Electronic Supplementary Material (ESI) for Dalton Transactions

Luminescence Mechanochromism in Cyclometallated Ir(III) Complexes Containing Picolinamine.†

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Supporting Information.

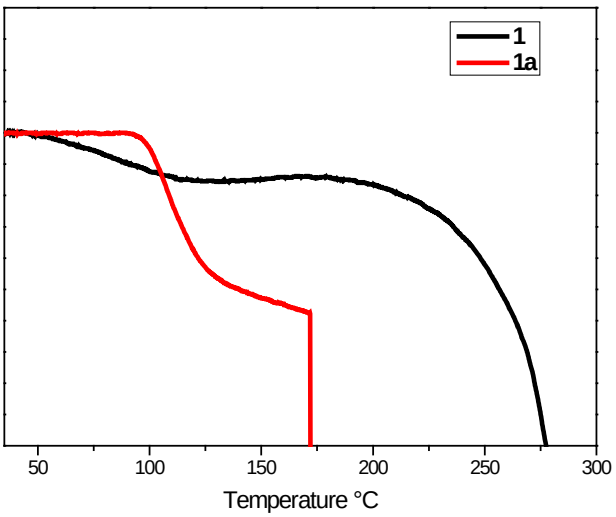

Figure S1. TGA traces of powder complex **1** (experimental mass loss 2.78% corresponds to one water molecule calcd. 2.72%) and crystals **1a** (experimental mass loss 6.54 % corresponds to one ethanol molecule calcd. 6.67%)

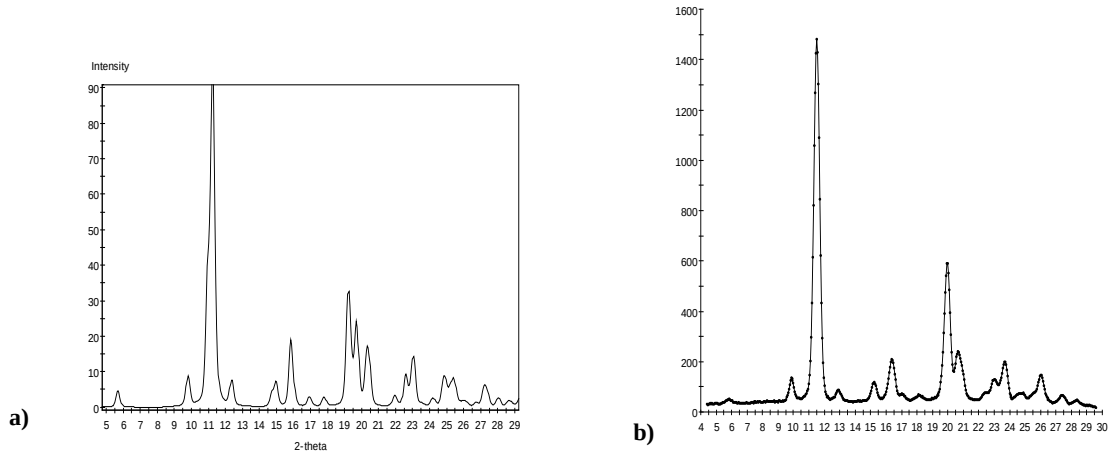

Figure S2. Simulated PXRD pattern of **2** (a) and collected on the yellow crystalline powder of **2** (b).

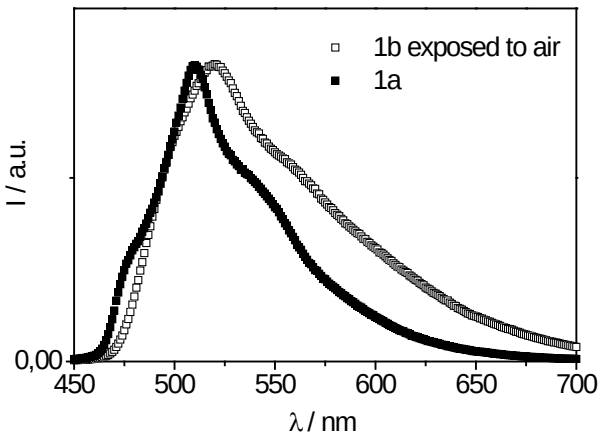

Figure S3. Emission spectrum of: (0) crystals **1b** after complete solvatomorphic transformation and (•) crystals **1a**

