

Supporting Information

Diazopyridine-Ni(II) Complexes Exhibiting Intra-Chain Ferromagnetic Interaction After Irradiation: Formation of Magnetic Gel

Koya Mori,¹Rumi Eguchi,¹ Satoru Karasawa,^{1,2,*} and Noboru Koga^{1,*}

¹.Graduate School of Pharmaceutical Sciences, Kyushu University, 3-1-1 Maidashi, Higashi-ku,
Fukuoka, 812-8582 Japan

².PRESTO, Japan Science and Technology Agency, Kawaguchi, 332-0012 Japan

*Corresponding authors

Tel ; +81-92-642-6593. Fax +81-92-642-6545

E-mail: karasawa@fc.phar.kyushu-u.ac.jp and koga@fc.phar.kyushu-u.ac.jp

Contents

- S1. Figure S1. Table 1. Crystallographic data collection and structural refinement information for **3**.
- S2. Figure S1. Molecular structures of **3**.
- Figure S1'. The chain structure of $[\text{Co}(\text{Br-hfpip})_2\text{D1py}_2]_n$
- S3. Figure S2. Strain dependence of G' and G'' for the gel of **2** (entry 16 in Table 2).
- S4. Figure S3. Absorption spectrum of **1** in 15 mM MTHF solution.
- S5. Figure S4. SEM image of **1** and counts vs width plot of the fibers in xerogel.
- S6. Figure S5. M vs *Irradiation* plots of **1**.
- S7. Figure S6. $\ln(\chi_{\text{mol}}T)$ vs T plot of the gel sample of **1** after irradiation. The solid line is the fitting the data from 50 – 15 K.

Table 1. Crystallographic data collection and structural refinement information for **3**.

3	
empirical formula	C ₅₂ H ₆₂ F ₁₂ N ₆ O ₄ Ni
formula weight	1121.78
crystal system	Monoclinic
space group	<i>P</i> 2 ₁ / <i>c</i> (no. 14)
<i>a</i> / Å	11.0039(6)
<i>b</i> / Å	45.083(3)
<i>c</i> / Å	11.3568(4)
β / °	105.098(4)
<i>V</i> / Å ³	5439.5(5)
μ / cm ⁻¹	1.303
<i>Z</i> (<i>Z'</i>)	4 (1)
crystal size / mm	0.80 x 0.80 x 0.3
<i>D</i> _{calc} / gcm ⁻³	1.370
<i>F</i> (000)	2336.00
radiation	CuK α
<i>T</i> / K	123
no. reflections	52833
measured	
no. unique	9928
reflections	
no. parameters	677
<i>R</i> ₁ (<i>I</i> > 2 σ (<i>I</i>)) ^a	0.0762
<i>wR</i> ₂ (all data) ^a	0.1895
GOF	1.022

$$^a R_1 = \sum ||F_0| - |F_c|| / \sum |F_0|; wR_2 = \{\sum w(F_0^2 - F_c^2)^2 / \sum w(F_0^2)\}^{1/2}$$

S2.

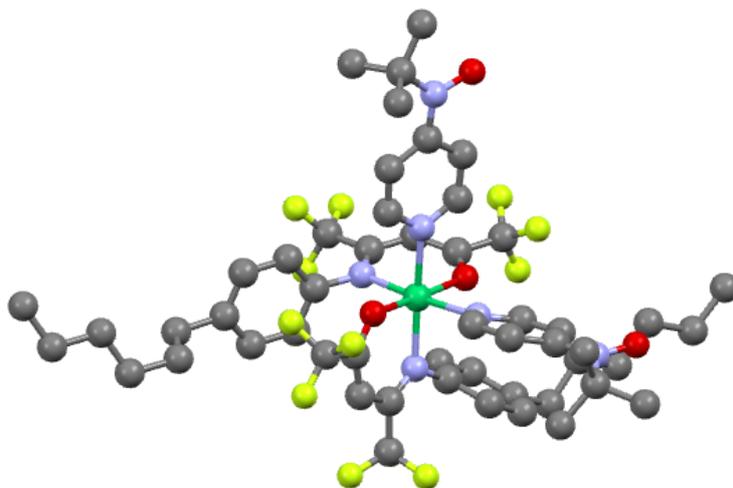


Figure S1. Molecular structures of **3**. Hydrogen atoms are omitted for sake of clarity. Color code; Ni (green), N (blue), O (red), F (yellow), and C (gray), respectively.

