Electronic Supplementary Material (ESI) for Dalton Transactions.

Tuning of Spin Crossover Properties in a Series of Mononuclear Cobalt(II) Complexes Based on Macrocyclic Tetradentate Ligand and Pseudohalide Coligands

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Experimental Section

Materials

The reactions and manipulations presented herein were performed under an argon atmosphere using standard Schlenk techniques if not otherwise stated. Solvents were dried using conventional drying methods and freshly distilled before use. The reagents were used as commercially available without further purification. The Ligand **L** was prepared according to a literature procedure reported elsewhere.[1]

Physical Methods

Physical methods including magnetic measurements and single-crystal X-ray diffraction studies (*vide infra*) were performed using a similar procedure described by Mondal *et*. al.[2] The elemental analyses of C, H, and N were studied with a Thermo Scientific Flash 2000 Organic Elemental Analyzer. Infrared (IR) spectra were recorded in the spectral range of 4000–400 cm^{-1} on a Bruker Tensor 27 spectrometer. UV-vis-NIR spectra were studied from 250–2000 nm on a Lambda 750 UV-vis-NIR spectrometer. Solution−state UV-vis-NIR spectroscopic studies were recorded with 1 cm quartz cuvettes, while Solid−state spectra were recorded using *ca*. 5% sample by weight in KBr. Thermogravimetric analysis (TGA) was measured using a Mettler Toledo TGA/SDTA851 analyzer from 27°C to 300°C (10 °C min^{-1}) under nitrogen atmosphere. Powder X-ray diffraction (PXRD) studies were performed with a PANalytical Empyrean diffractometer at 45 kV and 30 mA, under Cu−Kα radiation (λ = 1.54059 Å) and data analyses have been performed by PANalytical X'Pert HighScore Plus software.[3] Electrochemical measurements were done using a Metrohm Autolab PGSTAT101, where platinum has been used as a working electrode in DMF with 0.2 M $^{n}Bu_4NPF_6$ supporting electrolyte. The concentration of sample *ca*. 1 mM has been used. Ferrocene has been applied as an internal reference. To remove the adhering mother liquor from the crystalline complexes, it has been isolated from the mother liquor and soaked gently over filter paper, before any physical measurement.

Magnetic Measurements

The magnetic investigation was carried out with a Quantum Design MPMS−XL EverCool SQUID magnetometer, from 2−300 K, 2−375 K, and 2−400 K for **1**−**3**, respectively, under an external dc applied fields in the range of −5 T to 5 T. Polycrystalline samples of **1**−**3** (14.40, 18.21 and 26.74 mg, respectively)

placed in a polypropylene bag (2.8 × 0.75 × 0.02 cm) were subjected to measurements. The temperature dependence of magnetization was recorded under 2500 Oe and 10000 Oe external dc field. The isothermal magnetization was studied at 4 and 8 K. *M vs H* data were recorded at 100 K to examine the presence of ferromagnetic impurities which were observed to be absent. The magnetic data were corrected for the sample holder and the diamagnetic contribution.

X-ray Crystallography

Single–crystal X–ray structure diffraction studies of complexes **1**–**3** was performed with a Bruker SMART APEX CCD diffractometer equipped with graphite–monochromated Mo Kα radiation (λ = 0.71073 Å). The single crystal was mounted on crystal mounting loops using Paratone oil at 296 K and collected the data. For variable temperature measurements, the single crystal was slowly cooled to measure temperature using a sweep rate of 2 K/min, and collected data at 240 K (**2**) and 100 K (**1** and **2**). Data integration and reduction were carried out using SAINT software, and empirical absorption corrections were performed using SADABS program.[4] The structures were solved by direct methods and refined using full-matrix least-squares method on F2 with SHELXL-2014.[5] All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed to ideal positions and refined isotopically with riding model.

Figures and Tables

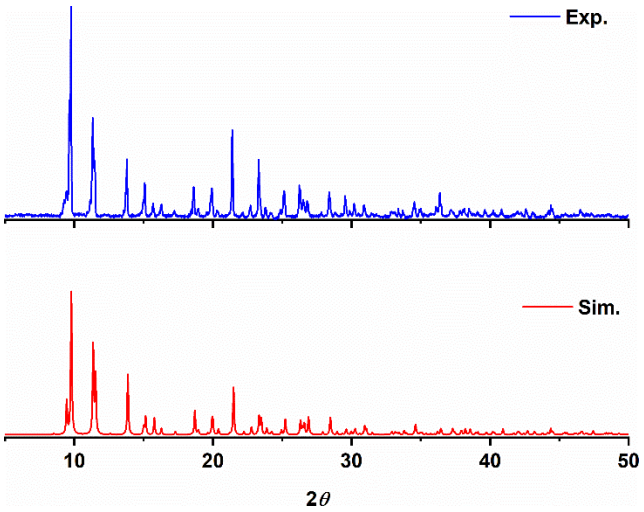


Fig. S1. Comparison of the room temperature experimental PXRD pattern and the 296 K simulated one for **1**.

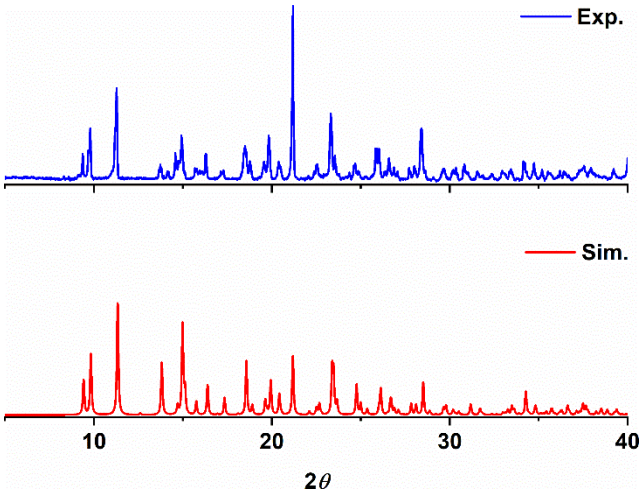


Fig. S2. Comparison of the room temperature experimental PXRD pattern and the 296 K simulated one for **2**.

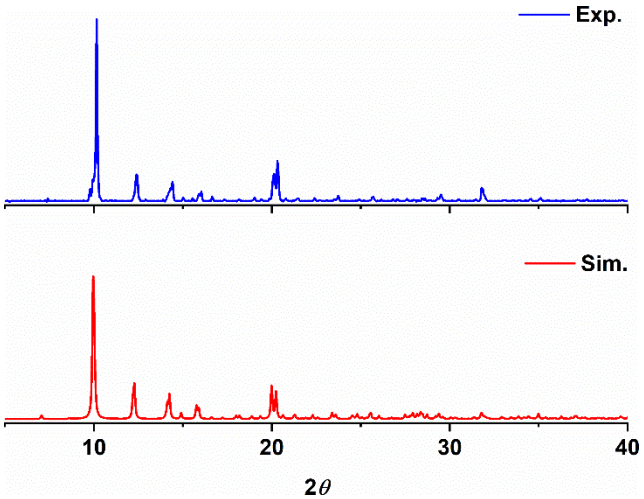


Fig. S3. Comparison of the room temperature experimental PXRD pattern and the 296 K simulated one for **3**.

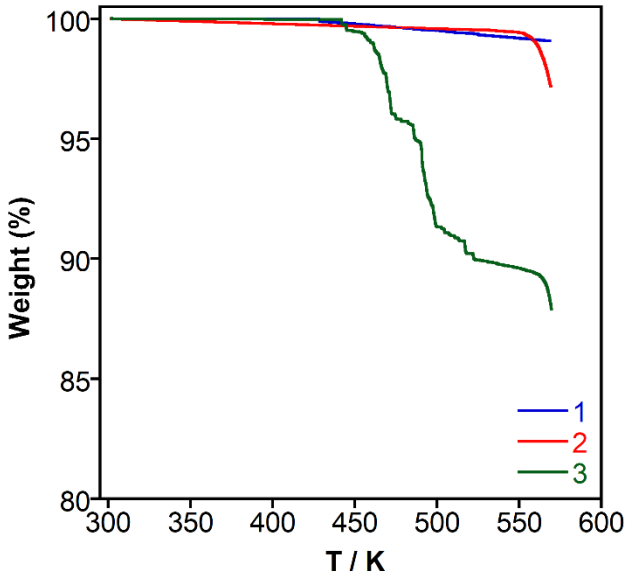


Fig. S4: TGA analysis for **1**–**3**.

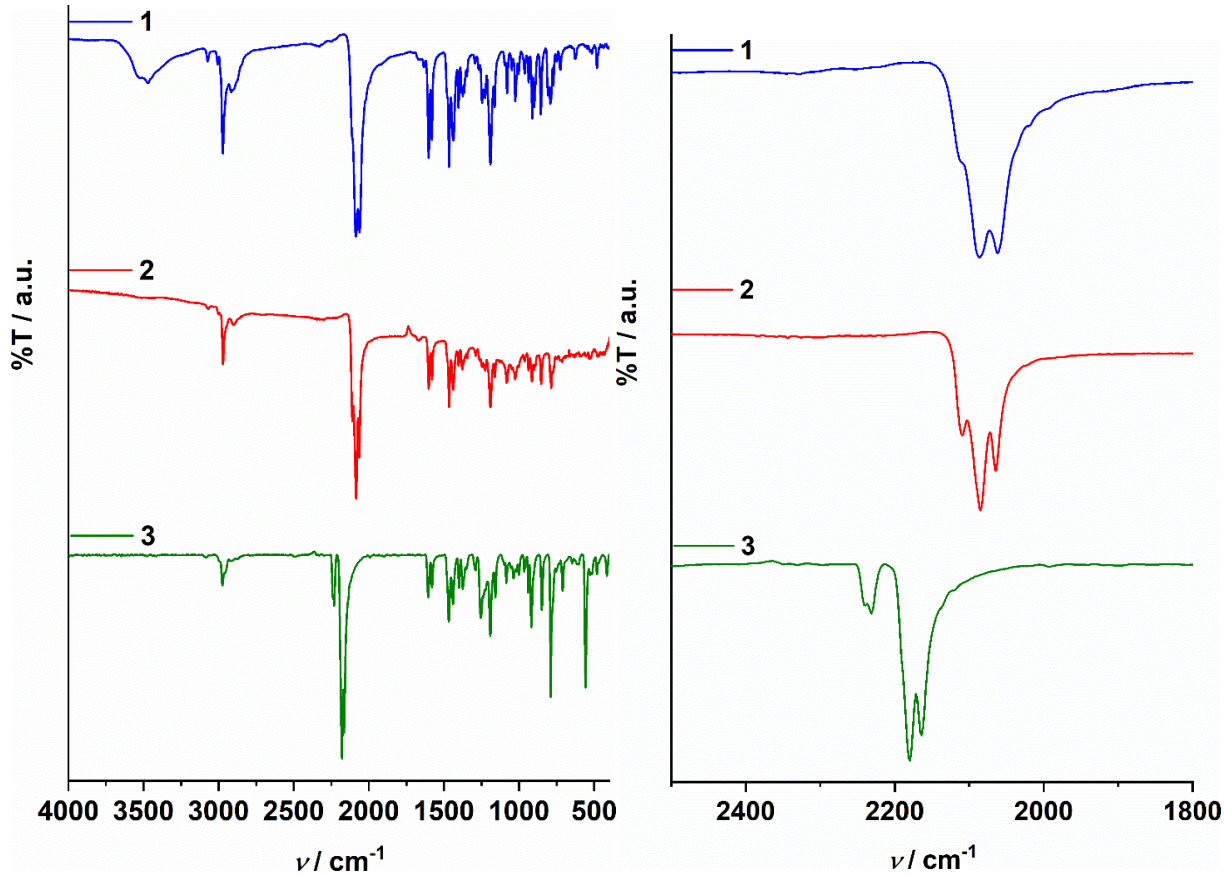


Fig. S5. Left: IR spectra of **1**, **2** and **3** at room temperature; Right: ν(C≡N) region of the IR spectra.

