Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information for

Terbium(III) bis-phthalocyaninato single-molecule magnet encapsulated in a single-walled carbon nanotube

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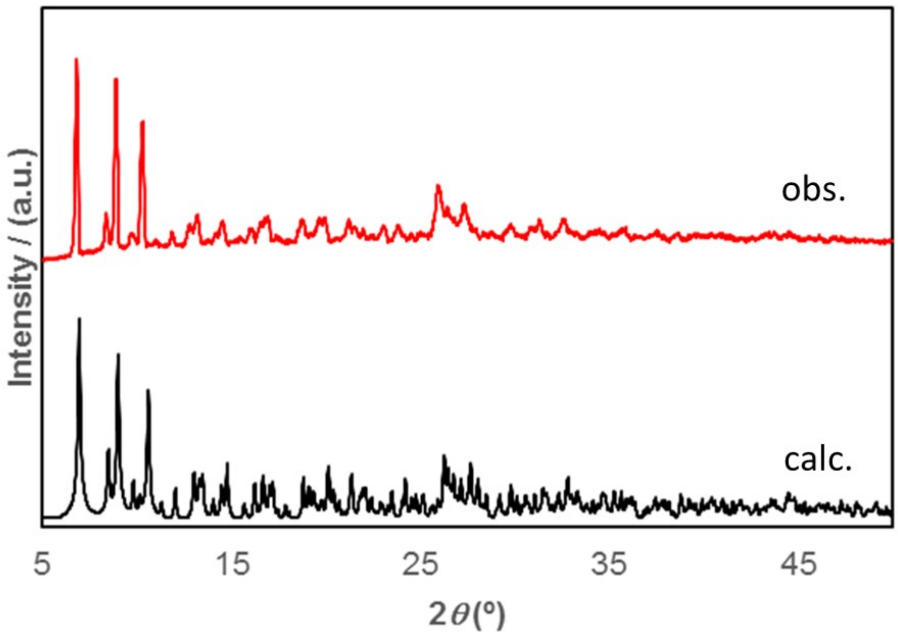


Fig. S1 PXRD pattern of $TbPc_2$ at 298 K.

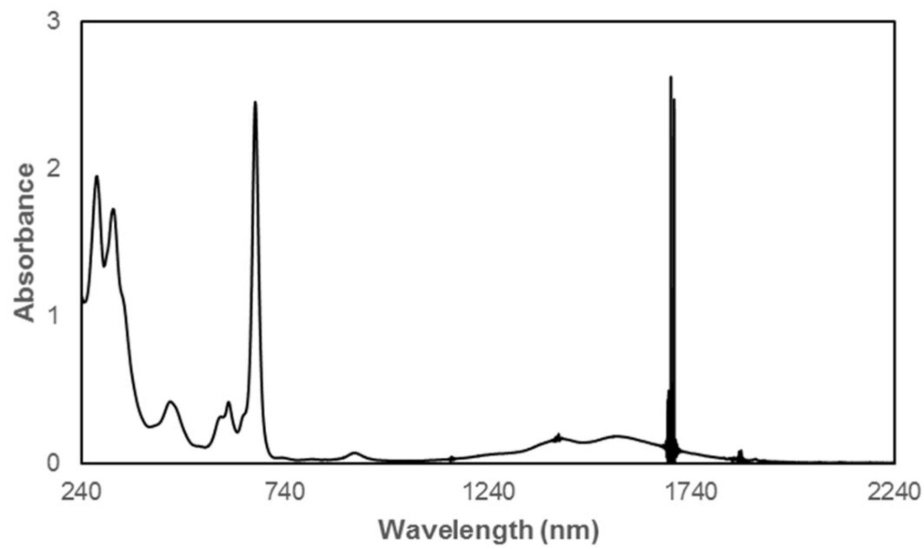


Fig. S2 UV-vis-NIR of $TbPc_2$ in CH_2Cl_2 at 298 K.

