Supporting Information

Doubly Reduced Phthalocyanine Complexes of V(IV), Cu(II), and Sn(II): Synthesis, Structure, and Spin Dynamics

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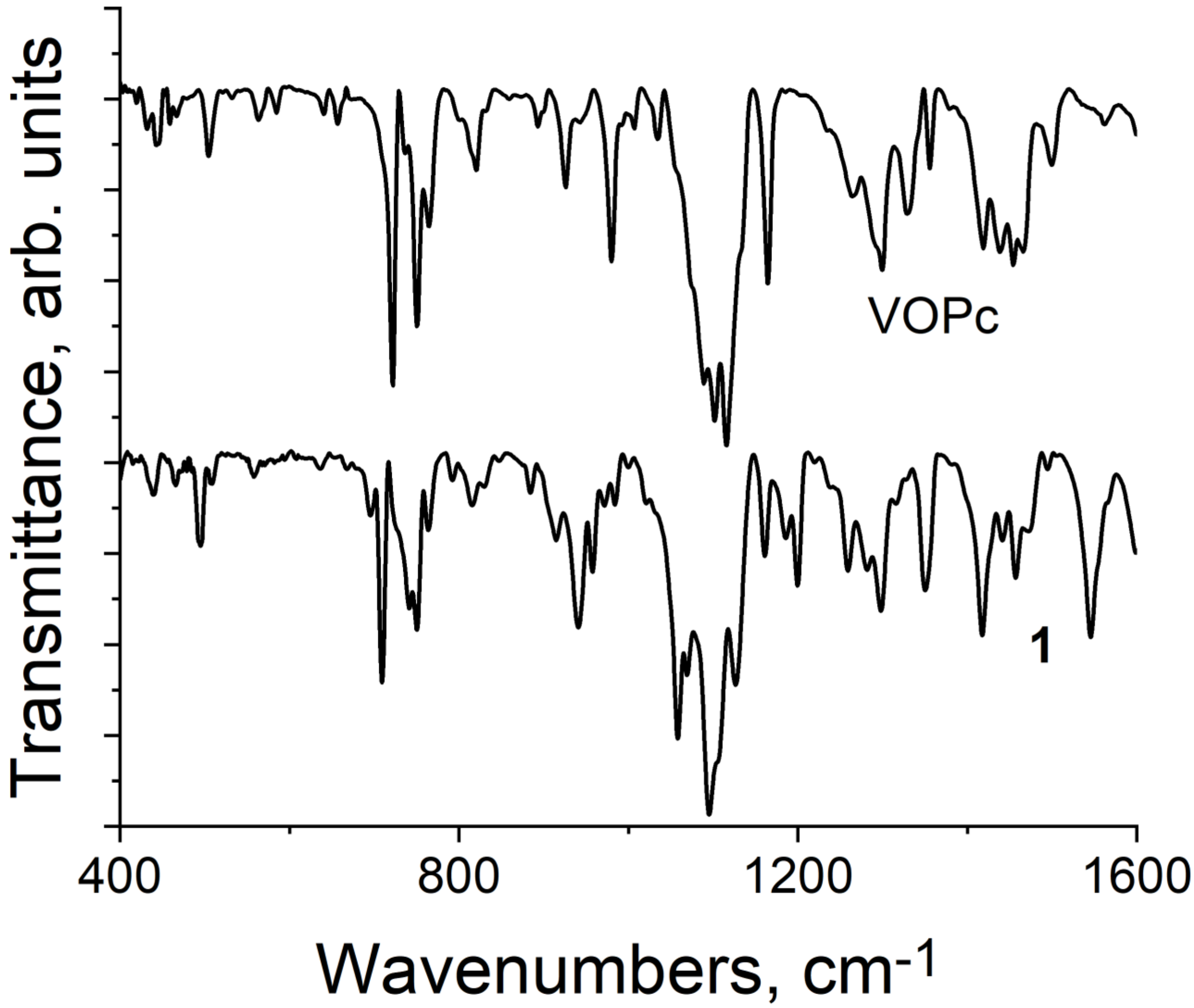

Figure S1. IR spectra of starting VOPc and complex **1** in KBr pellets prepared in anaerobic condition.