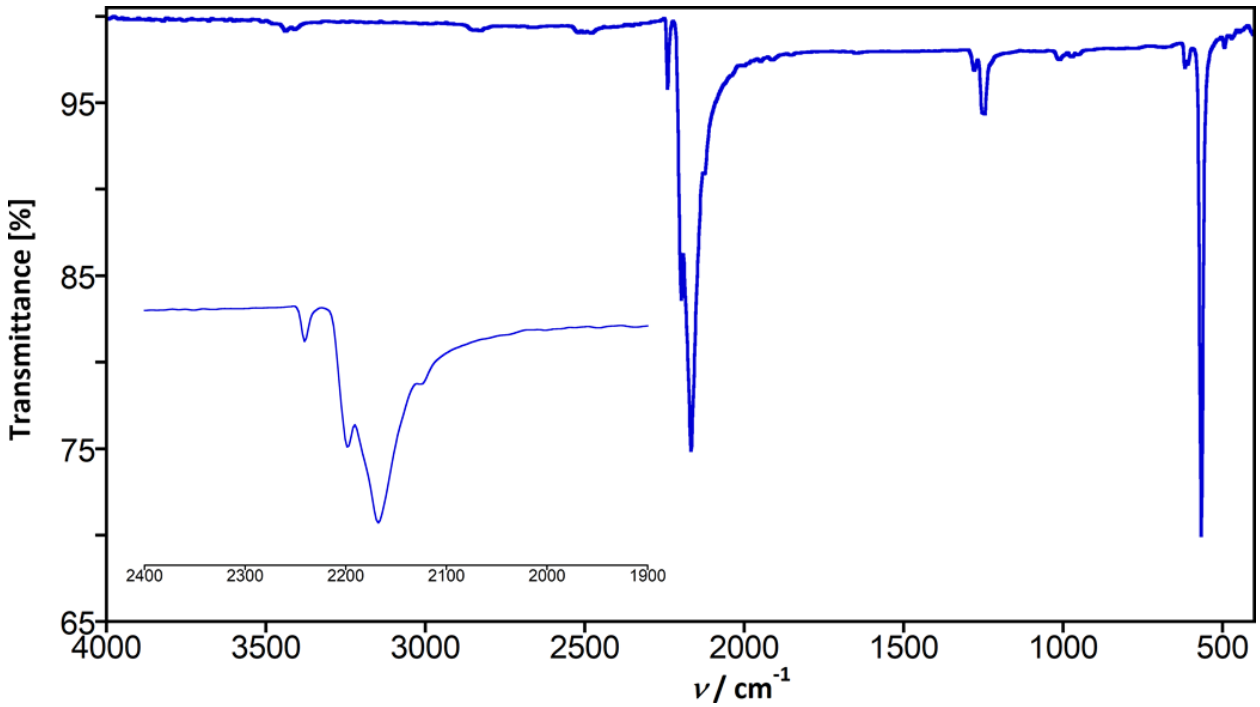


Fig. S6. IR spectrum of $Na[C(CN)_3]$ at room temperature. Inset: ν(C≡N) region of the spectrum.

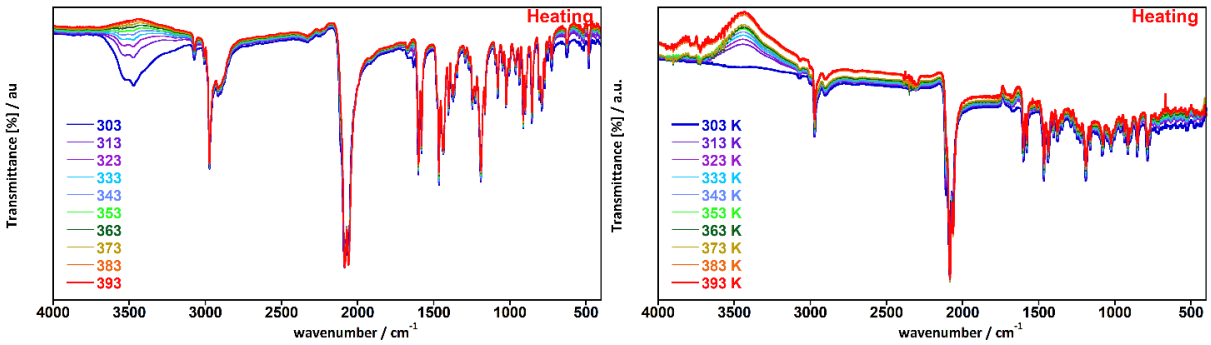


Fig. S7. Variable temperature IR spectra of **1** and **2** in heating mode.

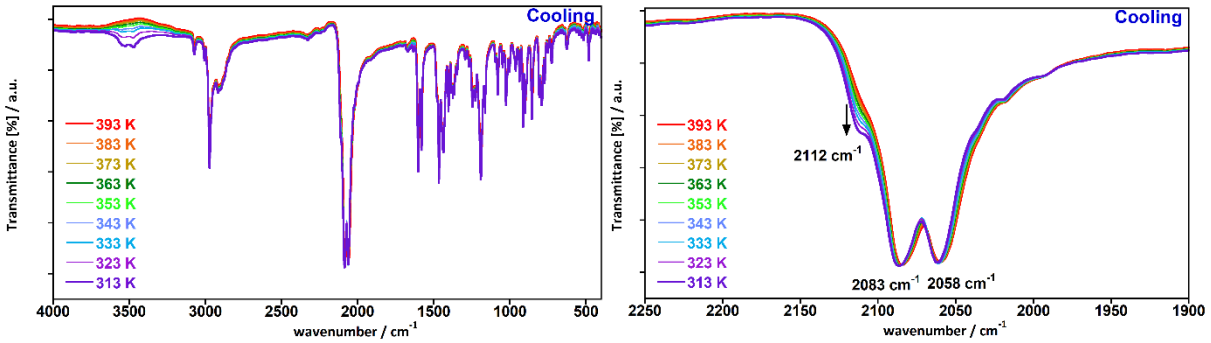


Fig. S8. Left: Variable temperature IR spectra of **1** in cooing mode. Right: Selected region of the spectra. Arrows indicate a change in intensities.

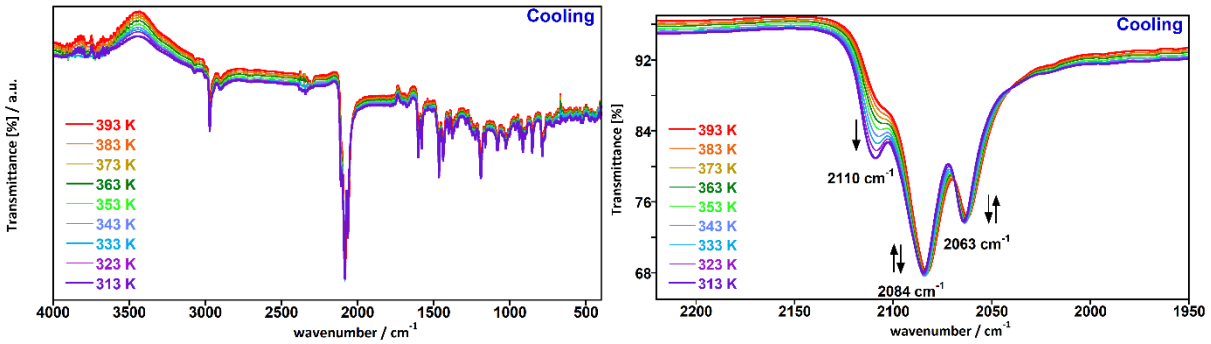


Fig. S9. Left: Variable temperature IR spectra of **2** in cooing mode. Right: Selected region of the spectra. Arrows indicate a change in intensities.

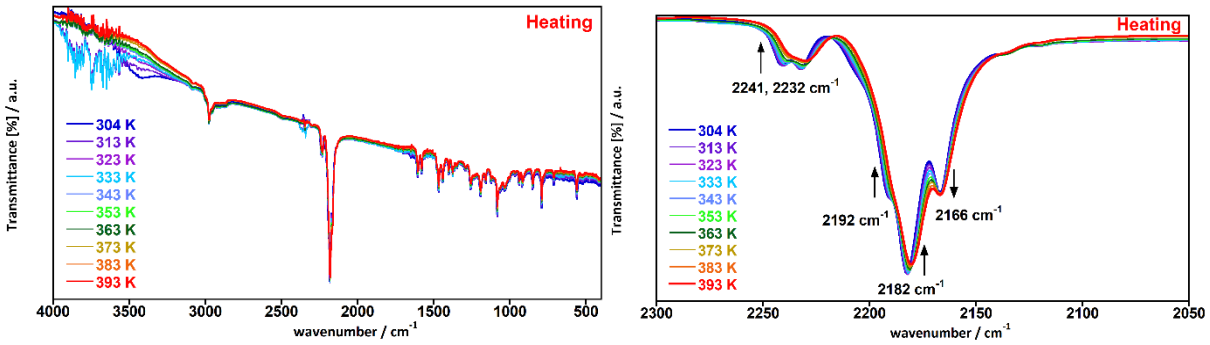


Fig. S10. Left: Variable temperature IR spectra of **3** in cooing mode. Right: Selected region of the spectra. Arrows indicate change in intensities.

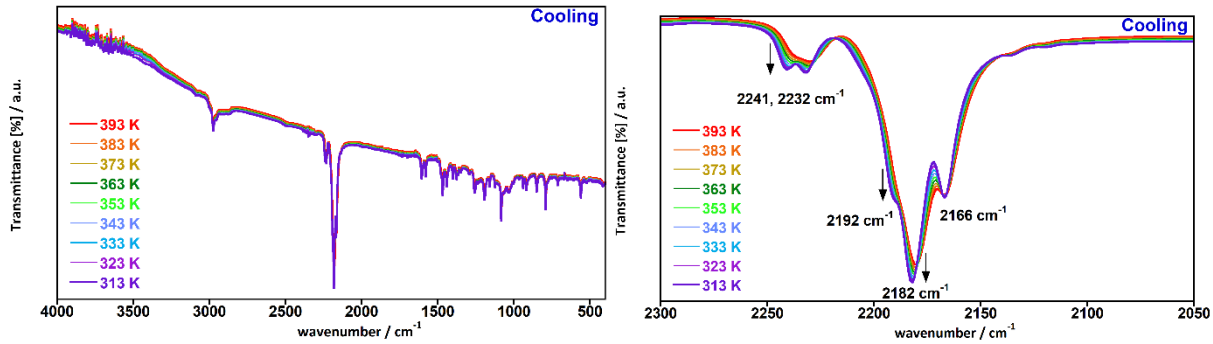


Fig. S11. Left: Variable temperature IR spectra of **3** in cooing mode. Right: Selected region of the spectra. Arrows indicate a change in intensities.

