

SUPPLEMENTARY INFORMATION

Thermosalient effect of naphthalene diimide and tetrachlorocobaltate hybrid and changes of color and magnetic property by ammonia vapor

Shunya Masuda, Sotaro Kusumoto,* Masaya Okamura, Shiro Hikichi, Ryuya Tokunaga, Shinya Hayami, Yang Kim, Yoshihiro Koide*

^a *Department of Material and Life Chemistry, Faculty of Engineering, Kanagawa University, 3-27-1 Rokkakubashi, Kanagawa-ku, Yokohama 221-8686, Japan.*

^b *Department of Chemistry, Graduate School of Science and Technology, Kumamoto University, 2-39-1 Kurokami, Chuo-ku, Kumamoto 860-8555, Japan.*

Corresponding author: S. Kusumoto
E-mail: kusumoto@kanagawa-u.ac.jp

Supplementary data

Table S1. Crystallographic data of **1**.

Compound	1
formula	C ₂₄ H ₁₆ Cl ₄ Co N ₄ O ₅
formula weight	641.14
crystal system	triclinic
space group	<i>P</i> -1
<i>a</i> / Å	9.6173(10)
<i>b</i> / Å	9.7060(10)
<i>c</i> / Å	14.232(2)
α / °	106.092(10)
β / °	93.459(10)
γ / °	93.474(8)
<i>V</i> / Å ³	1269.9(3)
<i>Z</i>	2
<i>T</i> / K	300
<i>R</i> ₁ [<i>I</i> > 2σ(<i>I</i>)]	0.1016
<i>wR</i> ₂ [<i>I</i> > 2σ(<i>I</i>)]	0.2801
<i>R</i> ₁ (all data)	0.1594
<i>wR</i> ₂ (all data)	0.3324
G.O.F.	1.067
CCDC	2263765

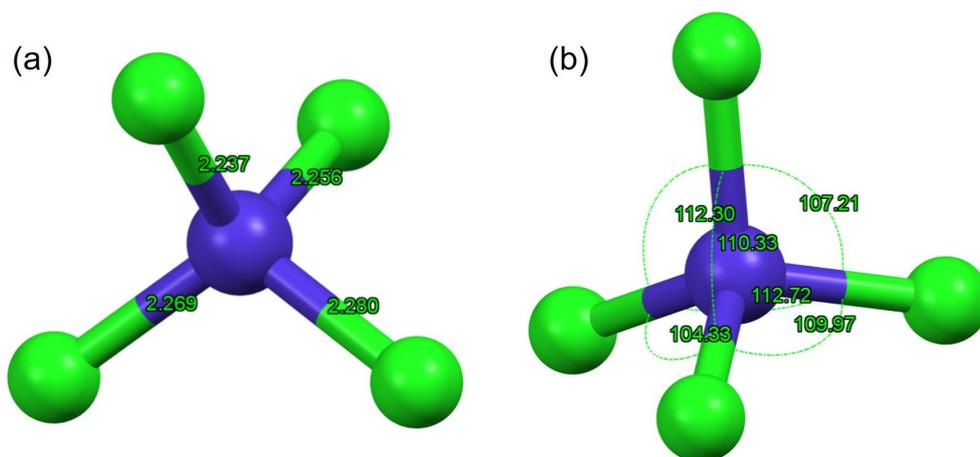


Figure S1 (a) The Co-Cl bond lengths and (b) the Cl-Co-Cl angles.

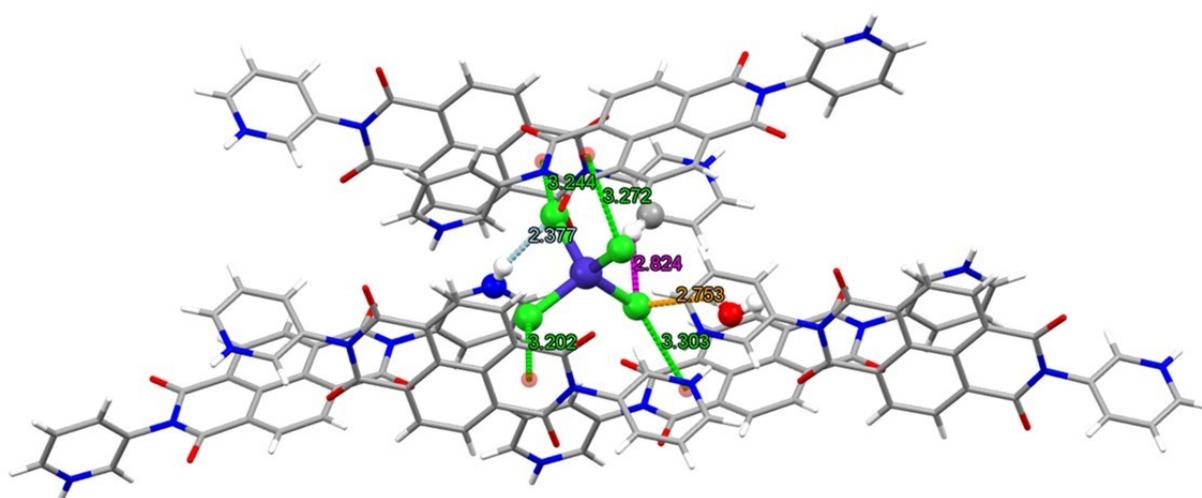


Figure S2 (a) Intermolecular interactions around $[\text{CoCl}_4]^{2-}$. Green dashed lines represent Cl... π , pink dashed lines represent C-H...Cl, light blue dashed lines represent N-H...Cl, and yellow dashed lines represent O-H...Cl.