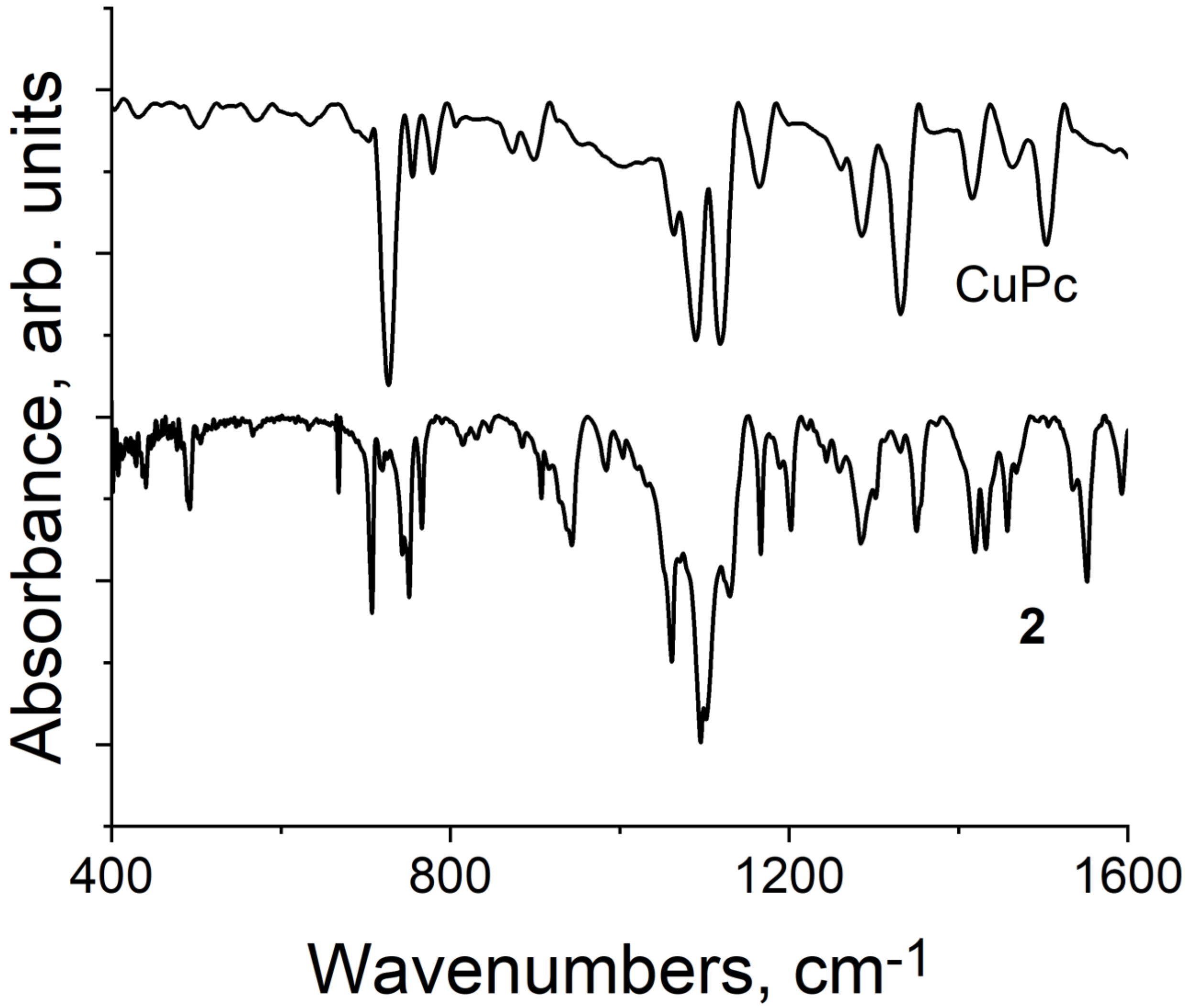

Figure S2. IR spectra of starting CuPc and complex **2** in KBr pellets prepared in anaerobic condition.

