Table 1S Crystal data of PNP[Fe(Pc)Cl_2]

Empirical formula	$C_{68}H_{46}Cl_2N_{10}FeP$
Formula weight	1160.91
Crystal system	triclinic
Space group	P1-
Unit cell dimensions	a = 10.501(6) Å
	b = 12.232(6) Å
	c = 12.938(6) Å
	α = 85.71(3)˚
	β = 68.16(4)˚
	γ = 66.19(4)˚
	V = 1405.7(12) $Å^3$
Z, Calculated density	1, 1.371 g cm^{-3}
Absorption coefficient	4.451 cm^{-1}
Reflections collected/unique	13709/6411 [R(int) = 0.043]
$R1$ [$I > 2\sigma(I)$]	0.0645
R, $wR2$ (all data)	0.0765, 0.1400
Goodness-of-fit indicator	0.995

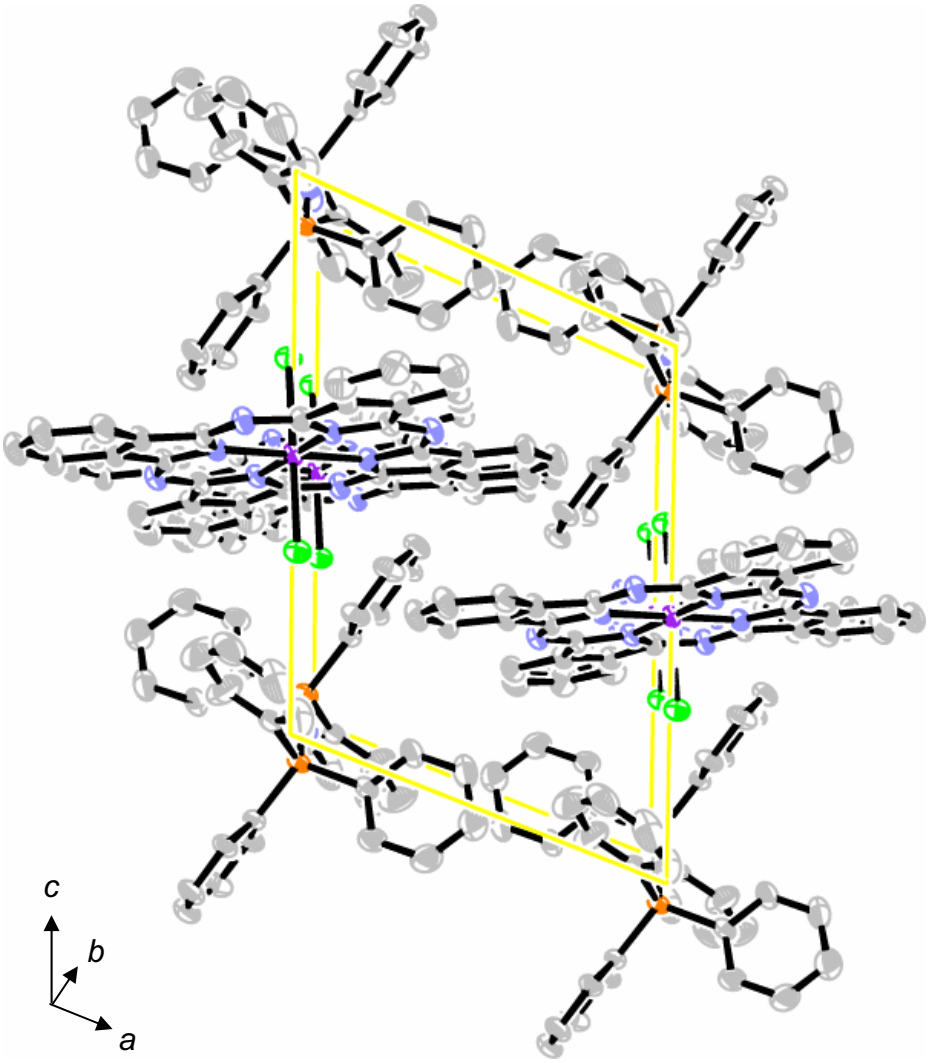

Fig. 1S Crystal structure of PNP[Fe(Pc)Cl_2]