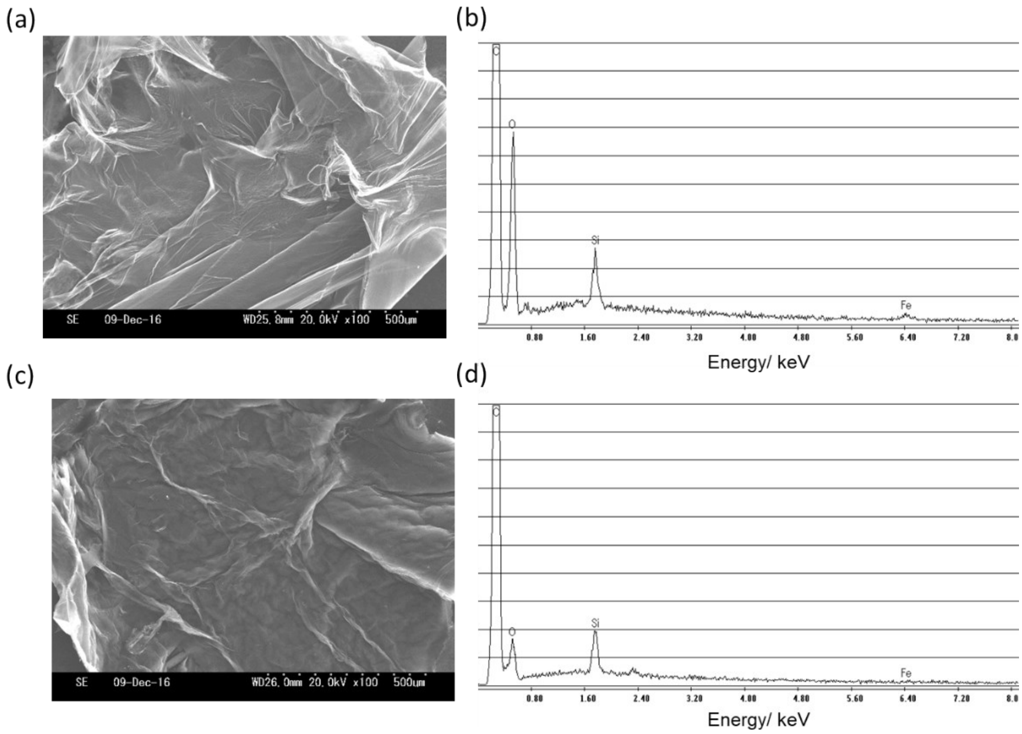
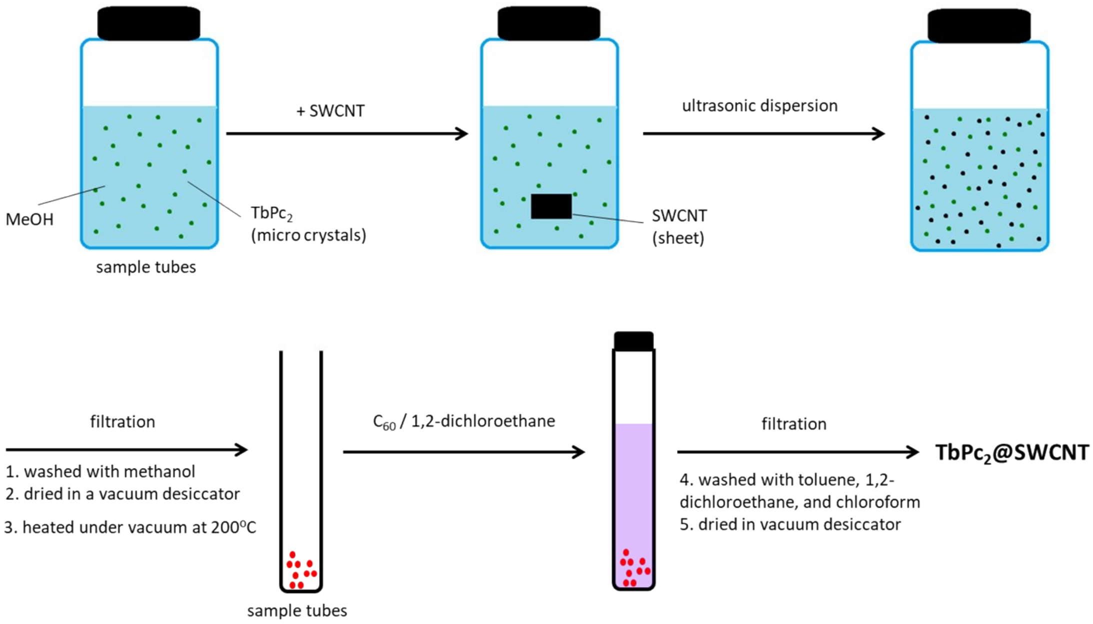


