Supporting Information

Ligand Radicals as Modular Organic Electron Spin Qubits

Jake McGuire,[†] *Haralampos N. Miras*,[†] *James P. Donahue*,[‡] *Emma Richards*,[§] *and Stephen Sproules*[†,*]

[†]WestCHEM, School of Chemistry, University of Glasgow, Glasgow G12 8QQ, United Kingdom

[‡]Department of Chemistry, Tulane University, 6400 Freret Street, New Orleans, Louisiana 70118, United States

[§]School of Chemistry, Cardiff University, Main Building, Park Place, Cardiff CF10 3AT, United Kingdom

Table S1. Crystallographic Data

compound	$PPh_4[Ni(adt)_2]$	$PPh_4[Pd(adt)_2]$	$PPh_4[Pt(adt)_2]\cdot CH_2Cl_2\cdot 2H_2O$
formula	$C_{56}H_{48}O_4PS_4Ni$	$C_{56}H_{48}O_4PS_4Pd$	$C_{57}H_{54}O_6PS_4Pt$
fw	1002.86	1050.55	1260.20
T, K	150(2)	150(2)	150(2)
λ, Å	0.71073	0.71073	0.71073
2θ range, deg	2.72 – 52.88	1.64 –52.74	1.62 – 52.98
crystal system	triclinic	triclinic	triclinic
space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$
a, Å	11.935(5)	14.424(5)	13.832(3)
b, Å	13.947(6)	15.323(6)	15.761(4)
c, Å	15.696(7)	25.029(9)	16.441(4)
α, deg	82.077(5)	86.403(5)	71.074(3)
β, deg	73.662(5)	89.534(5)	83.128(3)
γ, deg	79.995(5)	64.752(4)	80.342(3)
V, Å^3	2458(2)	4992(3)	3334(1)
Z	2	4	2
ρ, g cm^{-3}	1.355	1.398	1.255
μ, mm^{-1}	0.644	0.617	2.374
crystal size	0.08 × 0.10 × 0.20	0.15 × 0.17 × 0.18	0.05 × 0.05 × 0.10
color, habit	green block	orange block	orange block
reflections collected	35536	60789	56198
independent data	10095	20329	13795
restraints	0	0	0
parameters refined	595	1197	663
GoF[a]	1.077	1.047	1.061
R1,[b,c] wR2[c,d]	0.0262, 0.0704	0.0315, 0.0771	0.0577, 0.1866
R1,[b,e] wR2[d,e]	0.0325, 0.0784	0.0466, 0.0853	0.0713, 0.2031
largest diff. peak, e Å^{-3}	0.390	0.920	3.443
largest diff. hole, e Å^{-3}	-0.257	-0.493	-0.608

[a] GoF = $\{\Sigma[w(F_o^2 - F_c^2)^2]/(n-p)\}^{1/2}$, where n = number of reflections and p is the total number of parameters refined. [b] R1 = $\Sigma||F_o| - |F_c||/\Sigma|F_o|$. [c] R indices for data cut off at $I > 2\sigma(I)$. [d] wR2 = $\{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$, $P = (F_o^2 + 2F_c^2)/3$. [e] R indices for all data.

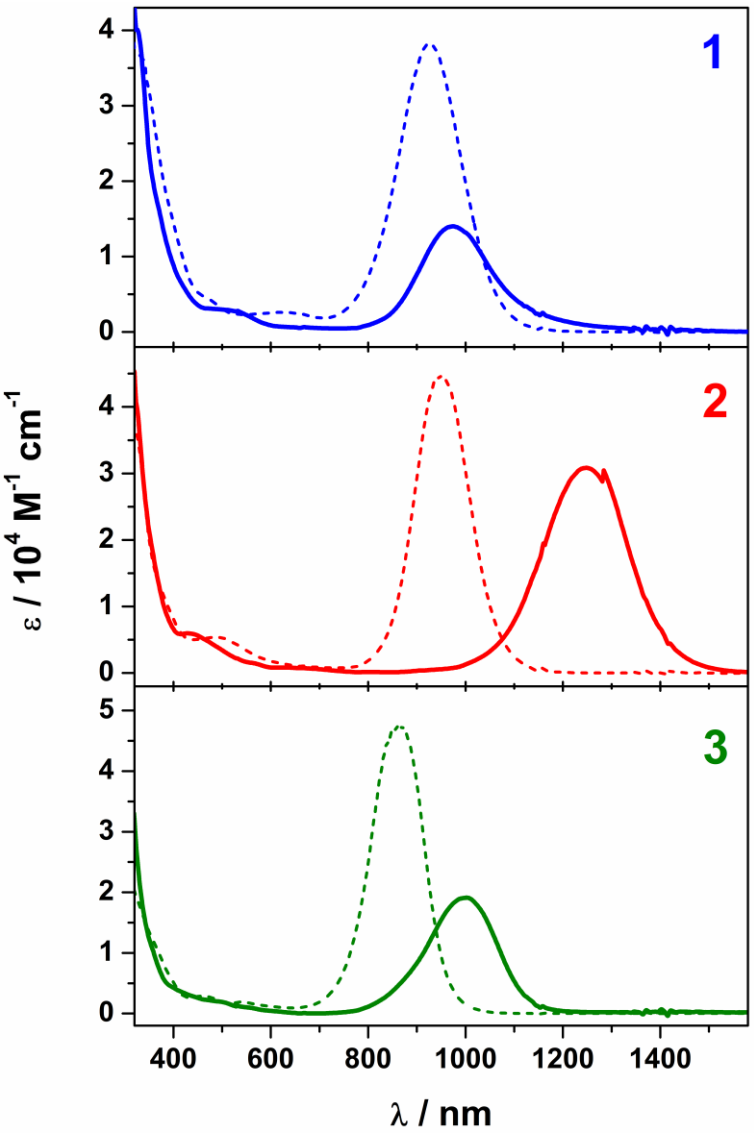

Figure S1. Comparison of the electronic spectra of **1**–**3** (solid lines) overlaid with spectra of the corresponding neutral complex (dashed lines) recorded in CH_2Cl_2 solution at ambient temperature.

Table S2. Comparison of Calculated and Experimental Metric Parameters[a]

	1		**2**		**3**	
	Exptl	Calcd	Exptl	Calcd	Exptl	Calcd
avg. M–S	2.1561(9)	2.154	2.278(1)	2.298	2.270(2)	2.295
avg. S–C	1.748(2)	1.752	1.742(2)	1.751	1.741(7)	1.753
avg. C–C	1.366(2)	1.382	1.372(3)	1.384	1.366(9)	1.382
avg. S–M–S	91.01(3)	90.4	88.46(2)	87.3	87.90(6)	87.3
α[b]	17.6	0.2	3.3	1.7	0	1.3

[a] Distances in angstrom; angles in degrees. [b] Dihedral angle between mean MS_2 planes.

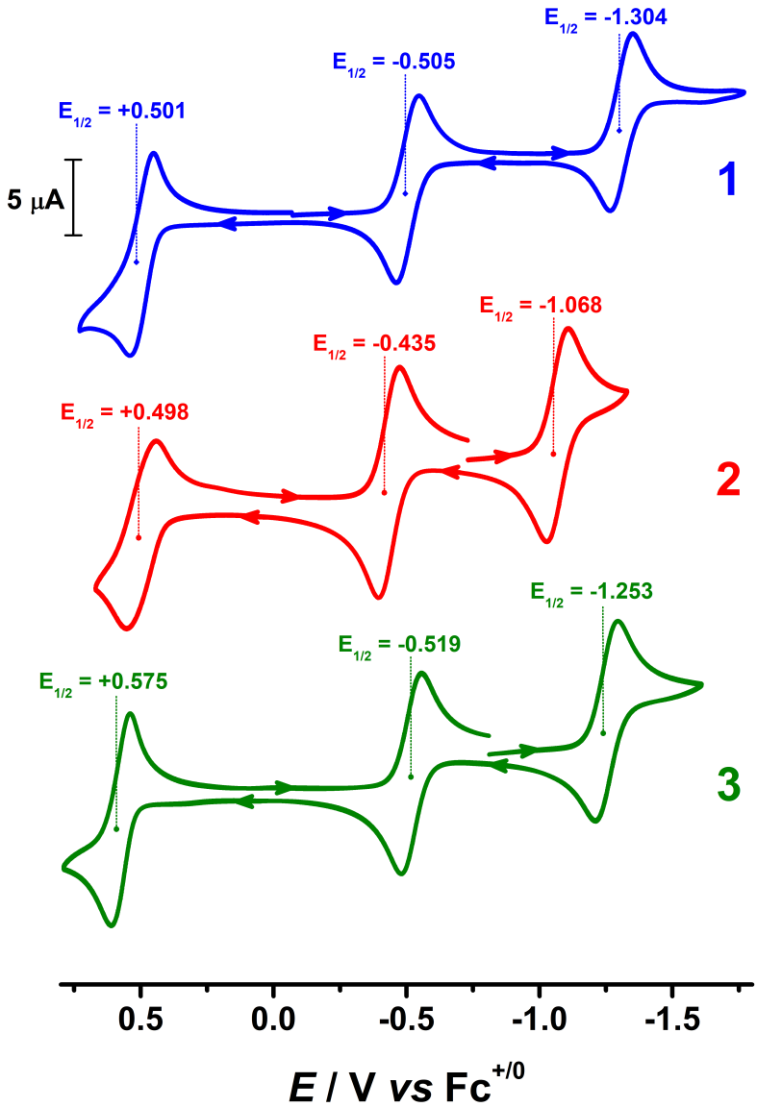

Figure S2. Cyclic voltammograms of **1**–**3** in CH_2Cl_2 solution (0.10 M $[N(^nBu)_4]PF_6$ supporting electrolyte at 22 °C at a scan rate of 100 mV s^{-1}. Potentials are referenced versus the $Fc^{+/0}$ couple.

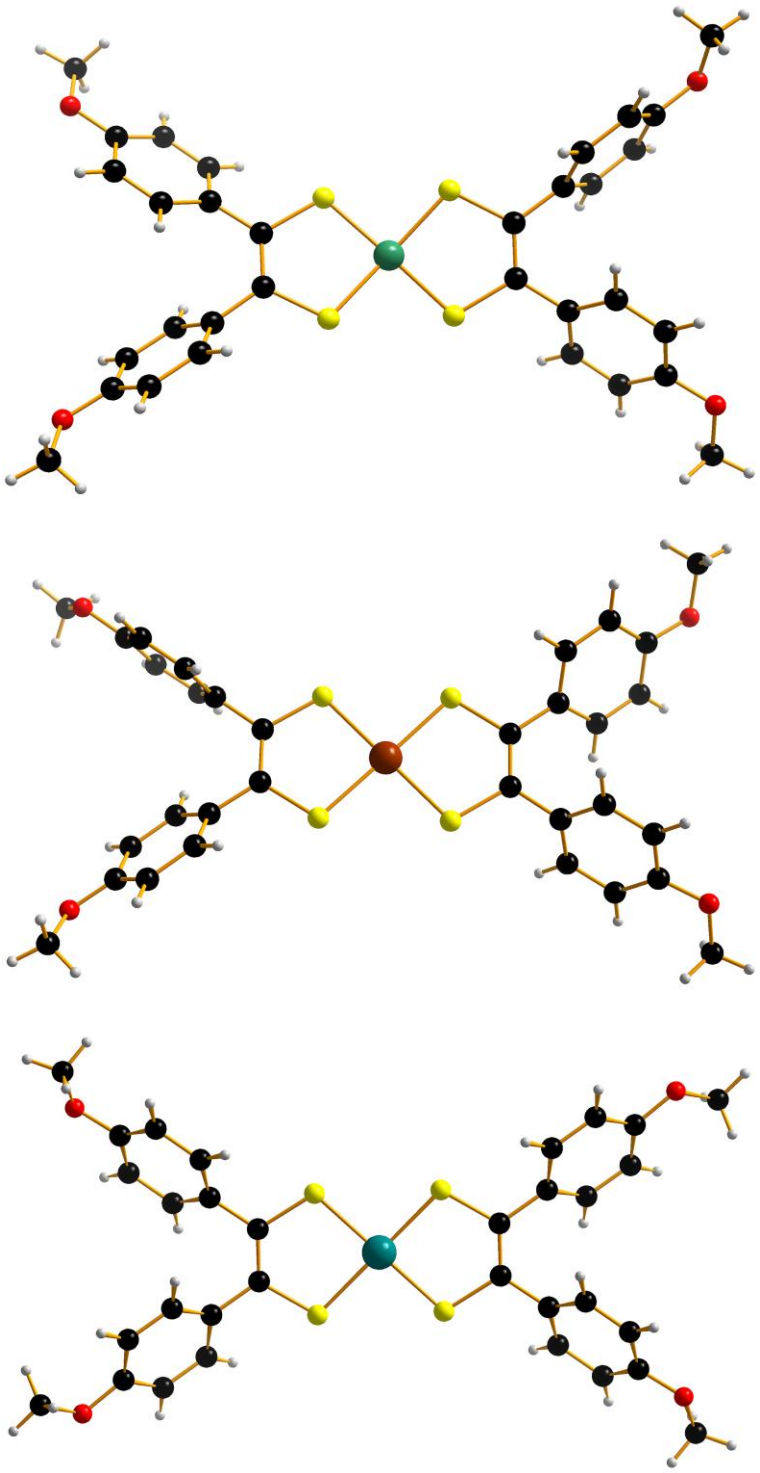

Figure S3. Structure of the anion in crystals of **1** (top), **2** (middle), and **3** (bottom)

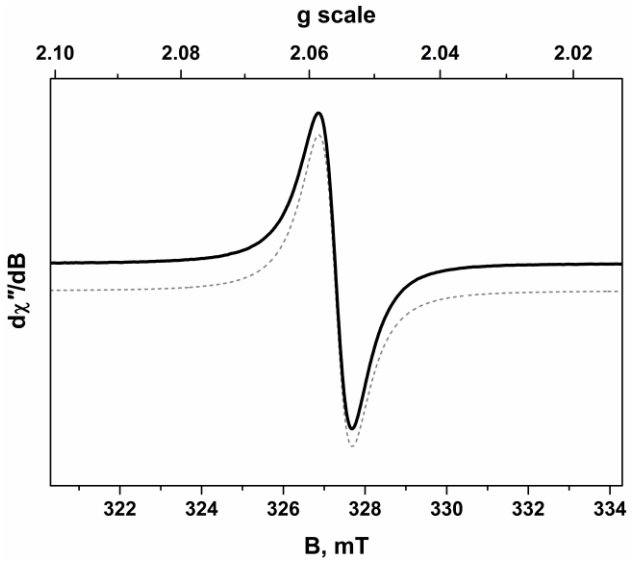

Figure S4. X-band EPR spectrum of **1** recorded in CH_2Cl_2 solution at 293 K (experimental conditions: frequency, 9.4176 GHz; power, 0.063 mW; modulation, 0.1 mT). Experimental data are represented by the black line; simulation is depicted by the dashed trace.

