Supporting Information for the manuscript

Field-Induced Slow magnetic Relaxation in Pseudooctahedral Cobalt(II) Complexes with Positive Axial and Large Rhombic Anisotropy†

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Table of Contents

Figure S1. The powder XPRD pattern of **1**

Figure S2. The powder XPRD pattern of **2**.
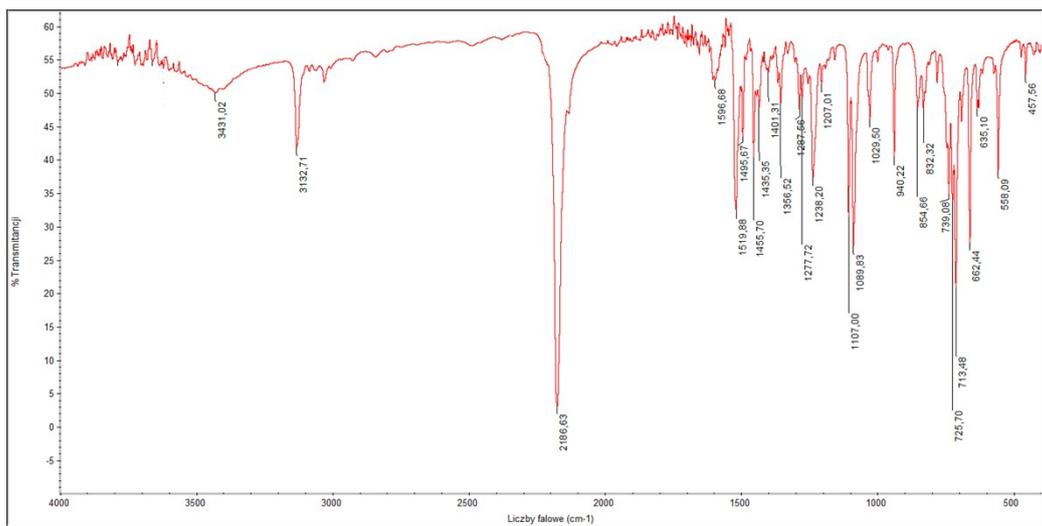
Figure S3. IR spectra of **1**
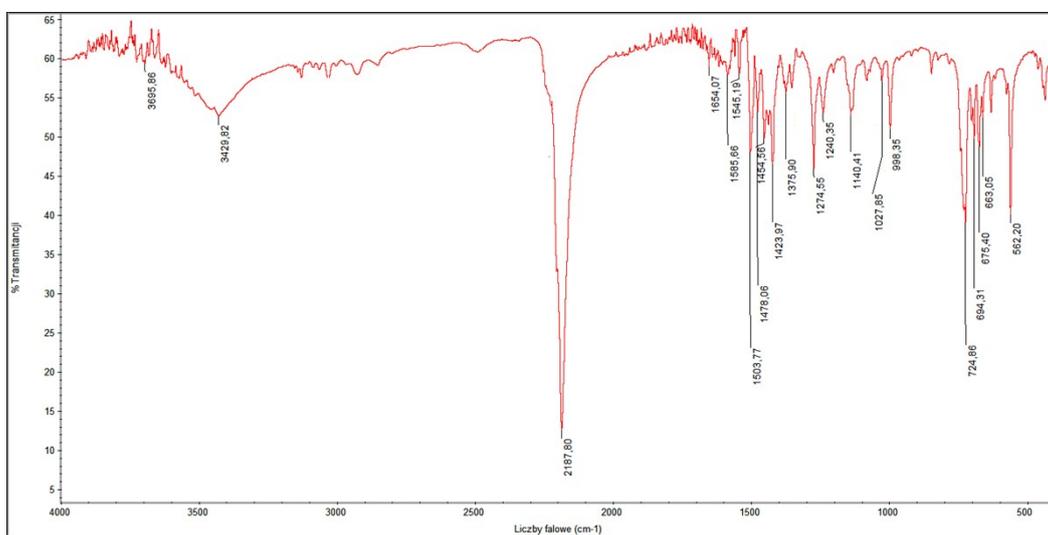
Figure S4. IR spectra of **2**
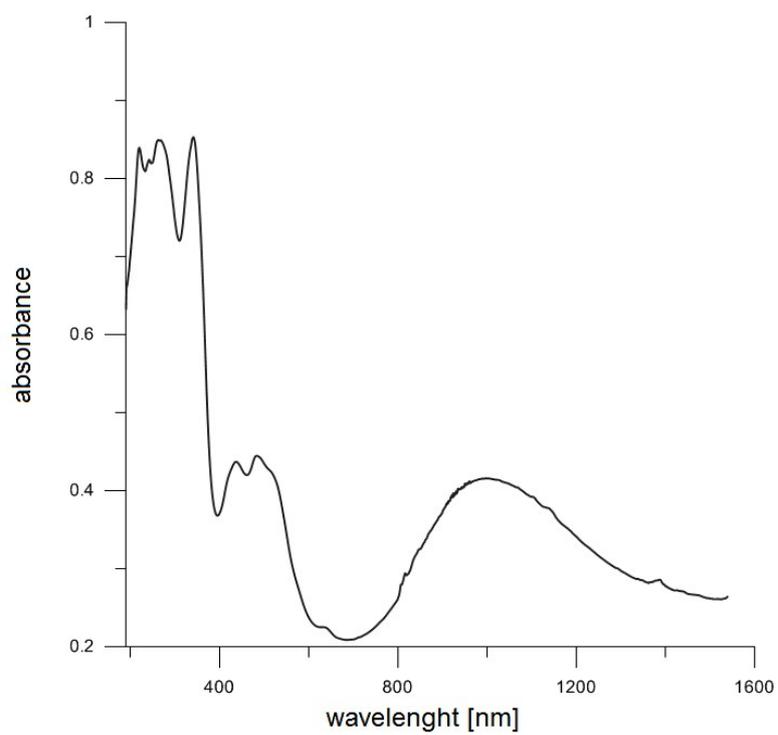
Figure S5. UV-ViS-NIR spectra for **1**
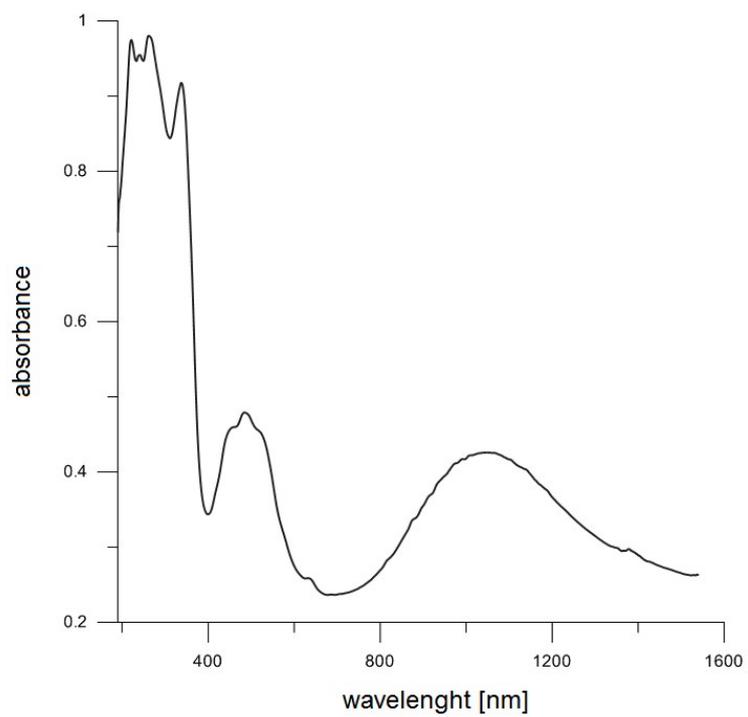
Figure S6. UV-ViS-NIR spectra for **2**
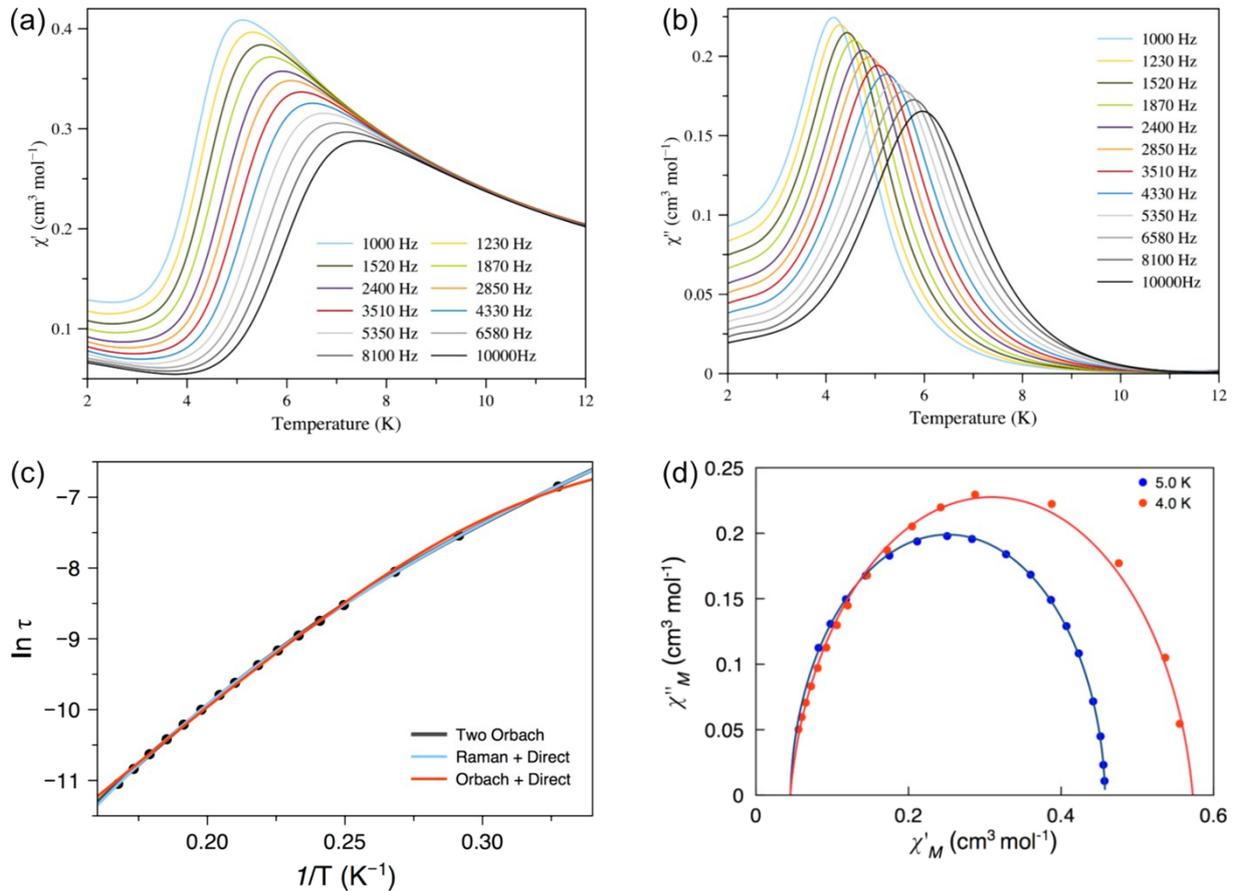
Figure S7. Frequency-dependence of the in-phase (a) and out-of-phase (b) ac susceptibilities for **1** under an applied static field H_{dc} = 