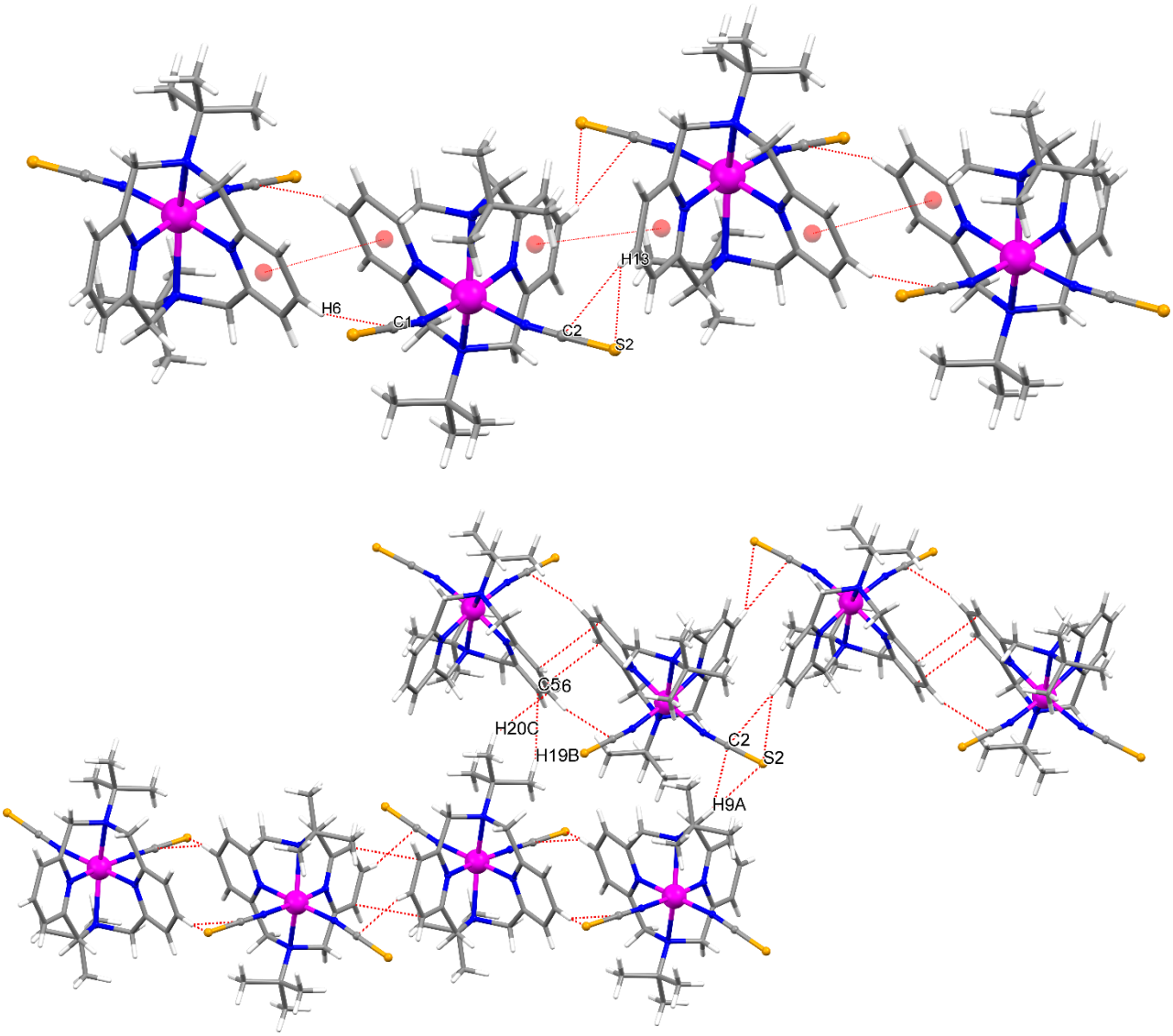


Fig. S12. Packing diagrams of **1** at 100 K showing the 1D supramolecular arrangement (top) and the supramolecular double chain (bottom) connected by intermolecular π···π, C-H···C and C-H···S (red dotted lines) interactions (Co: pink, C: gray, N: blue, S: orange, H: white).

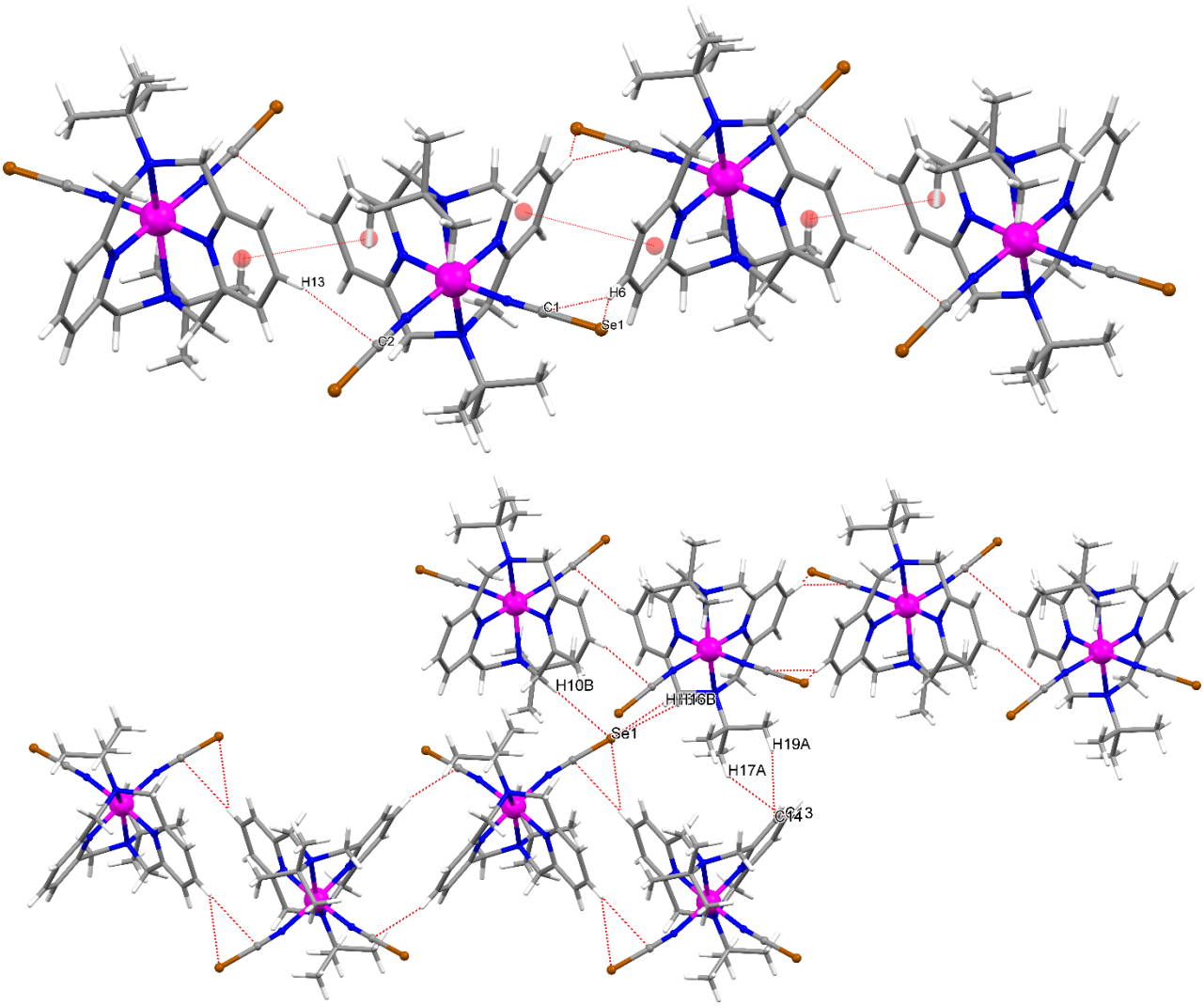


Fig. S13. Packing diagrams of **2** at 100 K showing the 1D supramolecular arrangement (top) and the supramolecular double chain (bottom) connected by intermolecular π···π, C-H···C and C-H···Se (red dotted lines) interactions (Co: pink, C: gray, N: blue, S: orange; Se: brown, H: white).

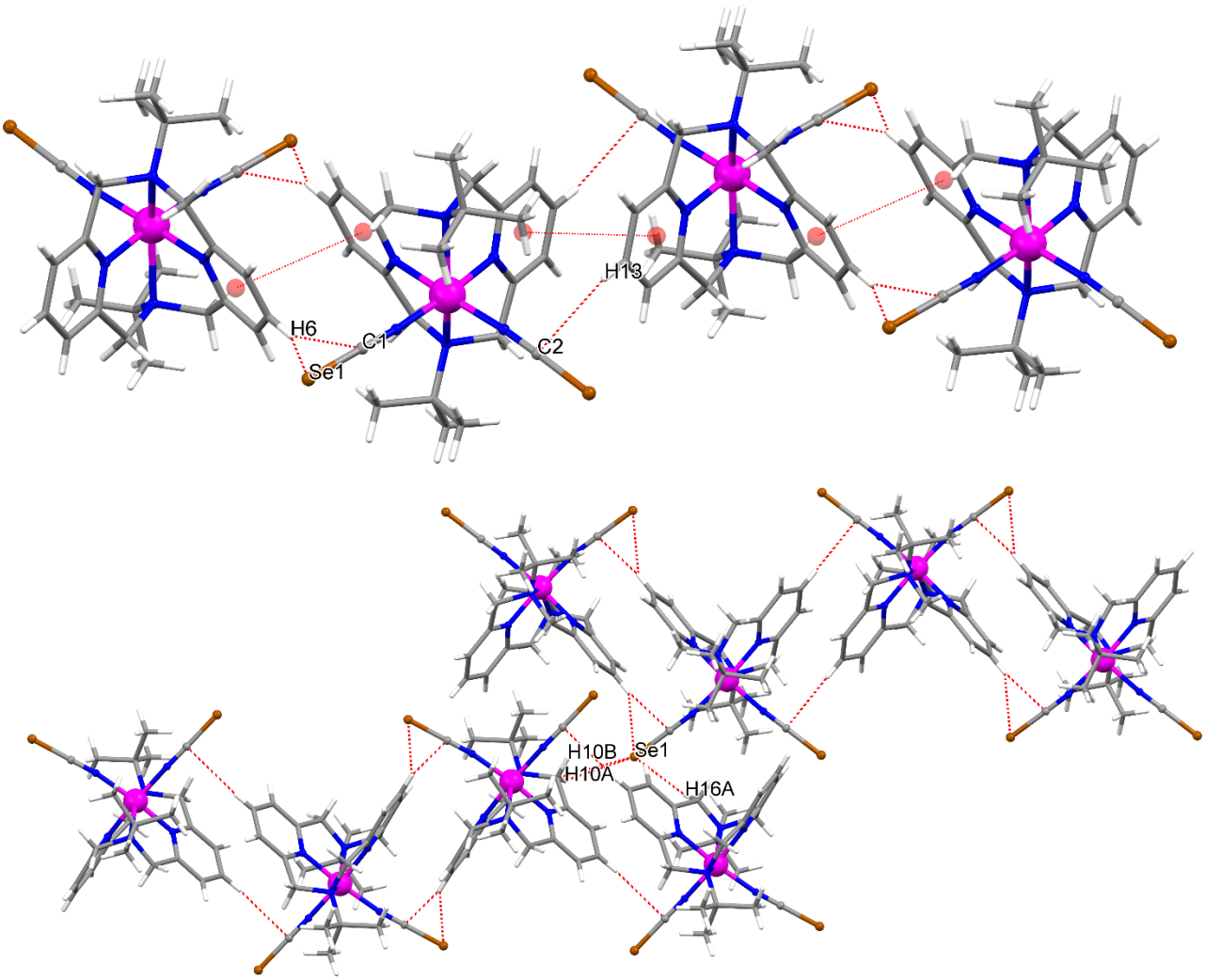


Fig. S14. Packing diagrams of **2** at 240 K showing the 1D supramolecular arrangement (top) and the supramolecular double chain (bottom) connected by intermolecular π···π, C-H···C and C-H···Se (red dotted lines) interactions (Co: pink, C: gray, N: blue, S: orange; Se: brown, H: white).