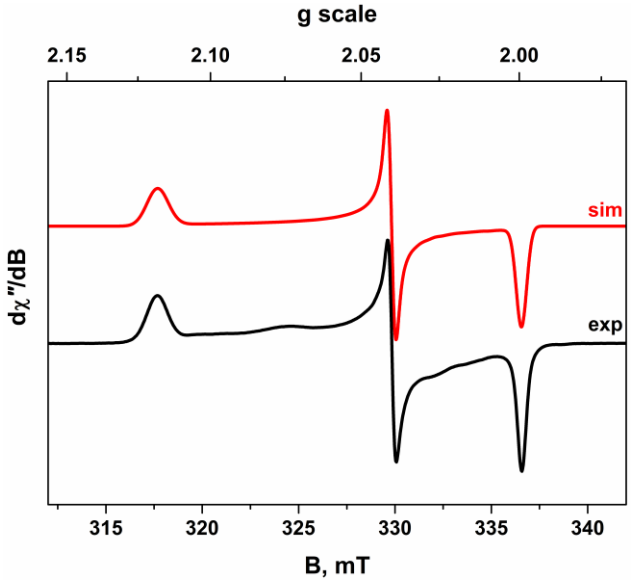

Figure S5. X-band EPR spectrum of **1** recorded in CH_2Cl_2/DMF solution at 130 K (experimental conditions: frequency, 9.4180 GHz; power, 0.63 mW; modulation, 0.2 mT). Experimental data are represented by the black line; simulation is depicted by the red trace.

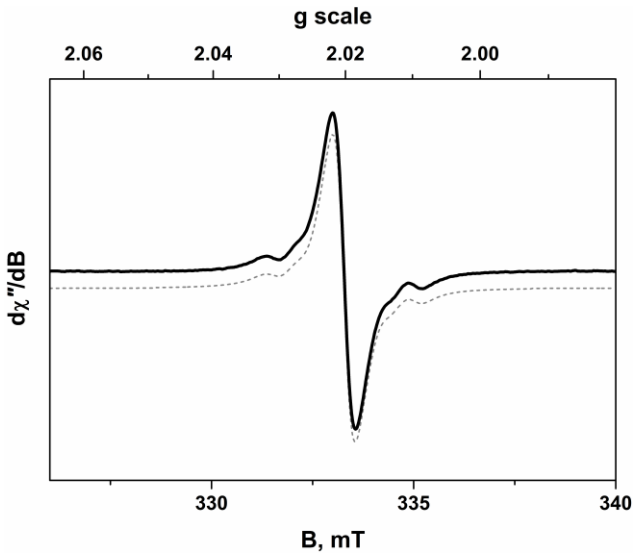

Figure S6. X-band EPR spectrum of **2** recorded in CH_2Cl_2 solution at 293 K (experimental conditions: frequency, 9.4236 GHz; power, 0.63 mW; modulation, 0.1 mT). Experimental data are represented by the black line; simulation is depicted by the dashed trace.

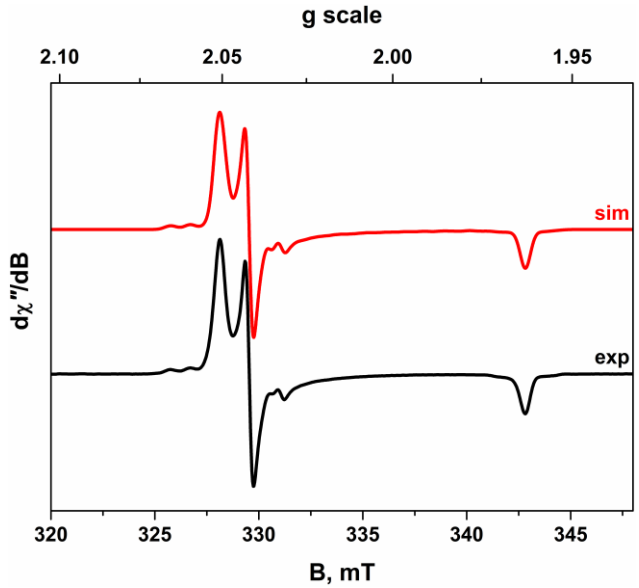

Figure S7. X-band EPR spectrum of **2** recorded in CH_2Cl_2/DMF solution at 130 K (experimental conditions: frequency, 9.4178 GHz; power, 0.2 mW; modulation, 0.3 mT). Experimental data are represented by the black line; simulation is depicted by the red trace.

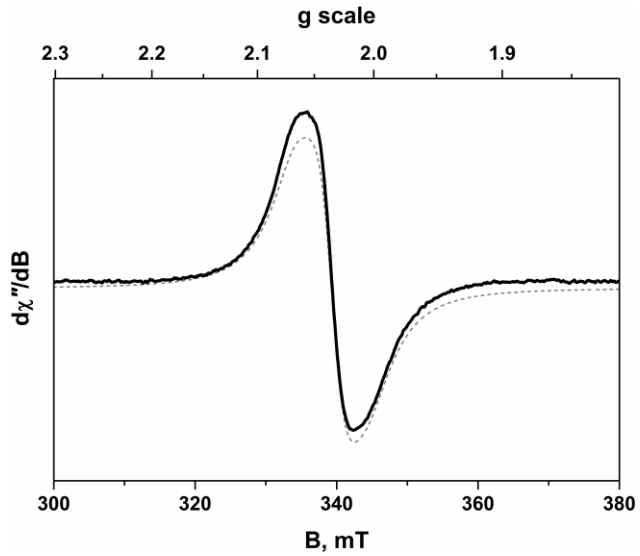

Figure S8. X-band EPR spectrum of **3** recorded in CH_2Cl_2 solution at 293 K (experimental conditions: frequency, 9.6647 GHz; power, 0.63 mW; modulation, 0.3 mT). Experimental data are represented by the black line; simulation is depicted by the dashed trace.

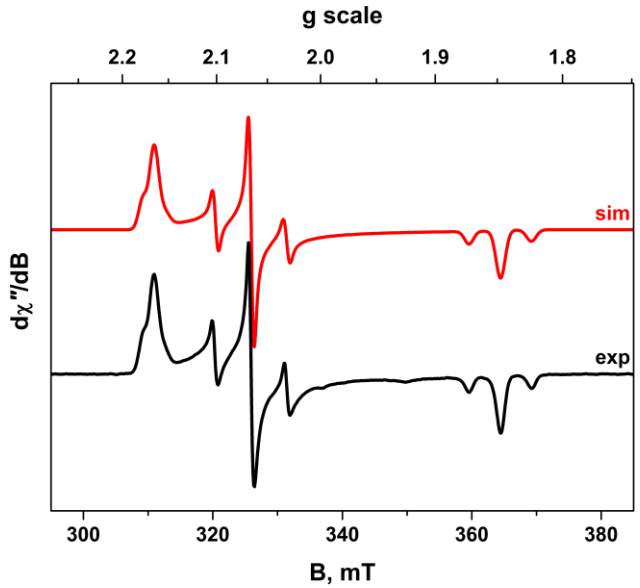

Figure S9. X-band EPR spectrum of **3** recorded in CH_2Cl_2/CH_3CN solution at 130 K (experimental conditions: frequency, 9.4230 GHz; power, 0.63 mW; modulation, 0.3 mT). Experimental data are represented by the black line; simulation is depicted by the red trace.

Table S3. EPR Spin Hamiltonian g- and A-Values ($\times 10^{-4}$ cm^{-1})[a] Derived from Simulation of Fluid (293 K) and Frozen Solution (130 K) Spectra

Compound	g_{iso}	a_{iso}	g_1	g_2	g_3	$\langle g \rangle$[b]	R_g[c]	Δg[d]	A_1	A_2	A_3	$\langle A \rangle$[e]
1	2.0559		2.1182	2.0402	1.9993	2.0526	0.66	0.1189				
2	2.0202	6.5	2.0508	2.0419	1.9628	2.0185	0.10	0.0880	9.0	5.9	4.6	6.5
3	2.0350	-73	2.1653	2.0654	1.8472	2.0260	0.31	0.3181	-33	-106	-83	-74

[a] The sign of the A-values is defined by the dominant Fermi-contact contribution. [b] $\langle g \rangle = (g_1 + g_2 + g_3)/3$. [c] Rhombicity, $R_g = (g_1 - g_2)/(g_1 - g_3)$. [d] Anisotropy, $\Delta g = g_1 - g_3$. [e] $\langle A \rangle = (A_1 + A_2 + A_3)/3$.

Table S4. Experimental Conditions,[a] Isotropic *g*- and *a*-Values ($\times 10^{-4}$ cm^{-1}),[b] and Coefficients for the Isotropic Liquids Line Shape Model[c]

compound	frequency[d]	power[e]	modulation[f]	g_{iso}	a_{iso}	*a*	*b*	*c*
1	9.4176	0.063	0.1	2.0559		6.8		
2	9.4263	0.63	0.1	2.0202	6.5	4.4	0.08	0.06
3	9.6647	0.63	0.3	2.0350	-73	44	-4	10

[a] All spectra are recorded in CH_2Cl_2 solution at ambient temperature. [b] The sign of a_{iso} is defined by the dominant Fermi-contact contribution.

[c] Kivelson line shape model, $\sigma_\upsilon = a + bM_I + cM_I^2$; coefficients in units $\times 10^{-4}$ cm^{-1}. [d] In GHz. [e] In mW. [f] In mT.

Table S5. Experimental Conditions,[a] *g*- and *A*-Matrices (*A*, 10^{-4} cm^{-1}),[b] Linewidth (W, 10^{-4} cm^{-1}) and Strain Coefficients (σ)

compound	ν[c]	g_1	g_2	g_3	A_1	A_2	A_3	W_1	W_2	W_3	σ_{g_1}	σ_{g_2}	σ_{g_3}	σ_{A_1}	σ_{A_2}	σ_{A_3}
1	9.4180	2.1182	2.0402	1.9993				6.4	2.0	2.3	0	0	0.0006			
2	9.4178	2.0508	2.0419	1.9628	9.0	5.9	4.6	1.7	1.7	2.6	-0.0007	0.0002	-0.0001	-0.25	-0.15	-1.5
3	9.4230	2.1653	2.0654	1.8472	-33	-106	-83	7.8	3.9	6.8	0.0009	0.0002	0.0007	-6	-4	-2

[a] All spectra recorded at 130 K in CH_2Cl_2/DMF. [b] The sign of the *A*-values is defined by the dominant Fermi-contact contribution. [c] ν = frequency in GHz.

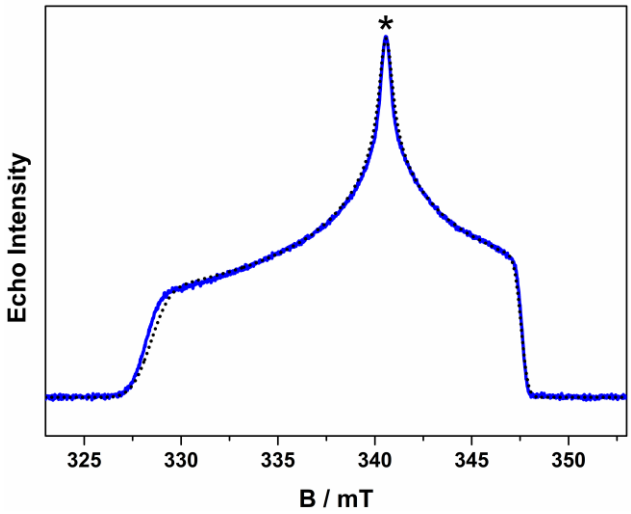

Figure S10. ESE detected EPR spectrum (blue line) and simulation (dashed line) of a 1 mM solution of **1** in 2% DMF-d_7/CD_2Cl_2 recorded at 10 K and 9.7437 GHz. Asterisk indicates field position for relaxation measurements.

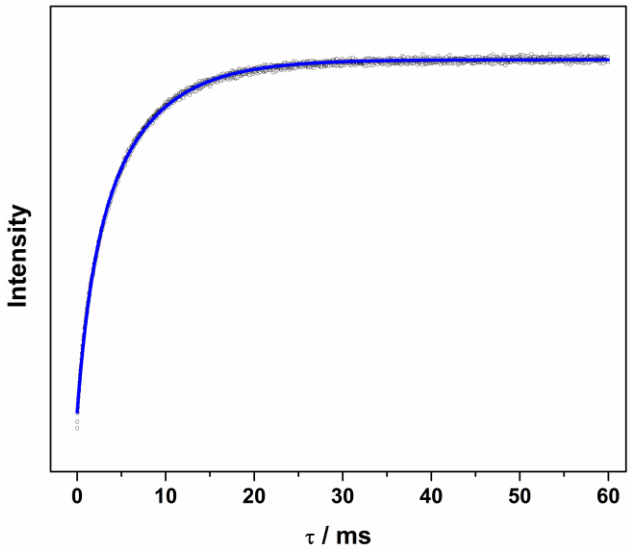

Figure S11. Inversion recovery data (open circles) and biexponential fit (blue line) of a 1 mM solution of **1** in 2% DMF-d_7/CD_2Cl_2 recorded at 10 K and 340.6 mT. Fit parameters: A_f = -0.23 ± 0.02, $T_{1,f}$ = 1.60 ± 0.02 ms, A_s = -0.42 ± 0.03, $T_{1,s}$ = 6.31 ± 0.03 ms.