1000 G with a ±5.0 G oscillating field at frequencies in the range 1.0-10 kHz. (c) Arrhenius plot (⤫) showing the best fits (solid lines) to three approaches: one with two Orbach processes (black), another one with one Raman plus one direct (blue), and the last one with one Orbach plus direct (red) relaxation processes. (d) Cole-Cole plots at 5.0 and 4.0 K.
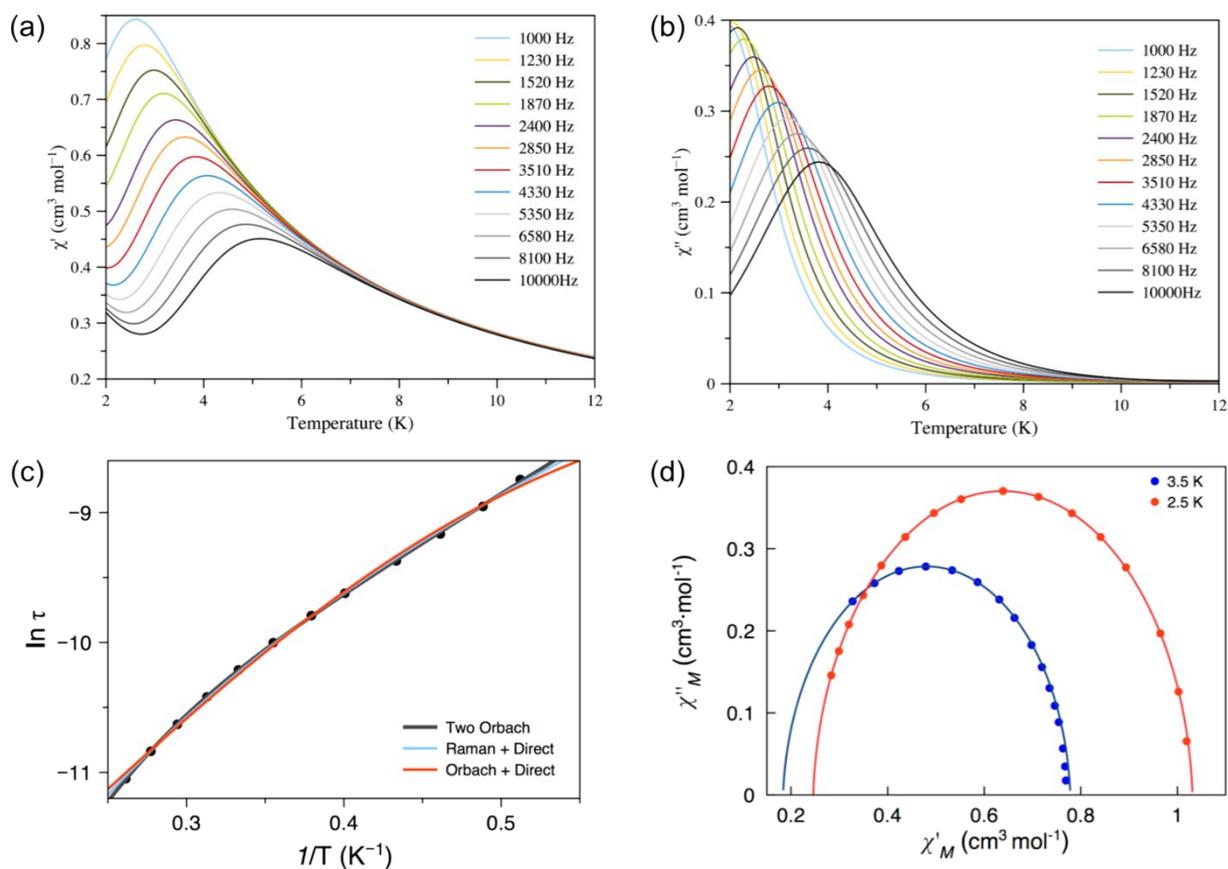
Figure S8. Frequency-dependence of the in-phase (a) and out-of-phase (b) ac susceptibilities for **2** under an applied static field H_{dc} = 1000 G with a ±5.0 G oscillating field at frequencies in the range 1.0-10 kHz. (c) Arrhenius plot (∞) showing the best fits (solid lines) to three approaches: one with two Orbach processes (black), another one with one Raman plus one direct (blue), and the last one with one Orbach plus direct (red) relaxation processes. (d) Cole-Cole plots at 3.5 and 2.5 K.