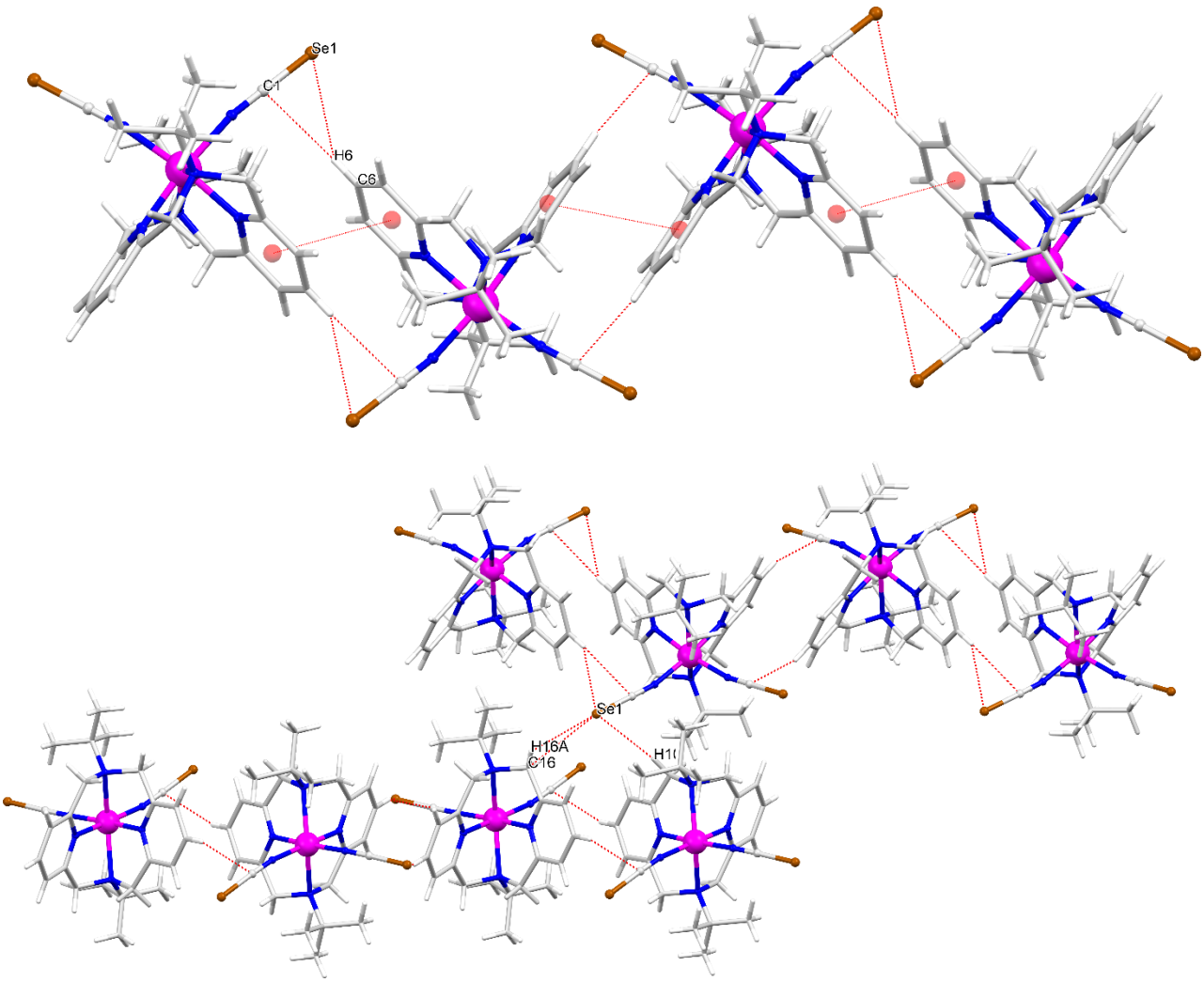


Fig. S15. Perspective view of the packing diagrams of **2** at 296 K displaying supramolecular 1D (top) and double chain (bottom) arrangements produced by several intermolecular π···π, C–H···C and C–H···Se (red dotted lines) interactions (Co, pink; C, gray; N, blue; Se, brown; H, white).

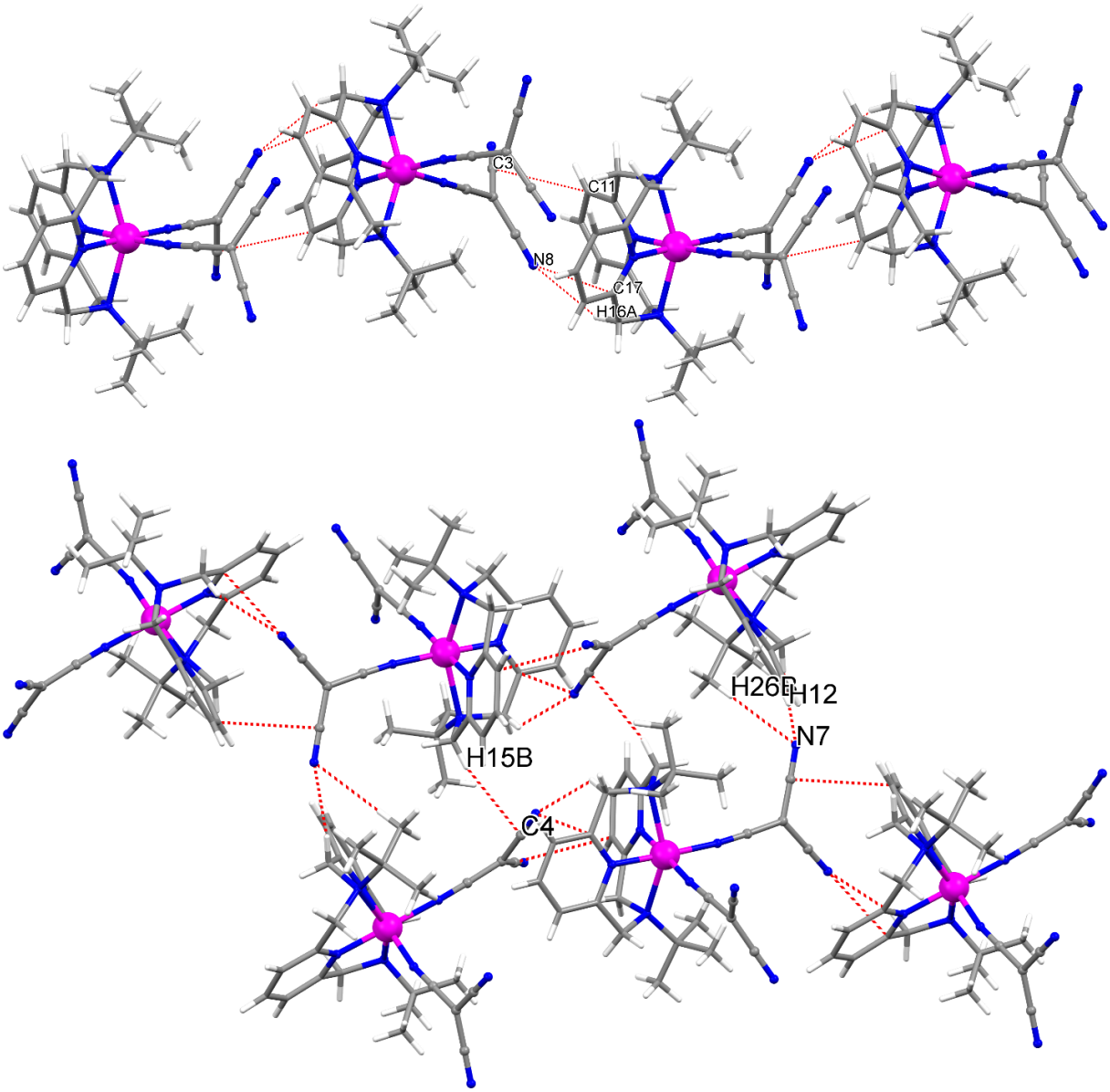


Fig. S16. Packing diagrams of **3** at 296 K showing the 1D supramolecular arrangement and the double layer supramolecular chain connected by intermolecular C-H···N and C-H···C (red dotted lines) interactions (Co: pink, C: gray, N: blue, H: white).

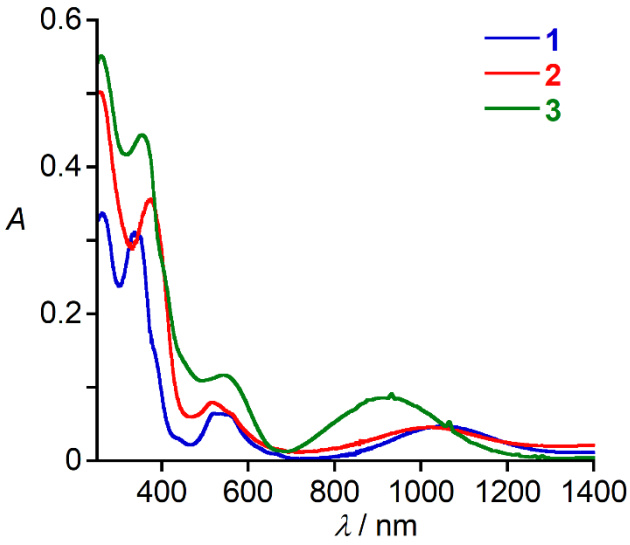


Fig. S17. Solid state UV-vis-NIR spectra of **1**–**3** at room temperature.