Fig. S3 SEM image of SWCNT (a, b) before and (c, d) after cleaning are shown together with elemental analysis by EDX.



Scheme S1 Synthetic procedures for $TbPc_2$ encapsulated in SWCNTs.

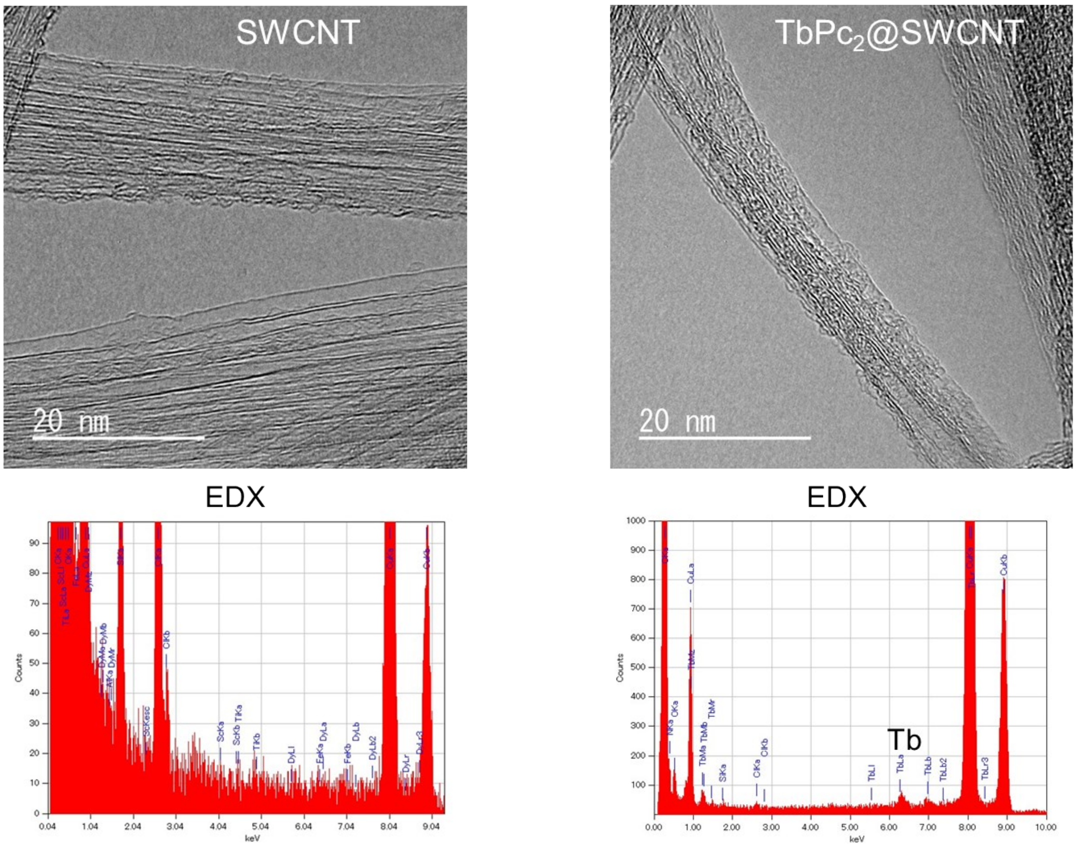


Fig. S4 TEM image and EDX of SWCNT (left) and $TbPc_2$@SWCNT (right).