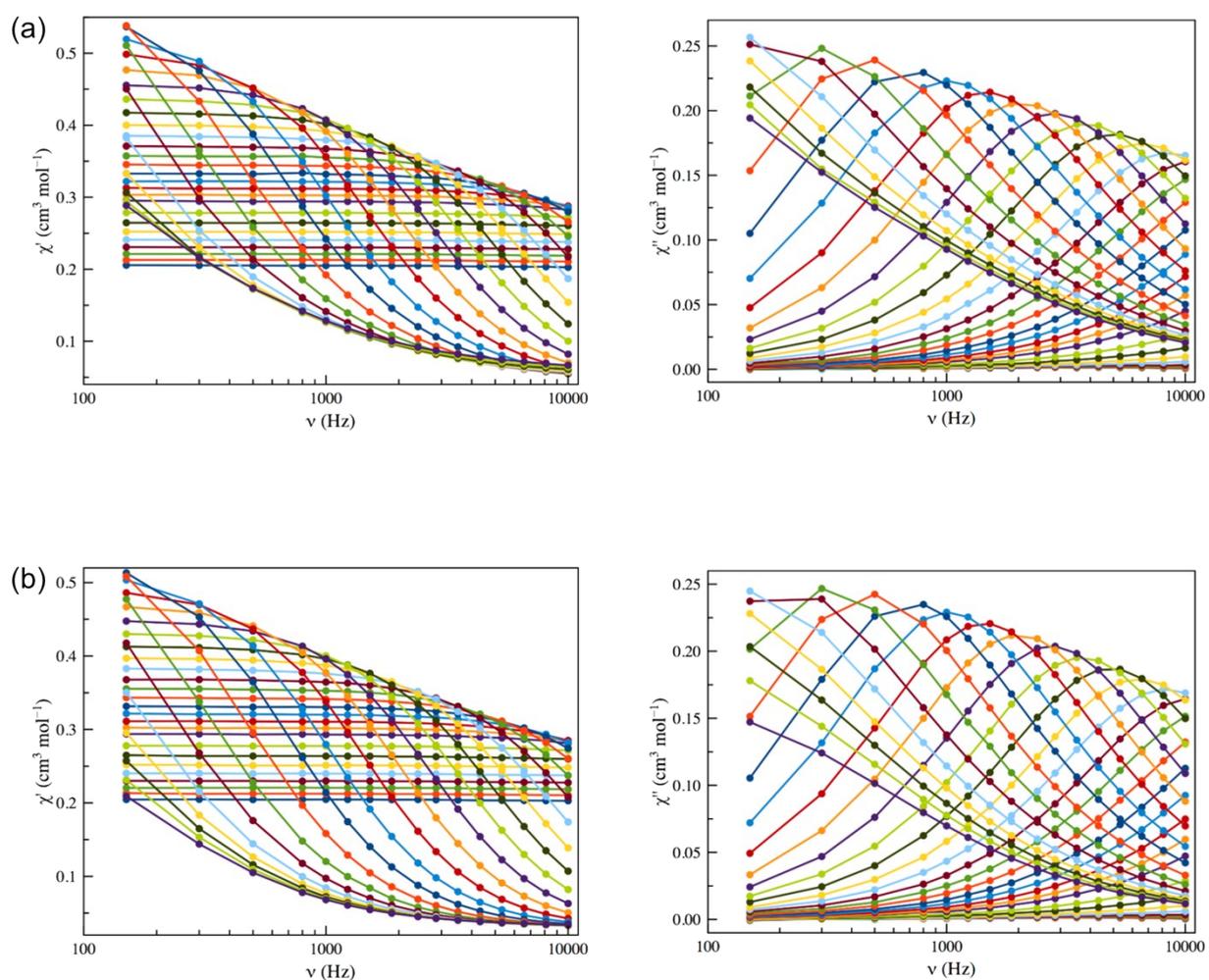
Figure S9. Frequency-dependence of the in-phase (left) and out-of-phase (right) ac susceptibilities for **1** under applied static fields H_{dc} = 1000 (a) and 2500 G (b) with a ±5.0 G oscillating field at temperatures in the range 2.0-12 K. Above and below 8 K, the intervals of the temperature are 0.5 and 0.25 K, respectively.
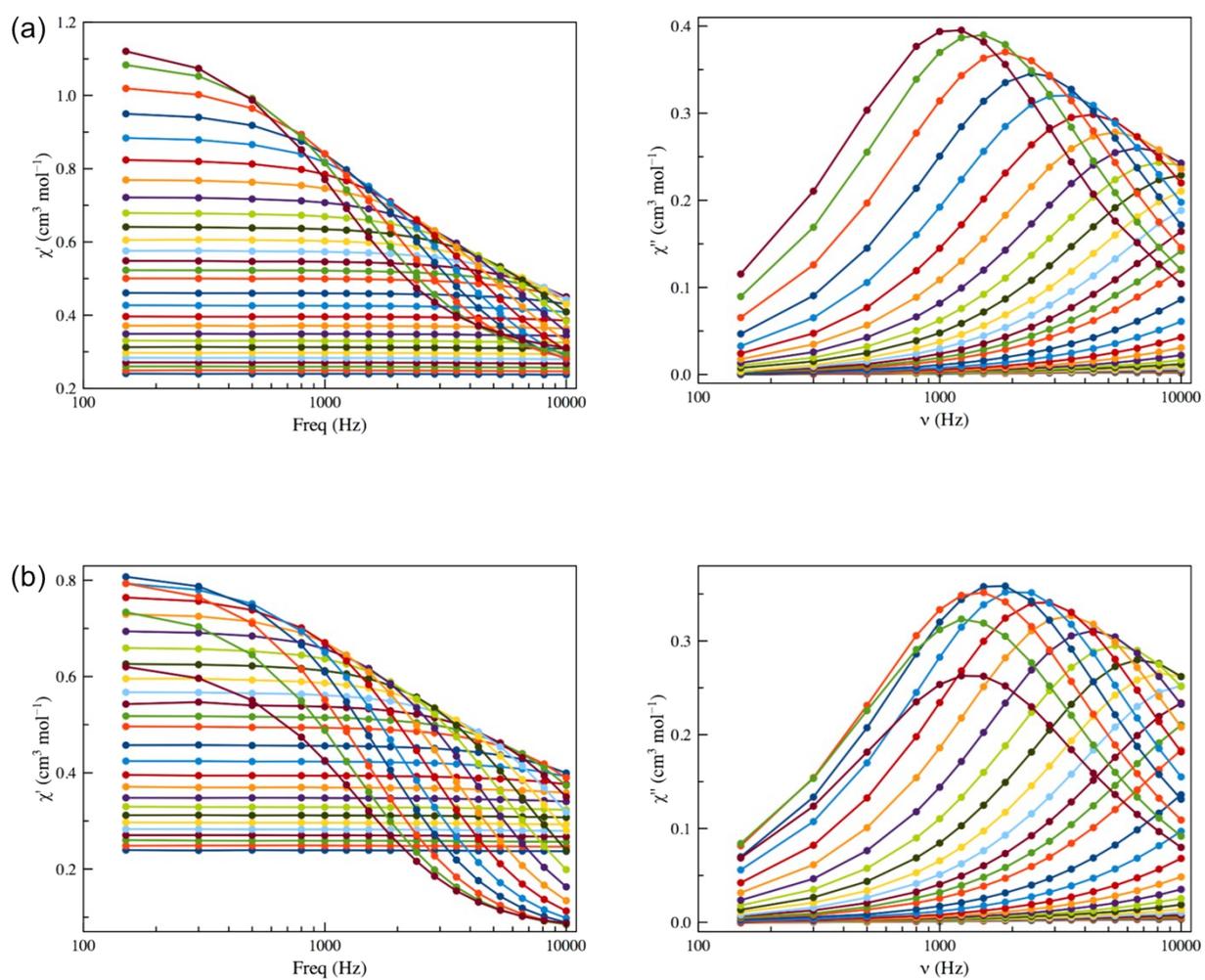
Figure S10. Frequency-dependence of the in-phase (left) and out-of-phase (right) ac susceptibilities for **2** under applied static fields H_{dc} = 1000 (a) and 2500 G (b) with a ±5.0 G oscillating field at temperatures in the range 2.0-12 K. Above and below 5.5 K, the intervals of the temperature are 0.5 and 0.25 K, respectively.