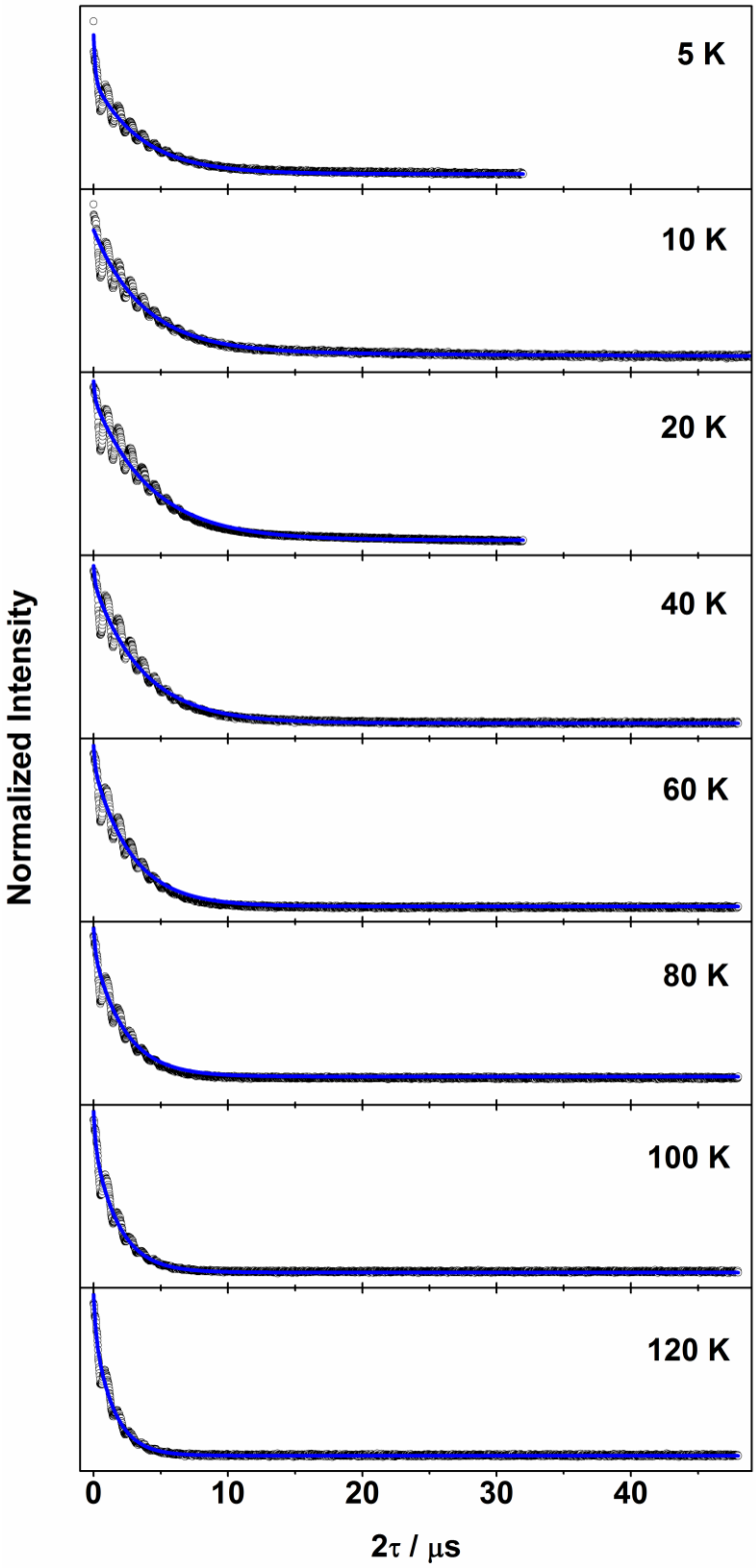

Figure S12. Hahn-echo decay curves (black line) and biexponential fit (blue line) of a 1 mM solution of **1** in 2% DMF-d_7/CD_2Cl_2 recorded at over the temperature range 5 – 120 K. Fit parameters are given in Table S6.

Table S6. Parameters of the biexponental fit functions for Hahn echo decay curves of **1**, B_0 = 340.6 mT

T	A_f	$T_{M,f}$ / µs	A_s	$T_{M,s}$ / µs
5	0.65(3)	0.13(1)	1.344(8)	3.58(3)
10	0.089(6)	0.09(1)	0.512(1)	4.89(1)
20	0.30(4)	0.10(2)	2.540(6)	4.23(1)
40	0.14(2)	0.10(2)	1.181(4)	3.66(2)
60	0.30(3)	0.11(2)	2.026(8)	2.84(1)
80	0.41(3)	0.13(2)	2.27(1)	2.32(1)
100	1.05(4)	0.15(1)	4.38(2)	1.86(1)
120	1.33(5)	0.17(1)	4.94(3)	1.49(1)

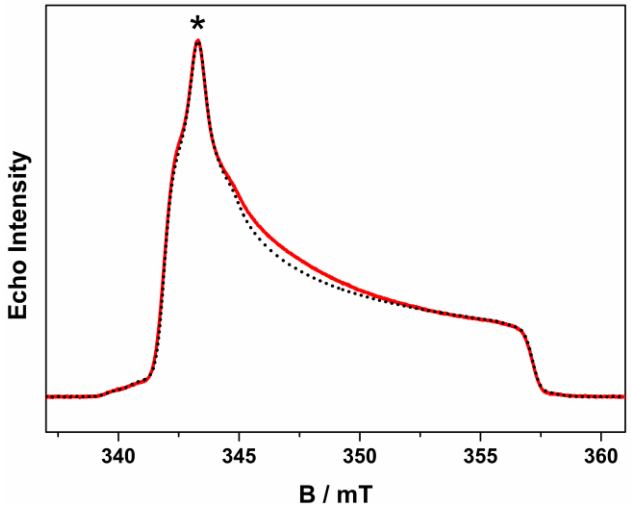

Figure S13. ESE detected EPR spectrum (red line) and simulation (dashed line) of a 1 mM solution of **2** in 2% DMF-d_7/CD_2Cl_2 recorded at 10 K and 9.8314 GHz. Asterisk indicates field position for relaxation measurements.

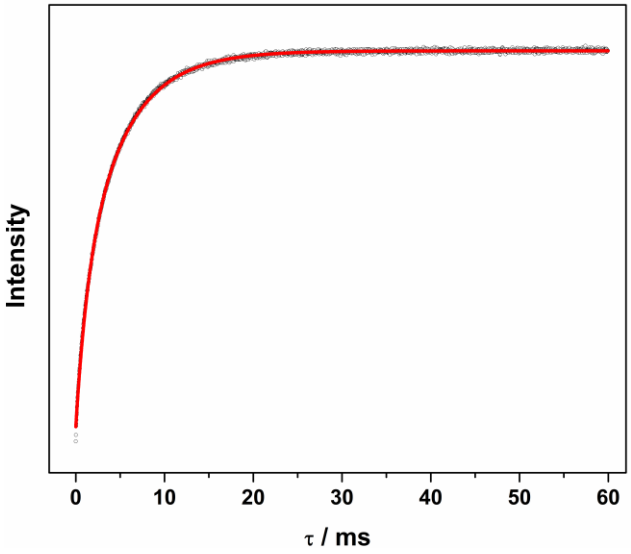

Figure S14. Inversion recovery data (open circles) and biexponential fit (red line) of a 1 mM solution of **1** in 2% DMF-d_7/CD_2Cl_2 recorded at 10 K and 343.3 mT. Fit parameters: A_f = -0.28 ± 0.02, $T_{1,f}$ = 1.32 ± 0.02 ms, A_s = -0.57 ± 0.01, $T_{1,s}$ = 4.99 ± 0.02 ms.

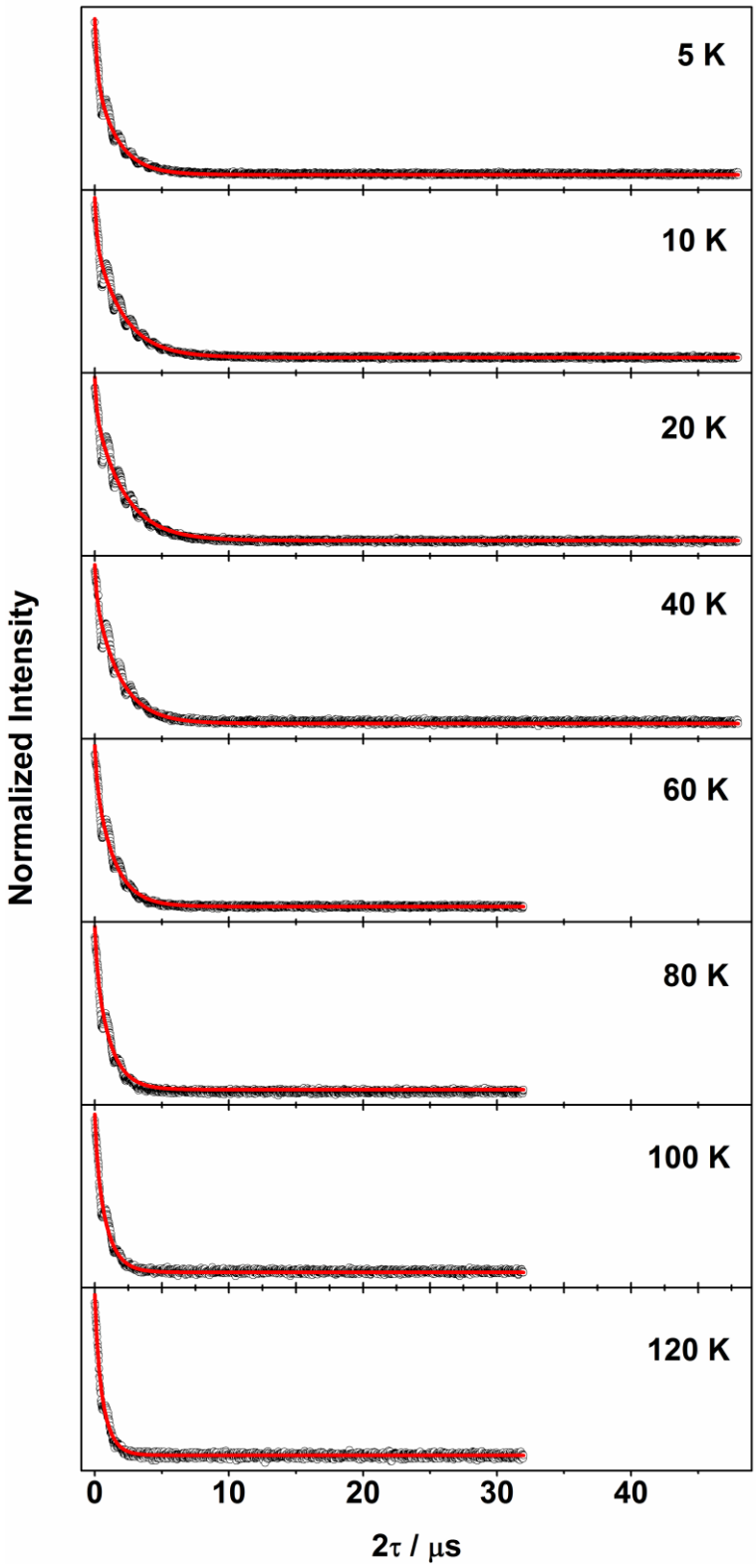

Figure S15. Hahn-echo decay curves (black line) and biexponential fit (blue line) of a 1 mM solution of **2** in 2% DMF-d_7/CD_2Cl_2 recorded at over the temperature range 5 – 120 K. Fit parameters are given in Table S7.

Table S7. Parameters of the biexponental fit functions for Hahn echo decay curves of **2**, B_0 = 343.3 mT

T	A_f	$T_{M,f}$ / µs	A_s	$T_{M,s}$ / µs
5	0.374(8)	0.181(8)	0.707(6)	1.61(1)
10	0.31(1)	0.15(1)	0.887(5)	2.08(1)
20	0.19(1)	0.14(1)	0.763(5)	2.17(1)
40	0.136(7)	0.14(1)	0.631(3)	1.81(1)
60	0.36(2)	0.15(2)	1.68(2)	1.39(1)
80	0.30(2)	0.17(2)	1.25(2)	1.13(1)
100	0.37(3)	0.19(2)	1.40(3)	0.91(1)
120	0.44(6)	0.23(3)	1.29(6)	0.73(2)

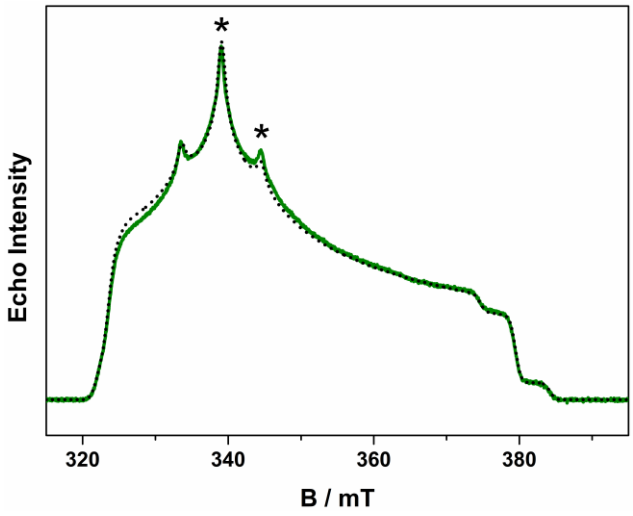

Figure S16. ESE detected EPR spectrum (green line) and simulation (dashed line) of a 1 mM solution of **3** in 2% DMF-d_7/CD_2Cl_2 recorded at 10 K and 9.8346 GHz. Asterisks indicate field positions for relaxation measurements.

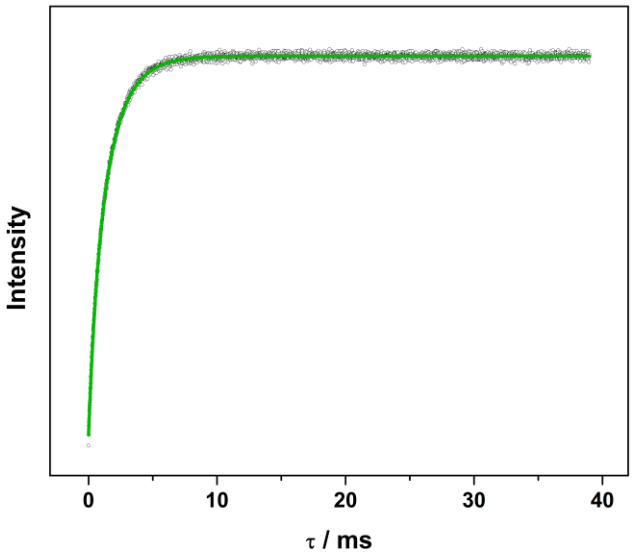

Figure S17. Inversion recovery data (open circles) and biexponential fit (red line) of a 1 mM solution of **3** in 2% DMF-d_7/CD_2Cl_2 recorded at 10 K and 339.1 mT. Fit parameters: A_f = -0.18 ± 0.01, $T_{1,f}$ = 0.56 ± 0.03 ms, A_s = -0.53 ± 0.01, $T_{1,s}$ = 1.64 ± 0.02 ms.

