Supporting Information for:

Probing Bistability in Fe^{II} and Co^{II} Complexes with an Unsymmetrically Substituted Quinonoid Ligand

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X-ray

Table S1. Crystal data and refinement details for **[1]**BF_4·$2CH_2Cl_2$and **[2]**BF_4·$2CH_2Cl_2$.

compound	**[1]**BF_4·2 CH_2Cl_2	**[2]**BF_4·$2CH_2Cl_2$
empirical formula	$C_{38}H_{40}BCl_6F_4FeN_5O_3$	$C_{38}H_{40}BCl_6CoF_4N_5O_3$
formula weight	970.11	973.19
T [K]	133(2)	140(2)
crystal size [mm³]	0.50 × 0.33 × 0.17	0.18 × 0.10 × 0.08
crystal system	monoclinic	monoclinic
space group	$P2_1/n$	$P2_1/n$
a [Å]	15.7289(6)	15.925(3)
b [Å]	15.3978(4)	15.360(3)
c [Å]	17.4980(7)	17.764(3)
α [°]	90	90
β [°]	94.213(3)	92.216(4)
γ [°]	90	90
V [Å³]	4226.4(3)	4342.0(14)
Z	4	4
ρ [g/cm³]	1.525	1.489
F(000)	1984	1988
μ [mm^{-1}]	0.798	0.824
T_{min} / T_{max}	0.7432 / 0.8680	0.6637 / 0.7452
θ-range [°]	1.681 - 25.698	1.685 - 25.112
hkl-range	±19, –18 - 17, ±21	–18 - 17, ±18, ±21
measured refl.	44734	34967
unique refl. [R_{int}]	7959 [0.0541]	7707 [0.0492]
observed refl. ($I > 2\sigma(I)$)	6992	5201
data / restraints / param.	7959 / 9 / 593	7707 / 8 / 580
goodness-of-fit (F^2)	1.112	1.059
$R1$, $wR2$ ($I > 2\sigma(I)$)	0.0695, 0.1725	0.0605, 0.1435
$R1$, $wR2$ (all data)	0.0784, 0.1779	0.0946, 0.1629
resid. el. dens. [e/Å³]	–0.930 / 0.894	–0.668 / 0.729

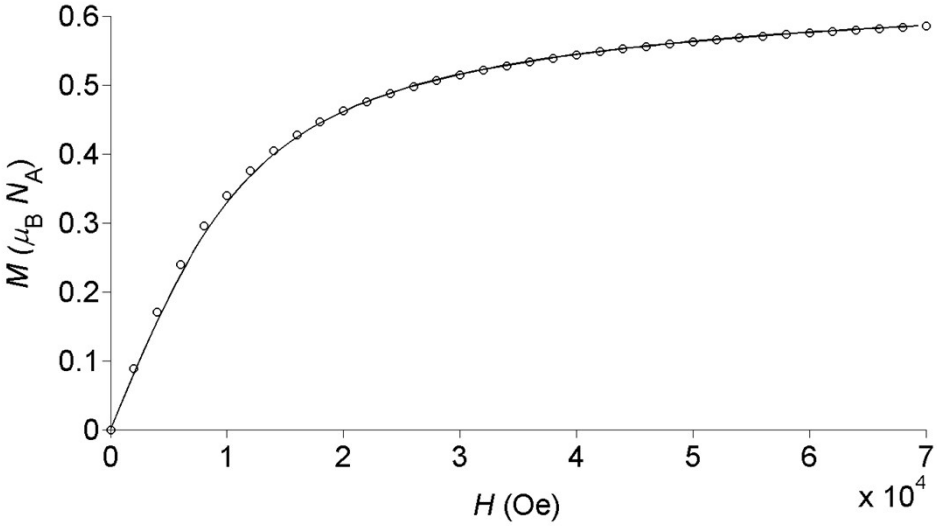

Fig. S1 Magnetization curve for **[1]**BF_4 measured at 1.8 K. The best fit with the parameters given in the text is shown as a solid line.