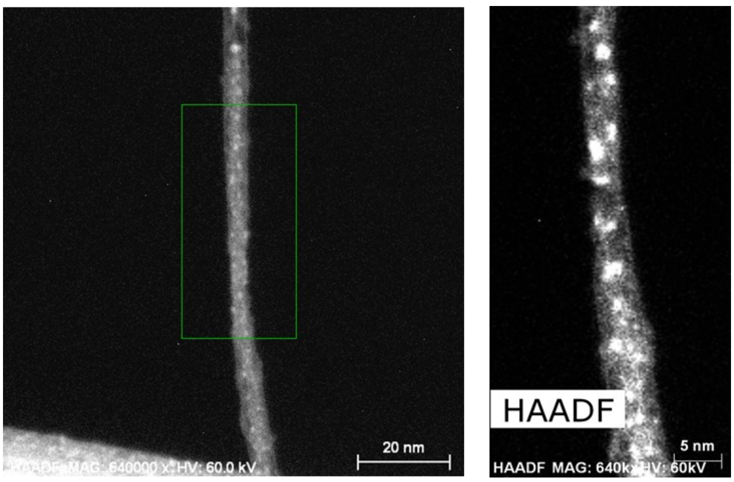


Fig. S5 HAADF–STEM images of $TbPc_2$@SWCNT. White spots are thought to be from Tb ions.

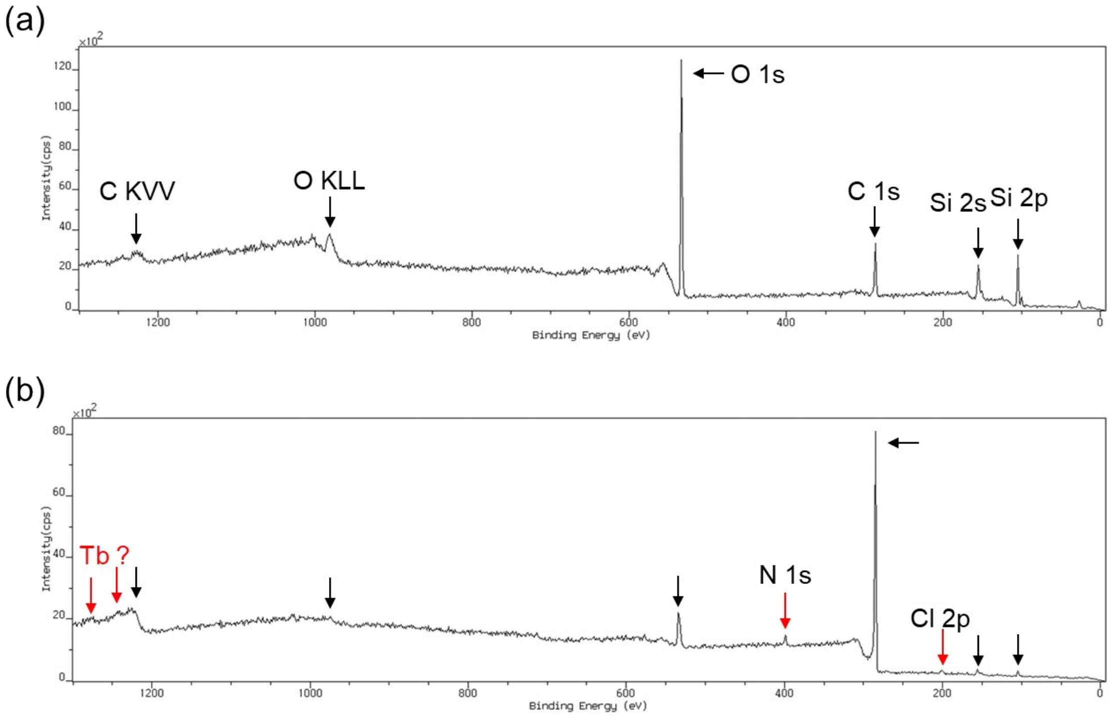


Fig. S6 (a) XPS spectrum of the background. (b) XPS spectrum of $TbPc_2$@SWCNT. Black arrows indicate the background.