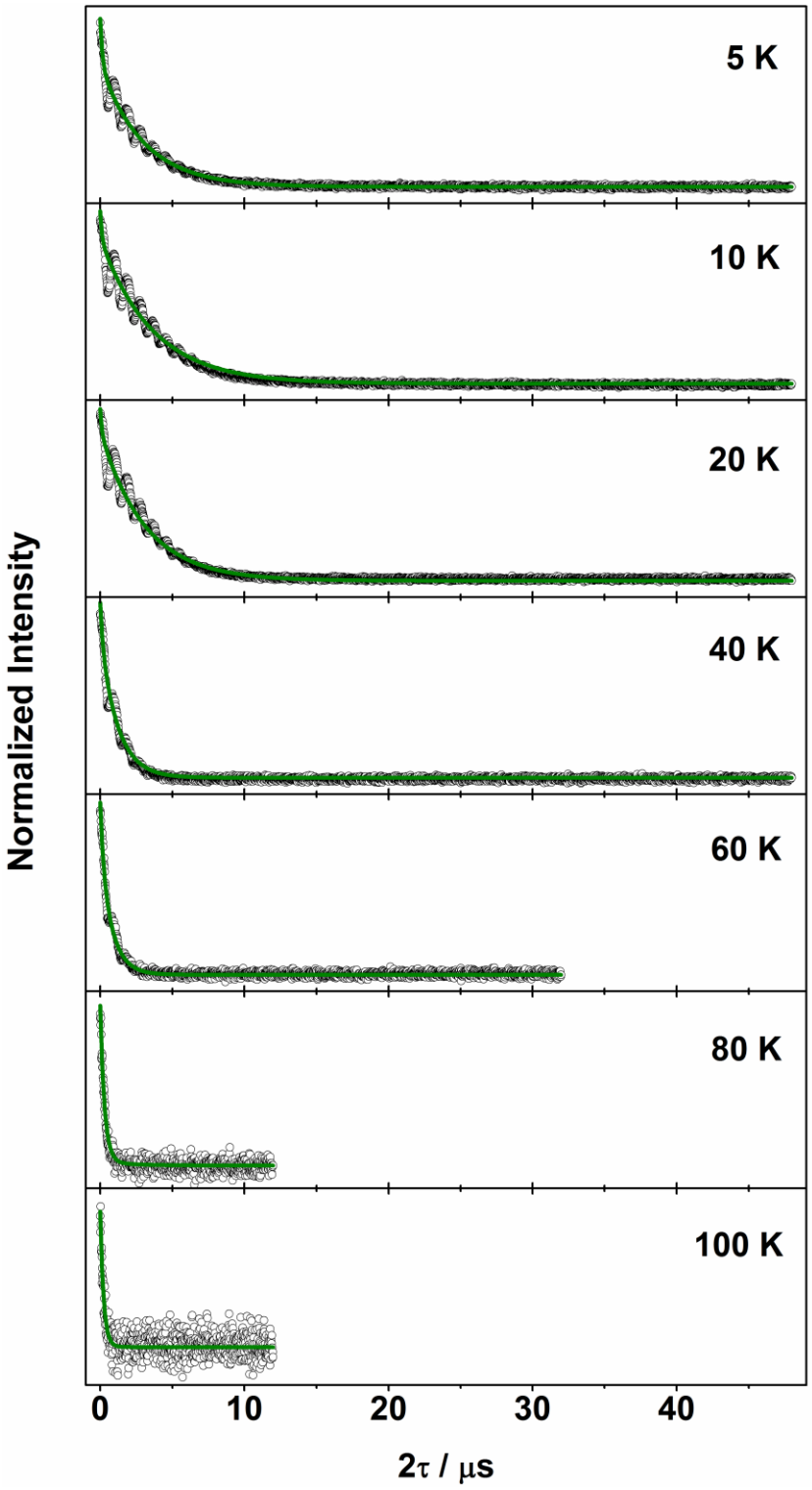

Figure S18. Hahn-echo decay curves (black line) and biexponential fit (green line) of a 1 mM solution of **2** in 2% DMF-d_7/CD_2Cl_2 recorded at B_0 = 339.1 mT over the temperature range 5 – 100 K. Fit parameters are given in Table S8.

Table S8. Parameters of the biexponental fit functions for Hahn echo decay curves of **3**, B_0 = 339.1 mT

T	A_f	$T_{M,f}$ / µs	A_s	$T_{M,s}$ / µs
5	0.167(6)	0.15(1)	0.450(2)	2.89(2)
10	0.092(8)	0.12(2)	0.491(2)	3.63(2)
20	0.12(1)	0.11(2)	0.825(3)	3.09(2)
40	0.36(2)	0.17(2)	1.56(2)	1.20(1)
60	0.81(7)	0.23(2)	1.90(8)	0.85(2)
80	1.03(6)	0.30(1)	3.0(3)	0.34(2)
100	1.54(4)	0.2(3)	4.0(2)	0.26(2)

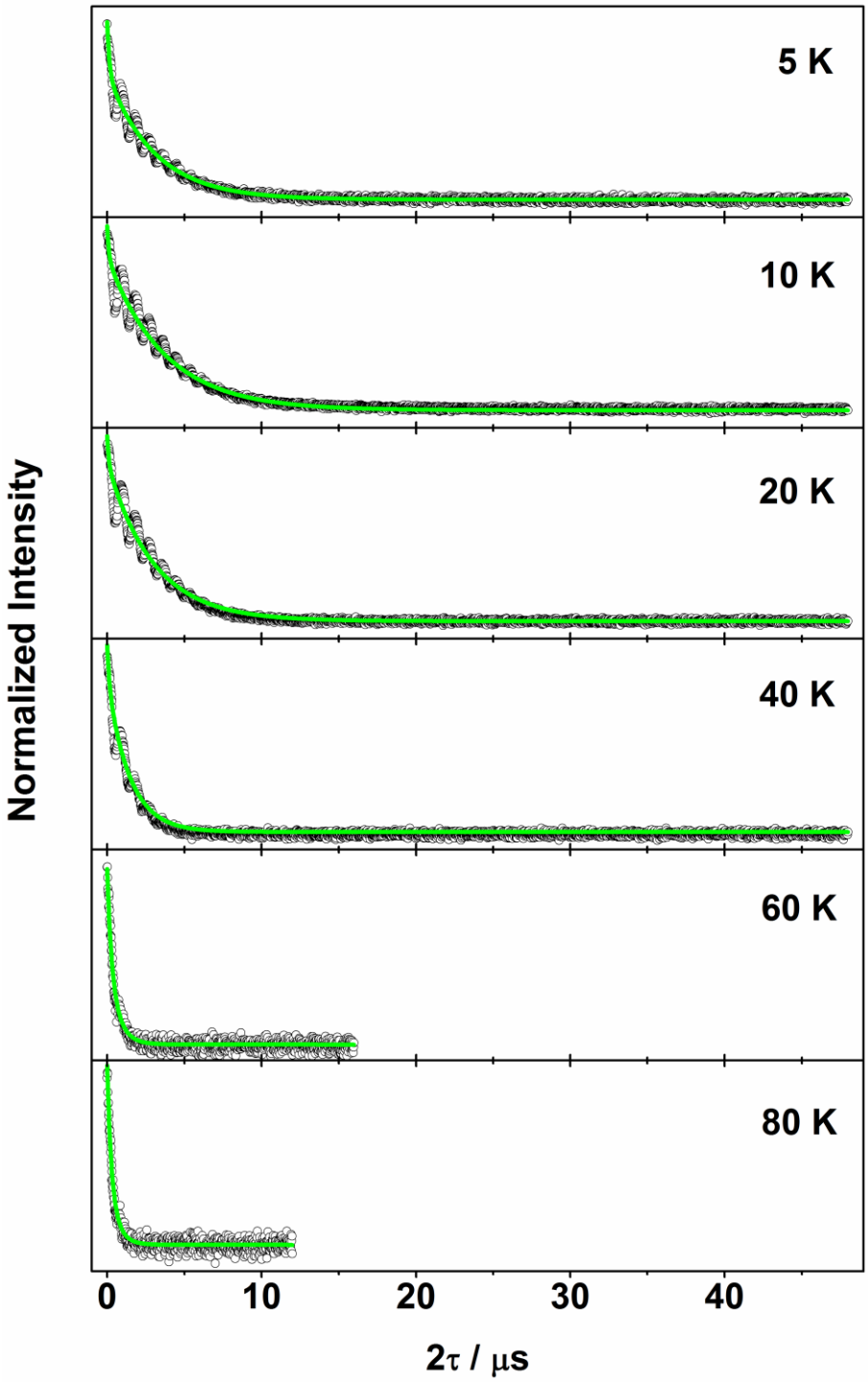

Figure S19. Hahn-echo decay curves (black line) and biexponential fit (green line) of a 1 mM solution of **2** in 2% DMF-d_7/CD_2Cl_2 recorded at B_0 = 344.5 mT over the temperature range 5 – 80 K. Fit parameters are given in Table S9.

Table S9. Parameters of the biexponental fit functions for Hahn echo decay curves of **3**, B_0 = 344.5 mT

T	A_f	$T_{M,f}$ / µs	A_s	$T_{M,s}$ / µs
5	0.157(6)	0.15(1)	0.386(2)	3.08(2)
10	0.099(8)	0.11(2)	0.491(2)	3.64(2)
20	0.15(2)	0.11(2)	1.068(4)	2.99(2)
40	0.29(2)	0.14(2)	1.33(1)	1.44(1)
60	0.36(2)	0.28(2)	3.11(8)	0.67(1)
80	6.0(2)	0.28(5)	3.0(2)	0.6(2)

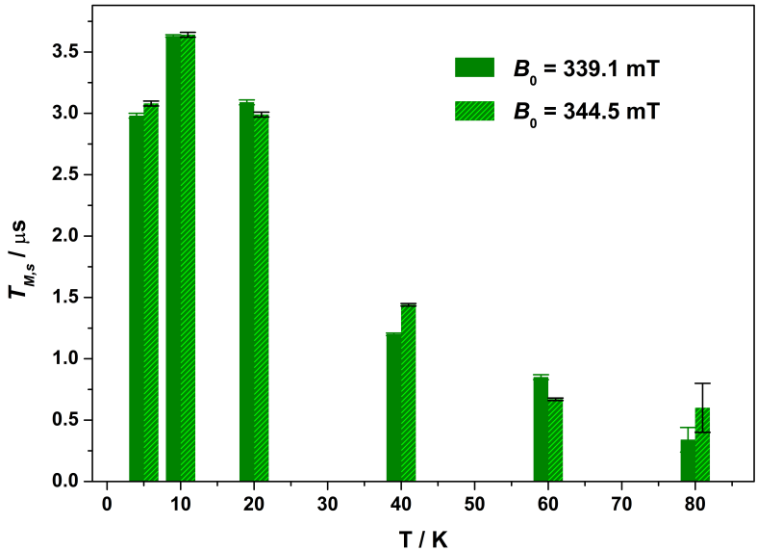

Figure S20. Temperature dependence of $T_{M,s}$ values for **3** comparing the B_0 = 339.1 mT corresponding to the maximum in the powder pattern (g_2) with B_0 = 344.5 mT corresponding to the high field hyperfine line of g_2 (see Figure S16). Error bars represent the standard deviation of the fit.

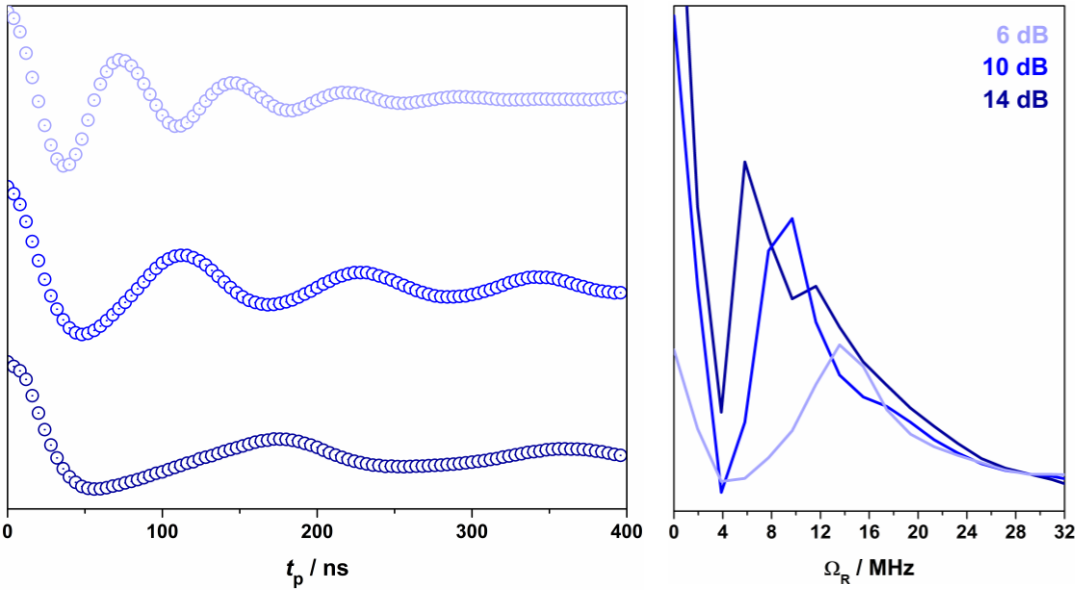

Figure S21. Rabi oscillations (left) and corresponding Rabi frequencies (right) for **1** B_0 = 340.6 mT and 10 K recorded variable power nutation measurements.