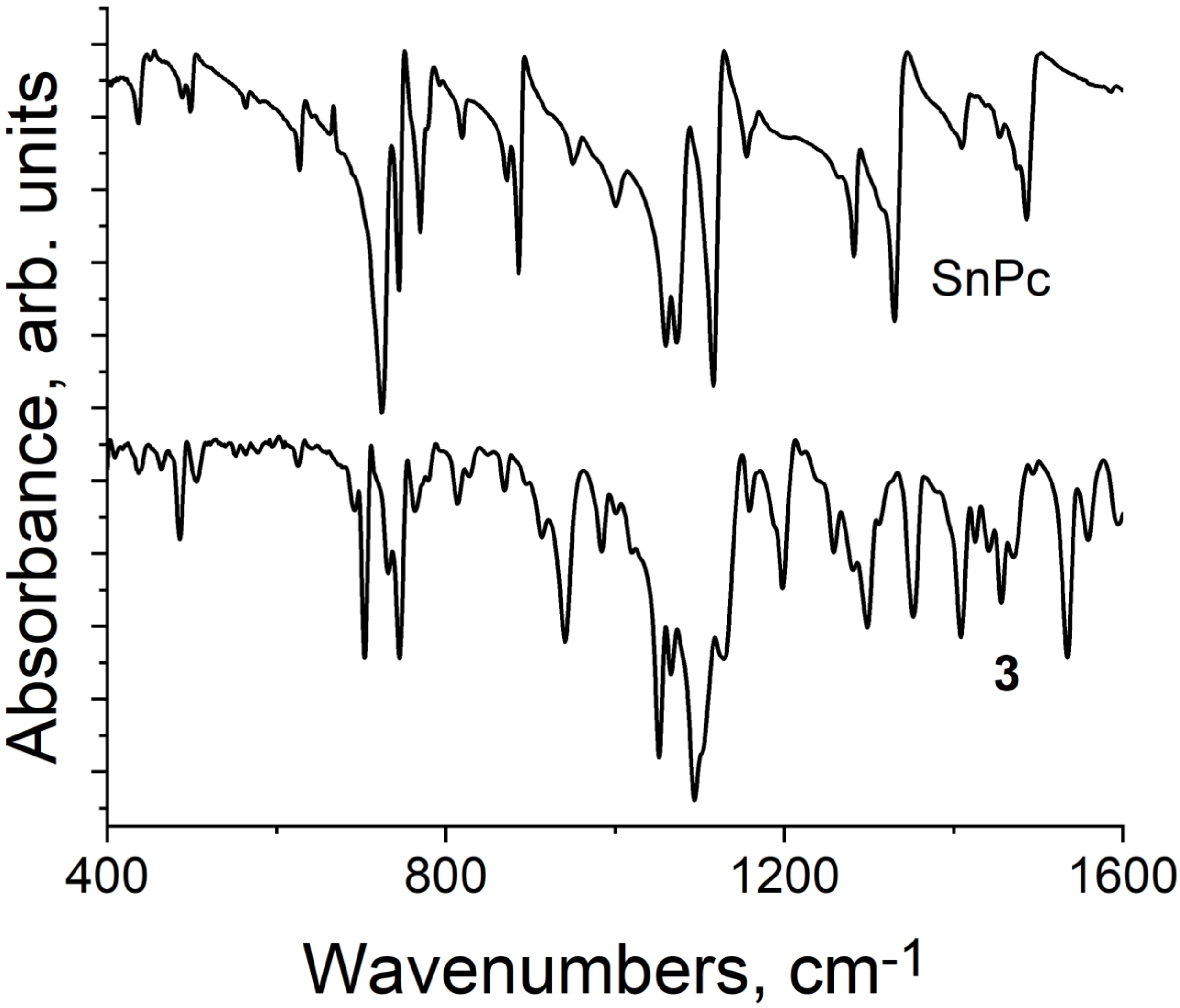

Figure S3. IR spectra of starting SnPc and complex **3** in KBr pellets prepared in anaerobic condition.