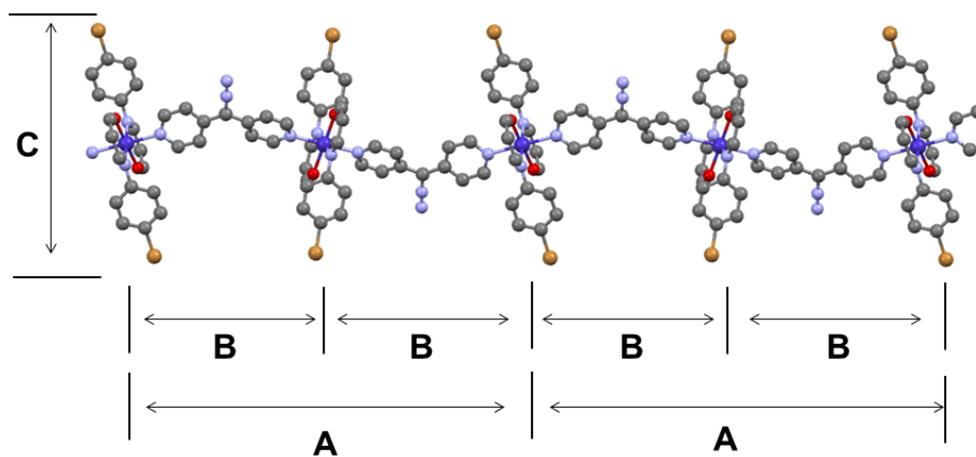


Figure S1'. The chain structure of $[\text{Co}(\text{Br-hfpip})_2\text{D1py}_2]_n$ reported previously.^[1] Capital letters of A, B, and C, represent the distances of one pitch (A), one unit (B), and the width of the chain, respectively. CF_3 groups and H atoms are omitted for a sake of clarity.

[1] S. Karasawa, N. Koga *Inorg. Chem.* **2011**, *50*, 2055.

S3.

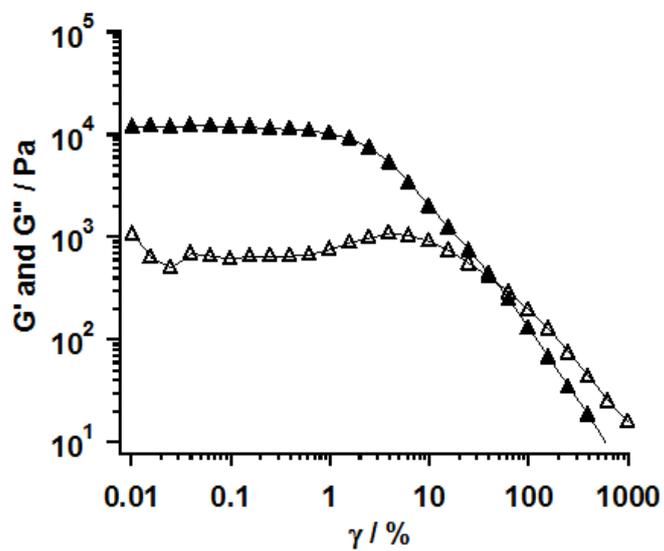


Figure S2. Strain dependence of G' and G'' for the gel of **2** (entry 16 in Table 2).

S4.

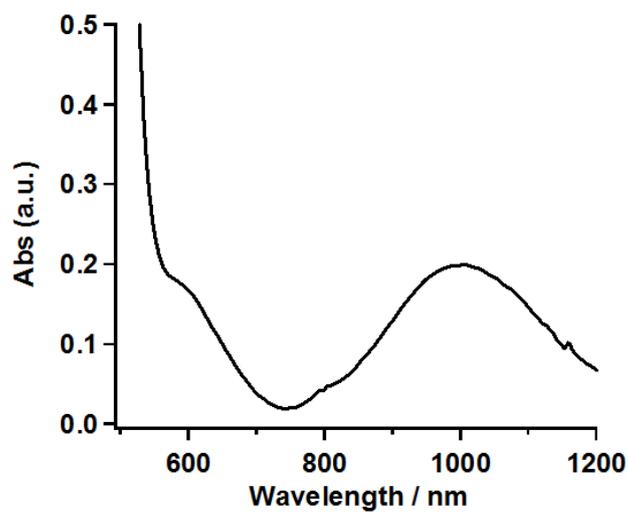
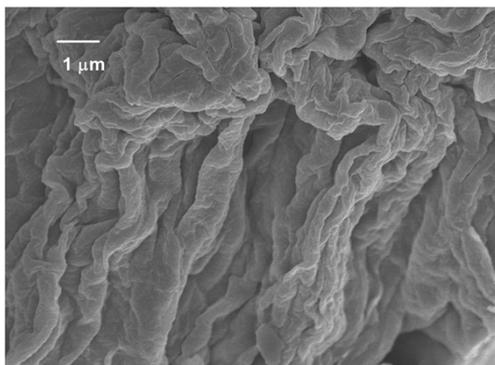


Figure S3. Absorption spectrum of **1** in 15 mM MTHF solution sample.

S5.