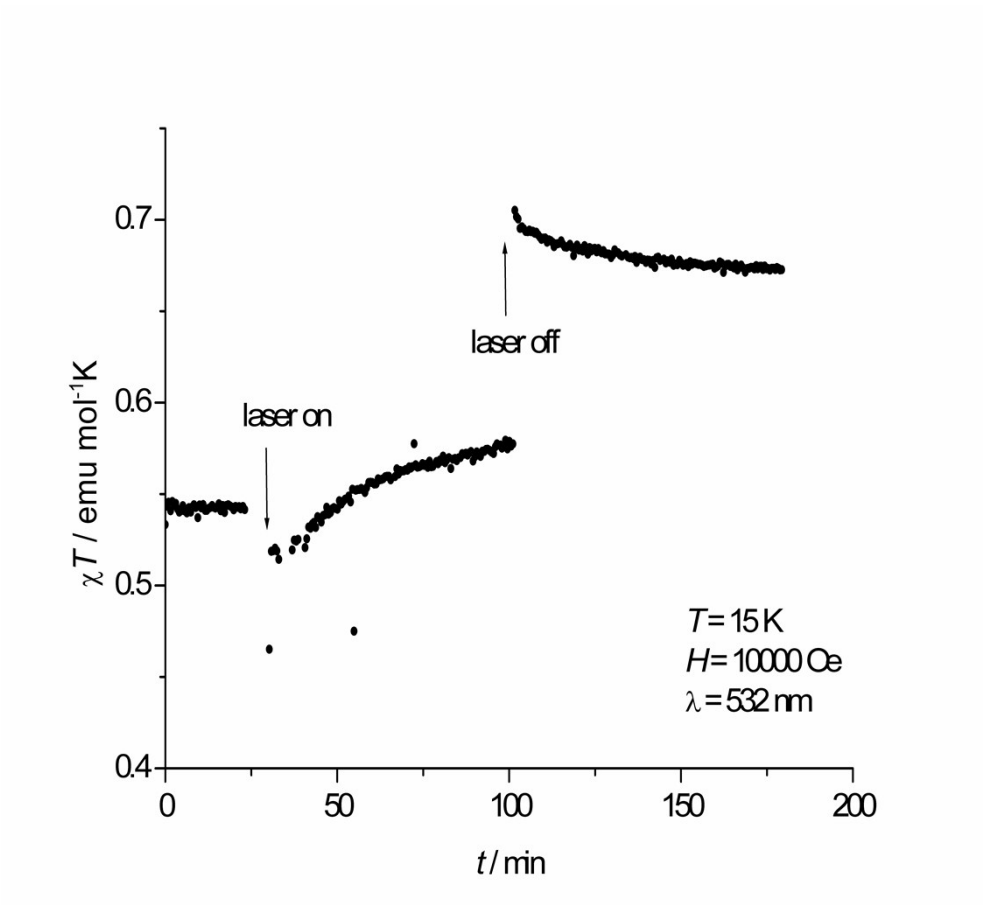

Fig. S2. Isothermal LIESST study of **[1]BF_4** at 15 K. The effect of sample heating due to laser irradiation can clearly be observed by jumps in χT on switching on and off the irradiation.