Table S1. IR spectra of starting metal phthalocyanines and complexes **1**–**3**.

Components	Cryptand(K^+)	$V^{IV}OPc$	**1**	$Cu^{II}Pc$	**2**	$Sn^{II}Pc$	**3**
Phthalocyanine		439w	439w	727s	708s	435w	-
		509w	495w*	755w	752s	498w	506w
		572w	-	779w	767m	627w	-
		639w	-	899w	908w	725s	704m
		723sw	709s	1005w	-	745m	732m*
		-	742m	1027w	1033w*	768m	745s
		755m	750m	1064m	1062s*	819w	814w
		776w	764w	1090s	1096s	887m	895w
		875w	884w	1119s	1120s	948w	941m
		899m	-	1165m	1167m	1001w	1001w
		963w	958w	1261w	-	1059s	1052s*
		1002s	-	1286m	1285m*	1072s	1066s*
		1079s	1058s	1332s	1351m*	1114s	1129s
		1120s	1127s	1416m	1420m	1156w	1159w*
		1161w	1161w*	1464w	1458m*	1283m	1258w*
		-	1200m	1504m	1552s	1329s	1281m*
		1288m	1282w	1610w	-	1407w	1409m
		1334s	1350m*	1861m	-	1454w	1456m*
		1418w	1418m	1894m	-	1486s	1471m*
		1464w	1457w*			1613w	1606w
		1478w	1473w				
		1498m	-				
		1610w	1599w				
			495w*				486w
Cryptand	476w		-		493m		506w
	528w		742m		-		-
	581w		915w		-		732m*
	735m		1021w		744m		914w
	922m		1069m		938m		1020w
	1038w		1095s		1033w*		1066s*
	1071m		1161w*		1071s		1094s
	1100s		1259w		1102s		1159w*
	1127s		1298m		1130s		1258w*
	1213w		1316w		1203m		1281m*
	1295m		1350m*		1285m*		1312w
	1329m		1441w		-		1352m
	1360s		1457w*		1351m*		1456m*
	1446m		-		1433m		1471m*
	1462m		1546m		1458m*		-
	1490w		2811w		-		1535m
	-		2876w		1535w		2804w
	2790w		2952w		-		2870m
	2877w				2868w		2949w
	2943w				2886w		