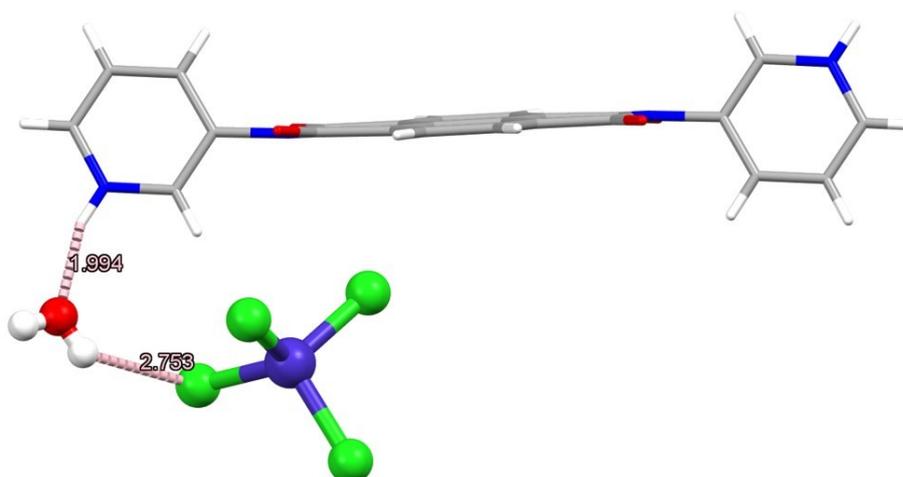


Figure S3 Intermolecular interactions around a water molecule.

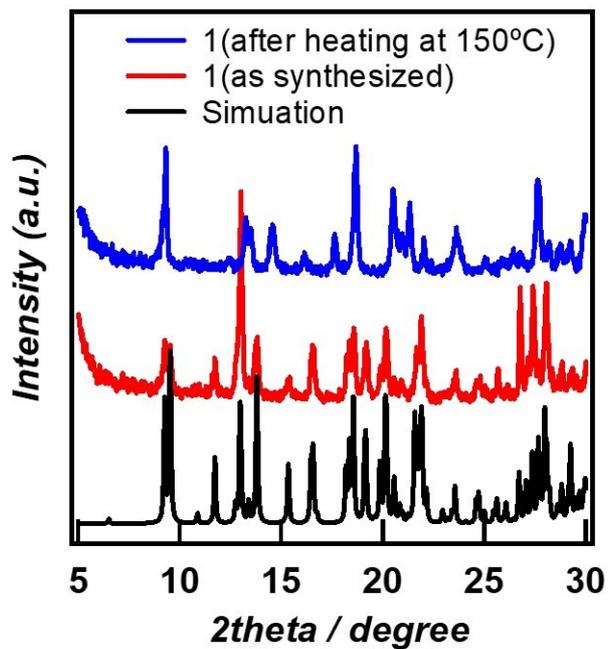


Figure S4 PXR D pattern for the simulation (black) and before (red) and after (blue) removal of water molecules.



Figure S5 A small vial (10 mL) containing approximately 20 mg of powder **1** was placed into a larger vial (50 mL) containing 5 mL of either ammonia or amine solution.