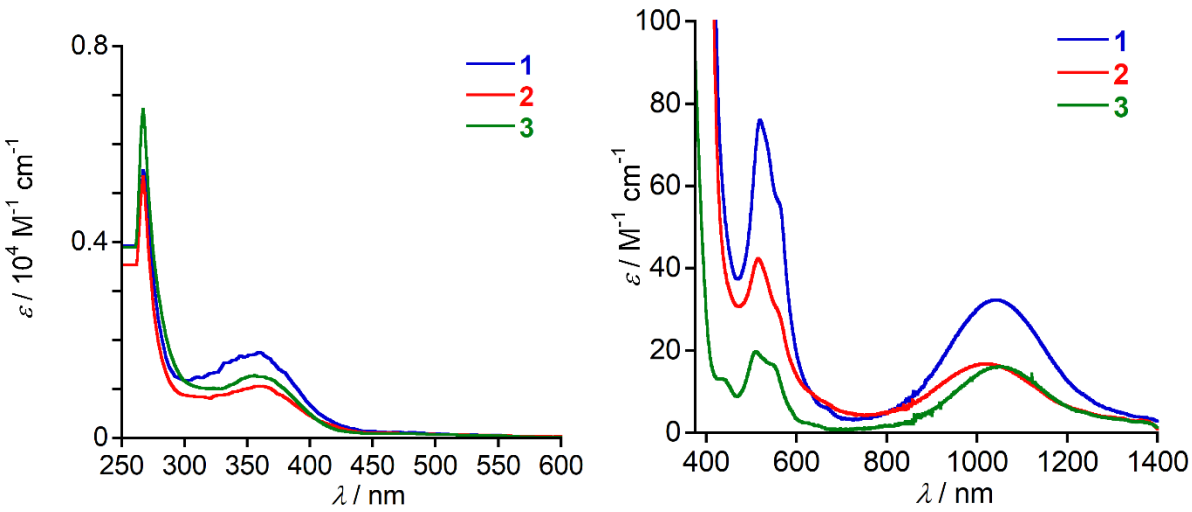


Fig. S18. UV-vis-NIR spectra of **1**, **2** and **3** in DMF at room temperature (left: dilute solution, right: concentrated solution).

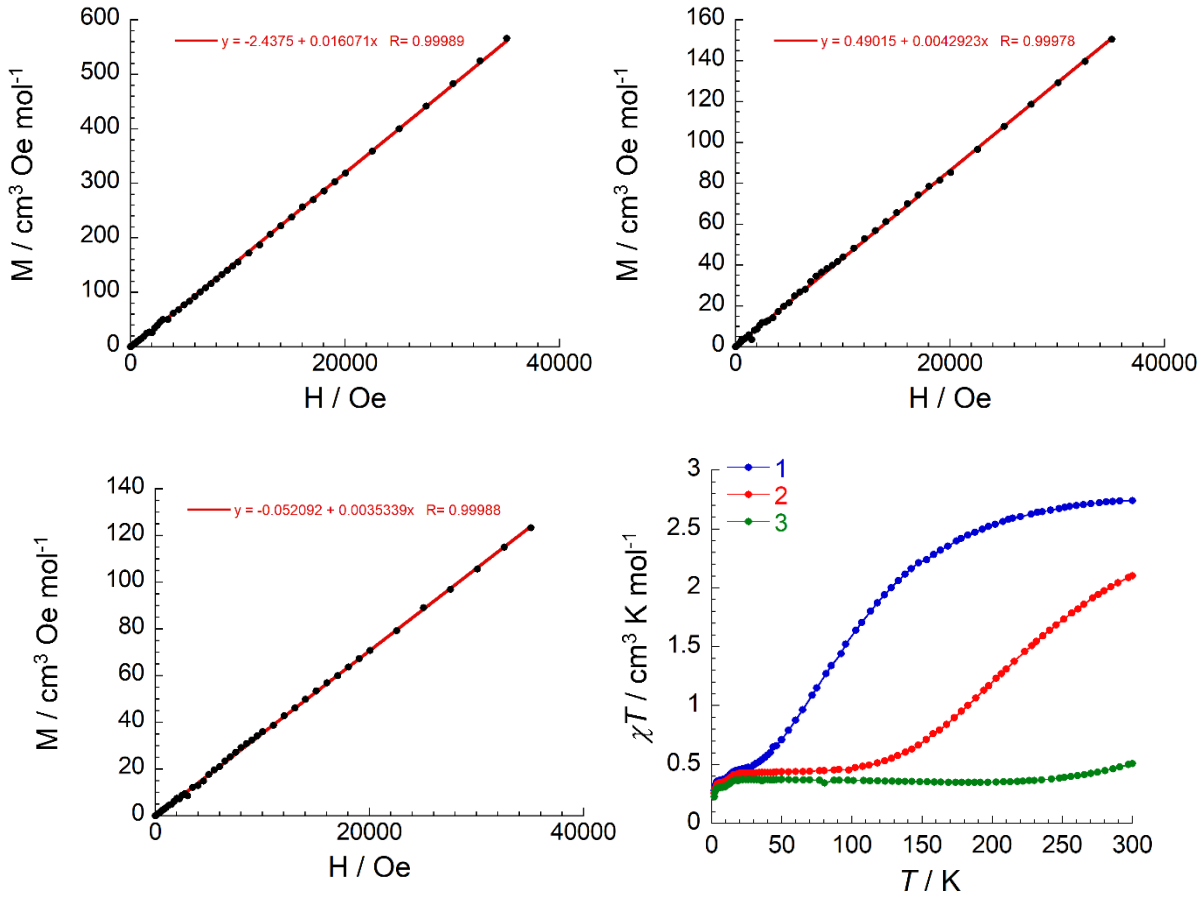


Fig. S19. Field dependence of the magnetization as *M vs H* plots for **1** (top, left), 2 (top, right) and **3** (bottom, left) at 100 K. The solid lines are the best fit. Bottom right: temperature dependence of χT for **1–3** at 2500 Oe

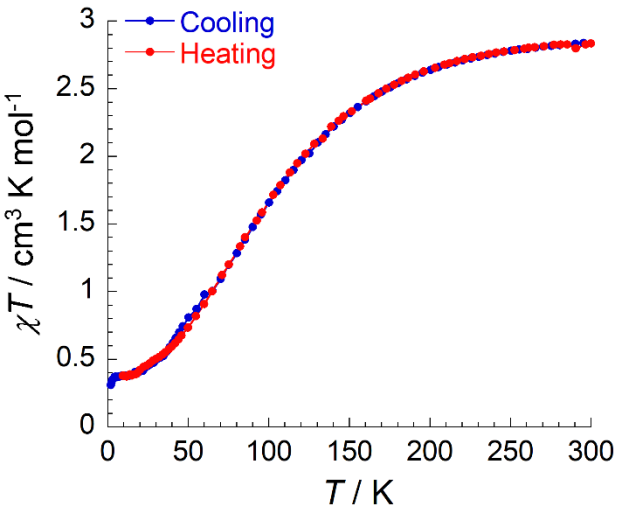


Fig. S20. Temperature dependence of χT product for **1** in cooling (blue) and heating (red) modes.

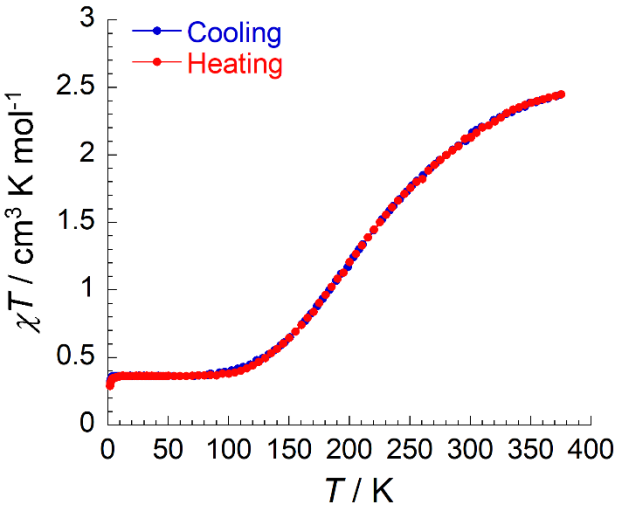


Fig. S21. Temperature dependence of χT product for **2** in cooling (blue) and heating (red) modes.

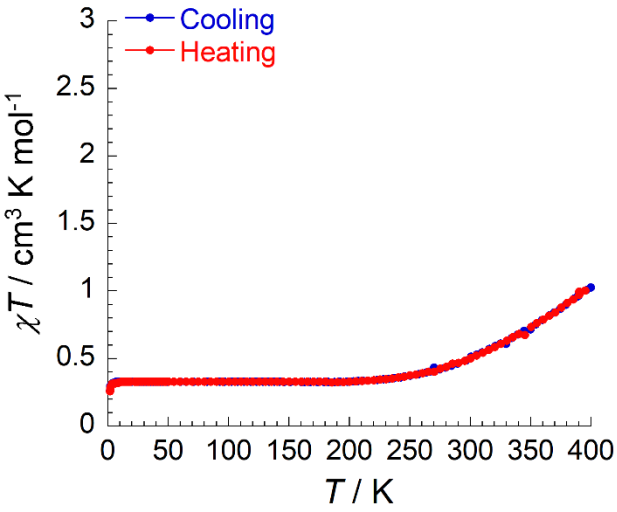


Fig. S22. Temperature dependence of χT product for **3** in cooling (blue) and heating (red) modes.

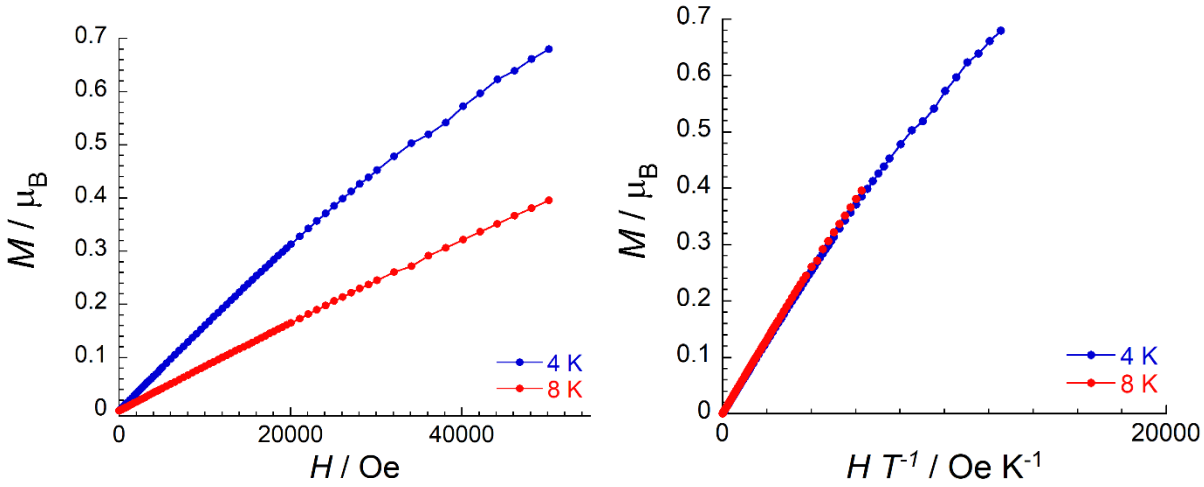


Fig. S23. Field dependence of the magnetization as *M* vs *H* (left) and *M* vs *H/T* (right) plots for **1** at 4 and 8 K. The solid lines are guide for the eyes.