* - bands are coincided

w – weak intensity, m –middle intensity, s – strong intensity

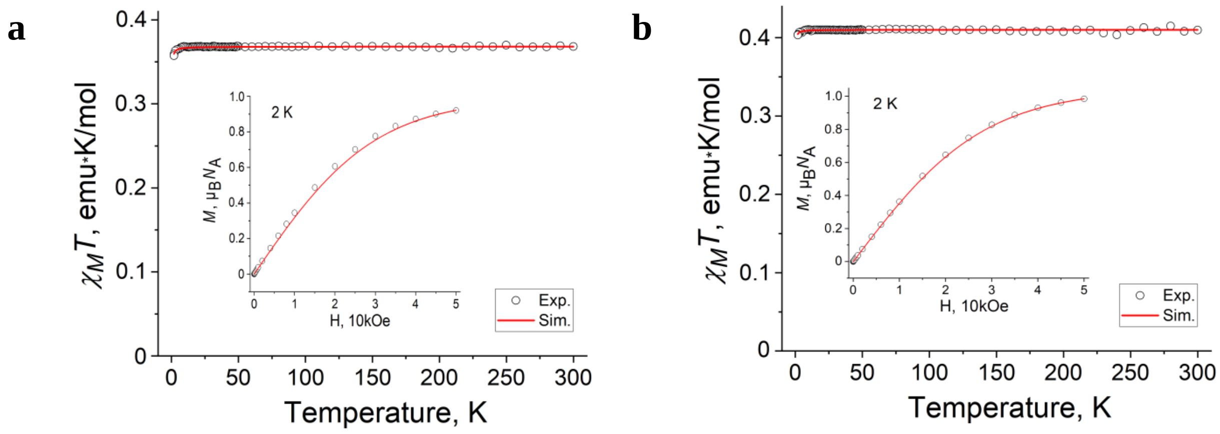

Figure S4. Temperature dependence of $\chi_M T$ measured at H = 1 kOe and magnetization *vs*. field measured at T = 2 K (open circles) for **1** (a) and **2** (b). Theoretical curves (solid red lines) obtained with PHI program[1] using parameters presented in the text.