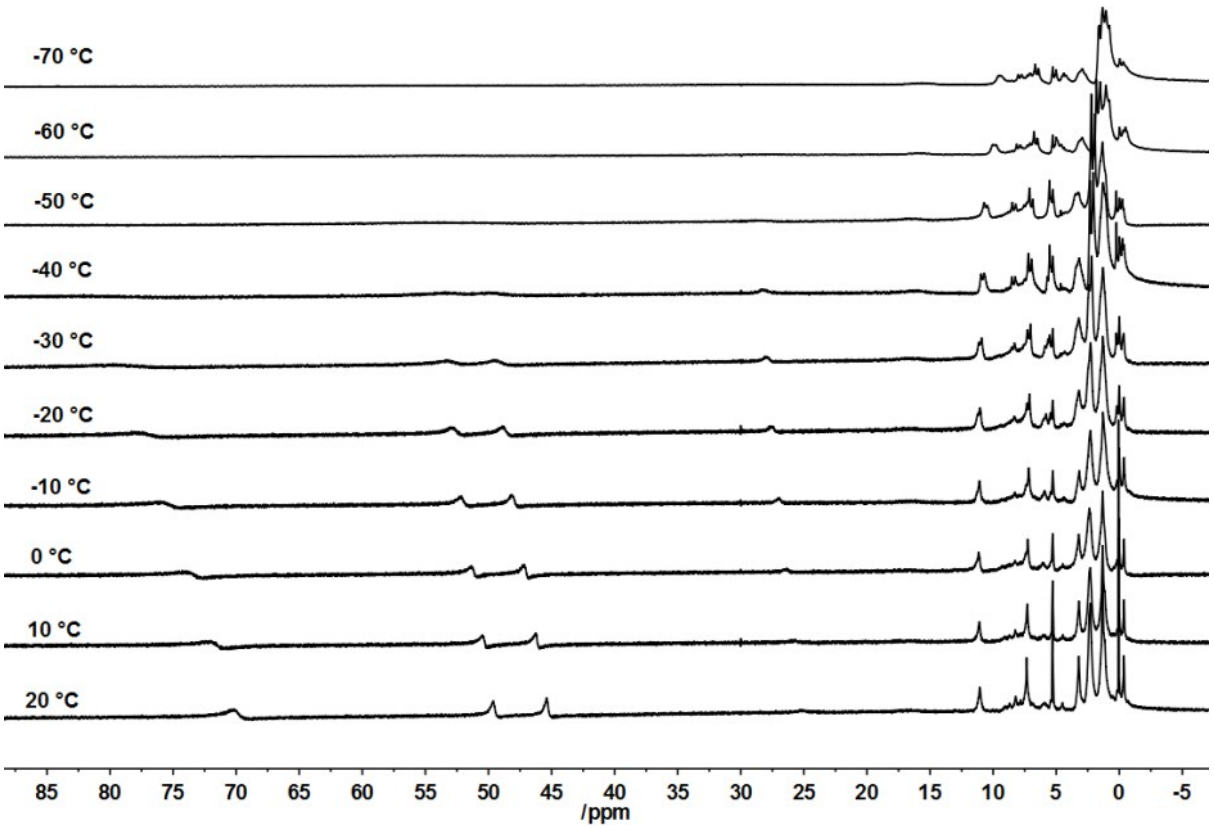

Fig. S3 ^{1}H-NMR of **[1]**$^{+}$ measured at 20 °C to -70 °C in CD_2Cl_2.