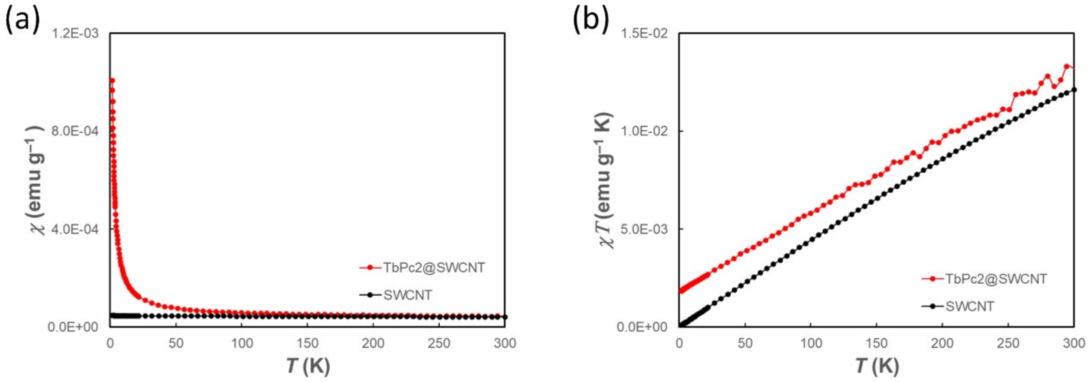


Fig. S7 Field-cooled (FC) measurements. Temperature (T) dependence of (a) χ and (b) χT for powder samples of SWCNT and $TbPc_2$@SWCNT at 1000 Oe.

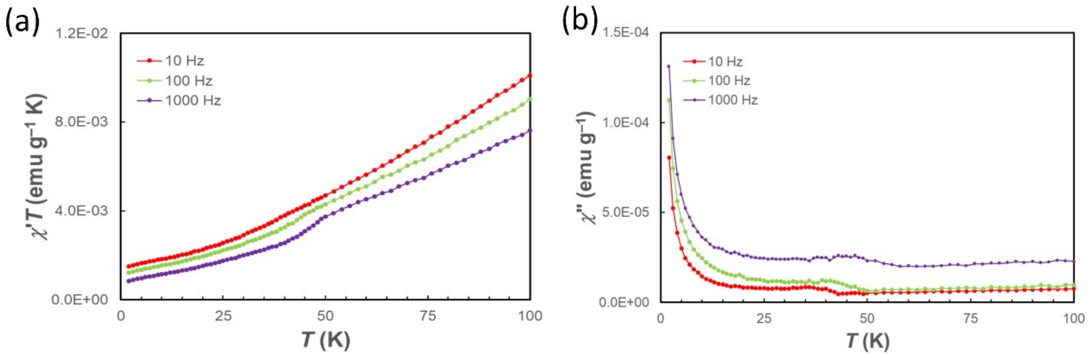


Fig. S8-1 Frequency (ν) and temperature (T) dependences of the (a) in-phase (χ_M') and (b) out-of-phase (χ_M'') ac magnetic susceptibilities of $TbPc_2$@SWCNT in an H_{dc} of zero. The increase in χ_M', the ac magnetic susceptibility, in the high temperature region is considered to be derived from the SWCNTs (Fig. S8-2a).