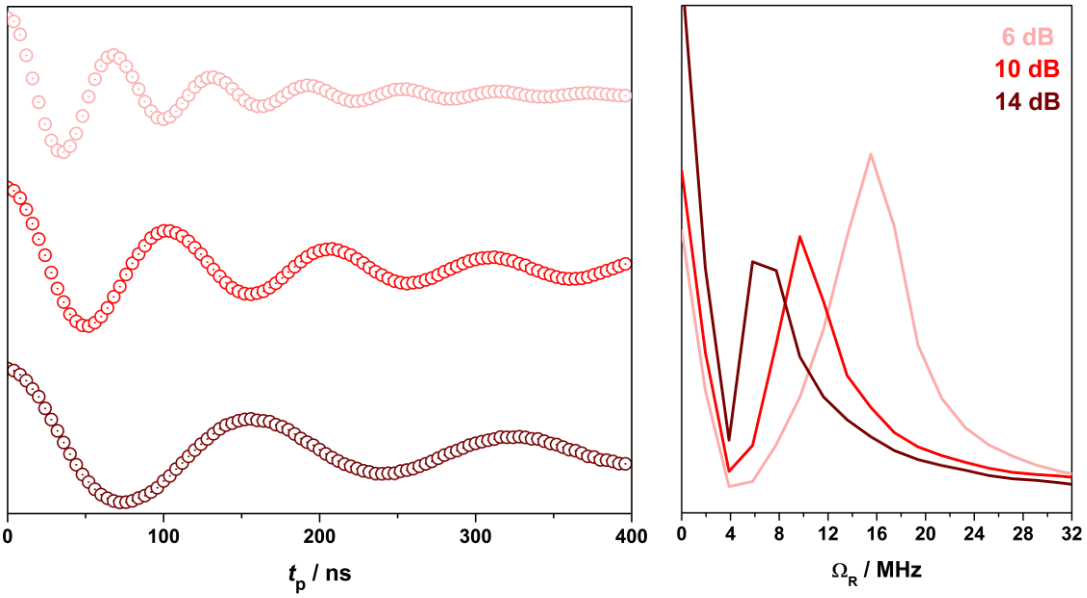

Figure S22. Rabi oscillations (left) and corresponding Rabi frequencies (right) for **2** B_0 = 343.3 mT and 10 K recorded variable power nutation measurements.

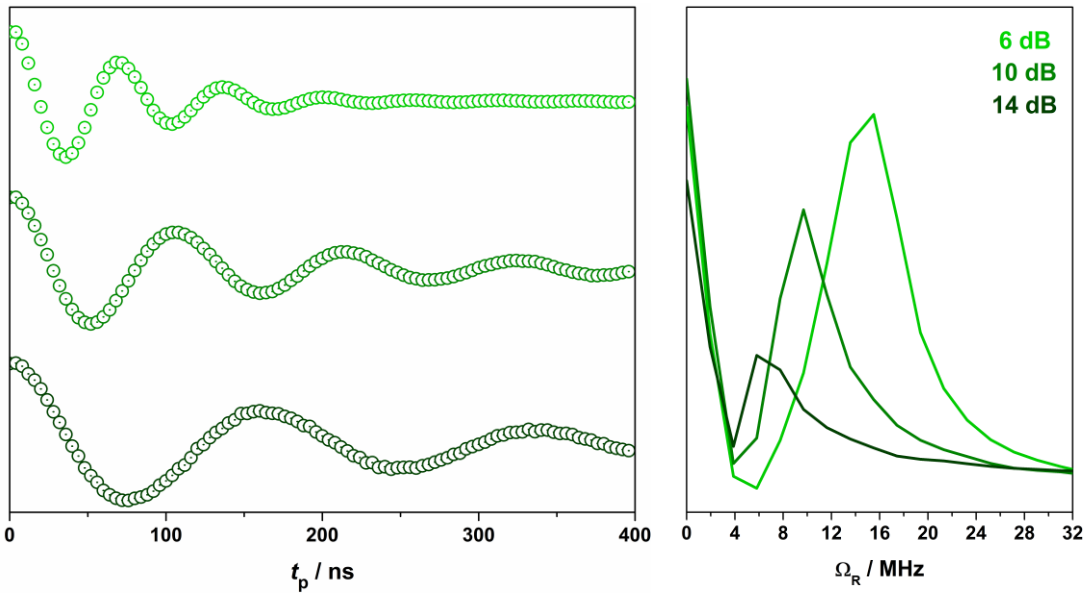

Figure S23. Rabi oscillations (left) and corresponding Rabi frequencies (right) for **3** at B_0 = 339.1 mT and 10 K recorded variable power nutation measurements.

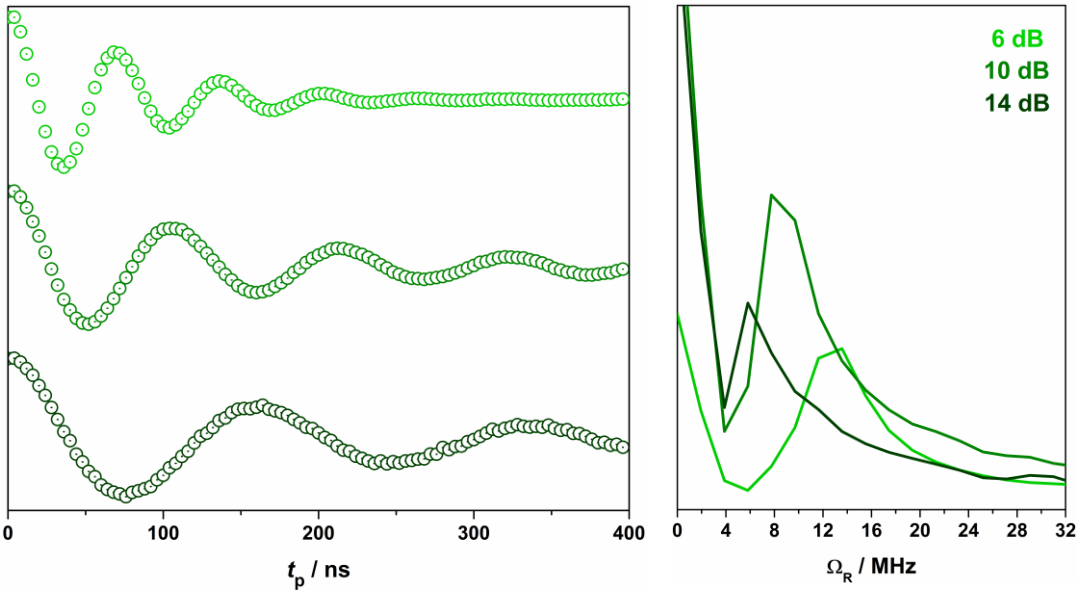

Figure S24. Rabi oscillations (left) and corresponding Rabi frequencies (right) for **3** at B_0 = 344.5 mT (corresponding to the high-field hyperfine line of g_2; Figure S16) and 10 K recorded variable power nutation measurements.

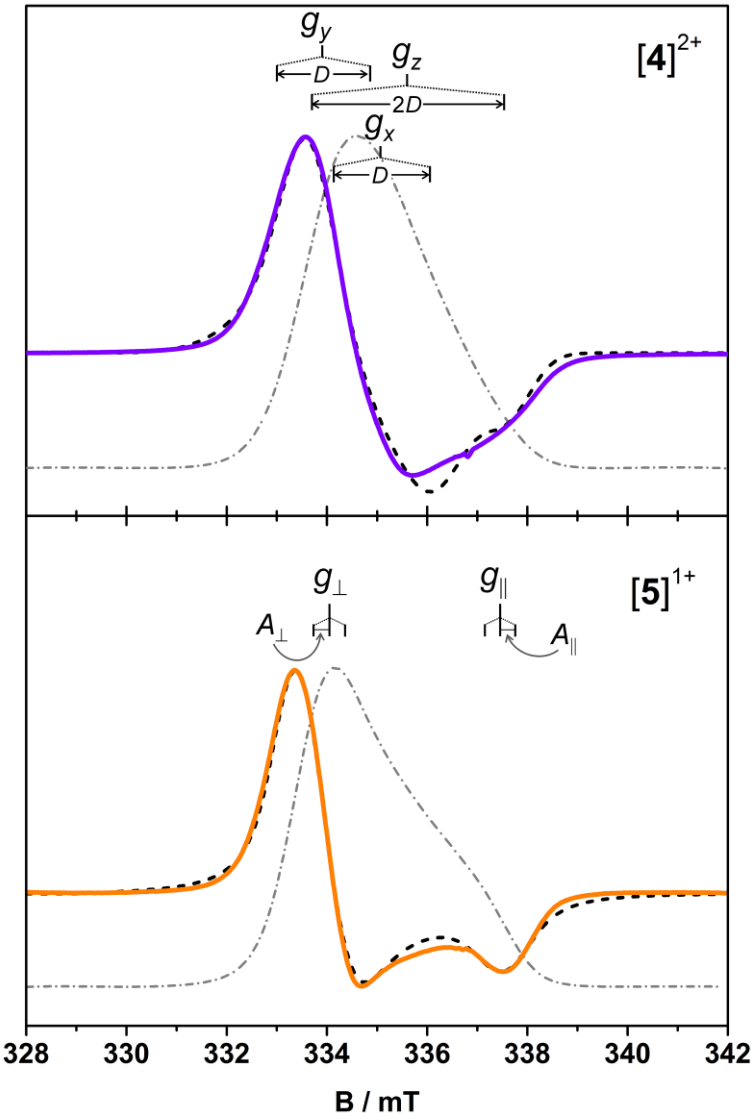

Figure S25. X-band EPR spectra of $[\mathbf{4}]^{2+}$ (top) and $[\mathbf{5}]^{1+}$ (bottom) recorded in CH_2Cl_2 solution at 130 K. Experimental data are shown as the solid line in each case, with the absorption spectrum shown beneath as a dashed gray line to indicate the field position of maximum intensity for pulsed EPR measurements. Simulations of each spectrum are depicted by the dashed black line with markings at field positions that correspond to the key spin-Hamiltonian parameters. For $[\mathbf{4}]^{2+}$ $S = 1$: $g_{x,y,z}$ = (2.010, 2.017, 2.007), $D = -18 \times 10^{-4}$ cm^{-1}, $E/D = 0.005$; $A_{x,y,z} = (3, 1, 1) \times 10^{-4}$ cm^{-1} ($4 \times {}^{31}$P $I = {}^1/_2$, 100% abundant – not resolved but used to improve the lineshape. For $[\mathbf{5}]^{1+}$ $S = {}^1/_2$: $g_{x,y,z}$ = (2.0205, 2.0158, 1.9954), $A_{x,y,z}$ = (3.0, 3.5, 3.5) $\times 10^{-4}$ cm^{-1} ($2 \times {}^{31}$P).

Table S10. Geometry Optimized Coordinates for $[Ni(adt)_2]^{1-}$

Ni	-0.00029825743218	-0.00003020622874	0.00020983146906
S	-1.98847849560950	-0.74664757447997	0.36008686322961
S	0.51124280411028	-1.82106437117618	-1.02937928165127
S	1.98923951503879	0.74467840489050	-0.35575411423935
S	-0.51340754331312	1.82325988482596	1.02501550081562
C	-2.04601520617188	-2.34779122132835	-0.34633465179148
C	-0.92490089574182	-2.82484885471497	-0.99768717572959
C	2.04627226194205	2.34671983488618	0.34864986208579
C	0.92357453427453	2.82597981887388	0.99558564419946
O	-6.92363300131926	-5.10915968964770	0.59025082485497
O	-0.43321255190888	-7.66722924425314	-3.93575926865271
C	-0.83839052417237	-4.09711101989070	-1.74921540519866
C	0.29869355519659	-4.92918449928982	-1.64960158463574
H	1.10856220736251	-4.64451711410756	-0.97581599862651
C	0.40539942895270	-6.10653688351866	-2.38231478488170
H	1.28697895446555	-6.74348030816725	-2.28989796718715
C	-0.62787133996282	-6.49318791654795	-3.25287257506160
C	-1.76418272594054	-5.67928716547397	-3.37660062809297
H	-2.57531623602556	-5.94455196739351	-4.05330067631088
C	-1.85571347561224	-4.49918666885172	-2.63306240396115
H	-2.73700699215406	-3.86889071663632	-2.75597314155047
C	-1.46837568308878	-8.09100491165358	-4.83418691919698
H	-1.11644189655521	-9.03316565383924	-5.26759306456755
H	-1.62759494229940	-7.35255766544797	-5.63552772797427
H	-2.41517096912247	-8.26264511944455	-4.29894728025893
C	-3.30090004190568	-3.10041981700179	-0.11951973195689
C	-3.28752753498875	-4.40892131514793	0.39382992942027
H	-2.33195934996031	-4.88572221898825	0.61560233722279
C	-4.46797558610501	-5.11425779329955	0.64453434196566
H	-4.41048012303446	-6.12233159890461	1.05141647996189
C	-4.55960351759103	-2.50934362637434	-0.36230745093740
H	-4.60272414432376	-1.49343543934022	-0.75790706359404
C	-5.74336983086918	-3.19859295144248	-0.12160615928833
H	-6.71091511131378	-2.73562285146561	-0.32310498181494
C	-5.70662736020664	-4.50960206009609	0.38289655675979
C	-6.92354515019206	-6.44988120558585	1.10113337130586
H	-7.97766406947984	-6.73586529672863	1.18307870667318
H	-6.45038923484756	-6.49748209778251	2.09420454165648
H	-6.40689716279201	-7.13816563573162	0.41364415714622
O	6.93144364180946	5.09953060069762	-0.57368861574645
O	0.42544900434970	7.67635002848869	3.91937081241461
C	0.83550621337586	4.10011564839349	1.74375269045409
C	-0.30073762225302	4.93262464381801	1.63823601056665
H	-1.10857466348135	4.64663117968030	0.96257743272742
C	-0.40909445151912	6.11201182362736	2.36741061757902
H	-1.28991384013622	6.74931383042922	2.27034750136841
C	0.62157057048958	6.50033492862429	3.24030957010255
C	1.75694838522016	5.68604621384028	3.36994028715894
H	2.56603345357797	5.95258939281743	4.04858904734039
C	1.85021036311168	4.50393211713167	2.62981116850631
H	2.73075322356713	3.87345937649390	2.75715838533279
C	1.45811600132839	8.10209688249572	4.81973200670031
H	1.10514703243550	9.04538551812633	5.24981591595426
H	1.61491523096581	7.36561012062384	5.62334899198054
H	2.40645595789532	8.27219320968272	4.28674052809228
C	3.30300947445694	3.09730365295773	0.12519677923819
C	3.29355950603033	4.40456811574003	-0.39133098038970

H	2.33959544002137	4.88210855367427	-0.61836457274981
C	4.47603639275741	5.10772890382177	-0.63866502214707
H	4.42160285530267	6.11489048366171	-1.04822121662966
C	4.55985892995304	2.50515358006201	0.37486158896188
H	4.59990154100647	1.49015966254573	0.77310953765511
C	5.74556800080864	3.19227332652975	0.13765307011594
H	6.71161497937321	2.72856015996095	0.34454532341176
C	5.71273716409094	4.50209020193072	-0.37019642394273
C	6.93538338420741	6.43924638253918	-1.08717597681197
H	7.99025245903876	6.72344658232895	-1.16563310418435
H	6.46611169062949	6.48571960272020	-2.08213759598867
H	6.41716537428365	7.12961001306090	-0.40296266867715