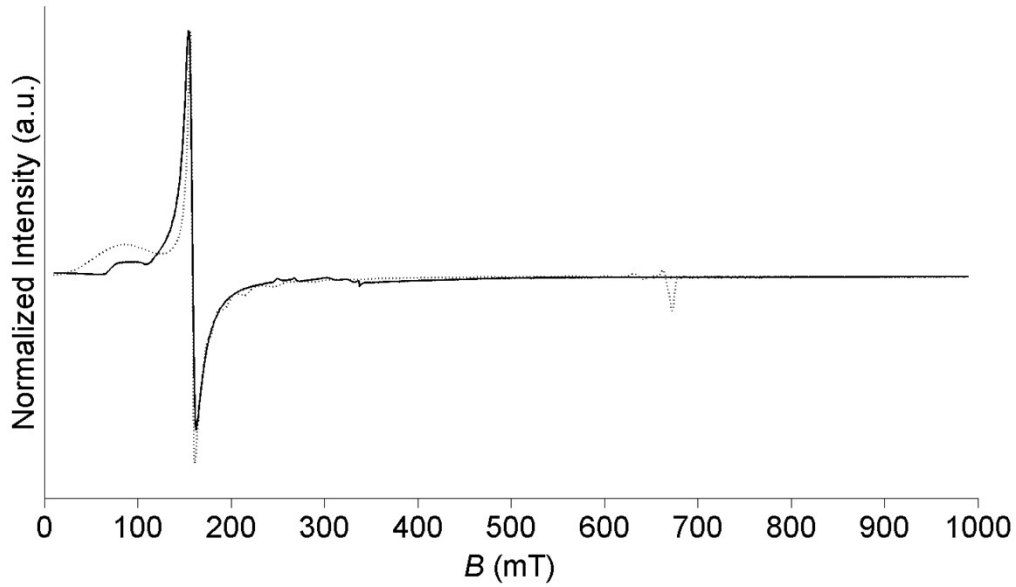

Fig. S4 X-band EPR measurement of **[1]**BF_4 recorded at 4 K. The best fit with the parameters given in the text is shown as a dotted line.

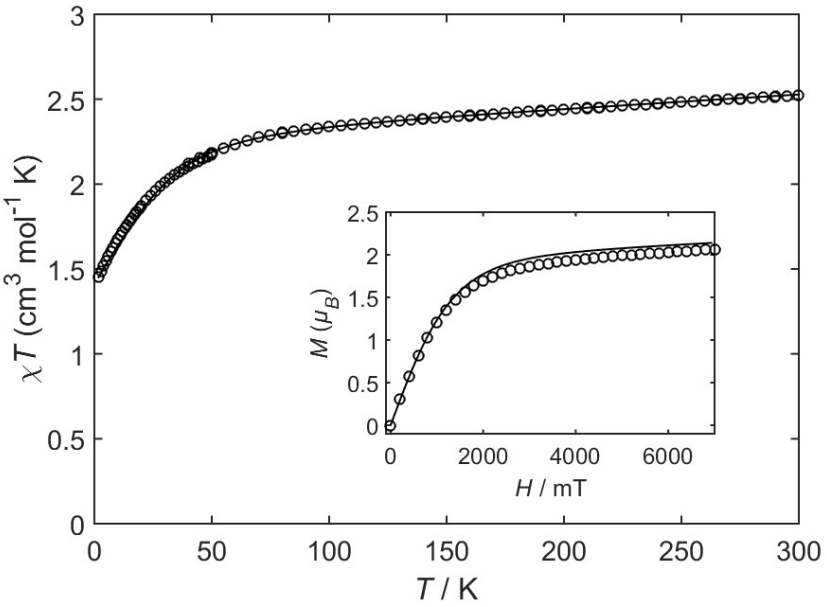

Fig. S5 χT as a function of T for the complex **[2]**BF_4 measured at 1000Oe. Inset: Magnetization curve for **[2]**BF_4 measured at 1.8 K. Simulations with the parameters given in the text are shown as solid lines.