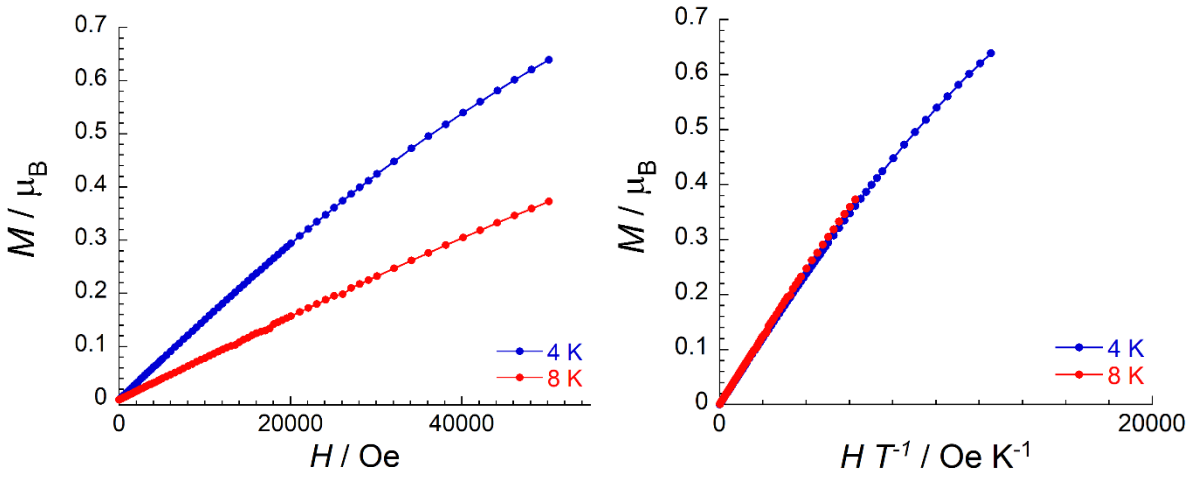


Fig. S24. Field dependence of the magnetization as *M* vs *H* (left) and *M* vs *H/T* (right) plots for **2** at 4, and 8 K. The solid lines are guide for the eyes.

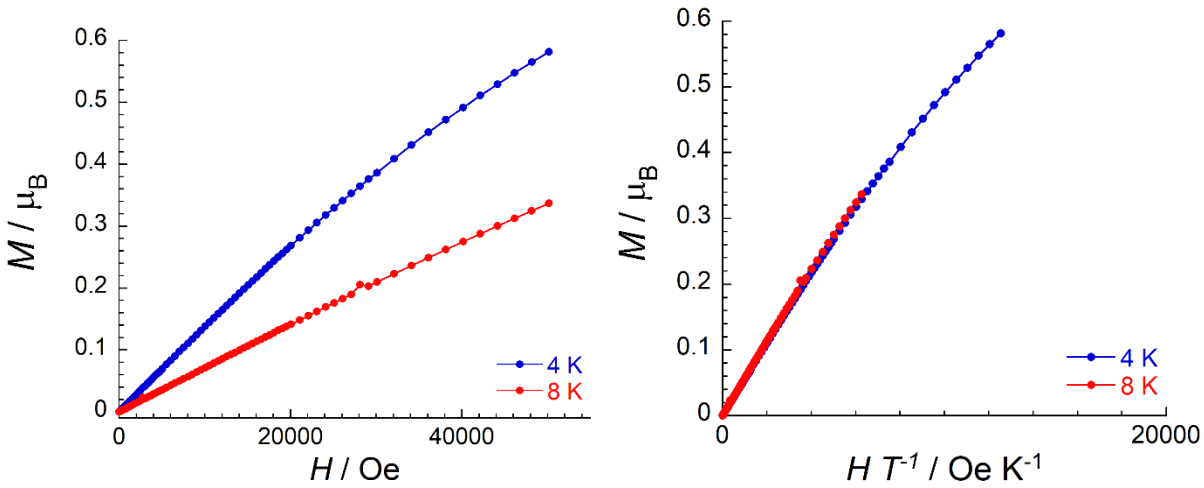


Fig. S25. Field dependence of the magnetization as *M* vs *H* (left) and *M* vs *H/T* (right) plots for **3** at 4 and 8 K. The solid lines are guide for the eyes.

The following equation deduced from the ideal solution model was applied to fit the spin crossover properties observed by magnetic studies.

$$X = X_{LS} + \frac{X_{HS} - X_{LS}}{1 + \exp\left[\Delta H/R\,(1/T - 1/T_{1/2})\right]}$$

X = χT product

X_{LS} = χT product for pure low-spin

X_{HS} = χT product for pure high-spin

ΔH = Enthalpy change associated to the spin crossover phenomenon

R = Ideal gas constant

Significant differences in the ΔH and ΔS values in **1**-**3** might be coming from the non-saturation nature of curves and/or presence of magnetic anisotropy (g > 2) in these systems.

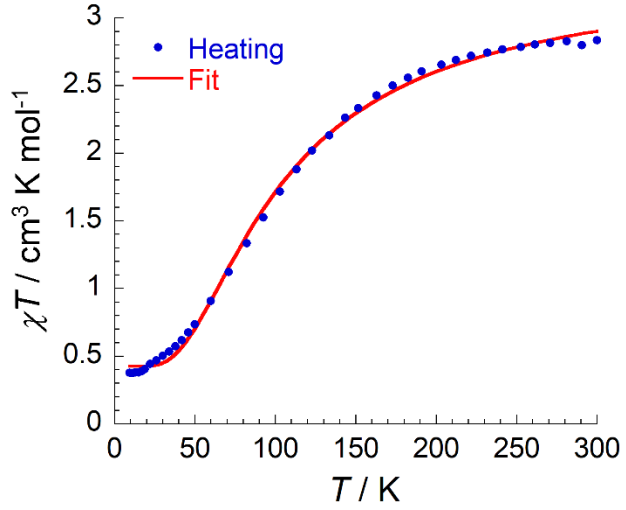


Fig. S26. χT *vs.* T data fit using the ideal solution model of **1**.

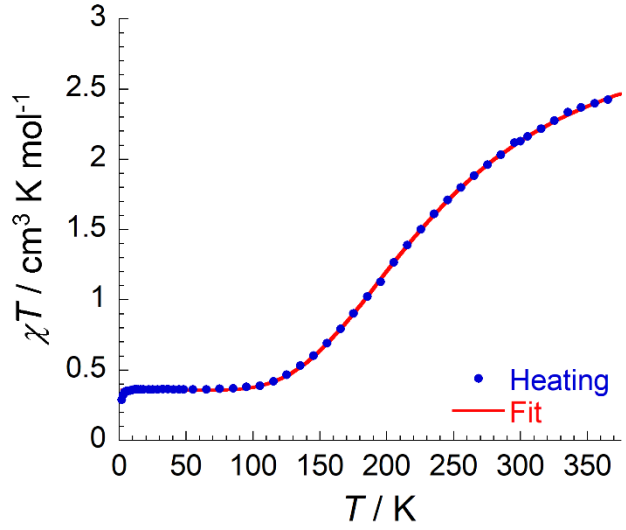


Fig. S27. χT *vs.* T data fit using the ideal solution model of **2**.

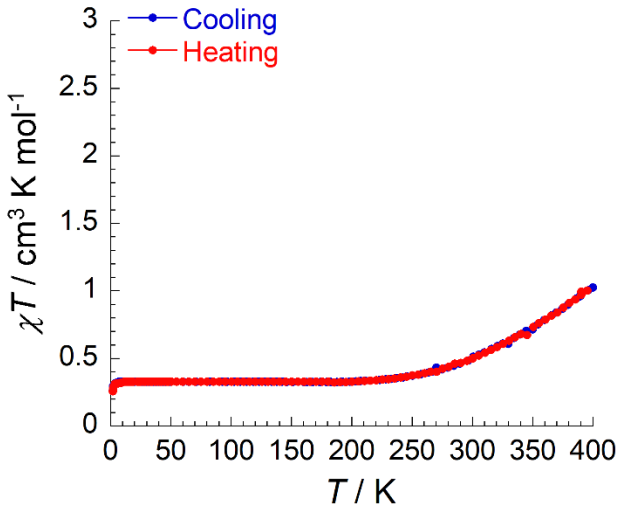


Fig. S28. χT *vs.* T data fit using the ideal solution model of **3**.

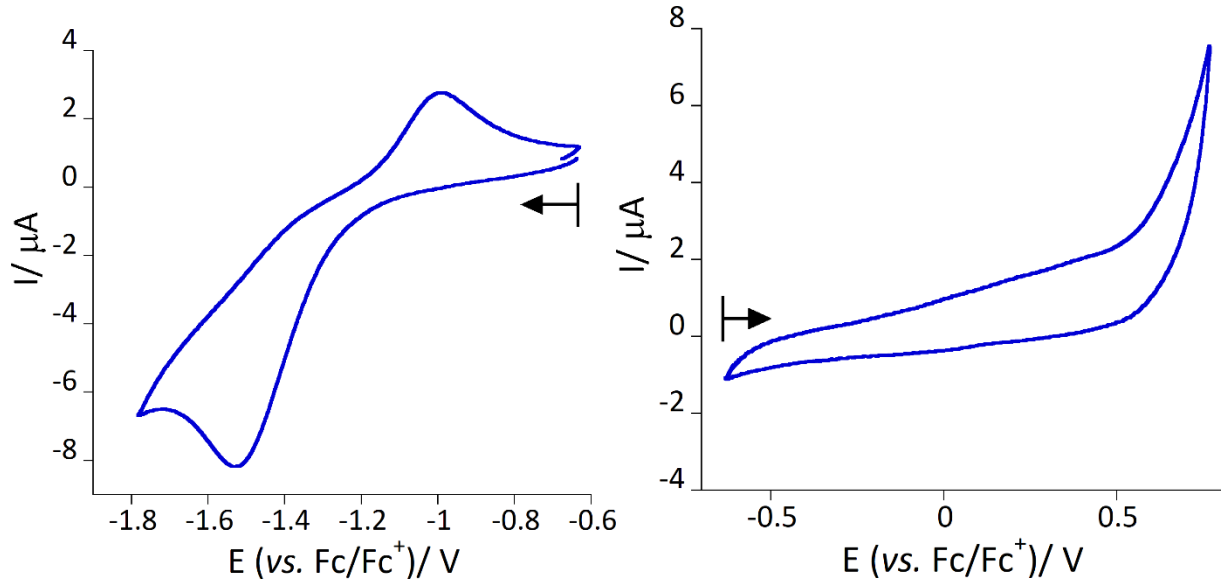


Fig. S29. Cyclic voltammograms for reduction (left) and oxidation (right) of the ligand **L** in 0.2 M (^{n}Bu$_4$N)PF$_6$/DMF with a scan rate of 100 mV/s.