Table S11. Geometry Optimized Coordinates for $[Pd(adt)_2]^{1-}$

Pd	0.56397426376863	4.71956681712097	0.68585414780852
S	-0.26236121898536	5.25719061627819	-1.38896401988043
S	-0.59930765700378	2.74482955401775	0.51627614993446
S	1.43199959790231	4.16200704407379	2.74065476391617
S	1.69175945268564	6.71279239344739	0.87316976311115
O	-3.16649114528073	4.22073327000115	-7.21548676460580
O	-5.00757357260908	-1.50211875466403	-1.93979932443916
O	5.28570742896870	4.58524753659836	8.04082310529316
O	5.12101421011305	11.48447420980631	3.87109674498637
C	-1.24521618641594	3.89259184371556	-1.87509215898249
C	-1.41509717634259	2.80857131487739	-1.03166526031725
C	2.42766714505970	5.52083310281567	3.21663610983731
C	2.51844937900947	6.64542672975510	2.41489784376474
C	-1.78864792256153	3.98572441223845	-3.25153441234396
C	-2.41770909240419	5.15732298832323	-3.70711255649432
H	-2.54515558542361	5.99439753214345	-3.01854474663473
C	-2.89648581552667	5.27818096930205	-5.01543100070587
H	-3.38762505040321	6.20165945688282	-5.31870111487931
C	-2.74148846959673	4.21060222250136	-5.91109479712740
C	-2.10566818502221	3.03334183276031	-5.47924878450842
H	-1.97411086928607	2.21286028421617	-6.18704882340848
C	-1.64095843526342	2.92712003404252	-4.17380292785284
H	-1.13816510092927	2.01159168610642	-3.86086894841490
C	-3.81083880243785	5.41062254147741	-7.69347570722102
H	-4.73181177699192	5.61978980567601	-7.12754984534021
H	-4.06204808993676	5.21098549624683	-8.74056832427153
H	-3.13670497276618	6.27959660030203	-7.63373905615349
C	-2.32244639220608	1.66672990560492	-1.29823537248086
C	-1.91272166345567	0.34251565375516	-1.06592760347350
H	-0.89417740694156	0.15446066132207	-0.72281674974127
C	-2.77058870660550	-0.74265642290615	-1.26999287670478
H	-2.40545999768915	-1.75219178816771	-1.08479409814825
C	-4.08244727666739	-0.51589796252698	-1.70987858743789
C	-4.51649324112618	0.80159068125544	-1.93710245869733
H	-5.54330957792815	0.97091648791850	-2.26544487262001
C	-3.64988982463567	1.86854349442353	-1.73453008606521
H	-4.00885025142838	2.88437759768565	-1.90371442208339
C	-4.60609533692190	-2.85770062082794	-1.69632151395135
H	-3.76285730812938	-3.14625377314331	-2.34297068027291
H	-5.48005677843085	-3.47307715138412	-1.93645849448932
H	-4.32808610466275	-3.00695597553343	-0.64127916967438
C	3.19021663145145	5.31639333711941	4.47151168223237

C	4.57091375781055	5.57018335908862	4.53903125156308
H	5.08847284307977	5.94593988294605	3.65560705205716
C	5.30657092543872	5.34168814773633	5.70504260019778
H	6.37642323453539	5.54658912580943	5.70782054990929
C	4.66188717440629	4.84379133904204	6.84699646651242
C	3.28340155616119	4.57533602139054	6.79934556456501
H	2.78815590597931	4.18834673114404	7.69172312605666
C	2.56670290473945	4.80415027953829	5.62993370745949
H	1.49667392657008	4.59121530607550	5.60811123495672
C	6.69610708441536	4.83512514150471	8.11898281106456
H	7.25156212816341	4.20939976581765	7.40337782491825
H	6.98765030348313	4.57052481794485	9.14106320393205
H	6.92400422921272	5.89680204066451	7.93355270819818
C	3.23388302060561	7.89005479371161	2.78506939872861
C	4.07039540271954	8.54788835619495	1.86719451036299
H	4.22449326917974	8.10968860432070	0.87963192286925
C	4.72086742316653	9.74380338187808	2.18619856465586
H	5.36751355088193	10.21283890801144	1.44566058953692
C	4.53466163050207	10.31758538952500	3.45177639943522
C	3.69090799430504	9.68326719687979	4.38038387738369
H	3.53744053537511	10.14501518325580	5.35734055805601
C	3.05534067290035	8.49320602665641	4.04900229051221
H	2.39396998323675	8.02247644882819	4.77740963310673
C	5.97448553212480	12.16822119482955	2.94255925979492
H	6.83174011021481	11.54056488779799	2.65244160214877
H	6.33361559151454	13.05830341903750	3.46983485109481
H	5.41981119233460	12.47238258571278	2.04122768946112

Table S12. Geometry Optimized Coordinates for $[Pt(adt)_2]^{1-}$

Pt	1.94107342218879	6.90043087076864	9.10656513302129
S	2.82568265320148	4.80133893623246	8.82630148870193
S	2.81685660275389	7.42350416933659	7.05337704055156
S	1.02480492645378	6.37110665789657	11.14266089679651
S	1.08416440047413	9.00931681600538	9.39240990131470
O	6.47494444447489	0.07105060580874	6.01082392918297
O	5.70606376617657	6.54543072265202	1.23548002007565
O	-2.67403511834867	7.05551982443765	16.52605098021474
O	-1.79926746704550	14.01818105530960	12.58395794877750
C	3.62373728649749	4.82661319660471	7.26620006327675
C	3.60810413239998	5.96766459566922	6.48769024930757
C	0.21516515309872	7.82388296123279	11.69075346081720
C	0.25545324340230	8.97996473388477	10.93508035771527
C	4.33943468544226	3.57510635318098	6.92005821156290
C	3.72428091270594	2.32068576911309	7.07091837254540
H	2.69045150998545	2.27343350001577	7.41666814447516
C	4.39587850220260	1.12863459445133	6.77948937622721
H	3.87494978260033	0.18019985756240	6.90374844249495
C	5.72271983569628	1.17376400916231	6.32855320396768
C	6.36145906973708	2.41770607691692	6.18341024624017
H	7.39910979902258	2.44321118692951	5.84700385403490
C	5.67945685328290	3.59286691876105	6.47563904678652
H	6.19627077340660	4.54754247026104	6.37112627580436
C	5.86134091220442	-1.21674055818430	6.16438139423107
H	5.56664644327510	-1.39541560052213	7.21018578047761
H	6.62386822759834	-1.94530682241341	5.86814635762643
H	4.98026628594430	-1.31874232712259	5.51160959147020

C	4.16770750114997	6.07307671955879	5.11810212715301
C	3.86033037845427	5.12940775911872	4.12359913152935
H	3.21049663446586	4.28769827563575	4.36687907835519
C	4.35217138225531	5.24570944938961	2.81995677063568
H	4.07884619331898	4.49502361540215	2.07954453977126
C	5.17396461715522	6.33125849909765	2.48149514370561
C	5.48928591153200	7.28952722087256	3.45970909750569
H	6.13070051721520	8.13058986435014	3.19014824513240
C	4.98934188769920	7.16063157304953	4.75107494826482
H	5.24517698011956	7.91155845428769	5.50067325235108
C	5.41404052342720	5.58058529053647	0.21470500761645
H	5.79289238712346	4.58376139414734	0.48881993373191
H	5.92925701432830	5.93542352790331	-0.68419944688486
H	4.33174149483635	5.52159690456909	0.01991565227075
C	-0.55009657311144	7.66263865832062	12.95052662895292
C	0.02925743312613	7.05759117519309	14.08635260139120
H	1.07132804800144	6.73675433946556	14.04680135057624
C	-0.69620590092178	6.87152945183754	15.25840376660480
H	-0.23497402045276	6.41065990339663	16.13376691226186
C	-2.03838934361436	7.28040187211286	15.33101212216926
C	-2.63967500086721	7.87281444956500	14.21090090239651
H	-3.68254218607718	8.18572155793851	14.23168167424686
C	-1.89611350229983	8.05558005220819	13.04193760065406
H	-2.38012685528780	8.50655159612676	12.17479094125965
C	-4.04657031581655	7.45859881186071	16.63148271544202
H	-4.15705751361966	8.54322827387583	16.47249551865487
H	-4.35262082922910	7.20397119449259	17.65193365799940
H	-4.67781364795413	6.91511334897039	15.91151224133194
C	-0.31275175690434	10.28454641680340	11.35222186800332
C	-0.05091030915332	10.82557203103185	12.62923190396668
H	0.56905690133397	10.26566153527105	13.33028023630421
C	-0.55419771980710	12.06381335357227	13.00913082007726
H	-0.33823751099025	12.47451730065007	13.99683015745673
C	-1.34266040522322	12.81155060913944	12.11717881749756
C	-1.60734793439487	12.30108058549650	10.83868074852149
H	-2.21348952735103	12.85723504899661	10.12469091784953
C	-1.09092002518680	11.05424823233192	10.47117543695121
H	-1.30860874937826	10.66584719486536	9.47490109226404
C	-2.60131461116717	14.81138610857647	11.69736747441540
H	-2.03623030417571	15.09636254354079	10.79606609802226
H	-2.86696449188001	15.71091510511651	12.26277970123457
H	-3.51799080951058	14.27683412737361	11.40288784465753

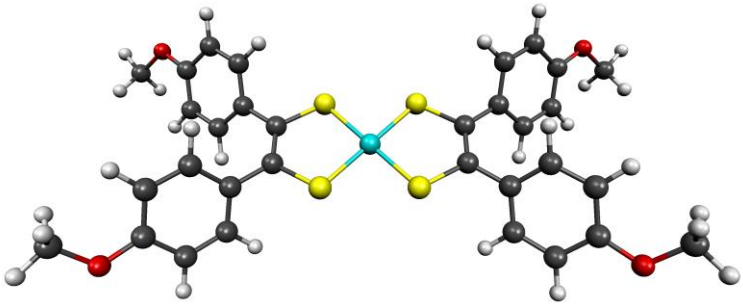

Figure S26. Geometry-optimized structure of $[Ni(adt)_2]^{1-}$

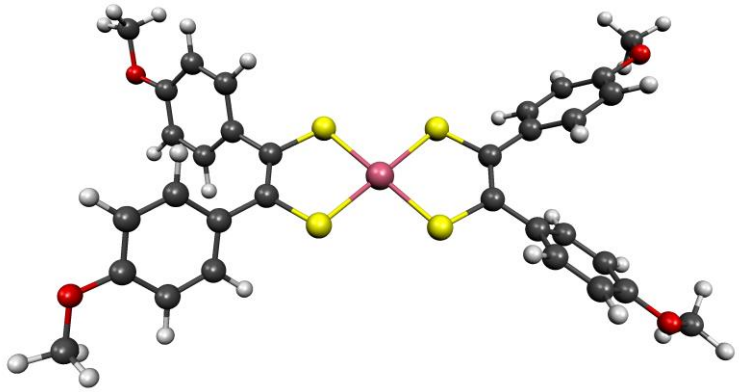

Figure S27. Geometry-optimized structure of $[Pd(adt)_2]^{1-}$

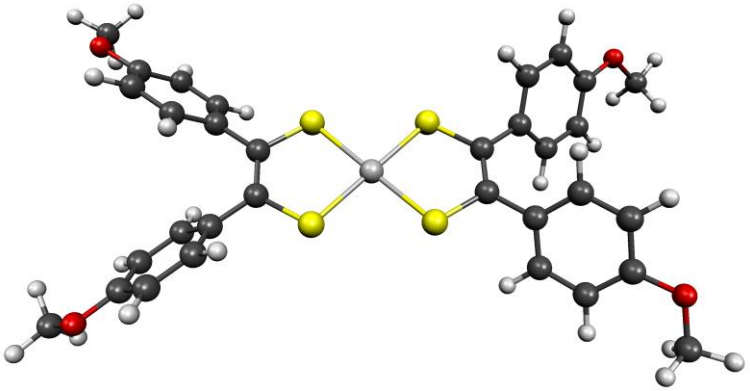

Figure S28. Geometry-optimized structure of $[Pt(adt)_2]^{1-}$

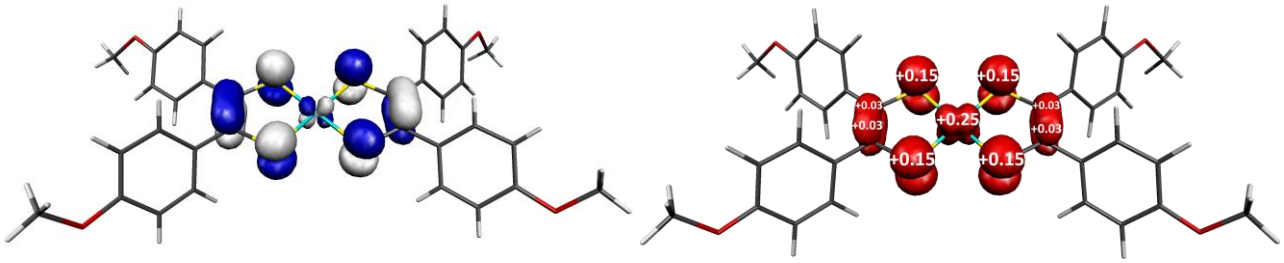

Figure S29. Depiction of the singly-occupied molecular orbital (left) and Mulliken spin population analysis (right) of $[Ni(adt)_2]^{1-}$

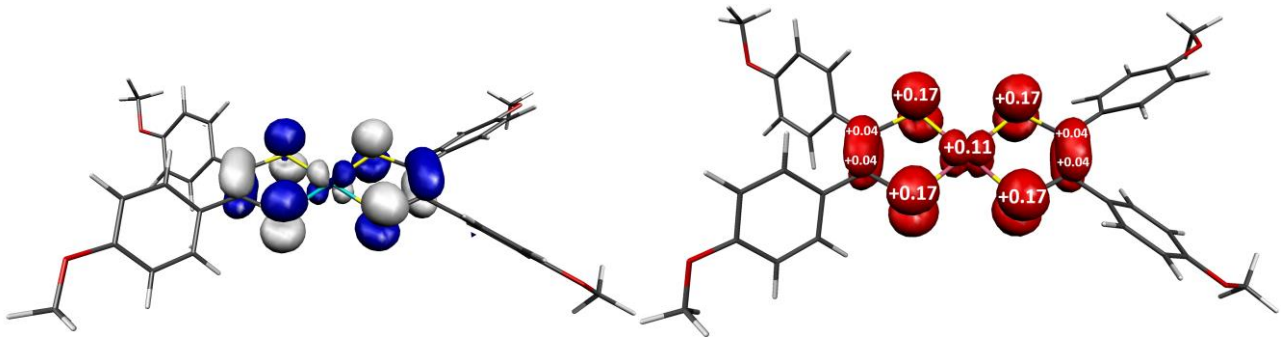

Figure S30. Depiction of the singly-occupied molecular orbital (left) and Mulliken spin population analysis (right) of $[Pd(adt)_2]^{1-}$