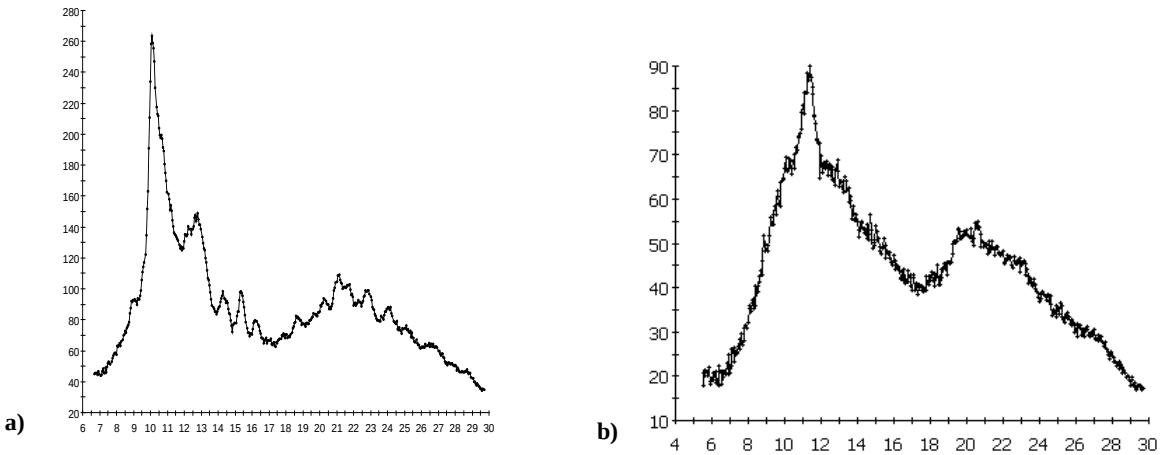

Figure S4. Measured PXRD patterns of a grinded sample of **1b** (a) and **2** (b).

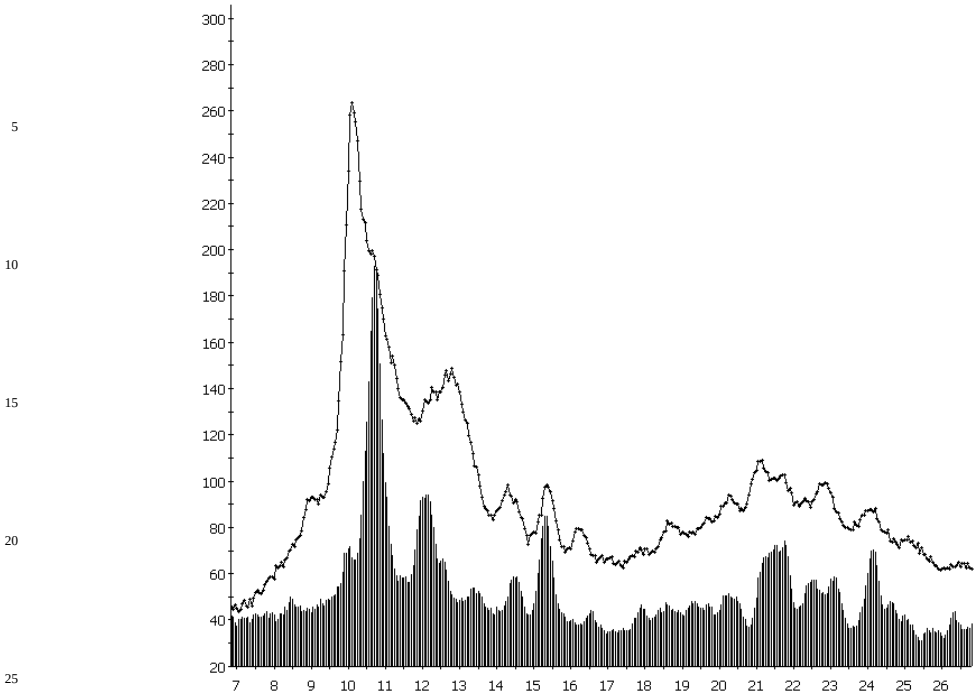

Figure S5. Measured PXRD pattern of a grinded sample of **1b** superimposed with the one measured on the orange **1b** crystals after transformation in air.

Table S1. Crystal data and selected structure refinement parameters for **1a**, **1b**, **2** and **3**.

