Electronic Supplementary Information

pH-Dependent structural diversity of a 2-pyridinemethanol Cu complex and its relatively strong magnetic exchange coupling *via* hydrogen bonding

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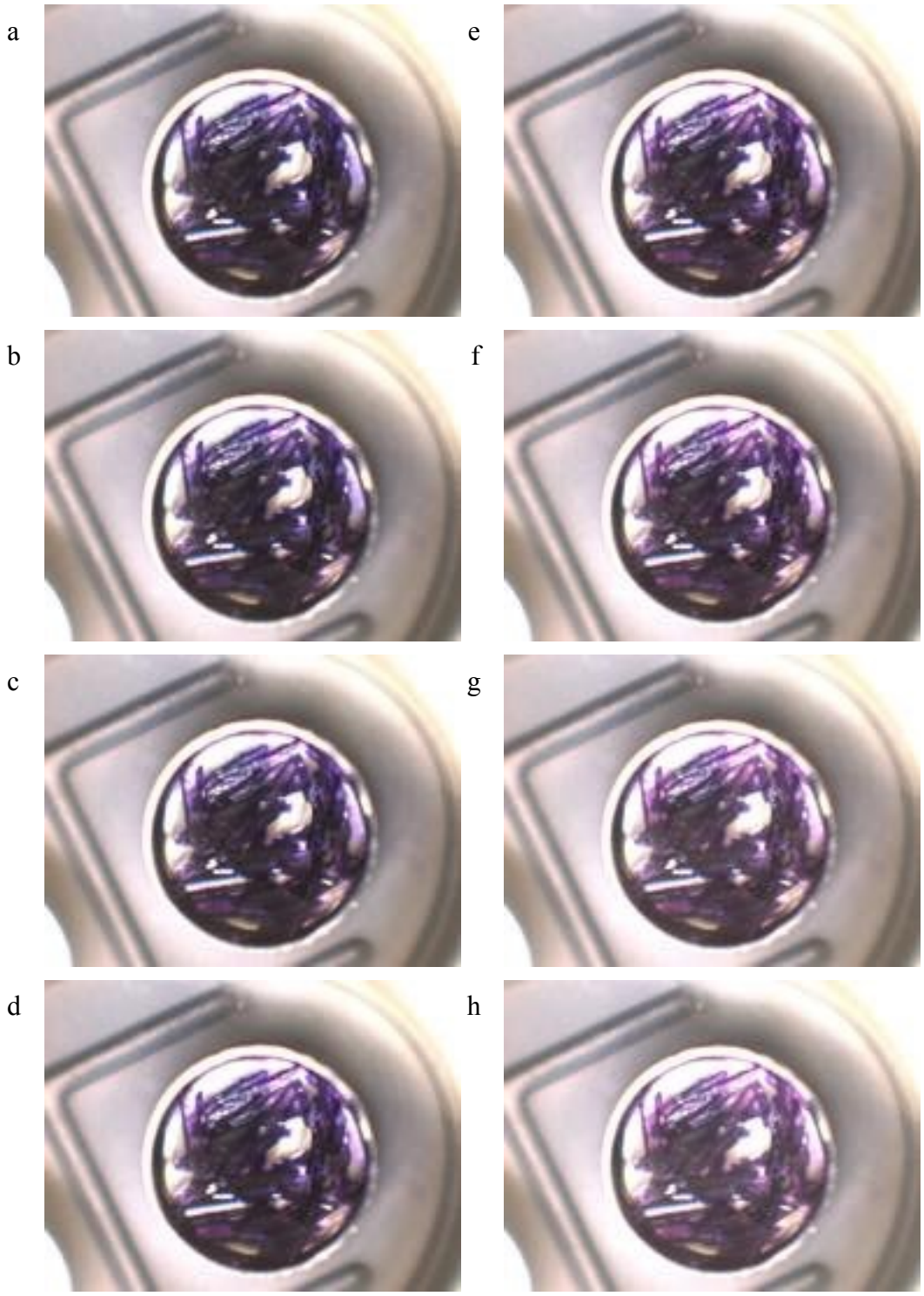

Figure S1 Color change of complex **1** on cooling (a : 293 K; b : 273 K; c : 253 K; d : 233 K; e : 213 K; f : 193 K; g : 173 K; h : 153 K)

