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Correction: New insight into the effects of N^ΔN ligand isomerization and methyl modification on the phosphorescence properties of Cu(I) complexes with (1-(2-pyridyl)pyrazole/imidazole) ligands

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Correction for 'New insight into the effects of N^ΔN ligand isomerization and methyl modification on the phosphorescence properties of Cu(I) complexes with (1-(2-pyridyl)pyrazole/imidazole) ligands' by Lu Shen et al., *New J. Chem.*, 2018, 42, 3660–3670, <https://doi.org/10.1039/C7NJ04879C>.

The authors regret that some of the data in Tables 7 and 8 in the main manuscript were incorrect. The corrected versions of Tables 7 and 8 are shown below. In Section 3.6.2 of the original article, the k_{nr}^d values calculated using eqn (4) were underestimated with respect to the experimental findings; therefore, the subsequent discussions focus on the k_{nr}^e values which were calculated using eqn (5). The corrected values for ΔE display the same trend as in the original article so the discussion of the relationship between the k_{nr} and the ΔE is still accurate in the original article and the overall conclusions of the article remain unchanged.

Table 7 Values of Huang–Rhys factors of the lf and hf modes, λ_M , and k_{nr} obtained at their respective optimized T₁ geometries

	S_M (cm ⁻¹)	S_S (cm ⁻¹)	λ_M (cm ⁻¹)	$\langle S_0 H_{SOC} T_1 \rangle$ (cm ⁻¹)	k_{nr}^d (×10 ³ s ⁻¹)	k_{nr}^e (×10 ³ s ⁻¹)	$k_{nr}^{exp.}$ (×10 ³ s ⁻¹)
py-pop	2.68	54.38	3592	42.49	5.98	160	612 ^a /27.5 ^c
py-ch3	3.00	36.19	4046	25.20	6.57	75	46 ^a
py-meta	1.08	125.48	1547	48.84	29.6	104	
py-para	0.95	160.65	1386	53.79	246	735	
cu-pyim	2.23	6.81	3296	36.38	93.8	713	48.3 ^b

Note: ^a Measured in CH₂Cl₂ in ref. 19. ^b Measured in PYD2 film in ref. 34. ^c Measured in crystalline powder in ref. 19. k_{nr}^d was calculated using eqn (4). k_{nr}^e was calculated by using eqn (5).

Table 8 Calculated reorganization energy, RMSD (root-mean-square deviation), Huang–Rhys factor and ΔE

	py-pop	py-ch3	py-meta	py-para	cu-pyim
λ /cm ⁻¹	9060	8219	9498	11210	4305
RMSD/Å	0.720	0.282	0.800	0.774	0.128
Huang–Rhys factor(S)	57.02	39.23	126.53	161.67	9.05
ΔE /cm ⁻¹	26221	26540	22883	22796	21614

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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