Supporting Information

Multi-Functional Molecular Rotators with Dielectric, Magnetic and Optical Responses

Norihisa Hoshino,* Takashi Takeda, and Tomoyuki Akutagawa*

Table S1. Transition temperatures from ordered phase to disordered phase in the heating process of adamanane derivatives.

		$T_{\rm trs}$	Molecular weight	Ref.
	adamantane	178	136.2	[1]
1	2-azaadamantane-N-oxyl	300	152.2	[2]
2	1-methyladamantane	212	150.3	[3]
3	2-adamantanone	205	150.2	[4]
4	1-cholroadamantane	243	170.7	[2]
5	1-bromoadamantane	311	215.1	[2]
6	2-chloroadamantane	237	170.7	[5]
7	2-bromoadamantane	277	215.1	[5]
8	1-hydroxyadamantane	357	152.2	[6]
9	2-hydroxyadamantane	389	151.2	[6]



Figure S1. Difference scanning thermoanalyses of a) 2-chloroadamantane (6) and b) 2bromoadamantane (7). The data were conducted using a Rigaku Thermo plus TG8120 differential scanning calorimeter at the rate of 5 K min⁻¹. The samples were used as received without further purification (Wako Chemical for 6 and TCI Chemical for 7).



Figure S2. Hydrogen bonding structures of a) 1-hydroxyadamantane thermoanalyses of 1-hydroxyadamantane (8), b) 2-hydroxyadamantane (9) and c) 2-azaadamatane-*N*-oxyl (1). Atomic coordinates of 8 and 9 were obtained from ref. [7] and [8].



Figure S3. Powder X-ray diffractions of **1** in the heating process at the rate of 1 K min⁻¹. The powder sample was sealed in a Lindemann glass capillary ($\varphi = 0.2$ mm) and Debye-Scherrer rings were recorded using Rigaku RAPID-II imaging plate area detector with a Cu-K α radiation.



Figure S4. Temperature dependent magnetic susceptibilities of **1**. The data were conducted using a MPMS-XL7 magnetometer in the range of $250 \sim 320$ K at the rate of 0.5 K min⁻¹.



Figure S5. A difference scanning thermoanalysis of **1**. The data were conducted using a Rigaku Thermo plus TG8120 differential scanning calorimeter.

References

[1] S.-S. Chang, E. F. Westrum JR. J. Phys. Chem. 1960, 64, 1547-1551.

[2] S. Matsumoto, T. Higashiyama, H. Akutsu, S. Nakatsuji, *Angew. Chem. Int. Ed.* **2011**, *50*, 10879-10883.

[3] T. Clark, T. Mc. O. Knox, H. Mackle, M. A. McKervey, J. Chem. Soc., Faraday Trans. 1 1977, 73, 1224-1231.

[4] I. S. Butler, H. B. R. Cole, D. F. R. Gilson, P. D. Harver, J. D. McFarlane, J. Chem. Soc., Faraday Trans. 2 1986, 82, 535.

[5] This work (fig. S1).

[6] M. B. Charapennikau, A. V. Blokhim, A. G. Kabo, G. J. Kabo, J. Chem. Thermodyn. 2003, 35, 145-157.

[7] J. P. Amoureux, M. Bee, C. Gors, V. Warin, F. Baert, *Cryst. Struct. Commun.* **1979**, *8*, 449.

[8] J. A. Kanters, R. W. W. Hooft, A. J. M. Duisenberg, J. Crystallogr. Spectrosc. Res. 1990, 20, 123-131.