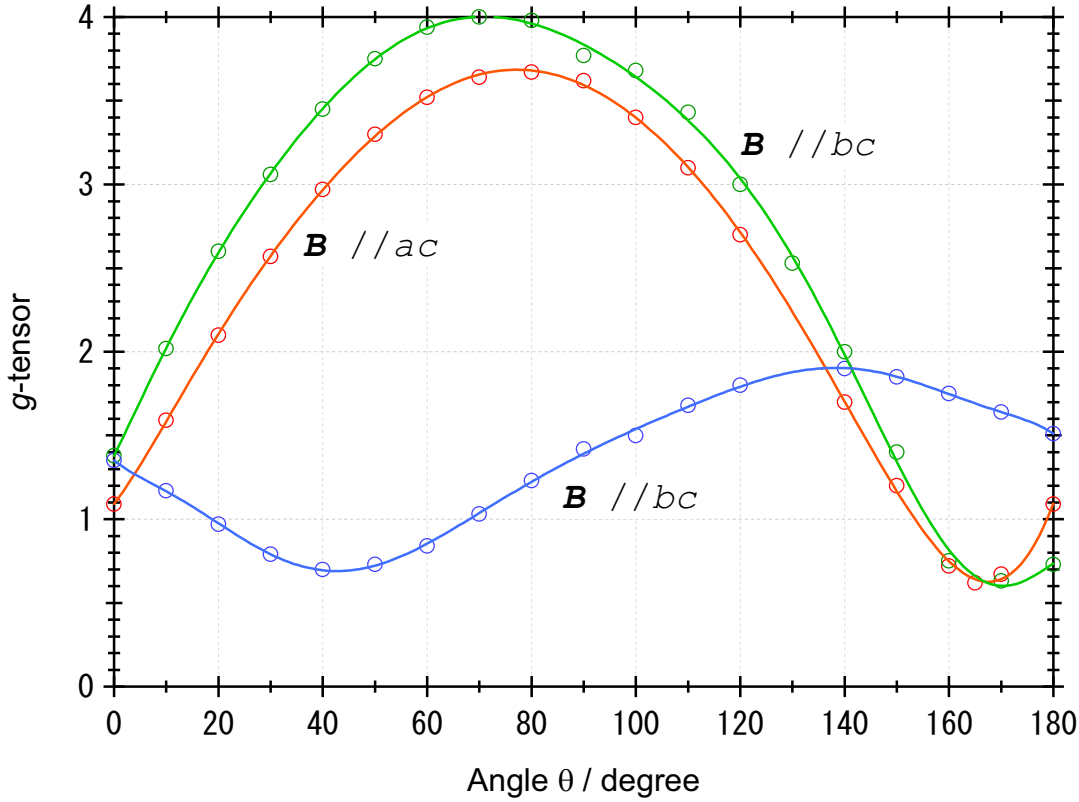

Fig. 2S Angular dependence of the ESR signal of PNP[Fe(Pc)Cl_2] measured at 5 K. The solid curves represent the best fit of the data points.

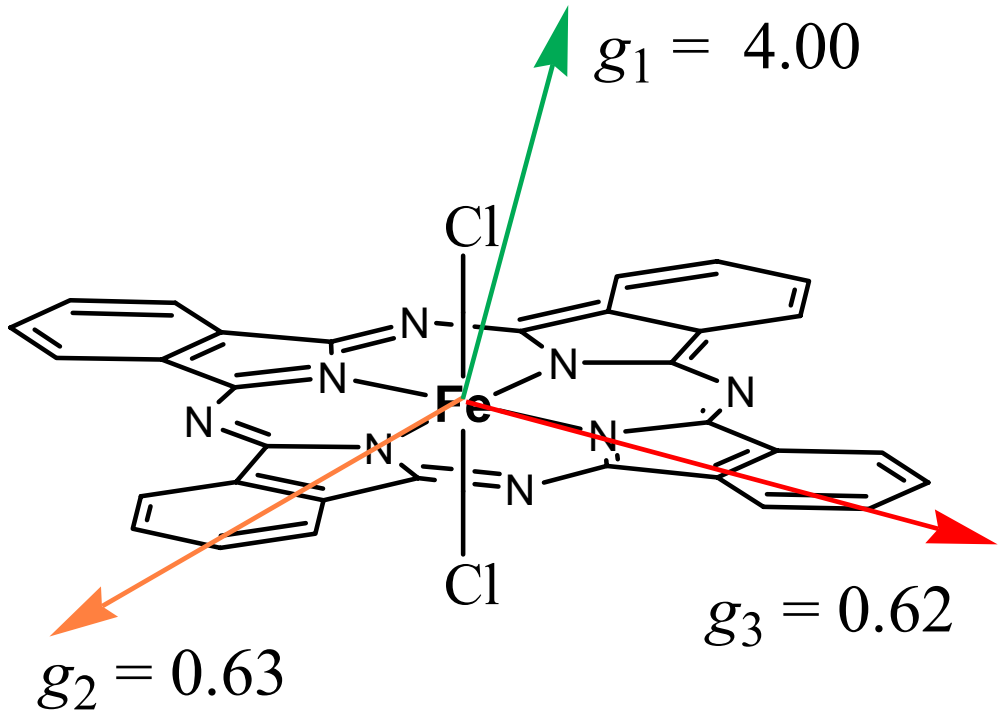

Fig. 3S Principal axes of the g-values of the molecular unit of $Fe(Pc)Cl_2$ derived from Fig. 2S.