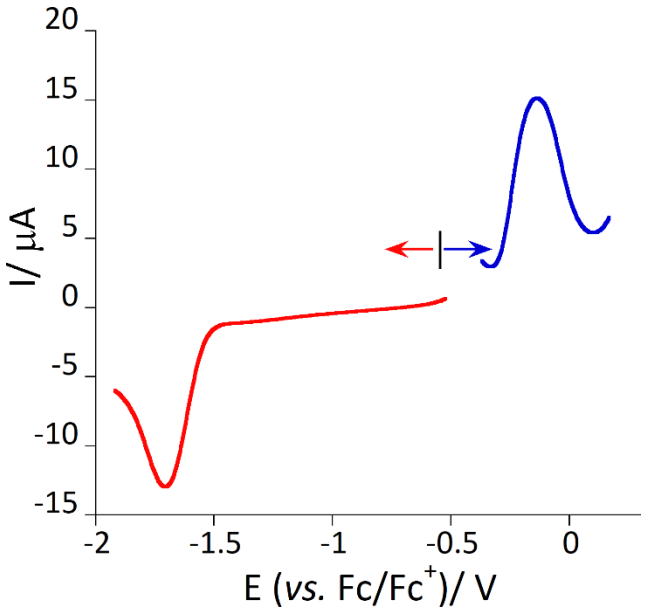


Fig. S30. Square wave voltammograms of **1** in acetonitrile containing 0.2 M (^{n}Bu$_4$N)PF$_6$ as an electrolyte. Arrows indicate open circuit potential along with the direction of the potential sweep.

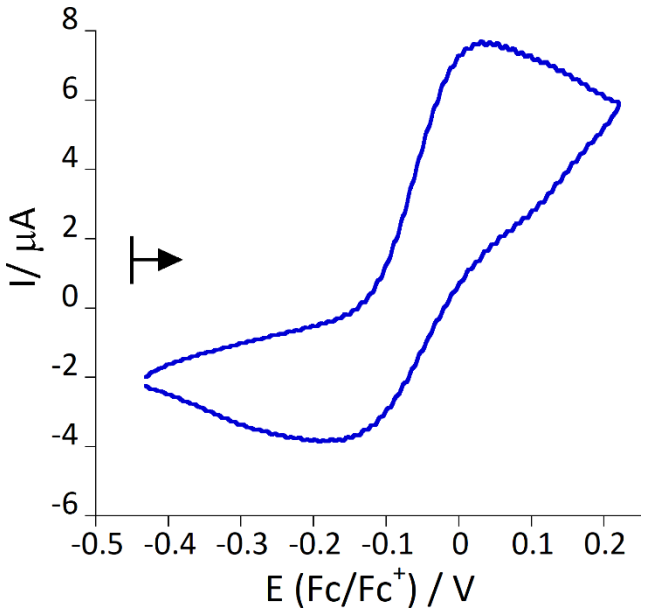


Fig. S31. Cyclic voltammogram for oxidation of **2** in 0.2 M (^{n}Bu$_4$N)PF$_6$/DMF with a scan rate of 0.1 V s^{-1}. Arrows indicate open circuit potential along with the direction of the potential sweep.

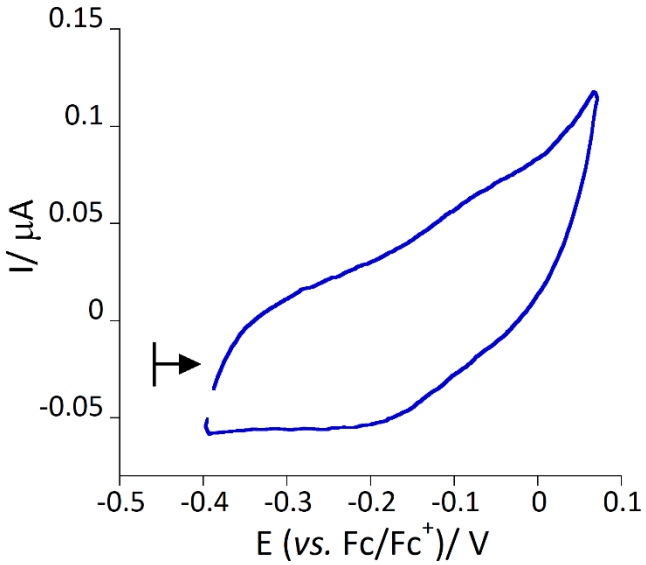


Fig. S32. Cyclic voltammogram for oxidation of **3** in 0.2 M (^{n}Bu$_4$N)PF$_6$/DMF with a scan rate of 0.1 V s^{-1}. Arrows indicate open circuit potential along with the direction of the potential sweep.

Table S1. X-ray Crystallographic Data for Complexes **1**−**3**.

	1		**2**			**3**
CCDC no	2004092	2004093	2004095	2004096	2004097	2004098
temp (K)	296	100	296	240	100	296
empirical formula	$C_{24}H_{32}CoN_6S_2$	$C_{24}H_{32}CoN_6S_2$	$C_{24}H_{32}CoN_6Se_2$	$C_{24}H_{32}CoN_6Se_2$	$C_{24}H_{32}CoN_6Se_2$	$C_{30}H_{32}CoN_{10}$
formula wt	527.61	527.61	621.41	621.42	621.42	591.59
cryst syst	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
space group	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/n$	$P2_1/c$
a (Å)	11.801(3)	11.6028(9)	11.725(4)	11.6923(6)	11.6185(15)	13.3379(2)
b (Å)	14.041(3)	13.9245(11)	14.041(4)	13.9860(7)	13.8515(19)	12.6230(2)
c (Å)	15.332(4)	15.2779(12)	15.673(4)	15.6498(8)	15.550(2)	18.7965(4)
α (deg)	90	90	90	90	90	90
β (deg)	90.076(10)	90.056(4)	90.133(14)	90.018(2)	90.276(7)	110.087(1)
γ (deg)	90	90	90	90	90	90
V, Å^3	2540.5(11)	2468.4(3)	2580.3(13)	2559.2(2)	2502.5(6)	2972.16(9)
Z	4	4	4	4	4	4
d_{calcd} (g cm^{-3})	1.379	1.420	1.600	1.613	1.649	1.322
μ (mm^{-1})	0.864	0.889	3.510	3.539	3.619	0.615
F(000)	1108	1108	1252	1252	1252	1236
θ_{max} (deg)	31.196	30.634	30.681	30.541	30.672	30.599
completeness (%)	97.0	99.8	99.2	90.1	99.8	98.5
no. of. rflns collected	8227	7612	8008	7814	7743	9147
no. of. Indep rflns	4665	5246	3235	3272	5904	5288
goodness of fit on F^2	1.017	1.09	0.976	0.974	1.014	0.999
final R indices (I>2σ(I))	R1 = 0.0462	R1 = 0. 0419	R1 = 0.0564	R1 = 0.0569	R1 = 0.0335	R1 = 0.0447
	wR2 = 0.1019	wR2 = 0.0864	wR2 = 0.1194	wR2 = 0.0937	wR2 = 0.0682	wR2 = 0.1035
final R indices (all data)	R1 = 0.0988	R1 = 0.0787	R1 = 0.1815	R1 = 0.1674	R1 = 0.0556	R1 = 0.0938
	wR2 = 0.1218	wR2 = 0.1026	wR2 = 0.1666	wR2 = 0.1239	wR2 = 0.0756	wR2 = 0.1247

$R1 = \sum||Fo| - |Fc||/\sum|Fo|$ and $wR2 = |\sum w(|Fo|^2 - |Fc|^2)|/\sum|w(Fo)^2|^{1/2}$

Table S2. Selected bond lengths (Å) and bond angles (°) in **1**–**3**.

Complex	**1**		**2**			**3**
	296 K	100 K	296 K	240 K	100 K	296 K
Co(1)-N(1)	2.409(2)	2.373(2)	2.385(5)	2.374(2)	2.363(2)	2.335(2)
Co(1)-N(2)	2.063(2)	1.987(2)	2.022(5)	1.991(3)	1.923(2)	1.925(1)
Co(1)-N(3)	2.345(2)	2.328(2)	2.316(5)	2.328(3)	2.330(2)	2.324(2)
Co(1)-N(4)	2.067(2)	1.988(2)	2.021(5)	1.993(3)	1.920(2)	1.919(2)
Co(1)-N(5)	2.029(2)	1.975(2)	2.013(6)	1.976(3)	1.917(2)	1.922(2)
Co(1)-N(6)	2.024(2)	1.971(2)	2.002(6)	1.979(3)	1.928(2)	1.937(2)
N(1)-Co(1)-N(2)	77.11(8)	77.78(6)	77.8(2)	78.3(1)	80.20(7)	81.03(7)
N(1)-Co(1)-N(3)	145.43(7)	149.20(6)	147.1(2)	148.73(9)	152.31(7)	150.78(6)
N(1)-Co(1)-N(4)	78.07(8)	78.80(6)	76.6(2)	79.5(1)	79.15(7)	78.82(7)
N(1)-Co(1)-N(5)	105.13(9)	97.29(7)	101.9(2)	99.7(1)	99.87(7)	102.51(7)
N(1)-Co(1)-N(6)	100.32(9)	100.32(9)	97.5(2)	104.2(1)	96.42(7)	96.62(8)
N(2)-Co(1)-N(3)	76.69(8)	79.30(7)	77.9(2)	78.6(1)	79.55(7)	77.97(7)
N(2)-Co(1)-N(4)	81.16(8)	83.32(7)	83.3(2)	84.0(1)	85.40(8)	89.14(7)
N(2)-Co(1)-N(5)	172.39(9)	91.59(8)	90.6(2)	90.7(1)	90.34(8)	89.57(8)
N(2)-Co(1)-N(6)	90.64(9)	173.85(8)	173.5(2)	174.1(1)	175.47(8)	177.60(8)
N(3)-Co(1)-N(4)	75.96(8)	78.34(7)	78.8(2)	77.4(1)	80.59(7)	80.76(7)
N(3)-Co(1)-N(5)	98.29(9)	103.66(7)	100.2(2)	101.4(1)	98.93(7)	97.44(7)
N(3)-Co(1)-N(6)	102.14(8)	99.68(7)	104.7(2)	97.1(1)	102.63(7)	104.40(8)
N(4)-Co(1)-N(5)	92.13(9)	174.12(8)	173.9(2)	174.7(1)	175.73(8)	177.97(8)
N(4)-Co(1)-N(6)	171.80(9)	90.53(8)	91.3(2)	91.1(1)	91.03(8)	90.87(8)
N(5)-Co(1)-N(6)	96.01(1)	94.54(8)	94.8(2)	94.2(1)	93.21(8)	90.49(8)
Co(1)-N(5)-C(1)	165.9(2)	167.0(2)	169.6(6)	169.2(3)	169.8(2)	173.1(1)
Co(1)-N(6)-C(2)	168.6(2)	169.0(2)	166.9(6)	167.2(3)	168.3(2)	171.4(1)
N(5)-C(A)-X(Y)	179.2(3)[a]	179.5(2)[a]	177.3(6)[c]	178.2(3)[c]	177.9(2)[c]	177.4(2)[e]
N(6)-C(B)-X(Z)	178.8(3)[b]	178.8(2)[b]	178.1(6)[d]	178.2(4)[d]	178.1(2)[d]	179.5(3)[f]

a: N(5)-C(1)-S(1); b: N(6)-C(2)-S(2); c: N(5)-C(1)-Se(1); d: N(6)-C(2)-Se(2); e: N(5)-C(1)-C(2); f: N(6)-C(5)-C(6)

Continuous Shape Measures (CShM) Analysis:

Continuous Shape Measures (CShM) analysis was carried out to determine the geometry around Co atom. Based on the values obtained, the idealized polyhedron was matched with the actual coordination spheres. The smallest value is symbolic of the proximity of the actual coordination sphere and idealized polyhedron.

