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An organometallic complex revealing an unexpected, reversible, temperature induced SC-SC transformation

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Supplementary Information

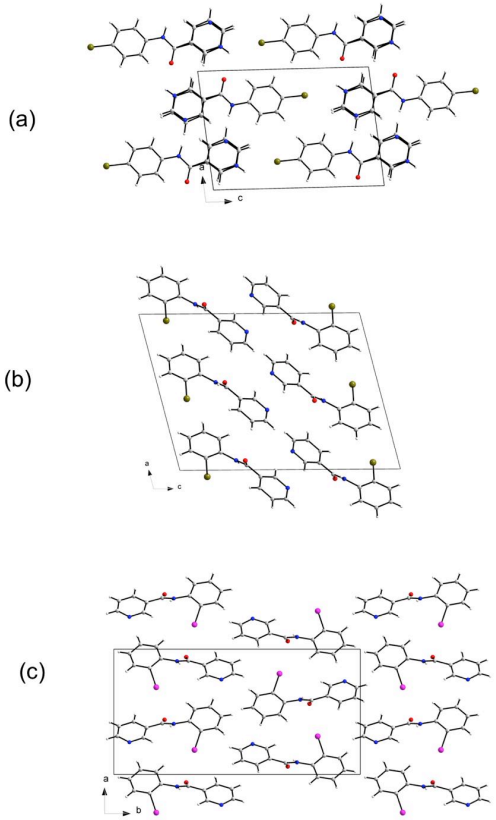

Fig. S1 The crystal structures of the ligands (a) *N*-(4-bromophenyl)nicotinamide (***p*-Br**), (b) *N*-(2-bromophenyl)nicotinamide (***o*-Br**), (c) *N*-(2-iodophenyl)nicotinamide (***o*-I**).

Table S1 Crystal and diffraction data for the free nicotinamide ligands.

	***p*-Br**	***o*-Br**	***o*-I**
	$C_{12}H_9BrN_2O$	$C_{12}H_9BrN_2O$	$C_{12}H_9IN_2O$
FW	277.12	277.12	324.11
T / K	150(2)	150(2)	150(2)
λ / Å	0.71073	0.71073	0.71073
System	Monoclinic	Monoclinic	Orthorhombic
Space grp	$P2_1$	$P2_1/a$	$Pna2_1$
a / Å	9.8494(18)	12.8722(4)	10.8408(5)
b / Å	3.8718(7)	4.9256(2)	21.2412(11)
c / Å	13.972(2)	17.5710(5)	4.8537(2)
α / °	90	90	90
β / °	96.018(10)	104.327(2)	90
γ / °	90	90	90
V / $Å^3$	529.87(16)	1079.41(6)	117.67(9)
Z	2	4	4
$\sigma_{calc}/Mg/m^3$	1.737	1.705	1.926
Size/ mm^3	0.35×0.05×0.01	0.30×0.15×0.15	0.30×0.1×0.08
Reflections	1386	3995	2630
Unique	1086	2464	2403
R(int)	0.0400	0.0369	0.054
Gof	1.160	1.031	1.054
R1 [I>2σ(I)]	0.0816	0.0355	0.0341
wR2	0.1692	0.0815	0.0731