Polymorphism in a π Stacked Blatter Radical: Structures and Magnetic Properties of 3-(Phenyl)-1-(pyrid-2-yl)-1,4-dihydrobenzo[*e*][1,2,4]triazin-4-yl

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Supplemental Information

Table 1. Crystallographic data for polymorphs **2**α and **2**β.

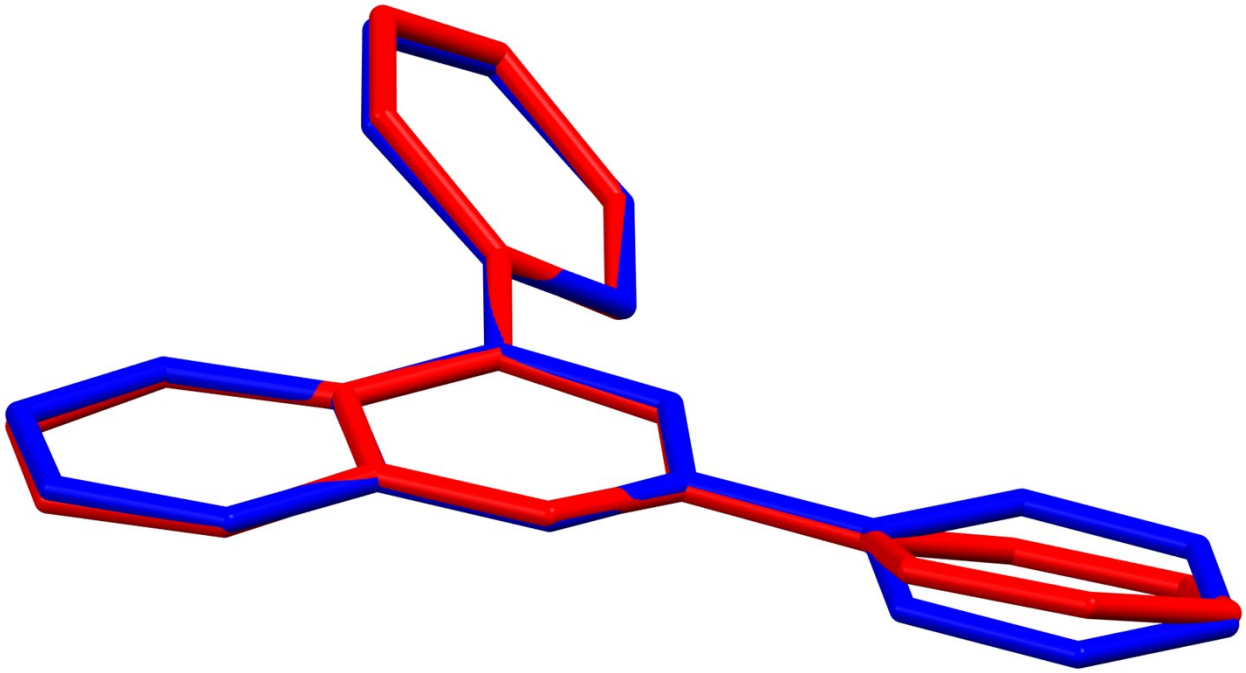
	2α	**2β**
	Crystal Data	**Crystal Data**
Formula	$C_{18}H_{13}N_4$	$C_{18}H_{13}N_4$
Formula weight, g.mol^{-1}	285.32	285.32
Crystal system	Orthorhombic	Monoclinic
Space group	*P 2$_1$ 2$_1$ 2$_1$*	*P-1 2$_1$/c$_1$*
a, *b*, *c*, Å	7.1656(3), 10.9705(4), 17.5843(6)	19.7893(9), 3.76820(10), 19.7322(8)
α, β, γ °	90, 90, 90	90, 114.594(5), 90
V, Å^3	1382.31(9)	1337.94(10)
Z	4	4
ρ_{calc}, g.cm^{-3}	1.371	1.416
μ(Mo Ka), mm^{-1}	0.671	0.693
F(000)	596	596
Crystal size, mm^3	0.224 × 0.053 × 0.035	0.193 × 0.085 × 0.026
	Data Collection	**Data Collection**
T, K	120.01(10)	120.00(10)
λ[a], Å	1.54184	1.54184
θ (min, max), °	4.751, 74.490	4.500, 76.649
Dataset (-*h*, *h*; -*k*, *k*; -*l*, *l*)	-8, 7; -12, 13; -20, 21	-24, 23; -4, 2; -24, 24
Meas./ indep. refl. (R_{int})	5012 / 2674 (0.0281)	9981 / 2797 (0.0267)
Obs. refl. [I>2σ(I)]	199	199
	Refinement	**Refinement**
R_1[b]	0.0388	0.0418
wR_2 [c]	0.1001	0.1196
Goodness of fit on F^2	1.040	1.030
Min, max resd density, *e*.Å^{-3}	-0.177/0.163	-0.266/0.222

[a] Graphite monochromator.