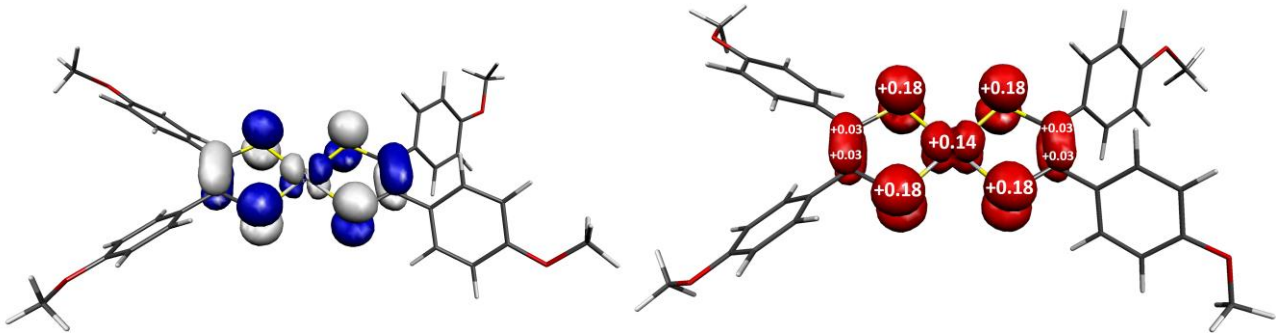

Figure S31. Depiction of the singly-occupied molecular orbital (left) and Mulliken spin poplation analysis (right) of $[Pt(adt)_2]^{1-}$

Table S13. Geometry Optimized Coordinates for [**4**]$^{2+}$

Ni	1.37771486412472	11.35356661673846	11.34033163562849
S	2.49908942284741	9.87330129838096	12.49248677317713
S	2.49103600858026	12.96182373311985	12.31412989074694
P	-0.11741336483122	9.89164994855657	10.72839592954049
P	0.61602296298384	12.73184605999638	9.81790485516629
O	6.02263026711480	7.67551194430161	17.59138699581222
O	7.43193095851857	15.71689816666264	15.64951272002040
C	3.54059161073799	10.78066747566682	13.56278915554207
C	3.61912319229321	12.19222638250413	13.39449555283057
C	-0.89461161107968	10.47679470582520	9.14996995936740
C	-0.60886345885707	11.80742581534385	8.76208040926016
C	-1.73312335704160	9.67123519771707	8.35394528679556
H	-1.94488344043324	8.63529292557763	8.66015073602809
C	4.22442104933534	10.01841263234510	14.61369151126291
C	4.66036519166104	8.68007840219840	14.38258443734232
H	4.53807685088905	8.24103139838325	13.38075692328322
C	5.26254977764816	7.93152758663224	15.38675010883872
H	5.62277303815920	6.90943372738403	15.20191232042742
C	5.43424454809973	8.48041958993471	16.68633064876931
C	4.98634970023109	9.79938928259069	16.94565485382587
H	5.08062340373456	10.24120344728382	17.94703904353819
C	4.40052138700332	10.54936776008768	15.92242409551948
H	4.03321401779268	11.55940013325577	16.15066896882273
C	6.23684655164184	8.14490022776741	18.92321566624585
H	6.89925256037528	9.03701019014388	18.93617795648400
H	6.72884967845218	7.31627788854491	19.46355264255831
H	5.27653057092795	8.39022097557742	19.42509215105997
C	4.61971880585250	13.06493876914024	14.02276344809701
C	4.28787300119512	14.39695815313973	14.40884718313765
H	3.24989165865201	14.74390365080423	14.29491548717732
C	5.24031953131755	15.25001104065570	14.95460512468525
H	4.97961702409901	16.26732879472758	15.27983533990399
C	6.58376644614823	14.81644017571465	15.11627452586835
C	6.94039959165216	13.50407972261582	14.71806529233485
H	7.97623794602992	13.14926474227390	14.80687662371880
C	5.96939653114613	12.64835138120448	14.18950546190714
H	6.27031196419790	11.64368846923957	13.86117727143920
C	8.79962406996999	15.36337537926257	15.85764582818639
H	8.89372358563368	14.50266594562724	16.55438520583489
H	9.27989592685996	16.25116039547123	16.30667880428570
H	9.30545770859604	15.11964869003447	14.89892254195384
C	-1.48130392230457	9.85745941478535	11.96506697983402
C	-1.14528247713301	9.50484418974959	13.29423178785909
H	-0.10420435654492	9.24942476654643	13.55021208713066
C	-2.13634685600468	9.48113512421274	14.28615900225035
H	-1.86788309753102	9.19692236875163	15.31492712466105
C	-3.46270043414588	9.82708130703500	13.97125918817501
H	-4.23599782826024	9.81615300765369	14.75456244824371
C	-3.79739925781590	10.19082982040140	12.65677138454830
H	-4.83350099836933	10.46410334785838	12.40516503480749
C	-2.81369915309482	10.20611032893815	11.65299371821671
H	-3.09457835937305	10.48568137323563	10.62698017622038
C	0.33806346659623	8.14167582745530	10.41050564974289
C	-0.47086027636182	7.06220096870931	10.82850959694008
H	-1.40180879357003	7.25067062670329	11.38493723239843
C	-0.07873025576244	5.74293822513672	10.54449776888796

H	-0.70918229675114	4.90416707011984	10.87624182541614
C	1.11729377726899	5.49487163054277	9.84965136745224
H	1.42413878070874	4.45989656691899	9.63476533958125
C	1.92894526383852	6.56760980939157	9.43938827854890
H	2.87264793341073	6.37355272055492	8.90742518943205
C	1.54656955038965	7.88748470712993	9.72214028375262
H	2.19434960916870	8.72532376694165	9.41967492790054
C	-0.24733616569438	14.25158114173660	10.37019334313583
C	-1.63872908806306	14.23473008684955	10.61785673637740
H	-2.23374069978748	13.33671958835957	10.39170577658417
C	-2.27181664009100	15.36581521724228	11.15654701288024
H	-3.35630599441894	15.34605456411878	11.34310995860531
C	-1.52436356217408	16.51694191773995	11.46034682560801
H	-2.02256459292942	17.40245798424193	11.88380203389868
C	-0.13882311043684	16.53442429265568	11.22653605603676
H	0.45064257502120	17.43252284286884	11.46644240172463
C	0.50323877569043	15.40726216534394	10.68897959285203
H	1.58966174302076	15.43047704082238	10.51535206837862
C	1.92405926441917	13.27479068520719	8.63999499937599
C	3.13861198360928	12.55457084738350	8.61682265132091
H	3.29359002876580	11.72451830496410	9.32496396561009
C	4.15492111356159	12.91532114494602	7.71723197104664
H	5.10238238171691	12.35521236384016	7.71062524569121
C	3.97019923997965	14.00062614427015	6.84372768796641
H	4.77318590481344	14.29113970754125	6.14890618694102
C	2.76671573391263	14.72816981957528	6.87055632622164
H	2.62742054041164	15.58969429695270	6.19972543863471
C	1.74433231704599	14.37085573703568	7.76508965527817
H	0.81806954679584	14.96455624766906	7.79734843831115
P	-2.79658789053248	12.11160173312833	5.21236548316313
P	-3.53057348934827	9.27144809206997	6.12331511016625
C	-2.02002399323144	11.52655299767055	6.79114592722257
C	-2.30563702569360	10.19586113984954	7.17892942052372
C	-1.18142246766120	12.33207496450988	7.58712174647121
H	-0.96983036538559	13.36810085532433	7.28107808522354
C	-1.43142003811122	12.14751917031445	3.97712310110148
C	-1.76635167709584	12.50096438103104	2.64789634414959
H	-2.80733554365836	12.75590184109066	2.39105851539135
C	-0.77435041894170	12.52603346119518	1.65694317850424
H	-1.04199278360692	12.81086246557245	0.62812923644724
C	0.55197060963987	12.18093993719288	1.97292768034277
H	1.32603896450276	12.19302773987997	1.19040266313364
C	0.88567420503061	11.81671881440742	3.28752984501650
H	1.92174324902298	11.54413714465164	3.54000661607700
C	-0.09903436885651	11.79984931949228	4.29029953098964
H	0.18116014071750	11.52022569009924	5.31648272439615
C	-3.25390449747648	13.86108860975746	5.53055759259230
C	-2.44577282841405	14.94147579531371	5.11340336673307
H	-1.51428295333734	14.75411786268107	4.55752570653154
C	-2.83928055789918	16.26026121328463	5.39773094812218
H	-2.20942115179651	17.09974549719343	5.06665755945536
C	-4.03579542267508	16.50693793828466	6.09221962476093
H	-4.34367664279693	17.54154269675468	6.30741907488297
C	-4.84655866504686	15.43327728293793	6.50182106528196
H	-5.79061209729733	15.62622874161537	7.03356085930179
C	-4.46287026400107	14.11387866824074	6.21862344386202
H	-5.10989121904371	13.27531555471150	6.52070502509754
C	-2.66762360670986	7.75155279685045	5.57081936147586
C	-1.27627308678950	7.76829262973644	5.32298905767490

H	-0.68098644950528	8.66597531437849	5.54975966324181
C	-0.64342827148751	6.63734109791491	4.78372719966936
H	0.44108697807354	6.65692514876007	4.59731268796426
C	-1.39126677495181	5.48682428863859	4.47856338375488
H	-0.89329070990934	4.60146733335838	4.05451497191039
C	-2.77695059257360	5.46984794678489	4.71153946706290
H	-3.36671918685797	4.57222543983523	4.47059811923925
C	-3.41865435885212	6.59664285337701	5.25030978185987
H	-4.50534297531177	6.57417561525838	5.42232163677293
C	-4.83876802089361	8.72911327262837	7.30120760518427
C	-6.05279057098572	9.45020881882914	7.32483316255496
H	-6.20724838951481	10.28067274236390	6.61707763065510
C	-7.06921587059855	9.08983260608500	8.22445515147908
H	-8.01628930143483	9.65059287684205	8.23144070058288
C	-6.88512948446875	8.00405459688929	9.09750086825249
H	-7.68823363278771	7.71381249913689	9.79230265295004
C	-5.68218392490894	7.27562667020241	9.07018707202398
H	-5.54345933606496	6.41369037645395	9.74061433543472
C	-4.65972231293842	7.63250264835910	8.17558204054400
H	-3.73391458407683	7.03812554798596	8.14285726521491
Ni	-4.29112273461371	10.64940443669872	4.59920402575785
S	-5.41032744568681	12.12929043290422	3.44467383078156
S	-5.40550982686471	9.04101244925921	3.62658314094477
O	-8.92721436237433	14.32493975883294	-1.65968381778846
O	-10.34434367718014	6.28618012662390	0.28815046474011
C	-6.45187016600885	11.22177742292477	2.37457304754212
C	-6.53186888936908	9.81047483785105	2.54433539400287
C	-7.13413672085671	11.98355378515568	1.32230356212516
C	-7.56954260895071	13.32234083702771	1.55172063054903
H	-7.44823173637429	13.76223569625354	2.55330559477860
C	-8.17010996519501	14.07034675624808	0.54616614562830
H	-8.52998103850610	15.09280895239428	0.72966794013911
C	-8.34051134365603	13.52044302857123	-0.75315035627293
C	-7.89304445690561	12.20100533130575	-1.01078652988361
H	-7.98637686777948	11.75835895924877	-2.01189585507440
C	-7.30894491325880	11.45156742412467	0.01382426487882
H	-6.94182281528259	10.44115952547807	-0.21309081390212
C	-9.14004584877026	13.85443214095380	-2.99133383452775
H	-9.80332901736275	12.96297196003652	-3.00429315315962
H	-9.63042964871647	14.68299847306621	-3.53322428228210
H	-8.17928693199527	13.60752127393404	-3.49157358833582
C	-7.53240990529286	8.93789600243353	1.91580573076269
C	-7.20083070950737	7.60546459758163	1.53088658615354
H	-6.16311295338671	7.25813988026843	1.64599075733858
C	-8.15316588677162	6.75247873236716	0.98484162938353
H	-7.89264458141503	5.73482284650955	0.66052062594309
C	-9.49623782686447	7.18659603531151	0.82155479489362
C	-9.85258261272682	8.49947099859012	1.21834097689758
H	-10.88815210923341	8.85471929604296	1.12825575680441
C	-8.88170611039890	9.35504746650058	1.74736837707254
H	-9.18238645154511	10.36019145002756	2.07443574510147
C	-11.71161495589584	6.64030953379625	0.07828858886184
H	-11.80448336406080	7.50038167192076	-0.61940746059619
H	-12.19196507516414	5.75236696451678	-0.37035290712458
H	-12.21826227127439	6.88529025374714	1.03625956651794

