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CORRECTION

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Correction: New insight into the effects of N^N 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^N 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.

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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	able 7 Values of Huang–Rhys factors of the lf and hf modes, λ_{M} , and k_{nr} obtained at their respective optimized T ₁ geometries										
	$S_{\rm M} \left({\rm cm}^{-1} \right)$	$S_{\rm S} ({\rm cm}^{-1})$	$\lambda_{\rm M} ({\rm cm}^{-1})$	$\langle S_0 H_{SOC} T_1 \rangle \text{ (cm}^{-1} \text{)}$	$k_{ m nr}^{ m d} (imes 10^3 \ { m s}^{-1})$	$k_{\rm nr}^{\rm e} (imes 10^3 {\rm s}^{-1})$	$k_{\rm nr}^{\rm exp.} \ (\times 10^3 \ {\rm s}^{-1})$				
ру-рор	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 CH_2Cl_2 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

	ру-рор	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
$\Delta E/\mathrm{cm}^{-1}$	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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