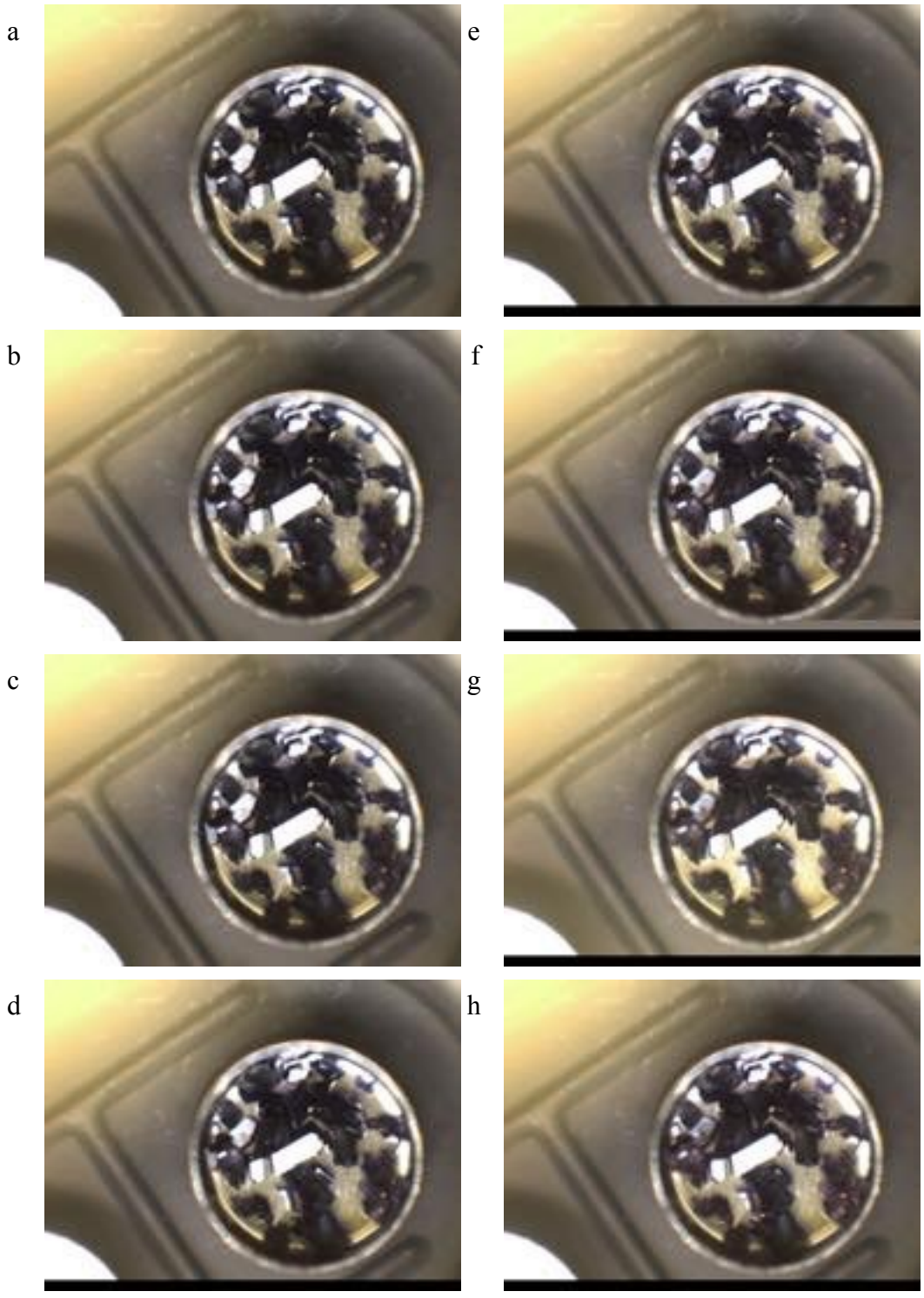

Figure S2 Photographs of complex **2** on cooling (a : 293 K; b : 273 K; c : 253 K; d : 233 K; e : 213 K; f : 193 K; g : 173 K; h : 153 K)

