.70279200	-1.96414800	1.14112400	N	-0.69408000	1.61789900	0.90459800
C	4.26712100	-0.41648300	2.55374700	O	-1.47441900	-0.08481800	-1.39146100
H	5.18743200	-0.56308200	3.11205100	C	-2.09413800	-1.87304000	0.83542500
C	3.35207300	0.56494300	2.94203300	N	-0.82584600	-1.51104100	1.04781600
H	3.56701800	1.18693800	3.80844500	N	-0.28554600	-2.35831800	1.94817400
C	2.17082000	0.75839800	2.23270700	N	-1.14937000	-3.22377300	2.31477000
H	1.48076500	1.53250600	2.55923400	N	-2.27663500	-2.94122900	1.64022500
C	1.85604700	-0.02235300	1.11332100	H	-3.08091400	-3.54218100	1.72924000