A co-crystal of 2-(1′-pyrenyl)-4,4,5,5-tetramethyl-4,5-dihydro-1H-imidazole-3-oxide-1-oxyl with octafluoronaphthalene

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Figure S1. Neat solid ATR-FTIR spectra of PyrNN2⋅OFN⋅DCM2, PyrNN, PyrNN2⋅HFB. F = fluoroarene component, Cl = DCM = dichloromethane. Literature spectra for HFB, OFN, DCM.

Figure S2. Magnetization versus field data for PyrNN2⋅OFN⋅DCM2 at 1.8 K, with Brillouin fitting function for S = 1/2.

Figure S3. χT vs T data with fitting to 1-D chain model for PyrNN2⋅OFN⋅DCM2 at 1000 Oe (dc).
Figure S1. Neat solid ATR-FTIR spectra of PyrNN$_2$·OFN·DCM$_2$, PyrNN, PyrNN$_2$·HFB. (F = fluoroarene component, Cl = DCM = dichloromethane); see also literature spectra for HFB, OFN, DCM on pages S2-S3.


See spectra from the SDBS site on the following two pages.
Figure S2. Magnetization versus field data for PyrNN$_2$·OFN·DCM$_2$ at 1.8 K, with Brillouin fitting function for $S = 1/2$. 

For the theoretical Brillouin curve of magnetization versus field at 1.8 K (solid red line), the following equation was used:

\[
M = N g \mu_B \cdot S \cdot B_S(x)
\]

\[
B_S(x) = \frac{2S + 1}{2S} \coth\left(\frac{2S + 1}{2S} x\right) - \frac{1}{2S} \coth\left(\frac{x}{2S}\right)
\]

\[
x = g \mu_B H / k_B T
\]

where $S = 1/2$ and $g = 1.9$ were used to fit the observed data. In the equation, $M$ is the molar magnetization, $H$ is external magnetic field, $T$ is temperature, and other terms are constants with the usual meanings.
Figure S3. $\chi T$ vs $T$ data with fitting to 1-D chain model for PyrNN$_2$·OFN·DCM$_2$ at 1000 Oe (dc).

1-D linear Heisenberg chain model for $S=1/2$ spin units


$$\chi T = \frac{ Ng^2 \beta}{4k} \cdot \frac{T}{T - \theta} \left[ 1 + A \cdot \left( \frac{J}{2kT} \right)^i + B \cdot \left( \frac{J}{2kT} \right)^i + C \cdot \left( \frac{J}{2kT} \right)^i + D \cdot \left( \frac{J}{2kT} \right)^i + E \cdot \left( \frac{J}{2kT} \right)^i \right]^{1/2}$$

$$H = -2J \sum_{N=1}^{\infty} S_i \cdot S_{i+N}$$

$A = 5.7979916$, $B = 16.902653$, $C = 29.376885$, $D = 29.832959$, $E = 14.036918$

and $F = 2.7979916$, $G = 7.0086780$, $H = 8.6538644$, $I = 4.5743114$

This fit was done for data where $T > 10$ K; the fitted results are $J/k = (-)0.96 \pm 0.03$ K, $g = 2.0093 \pm 0.002$. 

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