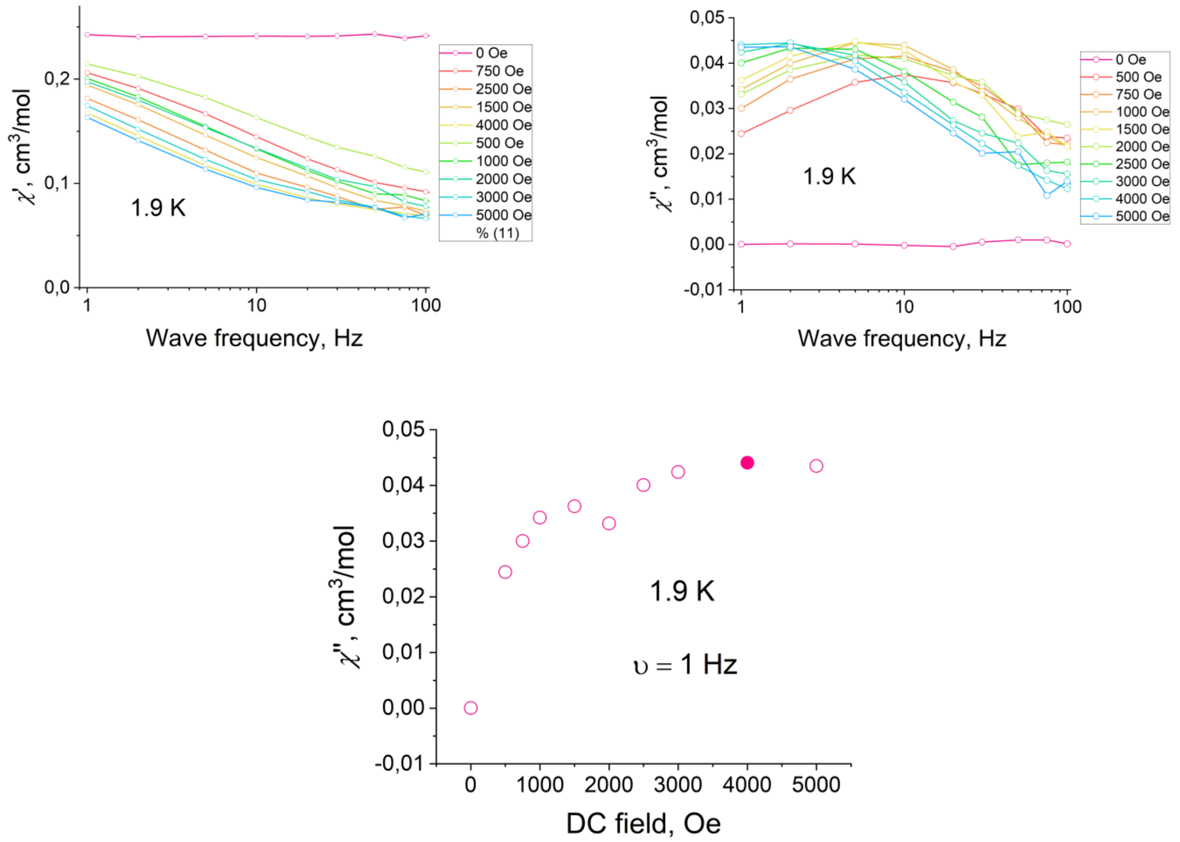

Figure S5. Frequency dependences of in-phase (χ') (top right) and out-of-phase (χ'') (top left) AC susceptibility for **2** at different applied static magnetic fields H_{DC} and T = 2 K. Field dependence of the out-of-phase (χ'') AC magnetic susceptibility at T = 1.9 K and frequency of 1 Hz (bottom).

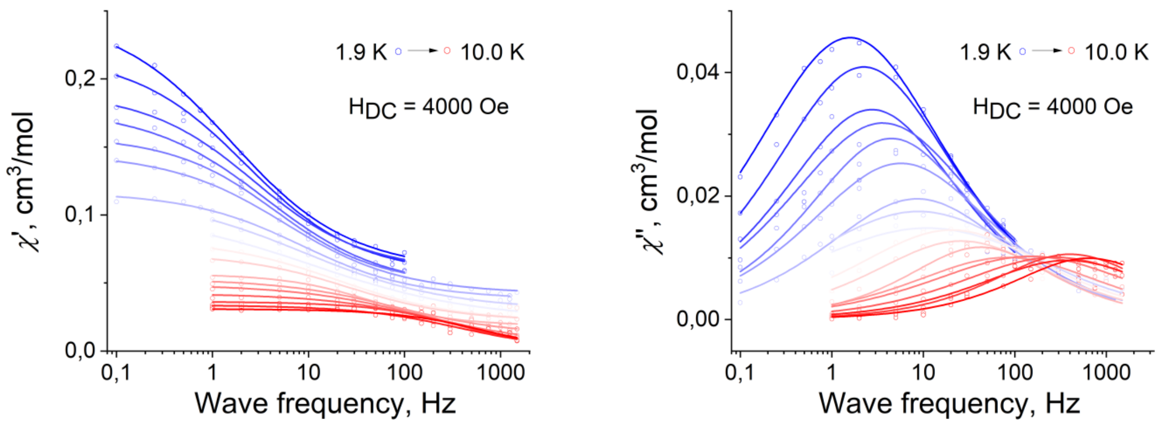

Figure S6. Frequency dependences of in-phase (χ') (left) and out-of-phase (χ'') (right) AC magnetic susceptibilities for **2** at applied static magnetic field H_{DC} = 4000 Oe and temperatures of 1.9 – 10.0 K. Solid lines represent the fitting of the data by the generalized Debye model.