Table S1 Crystallographic data for complex **1** at various temperature

Temp. / K	100(2)	150(2)	200(2)	250(2)	300(2)
Formula	C12H13CuF6N2O2P	C12H13CuF6N2O2P	C12H13CuF6N2O2P	C12H13CuF6N2O2P	C12H13CuF6N2O2P
Fw	425.75	425.75	425.75	425.75	425.75
Cryst. Syst.	orthorhombic	orthorhombic	orthorhombic	orthorhombic	orthorhombic
Space Group	*P*bcn	*P*bcn	*P*bcn	*P*bcn	*P*bcn
a / Å	8.6711(2)	8.7142(2)	8.7671(2)	8.8221(2)	8.8886(4)
b / Å	19.3370(4)	19.3795(4)	19.4257(4)	19.4655(4)	19.5247(8)
c / Å	8.7396(2)	8.7366(2)	8.7330(2)	8.7295(2)	8.7308(4)
V / Å^3	1465.40(6)	1475.41(6)	1487.29(6)	1499.09(6)	1515.21(12)
Z	4	4	4	4	4
D_{calc} / g cm^{-3}	1.930	1.917	1.901	1.886	1.866
F(000)	852	852	852	852	852
μ / mm^{-1}	1.679	1.667	1.654	1.641	1.623
Cryst. size / mm^3	0.44 × 0.21 × 0.19	0.44 × 0.21 × 0.19	0.44 × 0.21 × 0.19	0.44 × 0.21 × 0.19	0.44 × 0.21 × 0.19
θ range / º	3.142-27.439	3.140-27.444	3.137-27.461	3.135-27.457	3.130-27.455
Reflections collected	13321	13397	13444	13587	13770
Independent reflections	1683	1689	1699	1715	1735
R_{int}	0.0221	0.0224	0.0231	0.0238	0.0245
R_1* (I>2σ(I))	0.0240	0.0265	0.0279	0.0282	0.0312
wR_2* (I>2σ(I))	0.0672	0.0721	0.0747	0.0759	0.0832
GooF	1.092	1.092	1.112	1.122	1.140

* $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, w$R_2 = ((\Sigma(w(F_o^2-F_c^2)^2))/ \Sigma(wF_o^4))$

Table S2 Detail of π- π and Cu- π interaction at various temperature

Temperature / K	100(2)	150(2)	200(2)	250(2)	300(2)
distance between *Cg*(I) and *Cg*(J) / Å	4.0480(8)	4.0628(8)	4.0812(9)	4.0990(9)	4.1189(10)
α / °	9.40(6)	9.45(7)	9.55(7)	9.62(8)	9.69(8)
Cg(I)-prep / Å	3.5441(5)	–3.5542(6)	3.5666(6)	3.5767(6)	3.5904(7)
Cg(J)-prep / Å	3.5441(5)	–3.5542(6)	3.5666(6)	3.5768(6)	3.5904(7)
slippage / Å	1.956	1.968	1.984	2.002	2.019
distance between *Cg*(I) and Cu1% / Å	3.717	3.724	3.732	3.740	3.750
β / °	37.60	37.46	37.32	37.12	36.95
MeJ-prep / Å	2.945	–2.956	2.968	2.982	2.997

Ring (I) : 2-pyridyl ring of N1-C2-C3-C4-C5-C6. Ring (J) : 2-pyridyl ring of N1%-C2%-C3%-C4%-C5%-C6%. Symbol % means the equivalent atoms generated by the symmetry operator (1 − x, y , 3/2 − z) for 100, 150, 250 K or (1 − x, y, 1/2 − z) for 200, 300 K. α : dihedral angle between Ring (I) and Ring (J) β : angle *Cg*(I)-Cu1% vector and normal to plane I. *Cg*I-prep : perpendicular distance of *Cg*(I) from Ring (J) *Cg*J-perp : perpendicular distance of *Cg*(J) from Ring(I). MeJ-perp : perpendicular distance of *Cg*(I) from Cu1%. slippage : distance between *Cg*(I) and perpendicular projection of *Cg*(J) on Ring(I). *Cg*(I) and *Cg*(J) are the centroids of atoms N1-C2-C3-C4-C5-C6 and N1%-C2%-C3%-C4%-C5%-C6%, respectively.