[b] $R_1=\Sigma \| F_o | - | F_c \| / \Sigma | F_o |$.

[c] $wR_2=[\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[wF_o^2)^2]]^{1/2}$, $w=1/[\sigma^2(F_o^2) + (m\cdot p)^2 + n\cdot p]$, $p=[\max(F_o^2,0) + 2F_c^2]/3$.

Fig. S1 Structure overlay of polymorphs **2α** and **2β** (polymorph **2α** with red capped sticks and polymorph **2β** with blue capped sticks).



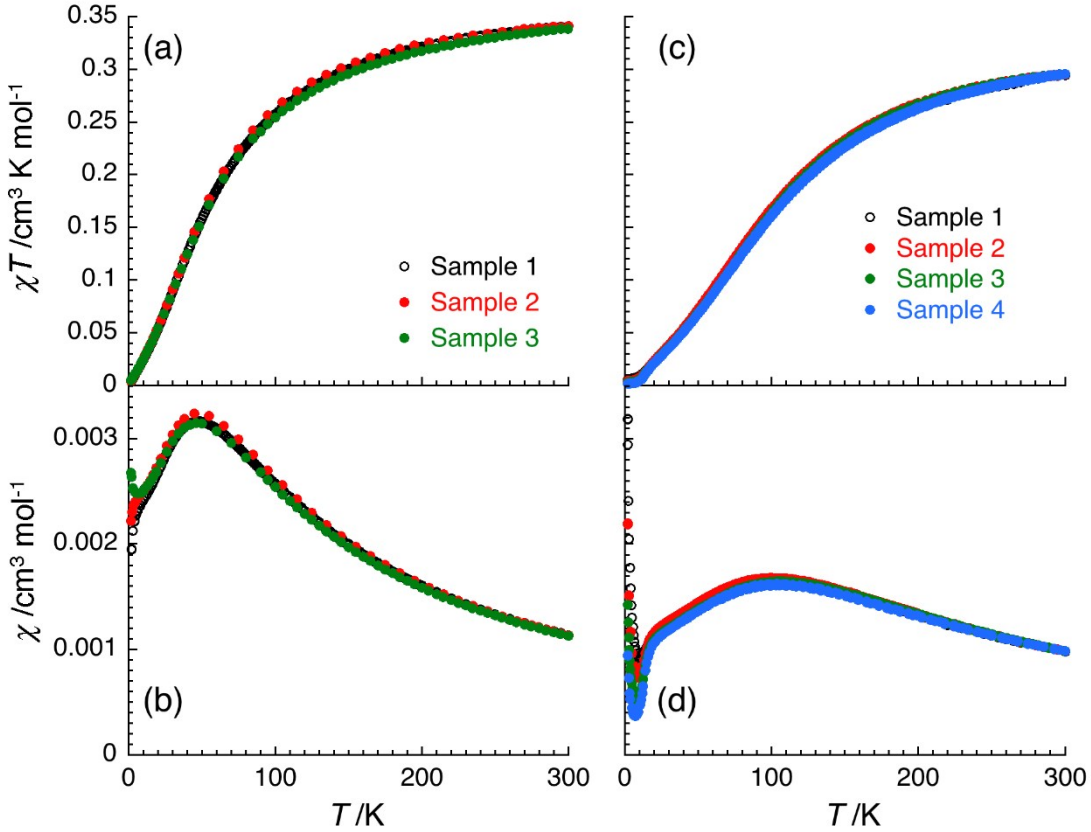


Fig. S2 Temperature dependence of (bottom) the magnetic susceptibility and (top) the χT product for polymorphs (left; at 0.5 T for sample 1 and 0.1 T for sample 2) **2**α and (right; at 0.1 T for sample 1; at 0.5 T for samples 2, 3 and 4) **2**β (χ is defined as M/H per mole of radical **2**). The best fit of the experimental data to the regular chain model of antiferromagnetically coupled quantum spins (see main text) leads for **2**α to J/k_B = –36.7(3) K (–25.5(2) cm^{-1}; between 300 and 15 K) for sample 1, J/k_B = –35.6(3) K (–24.7(2) cm^{-1}; between 300 and 14 K) for sample 2, J/k_B = –36.9(3) K (–25.6(2) cm^{-1}; between 300 and 16 K) for sample 3; and for **2**β to J/k_B = –72(3) K (–50(2) cm^{-1}; between 300 and 20 K) for sample 1, J/k_B = –70(3) K (–49(2) cm^{-1}; between 300 and 20 K) for sample 2, J/k_B = –72(3) K (–50(2) cm^{-1}; between 300 and 20 K) for sample 3 and , J/k_B = –73(3) K (–51(2) cm^{-1}; between 300 and 20 K) for sample 4 (with a fixed g factor of 2.05(5))