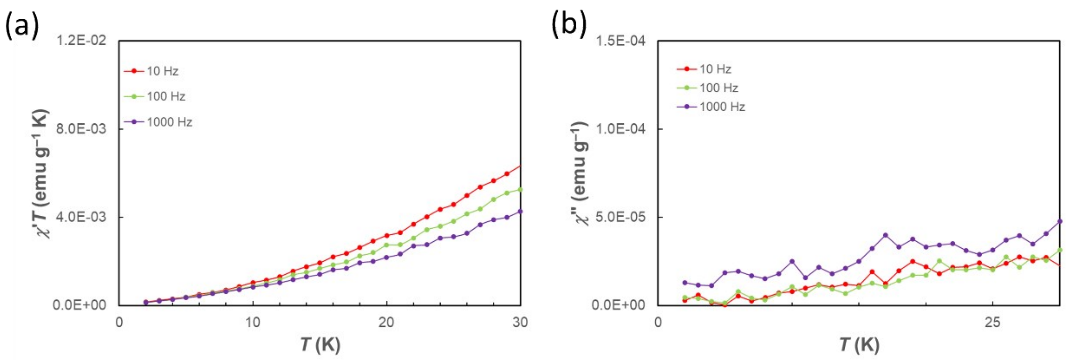


Fig. S8-2 Frequency (ν) and temperature (T) dependences of the (a) in-phase (χ_M') and (b) out-of-phase (χ_M'') ac magnetic susceptibilities of SWCNT in an H_{dc} of zero.

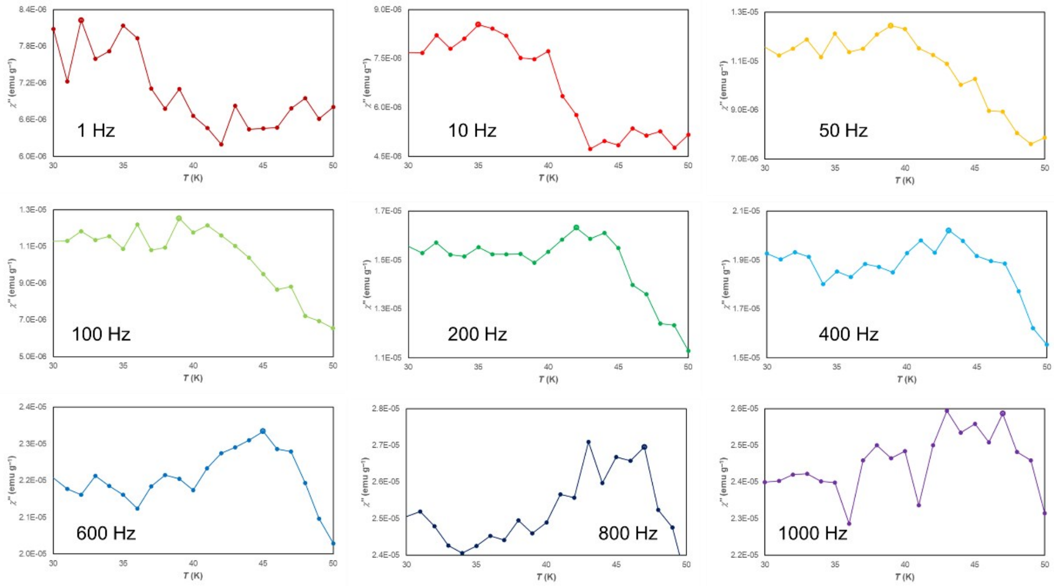


Fig. S9 Frequency (ν) and temperature (T) dependences of the out-of-phase (χ_M'') ac magnetic susceptibilities of $TbPc_2$@SWCNT in an H_{dc} of zero. Since the inclusion rate of $TbPc_2$ is low, the accuracy of the peak top temperature of χ'' has a large error at 1, 100, and 1000 Hz.

Table S1. Magnetic relaxation time (τ) estimated from the peak top temperature of χ'' in the frequency dependence of χ''

Peak top T of χ_M'' / K	ν/Hz	τ/s
31	1	0.15915
35	10	0.015915
38	50	0.0031831
40	100	0.0015915
42	200	0.00079577
44	400	0.00039789
45	600	0.00026526
47	800	0.00019894
47	1000	0.00015915