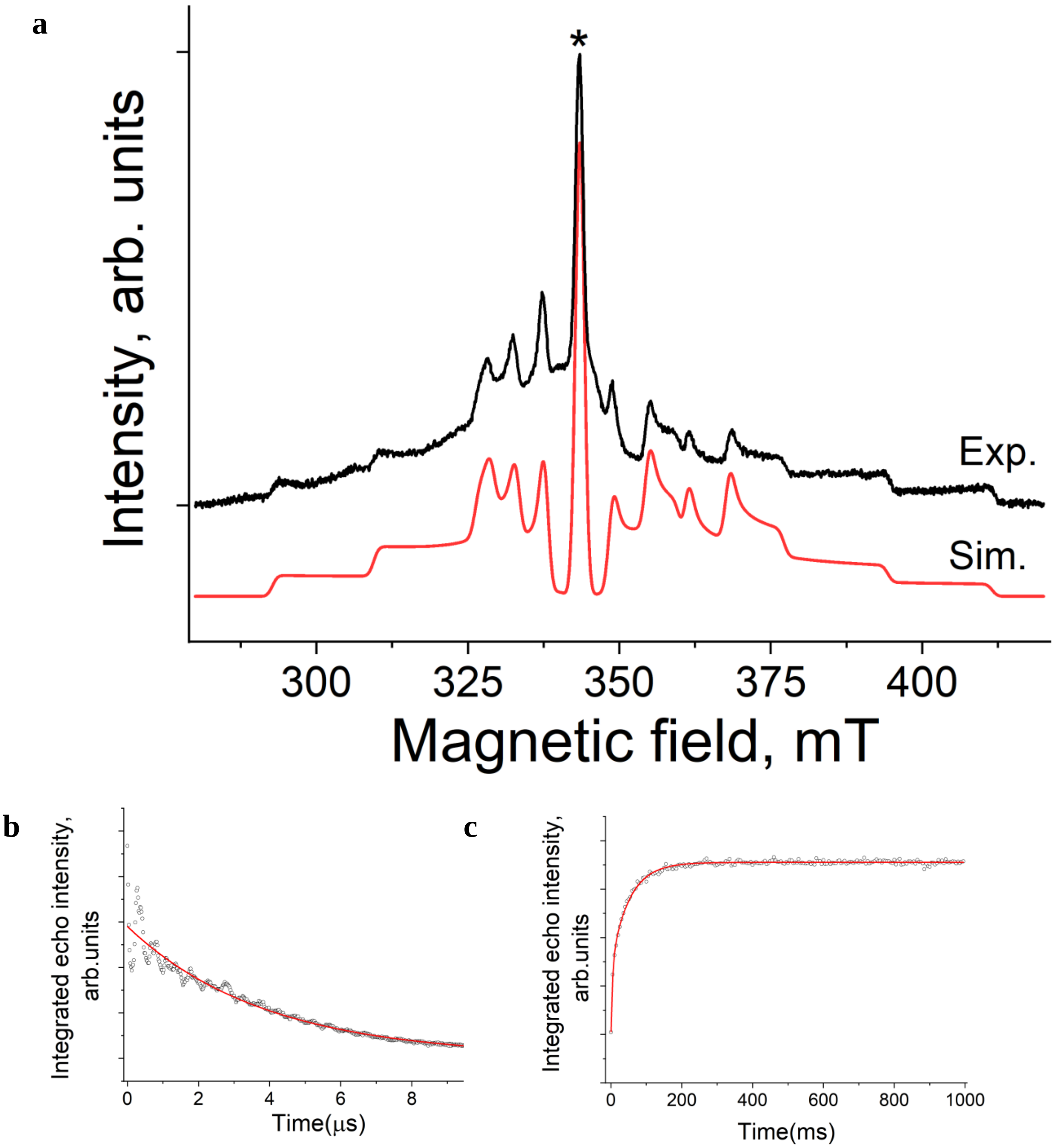

Figure S7. Glassy 1 mM toluene solution of **1**. (a) Echo detected X-band EPR spectrum at 10 K under microwave irradiation of 9.698 GHz (black), together with a simulation with parameters: *g*= [1.984; 1.966], *A* = [154; 467] MHz using EasySpin (red). The spectral position where the relaxation measurements were done (343.5 mT) is shown by asterisk (*). (b) Pulsed EPR echo decay traces at 10 K(black), together with a fitting using exponential equation with T_m = 3.9 μs (red). (c) Time dependence of saturation recovery at 10 K (black), together with a fitting using biexponential equation with $T_{1,1}$ = 51.1 ms and $T_{1,2}$ = 4.5 ms (red).