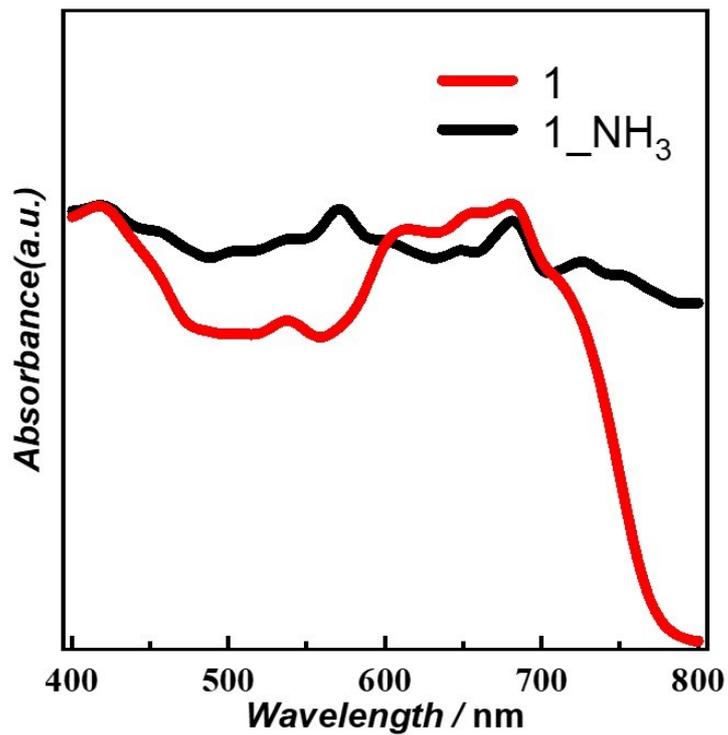


Figure S6 Solid-state UV-vis spectra of compounds 1 and 1_NH₃.

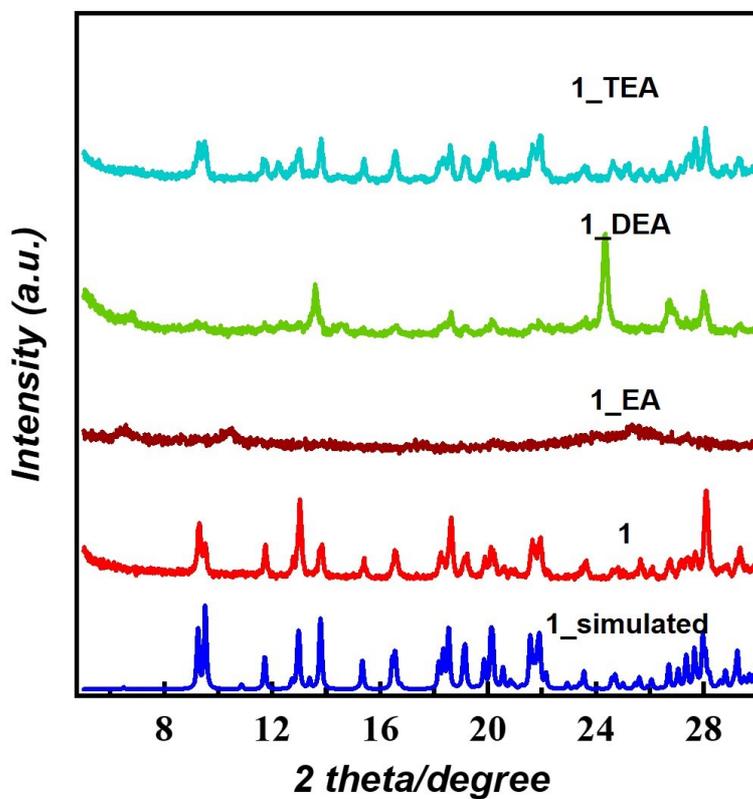


Figure S7 PXRD patterns for the samples before and after exposure to ammonia and amines.

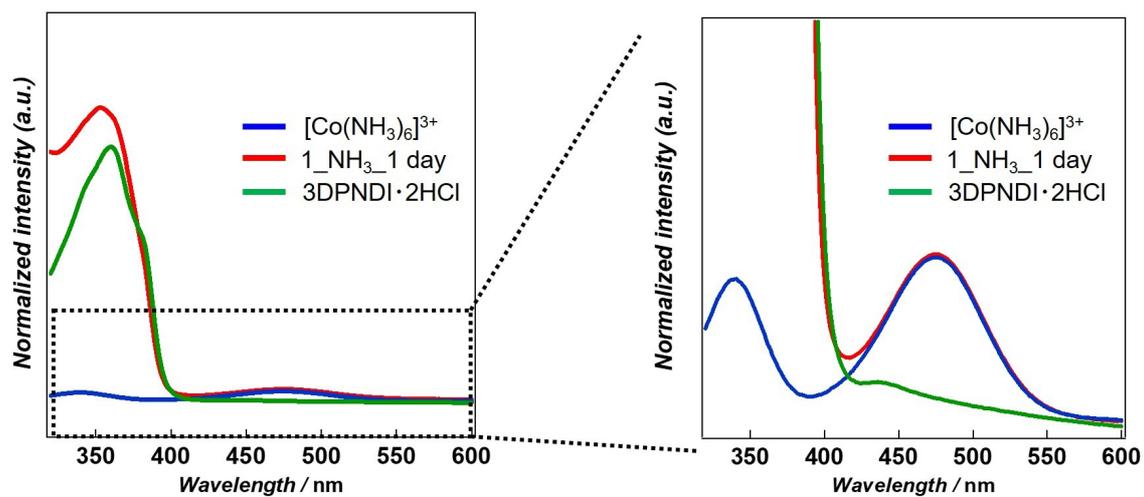


Figure S8 UV-vis spectra and their enlarged versions (on the right) of [Co(NH₃)₆]³⁺ (blue), 3DPNDI·2HCl (green), and 1_NH₃_1 day (red).