(a)



(b)

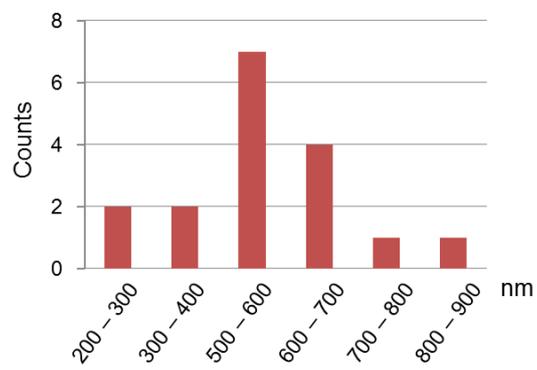
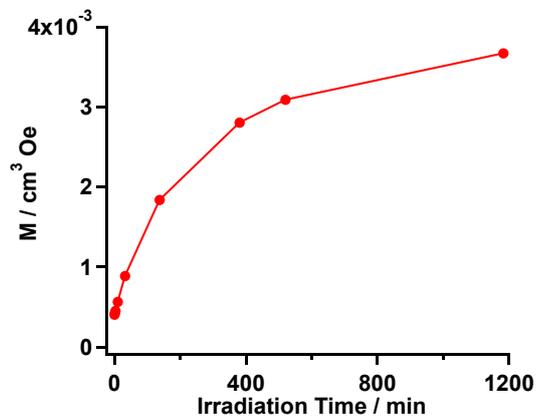


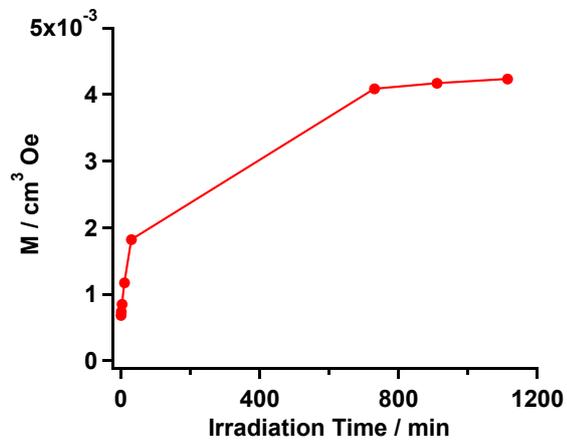
Figure S4. (a) SEM image of xerogel for **1**. (b) Counts vs width plot of the fiber in left image.

S6.

(a)



(b)



(c)

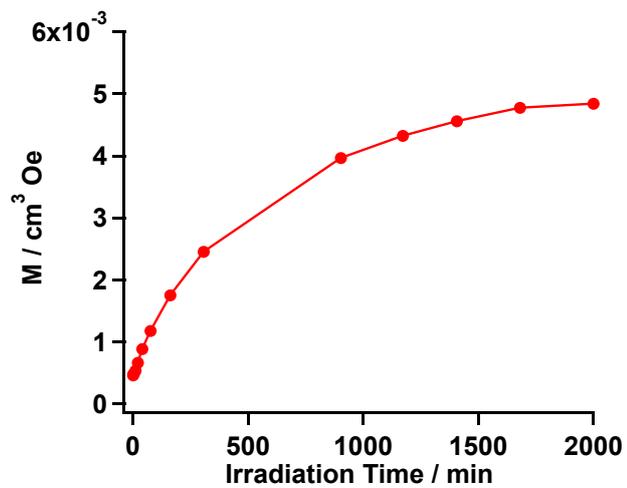


Figure S5. M vs Irradiation plots of **1**. Samples of the powder (a), 15 mM MTHF solution (b), and the gel (c).

S7.

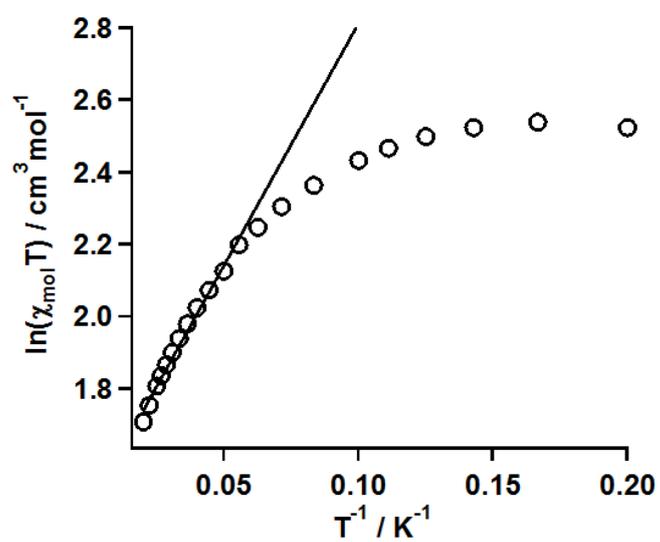


Figure S6. $\ln(\chi_{\text{mol}} T)$ vs T plot of the gel sample of **1** after irradiation. The solid line is the fitting the data from 50 – 15 K.