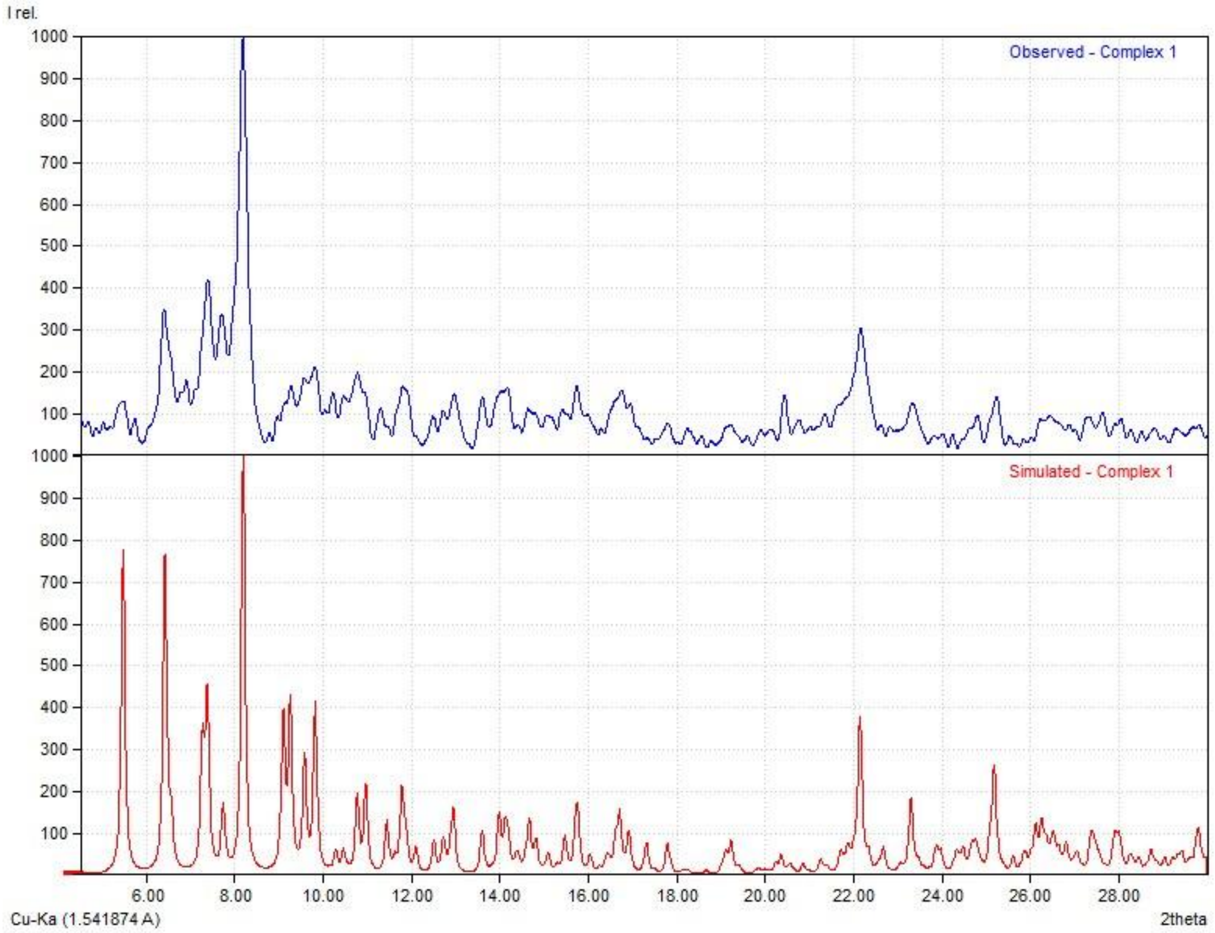

Figure S8. Powder X-ray diffraction pattern of polycrystalline sample of complex **1**: experimental (blue), and calculated from single crystal data (red).

References

(1) Chilton, N. F.; Anderson, R. P.; Turner, L. D.; Soncini, A.; Murray, K. S. PHI: A Powerful New Program for the Analysis of Anisotropic Monomeric and Exchange-Coupled Polynuclear *d* - and *f* -Block Complexes. *J. Comput. Chem.* **2013**, *34* (13), 1164–1175. https://doi.org/10.1002/jcc.23234.