Table S1. Selected magneto-structural parameters for mononuclear six-coordinate cobalt(II) complexes.

Compound	Co–N$_L$ [Å]	U$_{eff}$ [K]	τ [s]	D [cm^{-1}]	E[cm^{-1}]	Ref.
[Co(L^1)$_6$][BPh$_4$]$_2$·0.3CH$_3$CN	Co(1)–N(1)= 2.150; Co(1)–N(1)a= 2.150 Co(1)–N(3)= 2.183; Co(1)–N(3)a= 2.183 Co(1)–N(7)= 2.177; Co(1)–N(7)a= 2.177	21.6	1.5 · 10^{-6}	–	–	1
[Co(L^1)$_6$] [NO$_3$]$_2$	Co(1)–N(1)= 2.162	6.3	4.5 · 10^{-5}	–	–	1
[Co(L^2)(OAc)Y(NO$_3$)$_2$]	Co(1)–N(12)= 2.257(3); Co(1)–N(16)= 2.181(4) Co(1)–N(20)= 2.242(3); Co(1)–O(1)= 2.036(4) Co(1)–O(5)= 2.185(3); Co(1)–O(25)= 2.068(2)	22.58	8.9 · 10^{-7}	–	–	2
[Co(L^3)$_2$(L4)$_2$]	Co(1)–N(1)= 2.209; Co(1)–N(1)a= 2.209 Co(1)–O(1)= 2.001; Co(1)–O(1)= 2.001 Co(1)–O(1)a= 2.001; Co(1)–O(2)= 2.034	–	–	+74	1.21	3
[Co(L^3)$_2$(L5)]	Co(1)–N(1)= 2.110(4); Co(1)–N(2)= 2.115(3) Co(1)–O(1)= 2.071(2); Co(1)–O(2)= 2.012(3) Co(1)–O(3)= 2.069(3); Co(1)–O(4)= 2.065(3)	–	–	+24	−1.89	3
[Co(L^6)$_2$]·2ClO$_4$	Co(1)–N(1)= 2.194(3); Co(1)–N(2)= 2.056(3) Co(1)–N(3)= 2.225(3); Co(1)–N(4)= 2.204(3) Co(1)–N(5)= 2.070(3); Co(1)–N(6)= 2.187(3)	14.8	7.18 · 10^{-7}	61.1	−5.5	4
[Co(L^7)$_2$]·2ClO$_4$	Co(1)–N(1)= 2.169(2); Co(1)–N(2)= 2.059(2) Co(1)–N(3)= 2.174(2); Co(1)–N(4)= 2.160(2) Co(1)–N(5)= 2.066(2); Co(1)–N(6)= 2.147(2)	27.3	2.06 · 10^{-8}	68.1	−5.7	4
[Co(L^7)$_2$]·2ClO$_4$·MeOH	Co(1)–N(1)= 2.201(3); Co(1)–N(2)= 2.060(3) Co(1)–N(3)= 2.160(4); Co(1)–N(4)= 2.166(4) Co(1)–N(5)= 2.051(3); Co(1)–N(6)= 2.182(3)	22.6	3.44 · 10^{-7}	56.4	−10.5	4
[Co(L^8)$_2$]·2ClO$_4$	Co(1)–N(1)= 2.188(3); Co(1)–N(2)= 2.072(3) Co(1)–N(3)= 2.234(3); Co(1)–N(4)= 2.191(3) Co(1)–N(5)= 2.060(3); Co(1)–N(6)= 2.178(3)	30.8	2.07 · 10^{-7}	−66.4	10.2	4
[Co(L^9)$_2$]·2ClO$_4$·MeCN	Co(1)–N(1)= 2.144(5); Co(1)–N(2)= 2.078(5)	20.4	4.95 · 10^{-7}	62.9	−2.4	4