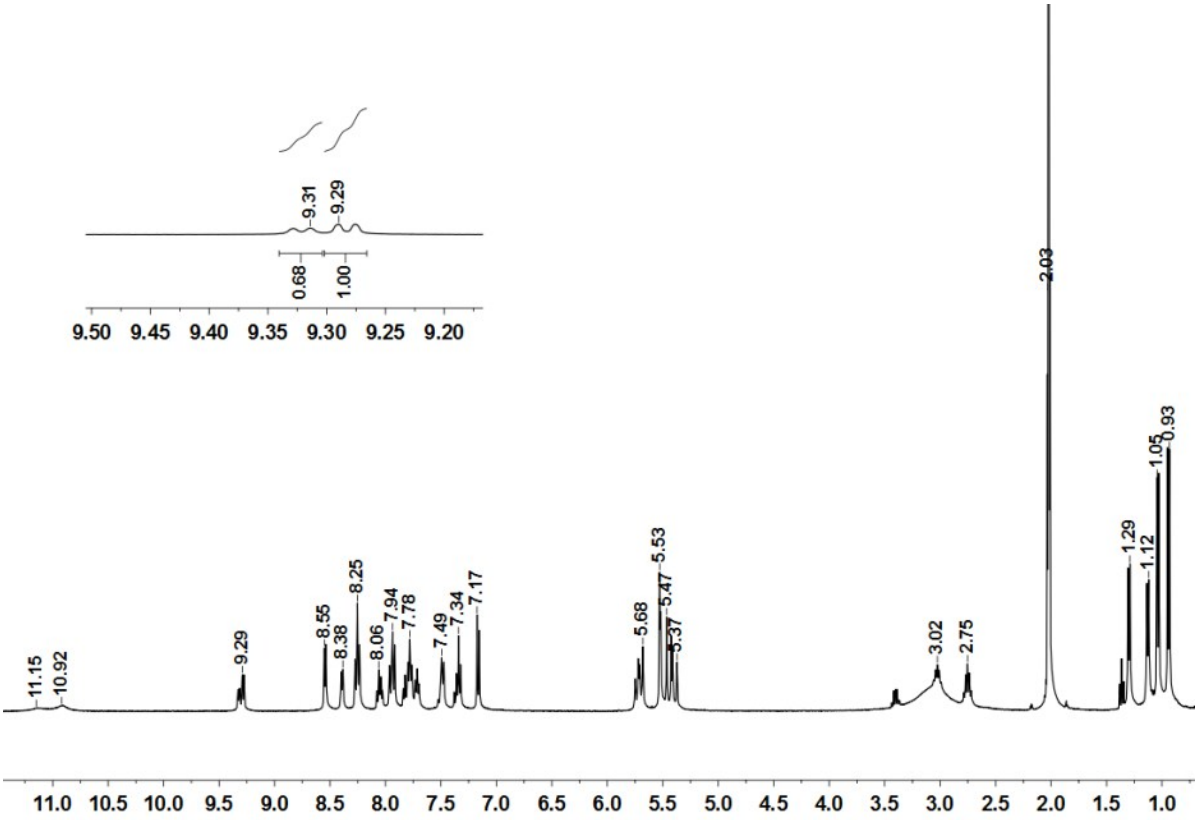

Fig. S6 ^{1}H NMR spectrum of **[2]**$^{2+}$ in acetone-d_6 measured after 12 h of dissolving the sample.