Compound	**1a**	**1b**	**2**	**3**
empirical formula	$C_{30}H_{30}ClIrN_4O$	$C_{28}H_{24}ClIrN_4$	$C_{28}H_{24}F_6IrN_4P$	$C_{28}H_{24}ClIrN_4O_4$
Crystal system	Monoclinic	Orthorhombic	Orthorhombic	Orthorhombic
Space group	P2(1)/c	P2(1)2(1)2(1)	pca(2)1	pca(2)1
Z	4	4	4	4
fw	690.23	644.16	753.68	708.16
a , Å	14.2312(13)	9.8167(17)	11.0809(13)	11.0556(10)
b , Å	11.7771(11)	13.747(3)	15.5306(18)	15.2516(15)
c , Å	19.2326(18)	20.447(4)	16.1226(19)	15.3882(14)
α, β, γ, deg	90, 104.770(4), 90	90, 90, 90	90, 90, 90	90, 90, 90
V, $Å^3$	3116.9(5)	2759.3(9)	2774.6(6)	2594.7(4)
D_c, g cm^{-3}	1.471	1.551	1.804	1.813
μ, □mm^{-1}	4.396	4.957	4.935	5.291
Independent reflections [R(int)]	6109 [0.0504]	4749 [0.0811]	4876 [0.0473]	5648 [0.0403]
Data/restraints/parameters	6109 / 0 / 361	4749 / 0 / 295	4876 / 1 / 358	5648 / 1 / 331
Goodness-of-fit on F^2	1.258	0.859	1.170	1.215
Absolute structure parameter	-	0.02(1)	0.087(8)	0.002(7)
[a]R1 [I > 2 σ (I)]	0.0372	0.0429	0.0261	0.0184
[b,c]wR2	0.1377	0.1017	0.0751	0.0474

$^a R1 = \sum ||F_o|-|F_c|| / \sum |F_o|$. $^b wR2 = \{ \sum [w(F_o^2-F_c^2)^2] / [(w(F_o^2)^2] \}^{1/2}$. $^c w = 1/[\sigma^2(F_o^2) + (aP)^2+bP]$ with $P = [F_o^2+2F_c^2]/3$, a = 0.0860 (**1a**), 0.0812 (**1b**), 0.0627 (**2**), 0.0216 (**3**) and b = 7.6815 (**1a**), 0.0000 (**1b**), 0.06647 (**2**), 1.2086 (**3**).

Table S2. Selected distances (Å) and angles (°) in **1a**-**3**

	1a	**1b**	**2**	**3**
Ir(1)-C(11)	2.026(7)	2.03(1)	2.041(5)	2.014(4)
Ir(1)-C(22)	2.022(8)	2.03(1)	2.046(6)	2.005(4)
Ir(1)-N(1)	2.101(6)	2.05(1)	2.072(4)	2.052(3)
Ir(1)-N(2)	2.065(6)	2.028(5)	2.072(5)	2.041(3)
Ir(1)-N(3)	2.229(5)	2.20(1)	2.207(5)	2.192(4)
Ir(1)-N(4)]	2.174(6)	2.15(1)	2.170(5)	2.124(2)
N(1)-Ir(1)-N(2)	172.8(2)	174.5(3)	174.1(2)	174.2(1)
N(1)-Ir(1)-N(3)	98.7(2)	97.5(3)	98.6(2)	98.8(1)
N(1)-Ir(1)-N(4)	88.8(2)	86.2(3)	87.1(2)	85.5(1)
N(2)-Ir(1)-N(3)	87.0(2)	86.6(3)	86.4(2)	86.8(2)
N(2)-Ir(1)-N(4)	96.7(3)	97.5(3)	97.0(2)	97.3(1)
N(4)-Ir(1)-N(3)	77.3(2)	77.9(3)	77.0(2)	77.6(1)
C(11)-Ir(1)-C(22)	90.0(3)	91.6(4)	87.4(2)	86.9(2)
C(11)-Ir(1)-N(1)	80.6(3)	80.5(4)	79.0(2)	79.6(1)
C(11)-Ir(1)-N(2)	94.1(3)	95.0(4)	96.1(2)	94.8(2)
C(11)-Ir(1)-N(3)	174.4(3)	174.4(4)	175.8(2)	177.0(1)
C(11)-Ir(1)-N(4)	97.1(3)	96.7(3)	99.4(2)	99.8(1)
C(22)-Ir(1)-N(1)	94.4(3)	96.6(4)	95.9(2)	97.7(1)
C(22)-Ir(1)-N(2)	80.6(3)	80.2(4)	80.4(2)	80.2(2)
C(22)-Ir(1)-N(3)	95.6(2)	93.9(4)	96.3(2)	95.9(1)
C(22)-Ir(1)-N(4)	172.6(2)	171.6(3)	172.9(2)	173.2(1)

Table S3. N-H···Cl interactions in **1a**.

	H···A	D···A	<(DHA)
N(3)-H(3a)···Cl(1)	2.646	3.46(1)	151.20
N(3)-H(3b)···Cl(1)^{i}	2.751	3.50(1)	141.85
O(1)-H(1a)···Cl(1)	2.273	3.09(1)	172.89
O(2)-H(2A)···Cl(1)^{ii}	1.879	2.69(1)	167.11

i = -*x*+2, *y*-1/2, -*z*+1/2

ii = -*x*+1, *y*-1/2, -*z*+1/2