Compound	Bond distances (Å)					
	Co(1)–N(3)= 2.185(5); Co(1)–N(4)= 2.150(5) Co(1)–N(5)= 2.081(4); Co(1)–N(6)= 2.152(5)					
[Co(L¹⁰)₂]·2ClO₄·H₂O	Co(1)–N(1)= 2.195(6); Co(1)–N(2)= 2.064(5) Co(1)–N(3)= 2.172(6); Co(1)–N(4)= 2.179(6) Co(1)–N(5)= 2.055(5); Co(1)–N(6)= 2.176(6)	8.0	$1.67 \cdot 10^{-6}$	74.9	−2.7	4
[Co(L¹¹)₂(H₂O)₂]	Co(1)–O(1)= 2.054; Co(1)–O(1)a= 2.054 Co(1)–O(2)= 2.045; Co(1)–O(2)a= 2.045 Co(1)–O(3)= 2.199; Co(1)–O(3)a= 2.199	14-17	–	57	17	5
[Co(L¹²)₂(tcm)₂]	Co(1)–N(1)= 2.133; Co(1)–N(1)a= 2.133 Co(1)–N(5)= 2.109; Co(1)–N(5)a= 2.109 Co(1)–N(10)=2.125; Co(1)–N(10)a=2.125	86.2	$1.37 \cdot 10^{-9}$	48.2	13	6
[Co(SCN)₂(L¹³)]	Co(1)-N(1)= 2.187; Co(1)-N(1)a= 2.187 Co(1)-N(4)= 2.162; Co(1)-N(4)a= 2.162 Co(1)-N(7)= 2.092; Co(1)-N(7)a= 2.092	89	$2.3 \cdot 10^{-10}$	–	–	7
[Co(L¹⁴)₂]	Co(1)-N(2)= 2.146; Co(1)-N(2)a= 2.146 Co(1)-N(4)= 2.151; Co(1)-N(4)a= 2.151 Co(1)-N(6)= 2.133; Co(1)-N(6)a= 2.133	38.59	$1.44 \cdot 10^{-7}$	–	36.8	8
α-[Co(L¹⁵)(PhCOO)₂]	Co(1)-N(1)= 2.116(2); Co(1)-N(2)= 2.097(2) Co(1)-O(1)= 2.048(2); Co(1)-O(2)= 2.313(2) Co(1)-O(3)= 2.085(2); Co(1)-O(4)= 2.215(2)	22.1	$6.51 \cdot 10^{-7}$	–	–	9
β-[Co(L¹⁵)(PhCOO)₂]	Co(1)-N(1)= 2.116(2); Co(1)-N(2)= 2.097(2) Co(1)-O(1)= 2.048(2); Co(1)-O(2)= 2.313(2) Co(1)-O(3)= 2.085(2); Co(1)-O(4)= 2.215(2)	17.1	$8.52 \cdot 10^{-7}$	+58.7	–	9
[Co(L¹⁶)₃(BC₆H₅)]Cl	Co(1)-N(1)= 1.928(2); Co(1)-N(2)= 1.919(2) Co(1)-N(3)= 2.071(2); Co(1)-N(4)= 2.023(2) Co(1)-N(5)= 1.975(2); Co(1)-N(6)= 2.031(1)	102	–	large negative value of D	–	10
[Co(L¹⁷)₂(L¹⁸)₂]	–	-	–	+24.17	6.90	11
[Co(L¹⁹)₂][Co(NCO)₄]·2H₂O	Co(1)-N(1)= 1.877(3); Co(1)-N(3)= 2.011(3) Co(1)-N(5)= 1.997(3) ; Co(1)-N(7)= 1.922(3) Co(1)-N(9)= 2.123(3);Co(1)-N(11)= 2.102(3)	11.7	$2.2 \cdot 10^{-9}$	4.30(3)	–	12

Et$_4$N[Co(L^{20})$_3$]	Co(1)-O(1)= 2.077(2); Co(1)-O(2)= 2.078(2) Co(1)-O(3)= 2.053(1); Co(1)-O(4)= 2.084(2) Co(1)-O(5)= 2.077(2); Co(1)-O(6)= 2.047(1)	20.6(5)	6.4(9) ·10^{-7}	+117.8	–	13
[Co(L^{21})$_2$(NCS)$_2$]	Co(1)-N(1)= 2.041(4); Co(1)-N(2)= 2.038(3) Co(1)-N(3)= 2.188(3); Co(1)-N(4)= 2.275(4) Co(1)-N(5)= 2.255(3); Co(1)-N(6)= 2.194(3)	17	(3.0−4.4) · 10^{-7}	+98	+8.4	14
[Co(oda)(L^{22})]	Co(1)-N(2)= 2.152(5); Co(1)-N(4)= 2.040(6) Co(1)-N(5)= 2.137(6); Co(1)-O(1)= 2.086(6) Co(1)-O(2)= 2.077(5); Co(1)-O(5)= 2.060(6)	4.2	2.5 · 10^{-5}	−7.44	–	15
[Co(L^{23})$_2$]$_2$[Co(NCS)$_4$] ·dmso·H$_2$O	Co(1)-N(1)= 1.929(7); Co(1)-N(2)= 1.888(5) Co(1)-N(3)= 1.943(8); Co(1)-N(6)= 1.947(5) Co(1)-N(7)= 1.908(5); Co(1)-N(8)= 1.942(5) Co(2)-N(11)= 1.921(8); Co(2)-N(12)= 1.903(5) Co(2)-N(13)= 1.956(7); Co(2)-N(16)= 1.931(5) Co(2)-N(17)= 1.897(5); Co(2)-N(18)= 1.927(5)	–	–	34.7	–	16
[Co(L^{24})$_4$Cl$_2$]	–	–	–	+106	–	17
[Co(L^{24})$_4$(SCN)$_2$]	–	27.7	1.16 · 10^{-6}	+90.5	–	17
[Co(L^{25})$_2$(py)$_2$(H$_2$O)$_2$] (polymorph 1)	Co(1)-N(1)= 2.151; Co(1)-N(2)= 2.130 Co(1)-O(1)= 2.109; Co(1)-O(1)= 2.109 Co(1)-O(1w)= 2.098; Co(1)-O(1w)= 2.098	∼20	1.37 · 10^{-7}	+91.5	–	18
[Co(L^{25})$_2$(py)$_2$(H$_2$O)$_2$] (polymorph 2)	Co(1)-N(1)= 2.151; Co(1)-N(2)= 2.151 Co(1)-O(1)= 2.136; Co(1)-O(1)= 2.136 Co(1)-O(1w)= 2.082; Co(1)-O(1w)= 2.082	∼20	3.4 · 10^{-8}	+117.4	–	18
[Co(L^{26})$_2$]	Co(1)-N(1)=2.070(3); Co(1)-N(1)a=2.070(3) Co(1)-N(3)= 2.159(3); Co(1)-N(3)a= 2.159(3) Co(1)-O(1)= 2.071(2); Co(1)-O(1)a= 2.071(2)	–	–	36.7	2.0	19
[Co(L^{27})$_2$L^{28}]·CH$_3$CN	Co(1)-O(1)= 2.061(4); Co(1)-O(2)= 2.061(4) Co(1)-O(3)= 2.061(4); Co(1)-O(4)= 2.043(4) Co(1)-N(6)= 2.255(4); Co(1)-N(7)= 2.083(4)	–	–	2.7	–	20