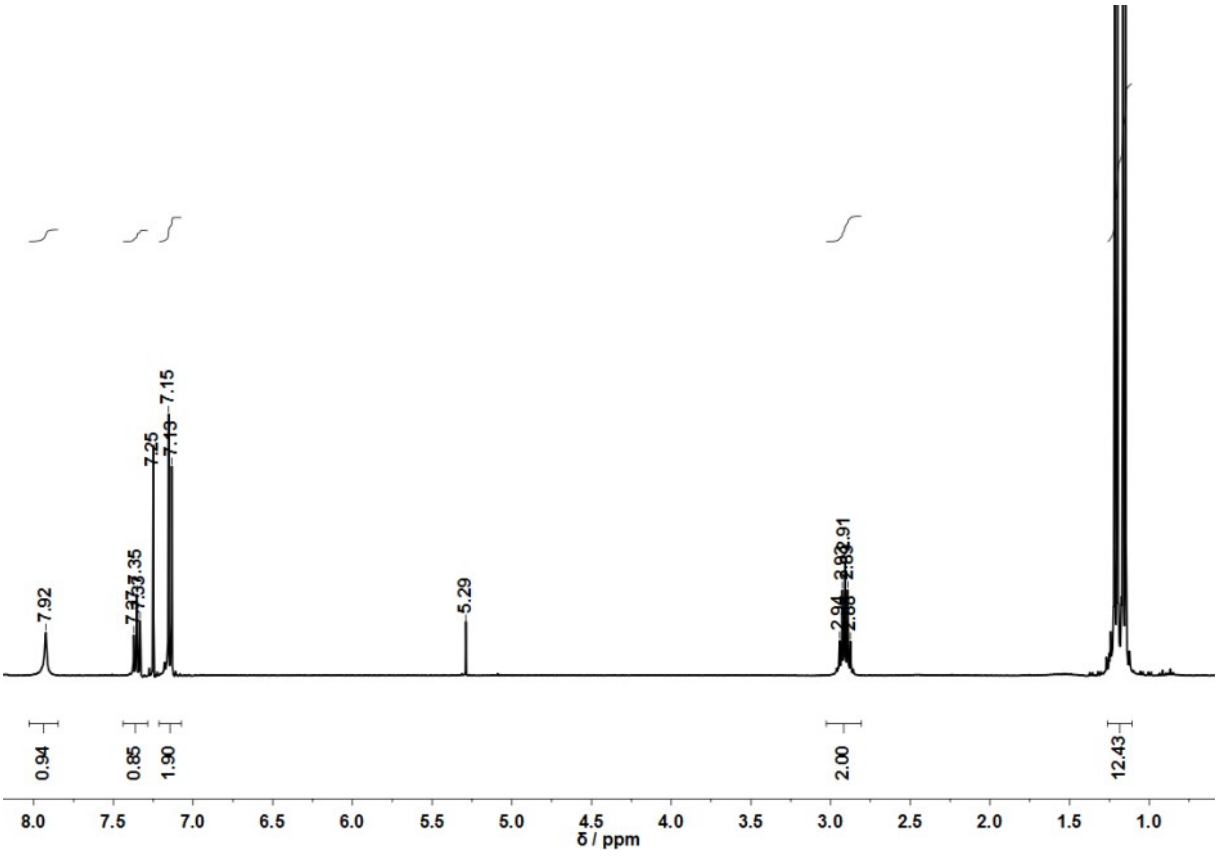

Fig. S7 ^{1}H NMR spectrum of $\mathbf{H_2L}$ in $CDCl_3$. Sample contains a residue of CH_2Cl_2.

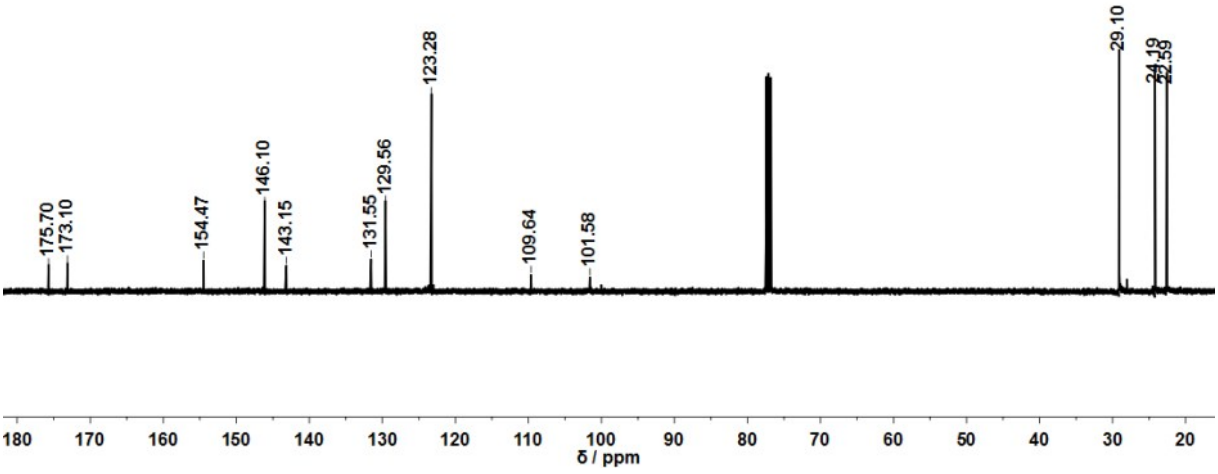

Fig. S8 ^{13}C NMR spectrum of $\mathbf{H_2L}$ in $CDCl_3$.