Supporting Information

Magnetoresistance effect in a conducting molecular crystal consisting of dicyano(phthalocyaninato)manganese(III)

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Crystallographic details

Crystal data and structure refinement are summerised as Table S1. One may notice that Goodness of fit is rather low. This often implies a twinning in crystal. In the case of non-merohedral twin, some reflections overlap the reflections from the second twin domain, giving rise to refinement parameters degraded. However, in the present measurement, we did not observe the second domain by using CCD area detector, which can easily find out the second domain if it presents. Whereas, in the case of merohedral twin, there is no possible "true" space group against the present $P4_2/n$ based on the list of International Tables C, Table 1.3.4.2 in the section of Twinning. In consequence, we conclude that the low Goodness of fit value is not related to the twinning.

We provide another possibility that we can see large temperature factors on Tetraphenylphosphonium. This implies that the cation has a rotational disorder. We consider the origin of the small goodness of fit might be come from the disorder, which has no influence on the discussion on the overlap integral between Pc rings.

Table S1. Crystal data and structure refinement for $TPP[Mn^{III}(Pc)(CN)_2]_2$.

Crystal data	
CCDC number	1517719
Chemical formula	$2(C_{34}H_{16}MnN_{10})\cdot C_{24}H_{20}P$
Formula weight	1578.29
Crystal description	Black needle
Crystal size (mm^3)	0.39 × 0.08 × 0.07
T (K)	293
Crystal system, space group	Tetragonal, $P4_2/n$ (No. 2)
a (Å)	21.7113 (11)
c (Å)	7.4439 (5)
V ($Å^3$)	3508.9 (3)
Z	2
d_{cal} ($g\ cm^{-3}$)	1.494
Radiation	MoKα
Wavelength (Å)	0.71069
μ (mm^{-1})	0.45
Max. and min. transmission	0.971, 0.898
θ range for data collection	$1.33° \leq \theta \leq 28.50°$
Index ranges	$0 \leq h \leq 29$, $0 \leq k \leq 29$, $0 \leq l \leq 9$,
No. of measured, independent and observed reflections	4372, 4372, 2390 ($I > 2\sigma(I)$)

Table S1. Crystal data and structure refinement for TPP[Mn^{III}(Pc)$(CN)_2$]$_2$. (Continued)

Refinement method	Full-matrix least-squares on F^2
R (all data)	R_1 = 0.0848, wR_2 = 0.0776
Goodness-of-fit	0.702
No. of reflections/parameters	4372/393
Largest difference peak and hole (e Å^{-3})	0.50 and −0.62

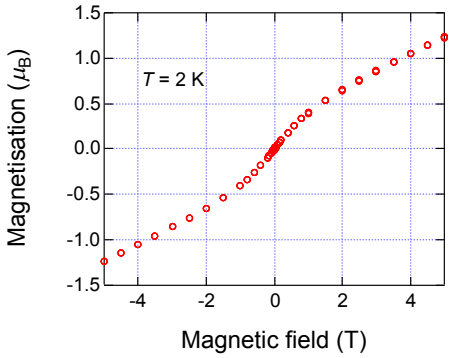

Figure S1. Magnetisation curve for TPP[Mn^{III}(Pc)$(CN)_2$]$_2$ at 2 K.