[Co(L²⁹)₂(H₂O)₂](tcap)₂	Co(1)-N(10)= 2.081; Co(1)-N(10)= 2.081 Co(1)-N(50)= 2.166; Co(1)-N(50)= 2.166 Co(1)-O(1)= 2.102; Co(1)-O(1)= 2.102	44.1	$1.04 \cdot 10^{-7}$	36.6	–	21
[Co(L²⁹)₂(H₂O)₂](nodcm)₂	Co(1)-N(10)= 2.112; Co(1)-N(10)= 2.112 Co(1)-N(50)= 2.146; Co(1)-N(50)= 2.146 Co(1)-O(1)= 2.118; Co(1)-O(1)= 2.118	12.3	$2.96 \cdot 10^{-5}$	39.8	–	21
[Co(L²⁹)₂(CH3OH)₂](pcp)₂	Co(1)-N(10)= 2.058; Co(1)-N(10)= 2.058 Co(1)-N(50)= 2.151; Co(1)-N(50)= 2.151 Co(1)-O(1)= 2.108; Co(1)-O(1)= 2.108	–	–	36.8	–	21
[Co(L²⁹)₂(nca)₂]	Co(1)-N(10)= 2.086; Co(1)-N(10)= 2.086 Co(1)-N(50)= 2.144; Co(1)-N(50)= 2.144 Co(1)-N(1)= 2.121; Co(1)-N(1)= 2.121	12.0	$2.19 \cdot 10^{-5}$	40.0	–	21
[Co(L²⁹)₂(NCSe)₂]	Co(1)-N(10)= 2.085; Co(1)-N(10)= 2.085 Co(1)-N(50)= 2.165; Co(1)-N(50)= 2.165 Co(1)-N(1)= 2.121; Co(1)-N(1)= 2.121	17.0	$7.76 \cdot 10^{-6}$	38.2	–	21
[Co(L²⁹)₂(ndcm)₂]	Co(1)-N(10)= 2.103; Co(1)-N(10)= 2.103 Co(1)-N(50)= 2.142; Co(1)-N(50)= 2.142 Co(1)-O(1)= 2.092; Co(1)-O(1)= 2.092	28.5	$1.63 \cdot 10^{-6}$	−69.7	–	21
[Co(L³⁰)₂]	Co(1)-N(1)= 2.036(2); Co(1)-N(2)= 2.040(2) Co(1)-O(1)= 2.146(1); Co(1)-O(2)= 2.078(1) Co(1)-O(3)= 2.185(1); Co(1)-O(4)= 2.158(1)	44.1(8)	$2.8(4) \cdot 10^{-9}$	–	–	22
[Co(L³¹)₃][CoBr₄]	Co(1)-O(1)= 2.081(3); Co(1)-O(2)= 2.125(3) Co(1)-O(3)= 2.103(3); Co(1)-O(4)= 2.093(3) Co(1)-O(5)= 2.102(3); Co(1)-O(6)= 2.101(3)	–	–	129	3	23
[Co(L³²)₂][ClO₄]₂	Co(1)-N(2)= 2.112(3); Co(1)-N(2)a= 2.112(3) Co(1)-N(2)= 2.107(3); Co(1)-N(2)a= 2.107(3) Co(1)-N(2)= 2.107(3); Co(1)-N(2)a= 2.107(3)	30.6(1)	$2.0(2)–3.3(7) \cdot 10^{-7}$	–	–	24
[Co(L³²)₂][BPh₄]₂·2MeCN	Co(1)-N(2)= 2.110(1); Co(1)-N(2)a= 2.110(1) Co(1)-N(2)= 2.104(1); Co(1)-N(2)a= 2.104(1) Co(1)-N(2)= 2.101(1); Co(1)-N(2)a= 2.101(1)	44.7(6)	$1.0(1)–1.5(2) \cdot 10^{-7}$	–	–	24

L¹= imidazole, **L²** =N,O Schiff base ligand, **L⁴**= pyridine, **L⁵**= 2,2'-bypiridine; **L⁶**=2,6-bis(oxazo-1-yl)pyridine, **L⁷** =2,6-bis(1,1'-dimetyhyloxazo-1-yl)pyridine; **L⁸**= 4-methylphenyl-2,6–bis(oxazo-1-yl)pyridine; **L⁹** =4-methylphenyl-2,6-bis(1,1'-dimetyhyloxazo-1-yl)pyridine; **L¹⁰** =4-pyridine-2,6-bis(1,1'-dimetyhyloxazo-1-yl)pyridine; **L¹¹**= acetylacetonate; **L¹²**= 4-amino- 3,5-bis(2-pyridyl)-1,2,4-triazole; **L¹³**=4-(α-diazobenzyl)pyridine; **L¹⁴**= bis-hydridotris(3,5-dimethylpyrazole; **L¹⁵**= neocuproine; **L¹⁶**= pyrazoloxime ;**L¹⁷** =1,1,1,5,5,5-hexafluoro-2,4-pentanedione; **L¹⁸**=4-methylpyridine; **L¹⁹**= 2,3,5,6-tetrakis-(2-pyridyl)pyrazine; L²⁰= hexafluoroacetylacetonate; **L²¹**= 2,9-dimethyl-1,10-phenanthroline; **L²²**= 4'-azido-2,2':6',2''-terpyridine; **L²³**=bis(2-pyrimidylcarbonyl)amide; **L²⁴**=4-benzylpyridine; **L²⁵**=3,5-dinitrobenzoic acid; **L²⁶**=o-[(1H-imidazol-2-yl)methylideneamino]phenol; **L²⁷**= hexafluoroacetylacetonate; **L²⁸**= O-donor ditopic ligand; **L²⁹**= 4-amino-3,5-bis(2-pyridyl)-1,2,4-triazole; **L³⁰**= 2,6-pyridinedimethanol; **L³¹** =bis(diphenylphosphanoxido)methane; **L³²**= tris(pyrazol-1-yl)methane

L³=
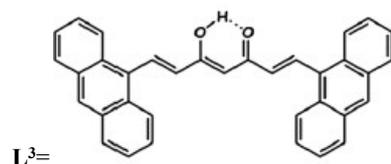
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Table S2. Energy of all calculated excited states and their contributions to the D and E values for the optimized geometries **1** and **2** obtained from CASSCF/NEVPT2 calculations.

	Compound **1**				Compound **2**		
Energy[a]	S	D[a]	E[a]	Energy[a]	S	D[a]	E[a]
961.4	4	30.143	30.025	254.2	4	52.644	52.644
1804.9	4	16.015	-16.104	874.7	4	36.415	-36.420
10590.8	4	3.998	-2.882	9493.7	4	4.934	-5.254
11068.6	4	2.844	2.809	9859.4	4	0.054	0.030
11477.2	4	0.147	-0.080	11623.6	4	-9.353	-0.030
22446.0	4	0.001	-0.001	21575.6	4	0.001	0.001
23584.2	4	0.071	0.014	22742.5	4	0.084	0.084
24042.9	4	0.074	-0.036	24357.5	4	0.004	-0.003
25950.5	4	0.005	0.004	24526.5	4	0.048	-0.049
9321.5	2	10.813	0.355	8366.2	2	-6.136	-6.136
10438.5	2	0.572	-0.147	10721.8	2	2.906	0.097
19031.8	2	-0.022	-0.016	17403.7	2	0.006	-0.000
19721.4	2	-0.658	-0.441	18945.8	2	-0.009	-0.009
19923.5	2	-0.507	-0.460	19492.6	2	-1.134	1.134
19981.6	2	-0.269	-0.006	19558.0	2	-1.249	-1.249
20246.6	2	-0.481	0.497	20151.2	2	-0.002	-0.002
20657.6	2	-0.341	0.350	20431.3	2	0.002	0.000
22774.0	2	-0.021	-0.008	22726.2	2	-0.230	0.239
23836.9	2	3.388	0.003	22984.8	2	2.348	0.004
23869.0	2	-0.098	-0.079	23172.2	2	-0.047	-0.047
28080.1	2	-0.109	0.102	27229.5	2	-0.000	-0.000
30361.8	2	-0.170	0.231	29510.2	2	-0.000	0.010
30884.3	2	-0.102	-0.102	30121.4	2	-0.004	-0.004
31201.8	2	0.000	-0.001	31253.2	2	0.479	0.000