Table S14. Geometry Optimized Coordinates for $[5]^{1+}$

Ni	10.84973298332259	9.96050024642930	3.55496329378698
S	9.46390668495712	11.18922634036232	2.39294438712532
S	9.95260410252496	10.68737419806108	5.41184585155346
P	12.15973868315295	9.64317853782454	1.83882159203120
P	11.85152257158329	8.31028861201714	4.58016854003435
O	5.26868780857288	16.21659791051481	1.46460556403688
O	5.24151303200552	13.28903337556705	9.19070186150623
C	8.49478270651472	12.05110145679508	3.55548955508272
C	8.64576786021872	11.73392636834269	4.93574671810861
C	14.98543102040669	6.58804661100078	1.59338991774436
H	15.70094281510736	6.18259580120090	0.86177720232501
C	14.16491450902189	7.66995399702506	1.23881269671092
H	14.23841507585312	8.11150131058598	0.23334218896559
C	13.24765944247506	8.18943453069427	2.17577897042096
C	13.14024981269727	7.60529400527806	3.45772626707370
C	13.97784092216792	6.52767036926663	3.81282430668941
H	13.90754201281827	6.07567674225462	4.81408007552111
C	14.89719473995281	6.02300415311769	2.87991587208301
H	15.54555996210579	5.17678528621959	3.15424923168274
C	7.61453849042544	13.10165937200650	3.02178147679050
C	6.97968719410044	12.94799422692866	1.76129041478691
H	7.10405071812859	12.00221108951223	1.21217257750486
C	6.18224543402253	13.95567212749084	1.20913790768597
H	5.69475191794009	13.78279510989221	0.24053319371294
C	6.01056498516903	15.17717270932683	1.90536275669322
C	6.65349271191164	15.35682063797596	3.15679254081528
H	6.52965291247972	16.31983388778397	3.67336446651070
C	7.43112043623335	14.34107839646698	3.70340570017651
H	7.93919217425583	14.51450383624215	4.66212225497470
C	4.60210965685541	16.11825923928449	0.20813988871847
H	5.32283723106917	15.97552673815025	-0.62565048958005
H	4.07036356080537	17.07649759886188	0.06736439668191
H	3.86376181448173	15.28708215972178	0.20215844513262
C	7.74337790523669	12.18143212861005	6.00761131777150
C	6.33947082662617	12.26438404204253	5.80700235511447
H	5.91742558184720	12.00833774956000	4.82498596942889
C	5.46967825442504	12.62104627741491	6.84285065908428
H	4.38907549383055	12.65196056865311	6.64586732389300
C	5.98673112190263	12.92235643706148	8.12601618899170
C	7.38666031021126	12.84023739259447	8.34567166236644
H	7.77211947209097	13.08542586551632	9.34593116118329
C	8.23994797598267	12.46667228714563	7.31263263012212
H	9.32331398172980	12.40955857325563	7.49764033778698
C	3.82757789459162	13.40150005752977	9.04938055340582
H	3.55397382879262	14.16722421091017	8.29148892932618
H	3.44384322187430	13.71391408363131	10.03722470028403
H	3.36717222992410	12.42895270416653	8.77011525425572
C	11.44354327124092	9.34235016983502	0.17535335525202
C	10.23286559058449	8.61696574440803	0.10489359971203
H	9.72358075912122	8.31061677510946	1.03219772304284
C	9.67461901889433	8.30217691628395	-1.14356796122323
H	8.72948446821082	7.74071838641092	-1.19354621192992
C	10.31507187061994	8.71366658558590	-2.32539531283001
H	9.87444391126320	8.46901065855223	-3.30375562953571
C	11.51429876366080	9.44383665569213	-2.25913976298811
H	12.01300787410015	9.77217654180454	-3.18355306583392
C	12.08077097710667	9.76151246356556	-1.01345951181211

H	13.01531143501078	10.34122368340900	-0.96846346904977
C	13.29789145860254	11.07953843883111	1.67496360152516
C	12.78629498197391	12.29890914561918	1.17005411034444
H	11.73698162249131	12.36580466244565	0.84319476831355
C	13.61439255315907	13.42839565473346	1.09133308954785
H	13.21151140413866	14.37034807024827	0.68914733050532
C	14.94983695751750	13.36081721292367	1.52820914855857
H	15.59547116637483	14.25020491910003	1.46581925469176
C	15.45665316049494	12.15738535191664	2.04603663150324
H	16.49966068380203	12.09939479082175	2.39223553943112
C	14.63627765595442	11.01876444779119	2.12262749825506
H	15.04547430881787	10.08108469281682	2.52676080799827
C	10.66128392928032	6.93964797521996	4.87495201894736
C	10.58224096129594	5.83395090839825	3.99890545657067
H	11.28022586023372	5.74106840339763	3.15286495750125
C	9.61348151528290	4.83780816013650	4.20759354606855
H	9.56481013164112	3.97516403430195	3.52517039431700
C	8.71506843439300	4.93871919848311	5.28277975662107
H	7.95974208391102	4.15443863560120	5.44606851003047
C	8.78086022459558	6.04516460909236	6.14885452936879
H	8.07636467248488	6.13204710252011	6.99042322638441
C	9.74181232662699	7.04688513314596	5.94506082412874
H	9.77327226855955	7.91871268268243	6.61663436774249
C	12.70575258241269	8.62487825216012	6.17494015952703
C	12.84508582732185	7.63446231687895	7.17278721834130
H	12.37974139881212	6.64507497785350	7.04474949343458
C	13.57042325626884	7.91798651877019	8.34188761811766
H	13.67666070232485	7.14455116357112	9.11831510215909
C	14.15438833725481	9.18387572727575	8.52321001058893
H	14.71807780247393	9.40188251588992	9.44316038328233
C	14.01062916246897	10.17377769071573	7.53546430529371
H	14.45865663028728	11.16861068127802	7.67934148569870
C	13.28532051836306	9.89953192312367	6.36534037330046
H	13.15517239816321	10.67927806130485	5.59798406299547

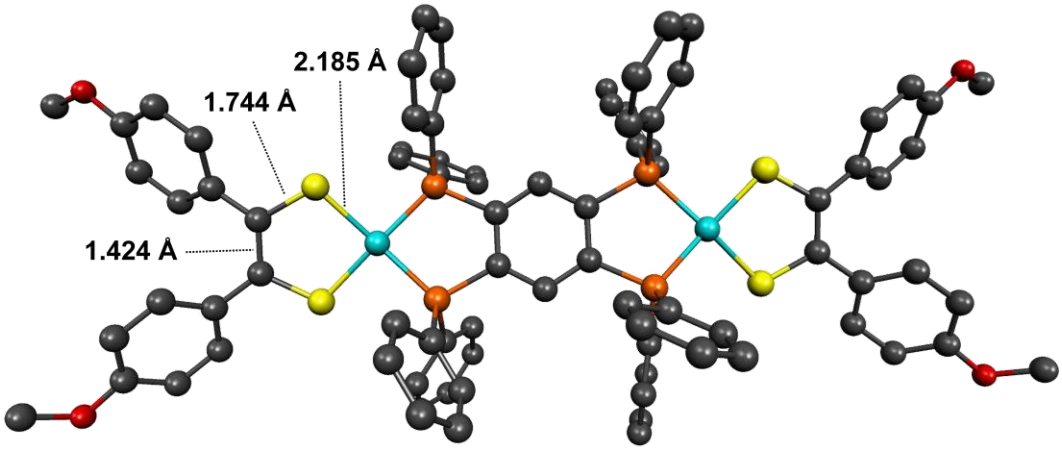

Figure S32. Geometry-optimized structure of [**4**]$^{2+}$

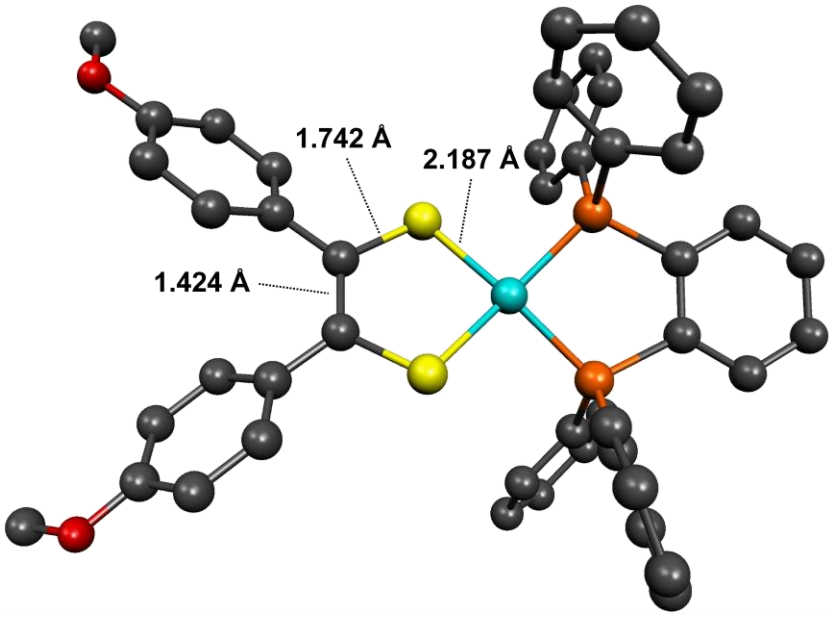

Figure S33. Geometry-optimized structure of [**5**]$^{1+}$

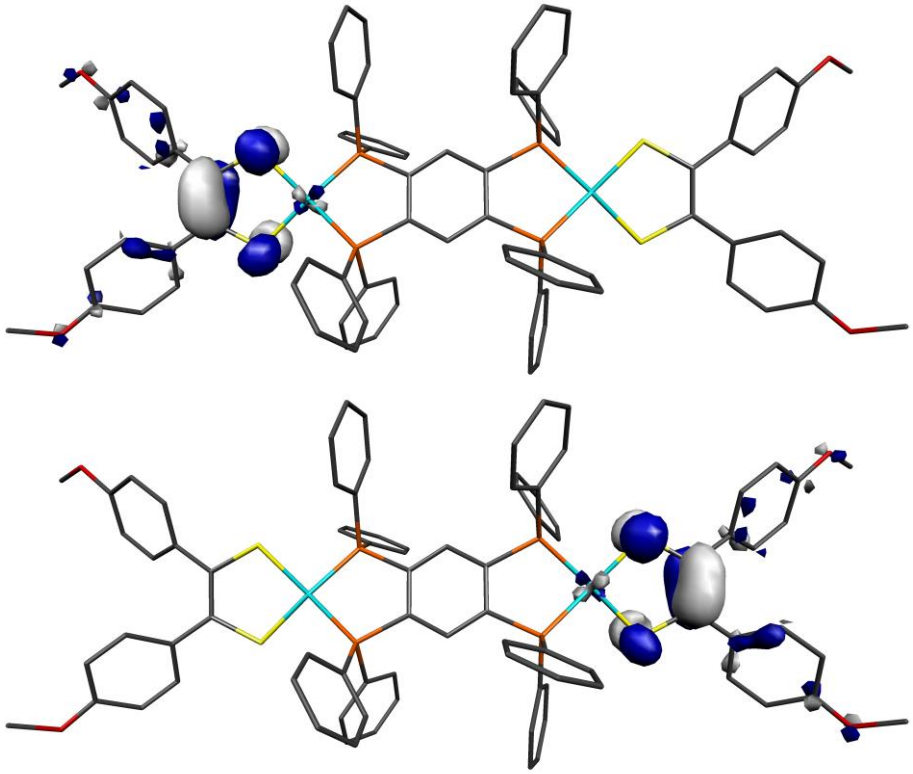

Figure S34. Depiction of the magnetic orbitals of [**4**]$^{2+}$

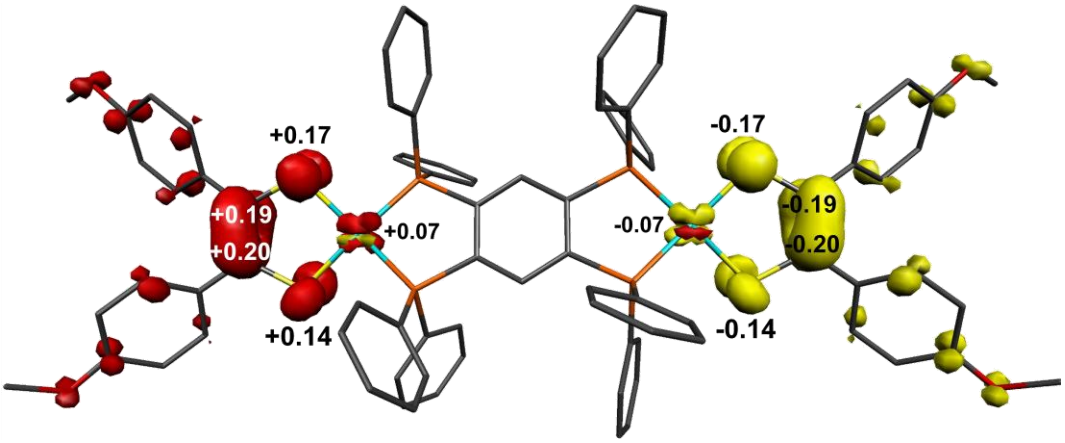

Figure S35. Mulliken spin distribution for [**4**]$^{2+}$

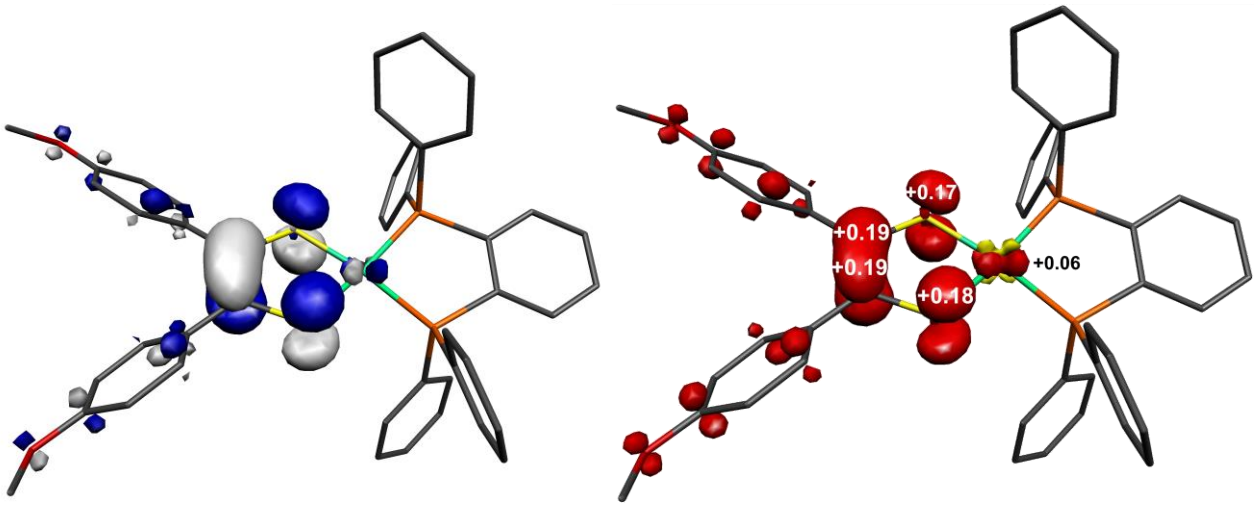

Figure S36. Depiction of the singly-occupied molecular orbital (left) and Mulliken spin population analysis (right) of [**5**]$^{1+}$