32528.6	2	-0.324	0.233	31659.2	2	-0.665	0.667
32745.3	2	-0.442	-0.384	31911.7	2	-0.003	0.003
33244.1	2	-0.015	-0.014	32719.1	2	-0.493	-0.493
33763.4	2	1.893	0.063	33611.6	2	0.967	0.019
34970.2	2	-0.038	-0.014	33779.1	2	-0.836	-0.839
36926.8	2	0.022	0.155	36015.0	2	1.412	0.006
37142.4	2	-0.324	-0.314	36775.9	2	-0.404	0.423
37590.5	2	-0.038	0.062	36842.4	2	-0.003	-0.003
39650.3	2	-0.172	-0.052	38823.8	2	-0.090	-0.090
39857.0	2	-0.206	0.123	39387.2	2	-0.000	-0.000
40244.7	2	0.026	-0.001	39550.9	2	-0.000	0.000
40500.1	2	0.002	0.002	39668.0	2	-0.006	0.009
40729.8	2	0.087	0.047	39745.4	2	-0.228	-0.228
44267.1	2	-0.028	0.008	43772.9	2	-0.114	0.122
44738.3	2	-0.037	0.018	43852.1	2	-0.003	0.001
45092.9	2	-0.020	-0.031	44999.0	2	0.189	0.001
47933.3	2	-0.070	-0.051	47101.3	2	-0.061	-0.061
48191.0	2	-0.062	0.055	47542.9	2	-0.000	-0.000
48447.2	2	-0.011	-0.002	47761.6	2	-0.063	0.063
48556.2	2	-0.001	0.000	47780.5	2	-0.001	-0.001
66480.1	2	-0.000	-0.003	65771.4	2	0.045	0.002
67358.4	2	0.009	-0.000	66864.7	2	-0.000	-0.000
67949.0	2	0.016	0.001	67031.8	2	-0.001	0.001
68039.6	2	0.014	0.000	67366.1	2	0.003	0.000
68427.2	2	0.137	0.004	67615.4	2	-0.084	-0.084

[a]Values in cm^{-1}.

Table S3. Energies of the low-lying Kramers doublets corresponding to the ground and first excited states, which should be related to those generated from a 1st order spin-orbit coupling, for the optimized geometries **1** and **2** obtained from CASSCF/NEVPT2 calculations.

Compound **1**		Compound **2**	
Kramers doublet	Energy[a]	Kramers doublet	Energy[a]
Ground	0.0	Ground	0.0
1st	136.1	1st	205.8
2nd	1048.8	2nd	534.7
3rd	1266.9	3rd	842.7
4th	2035.4	4th	1315.1
5th	2122.2	5th	1411.2

[a]Values in cm^{-1}.

Table S4. Selected ac magnetic data at different applied dc fields for **1** and **2**.

Compound	H_{dc}[a]	τ_{01}[b] x 10^8 (s) τ_{02} x 10^6 (s)	E_{a1}[b] (cm^{-1}) E_{a2} (cm^{-1})	A[c] (s^{-1} K^{-1})	B[c] (s^{-1} K^{-n})	n[c]
Two Orbach model						
1	1000	2.41 5.01	27.9 11.6			
	2500	2.49 5.56	27.8 11.3			
2	1000	2.89 3.36	19.7 5.2			
	2500	0.0007 1.0	51.1 8.9			
Raman + Direct model						
1	1000			22.1	0.68	6.40
	2500			31.3	0.69	6.38
2	1000			-3500.0	829.4	3.22
	2500			-2600.2	721.8	3.12
Orbach + Direct model						
1	1000	7.6	22.5	216.3		
	2500	7.8	22.5	223.3		
2	1000	80	8.5	2128.4		
	2500	61	10.2	703.7		

[a]Applied dc field in G. [b]The values of the pre-exponential factor (τ_0) and activation energy (E_a) are calculated through the Arrhenius law (see text). [c]The values of the coefficients of direct (A) and Raman (B and n) processes for the relaxation of the magnetization (see text).

Table S5. Main parameters extracted from the Cole-Cole plots for **1** and **2**.

Compound	H_{dc}[a]	α[b]	χ_S[b] (cm^3 mol^{-1})	χ_T[b] (cm^3 mol^{-1})	τ[b] x 10^5 (s)
1	1000	0.093 (4 K) 0.023 (5 K)	0.573 (4 K) 0.458 (5 K)	0.045 (4 K) 0.045 (5 K)	22.0 (4 K) 7.1 (5 K)
	2500	0.071 (4 K) 0.019 (5 K)	0.555 (4 K) 0.450 (5 K)	0.026 (4 K) 0.029 (5 K)	22.6 (4 K) 7.6 (5 K)

2	1000	0.038 (2.5 K)	1.032 (2.5 K)	0.246 (2.5 K)	3.9 (2.5 K)
		0.042 (3.5 K)	0.778 (3.5 K)	0.183 (3.5 K)	1.9 (3.5 K)
	2500	0.032 (2.5 K)	0.807 (2.5 K)	0.066 (2.5 K)	8.6 (2.5 K)
		0.032 (3.5 K)	0.738 (3.5 K)	0.051 (3.5 K)	4.2 (3.5 K)

[a]Applied dc field in G. [b]The values of the α parameter, adiabatic (χ_S) and isothermal (χ_T) susceptibilities, and relaxation time are calculated from the experimental data at different temperatures through the generalized Debye law (see text).

Table S6. XYZ coordinates (in angstroms) for the optimized molecular geometry of **1** using a PBE functional.

Atom	x	y	z
Co	-0.001954	0.002460	0.000675
N	-0.014889	-2.142142	-0.159297
N	0.011460	2.146873	0.160226
N	-0.299229	-4.213548	-0.963953
N	0.299442	4.218338	0.963428
N	-2.110150	-0.102301	0.313897
N	2.106295	0.106894	-0.312170
N	-4.321655	-0.017105	-0.019946
N	4.317653	0.017460	0.021374
N	0.369752	-0.149761	2.004394
N	-0.373313	0.153952	-2.003147
N	-3.445592	-2.336942	-3.680244
N	3.443025	2.340140	3.679781
N	1.181110	-0.502317	6.545962
N	-1.183798	0.507019	-6.544663
C	0.087702	-3.054315	0.899493
C	-0.094042	3.058819	-0.898474
C	-0.091331	-4.343595	0.412871
C	0.087253	4.348122	-0.412759
C	-0.244997	-2.871667	-1.269829
C	0.245520	2.876570	1.269823
C	-0.572129	-5.310721	-1.922301
C	0.576560	5.315636	1.920422
C	-1.857681	-6.062672	-1.616270
C	1.863157	6.064558	1.611271
C	-1.812103	-7.329286	-0.985560
C	1.819200	7.330421	0.978951
C	-3.003194	-8.018704	-0.673962
C	3.011228	8.016885	0.664446
C	-4.251788	-7.443287	-0.990080
C	4.259139	7.439212	0.979168
C	-4.303167	-6.182583	-1.624503
C	4.308919	6.179236	1.615162
C	-3.114499	-5.493158	-1.940323
C	3.119312	5.492804	1.933967
C	-2.749383	-0.721996	1.394044
C	2.746379	0.728900	-1.390462
C	-4.124253	-0.677074	1.198520
C	4.121194	0.681353	-1.195134
C	-3.082574	0.317150	-0.519901
C	3.078095	-0.316490	0.520350
C	-5.623432	0.296533	-0.653646
C	5.618938	-0.300080	0.654061
C	-6.560593	-0.897211	-0.738843
C	6.558332	0.891722	0.742081

C	-7.700878	-0.964617	0.097616
C	7.700814	0.957063	-0.091526
C	-8.582972	-2.063824	0.023024
C	8.585153	2.054284	-0.014170
C	-8.331170	-3.106043	-0.893339
C	8.333353	3.096605	0.902070
C	-7.195319	-3.044194	-1.730710
C	7.195259	3.036854	1.736553
C	-6.310085	-1.949146	-1.655634
C	6.307844	1.943765	1.658757
C	0.905684	0.100741	3.049204
C	-0.909182	-0.096605	-3.047976
C	1.635281	0.514093	4.176108
C	-1.638258	-0.510094	-4.175156
C	2.630076	1.506888	3.953620
C	-2.632749	-1.503343	-3.953316
C	1.390753	-0.035271	5.468457
C	-1.393572	0.039680	-5.467311
H	0.274379	-2.717355	1.923065
H	-0.284189	2.721713	-1.921357
H	-0.106221	-5.316220	0.914042
H	0.100935	5.320614	-0.914226
H	-0.376557	-2.484899	-2.284066
H	0.380223	2.490045	2.283736
H	-0.835772	-7.785272	-0.744241
H	0.843441	7.788159	0.738641
H	-2.954945	-9.005984	-0.186359
H	2.964261	9.003627	0.175631
H	-5.183893	-7.978887	-0.746873
H	5.191953	7.972524	0.733661
H	-5.275448	-5.729867	-1.878019
H	5.280662	5.724724	1.867562
H	-3.171588	-4.514222	-2.451024
H	3.175114	4.514523	2.446057
H	-2.179023	-1.152529	2.221887
H	2.176604	1.162826	-2.216945
H	-4.960062	-1.063874	1.789106
H	4.957568	1.068668	-1.784575
H	-2.935367	0.841986	-1.468366
H	2.930025	-0.843990	1.467207
H	-7.906162	-0.143992	0.807149
H	7.905981	0.136405	-0.801049
H	-9.468815	-2.102490	0.677595
H	9.472692	2.091324	-0.666534
H	-9.021487	-3.962858	-0.958681
H	9.025352	3.951897	0.969533
H	-6.998698	-3.848379	-2.458713
H	6.998549	3.841095	2.464467
H	-5.425518	-1.924220	-2.318270
H	5.421589	1.920564	2.319185

H	-6.107824	1.119426	-0.080718
H	6.101801	-1.122460	0.079109
H	-5.389316	0.685229	-1.668121
H	5.384240	-0.690886	1.667617
H	0.295606	-6.006946	-1.912892
H	-0.289728	6.013664	1.912137
H	-0.620664	-4.842040	-2.928108
H	0.626095	4.847647	2.926500

Table S7. XYZ coordinates (in angstroms) for the optimized molecular geometry of **2** using a PBE functional.

Atom	x	y	z
Co	-0.027665	0.025877	-0.005288
N	-2.216215	-0.037112	-0.007247
N	-0.064170	2.213834	0.002011
N	-4.411451	0.113908	-0.426806
N	-0.313796	4.398562	0.429966
N	0.007658	-2.166614	0.005643
N	2.166106	0.090320	-0.018833
N	0.271995	-4.348619	0.440373
N	4.357658	-0.069445	-0.456181
N	-0.016104	0.030761	1.992978
N	-0.035077	0.017844	-2.003540
N	-2.434232	0.706864	-5.673721
N	-0.809661	2.384174	5.671807
N	1.579253	-1.613093	5.829040
N	1.662046	-1.506821	-5.845379
C	-2.903683	-0.886205	0.871202
C	0.750054	2.942325	-0.876246
C	-4.264401	-0.802316	0.623264
C	0.605015	4.296930	-0.623216
C	-3.147303	0.570145	-0.786147
C	-0.711085	3.113645	0.785934
C	-2.924475	1.581369	-1.860122
C	-1.707210	2.842292	1.863031
C	-5.685434	0.558020	-1.006143
C	-0.806503	5.648591	1.021719
C	-6.189654	1.896878	-0.472268
C	-2.164148	6.108363	0.495004
C	-5.821338	2.372220	0.808297
C	-2.633481	5.728319	-0.784282
C	-6.334950	3.594453	1.291749
C	-3.873825	6.204157	-1.260564
C	-7.226732	4.351593	0.503443
C	-4.655670	7.068598	-0.465986
C	-7.598738	3.883361	-0.775041
C	-4.193819	7.451518	0.811649
C	-7.079000	2.666062	-1.261402
C	-2.958033	6.970089	1.290520
C	-0.813892	-2.902992	-0.859230
C	2.863700	0.944428	0.846818
C	-0.659335	-4.255742	-0.602305
C	4.221990	0.854715	0.588187
C	0.666820	-3.059967	0.786607
C	3.088833	-0.524209	-0.801817
C	1.669799	-2.776684	1.854412
C	2.851867	-1.538949	-1.869642

C	0.778905	-5.594954	1.027604
C	5.626688	-0.524032	-1.038141
C	2.130613	-6.050840	0.482466
C	6.129167	-1.859708	-0.494702
C	2.580734	-5.671385	-0.803864
C	5.769468	-2.319920	0.793811
C	3.815411	-6.145028	-1.296782
C	6.282899	-3.538714	1.286056
C	4.610534	-7.006219	-0.511918
C	7.165374	-4.307484	0.498523
C	4.167792	-7.388457	0.772659
C	7.528576	-3.854390	-0.787894
C	2.937617	-6.909523	1.267984
C	7.009313	-2.640394	-1.282826
C	0.106224	0.130278	3.182220
C	-0.133590	-0.109323	-3.192366
C	0.253557	0.260808	4.567632
C	-0.262663	-0.262870	-4.577208
C	0.974789	-0.740622	5.281369
C	0.766417	-0.940370	-5.294481
C	-0.318535	1.399727	5.206152
C	-1.427758	0.258970	-5.211585
H	-2.368271	-1.488237	1.610537
H	1.374237	2.437057	-1.618419
H	-5.124795	-1.299075	1.082499
H	1.061310	5.180442	-1.080538
H	-5.122509	1.788050	1.430196
H	-2.029986	5.050627	-1.411091
H	-6.033750	3.956358	2.288150
H	-4.230408	5.894742	-2.256370
H	-7.625945	5.306169	0.882168
H	-5.624122	7.438488	-0.839323
H	-8.290548	4.470786	-1.400550
H	-4.800363	8.122091	1.442038
H	-7.365308	2.310946	-2.266592
H	-2.607413	7.264924	2.294825
H	-1.452077	-2.407177	-1.595942
H	2.339431	1.556506	1.585963
H	-1.115706	-5.142900	-1.052394
H	5.087232	1.351383	1.038284
H	1.966526	-4.996981	-1.423794
H	5.078542	-1.726527	1.415833
H	4.156362	-5.836982	-2.298439
H	5.989336	-3.888067	2.289162
H	5.574353	-7.374578	-0.898479
H	7.564599	-5.259210	0.884284
H	4.784812	-8.056681	1.395318
H	8.213158	-4.450981	-1.412677
H	2.601739	-7.204436	2.277334
H	7.289326	-2.296885	-2.293849

H	1.275523	-2.981456	2.878510
H	3.043079	-1.137224	-2.893415
H	2.590057	-3.390444	1.719052
H	3.504078	-2.431958	-1.731286
H	1.950785	-1.707371	1.814773
H	1.795354	-1.864978	-1.832844
H	0.839291	-5.467603	2.131037
H	5.509510	-0.584297	-2.142684
H	0.006404	-6.376438	0.842669
H	6.375939	0.277593	-0.844041
H	-3.148247	1.181718	-2.878524
H	-1.312703	3.077802	2.880833
H	-3.562997	2.481702	-1.704394
H	-2.634783	3.442441	1.714772
H	-1.863574	1.895505	-1.847705
H	-1.976221	1.769119	1.847072
H	-5.573923	0.608214	-2.111794
H	-0.851083	5.523626	2.126185
H	-6.430682	-0.244502	-0.800755
H	-0.033494	6.426364	0.823811