Table S3: CShM analysis data for complexes **1**–**3**.

Complex	Temp.	Structure				
		HP - 6	PPY - 6	**OC - 6**	TPR - 6	JPPY - 6
[Co(**L**)$(NCS)_2$] (**1**)	296 K	33.304	24.436	**2.428**	12.549	29.346
	100 K	33.363	24.915	**2.263**	12.705	29.803
[Co(**L**)$(NCSe)_2$] (**2**)	296 K	33.362	24.258	**2.365**	12.305	29.207
	240 K	33.329	24.601	**2.317**	12.389	29.604
	100 K	33.487	25.480	**2.277**	12.837	29.794
[Co(**L**)$((C(CN)_3)_2$] (**3**)	296 K	33.047	24.002	**2.551**	11.356	28.737

HP – 6: Hexagon (D6h), PPY – 6 = Pentagonal pyramid, OC – 6: Octahedron (Oh), TPR – 6: Trigonal prism (D3h), JPPY – 6 = Johnson pentagonal pyramid J2 (C5v);

Table S4. Short intra–and inter molecular interactions in **1**–**3**.

	T / K	D-H···A	D-H / Å	H···A / Å	D···A / Å	∠D-H···A / °
1	**296**	C6-H6···C2	0.930	2.826	3.680	153.1
		C6-H6···S2	0.930	2.958	3.769	146.5
		C13-H13···C1	0.930	2.761	3.647	159.6
		C10-H10B···S2	0.970	2.950	3.520	118.7
		C22-H22B···C13	0.960	2.889	3.730	146.9
	100	C6-H6···C1	0.93	2.719	3.600	158.5
		C13-H13···C2	0.93	2.773	3.621	152.1
		C13-H13···S2	0.93	2.9157	3.714	144.8
		C20-H20C···C6	0.960	2.846	3.676	145.4
		C19-H19B···C5	0.960	2.880	3.801	161.0
		C9-H9A···S2	0.970	2.8522	3.710	126.5
		C9-H9A···C2	0.970	2.871	3.535	147.9
2	**296**	C6-H6···C1	0.93	2.844	3.696	152.9
		C6-H6···Se1	0.93	3.002	3.799	144.8
		C10-H10B···Se1	0.97	2.9865	3.866	151.5
		C16-H16B···Se1	0.97	3.040	3.579	116.4
	240	C6-H6···C1	0.93	2.834	3.687	153.0
		C6-H6···Se1	0.93	2.995	3.782	143.3
		C13-H13···C2	0.93	2.836	3.712	157.6
		C10-H10A···Se1	0.97	3.0269	3.558	115.8
		C10-H10B···Se1	0.97	3.2678	3.558	99.4
	100	C6-H6···C1	0.93	2.804	3.648	151.5
		C6-H6···Se1	0.93	2.964	3.737	141.5
		C13-H13···C2	0.93	2.794	3.665	156.3
		C10-H10B···Se1	0.97	2.9236	3.797	150.4
		C16A-H16B···Se1	0.97	3.002	3.500	113.22
		C17-H17A···C13	0.960	2.866	3.703	146.2
		C19-H19A···C14	0.960	2.891	3.815	161.9
		C16A·····Se1	-	-	3.500	-
3	**296**	C16-H16···N8	0.970	2.629	3.321	136.31
		C9-H9B···N7	0.970	2.512	3.430	157.9
		C26-H26B···N7	0.960	2.705	3.605	156.3
		C15-H15B···C4	0.970	2.894	3.847	167.7
		C3·····C11	-	-	3.382	-
		C17·····N8	-	-	3.150	-

Table S5. Spin crossover behaviors for mononuclear cobalt(II) complexes

Complex	$T_{1/2}$ (K)[a]	T (K)[b]	Co–N (Å)	Spin State	Ref.
$[Co(\mathbf{L})(NCS)_2]$	168 K Gradual and complete	296 100	2.063(2)-2.409(2) 1.987(2)-2.373(2)	HS HS/LS	This work
$[Co(\mathbf{L})(NCSe)_2]$	255 K Gradual and incomplete	296 240 100	2.013(6)-2.385(5) 1.999(3)-2.374(2) 1.920(2)-2.363(2)	HS/LS HS/LS LS	This work
$[Co(\mathbf{L})(C(CN)_3)_2]$	Incomplete Mainly LS	296	1.919(2)-2.335(3)	LS	This work
$[Co(\mathbf{L})(N(CN)_2)_2]$	238 K Gradual and complete	280 100	1.998(3)-2.349(3) 1.907(2)-2.341(2)	HS LS	1a
$[Co^{II}(L1)]$	~ 250 Gradual and incomplete	295 30	1.9533(17)-2.0440(18) 1.8850(13)-2.1472(12)	HS LS	6
$[Co^{II}(L2)]$	>300 Gradual and incomplete	140	1.881(2)–2.042(2)	LS	6
$[Co^{II}(L3)]$	~265, incomplete. ~220, incomplete. ~175, almost complete	300 30	1.939(2)–2.080(3) 1.8965(8)–2.1435(8)	HS LS	7
$[Co^{II}(dpzca)_2]$	$T½\downarrow$ = 168 $T½\uparrow$ = 179 $\Delta T½$ = 11 K, Abrupt and hysteretic	298 90	2.049(3)–2.145(3) 1.91(1)–2.20(1) Å	HS LS	8
$[Co^{II}(L4)_2](ClO_4)_2$.MeOH	>200 Gradual and incomplete	298 123	2.015(7)–2.123(5) 1.883(9)–2.252(6)	HS LS	9
$[Co^{II}(L5)(dbsq)](B(p\text{-}PhCl)_4)$	>200 Gradual and incomplete	100 400	1.931(2)–2.368(2) 1.986(4)–2.371(3)	HS LS	10
$[Co^{II}(L6)_2](NO_3)_2$	>218 Gradual and incomplete, and ferromagnetic coupling	123 273 353	1.959(3)–1.986(3) 2.040(2)–2.056(2) 2.056(3)–2.073(4)	LS HS/LS HS	10
$[Co^{II}(L7)_2](B(C_6F_5)_4)_2.CH_2Cl_2$	>200. Gradual and incomplete, anti- and ferromagnetic coupling	123 273	1.977(2)–1.992(2) 2.078(4)–2.093(3)	LS HS	11
$[Co^{II}(papl)_2]$	~150 Gradual	147 325	1.865(2)–2.048(2) 1.909(2)–2.042(1)	LS HS	12

$[Co(tppz)_2](dca)_2$	400 Incomplete	125 330	1.855(5)- 2.155(4) 1.870(3)- 2.128(2)	quasi LS	13
$[Co^{II}(L8)_2][BDS]\cdot 2H_2O$	Abrupt, hysteretic, $T_{1/2}\downarrow$= 226 K, $T_{1/2}\uparrow$ = 260 K , $\Delta T½$ = 20 K	300 260 230 200	1.887(4)- 2.132(4) 1.883(2)- 2.140(2) 1.874(2)- 2.143(3) 1.874(3)- 2.147(3)	LS LS LS LS	14
$Co^{II}(L8)_2][BDS]$	abrupt and complete SCO transition with a wide thermal hysteresis loop $T_{1/2}\downarrow$ = 235 K, $T_{1/2}\uparrow$ = 267 K, $\Delta T½$ = 35 K	300 260 230 200	1.981(5)- 2.134(5) 1.950(5)- 2.130(5) 1.858(5)- 2.136(5) 1.871(3)- 2.143(3)	HS HS LS LS	14
$[Co(terpy)_2](ClO_4)_2 \cdot 0.5H_2O$	$T_{1/2} \approx$ 180 K	243	$Co–N_{central}$ = 2.02 $Co–N_{distal}$ = 2.14	HS	15
$[Co(terpy)_2](BF_4)_2$	$T_{1/2}$ = 270 K	375 30	2.030(4)- 2.160(3) 1.907(3)- 2.132(2)	HS LS	16
[Co(4-terpyridone)$_2$](ClO_4)$_2$.H_2O	172.4 K almost complete and relatively cooperative spin conversion	293	2.106(5)- 2.153(6)	HS	17
[Co(4-terpyridone)$_2$](BF_4)$_2\cdot H_2O$ (2 Polymorphs)	152 K Poorly cooperative	293 293	1.892(6)- 2.036(7) 1.949(4)- 2.158(5)	HS:LS HS:LS	18
[Co(4-terpyridone)$_2$]$X_p\cdot_n S$ X = $[BF4]^-$ (p = 1) and $[SiF_6]^{2-}$ (p = 0.5) and S = CH_3OH	Incomplete at high temperature	293 105	1.894(2)- 2.171(2) 1.871(3)- 2.183(3)	HS:LS LS	18
[Co(OH-terpy)$_2$](CF_3SO_3)$_2\cdot$ H_2O	Tc↓ = 155.6 K; Tc↑ = 188.5 K	293	1.991(13)- 2.165(14)	HS HS	19
[Co(C5C12C10-terpy)$_2$](BF_4)$_2$	$T_{1/2}\uparrow$= 288 K; $T_{1/2}\downarrow$ = 284 K; ΔT = 4 K	-	-	-	20

[Co(C16-terpy)$_2$](BF$_4$)$_2$·MeOH	260 K	130	1.99-2.13	LS: HS	21
[Co(C16-terpy)$_2$](BF$_4$)$_2$	$T_{1/2}\downarrow$ = 217 K; $T_{1/2}\uparrow$ = 260 K; ΔT = 43 K	-	-	-	21
[Co(C14-terpy)$_2$](BF$_4$)$_2$·MeOH	T_1 = 50 K (steep); $T_2\uparrow$ = 206 K; $T_2\downarrow$ = 184 K; $T_{1/2}$ = 175 K (Gradual)	190 190 10	2.020(4)- 2.167(4) 1.945(3)- 2.144(4) 1.8443(3)- 2.137(4)	HS IS LS	22
[Co(C14-terpy)$_2$](BF$_4$)$_2$	$T_{1/2}\downarrow$ = 250 K; $T_{1/2}\uparrow$ = 307 K; ΔT = 57 K	-	-	-	22
[Co(C12-terpy)$_2$](BF$_4$)$_2$·EtOH·0.5H$_2$O	$T_{1/2}$ = 49 K; $T_{1/2}$ = 128 K	180	1.99-2.11	HS	23
[Co^{II}(Ar)(NHAr')]	229 K	90 240	1.875(3) 1.880(2)	LS HS	24
[Co^{II}(3,4-lut)$_4$Br]Br	T½ ≈ 210 K Gradual	296 123	2.110(4)–2.136(4) 1.9686(18)–1.9677(18)	HS LS	25

a: spin crossover temperature; b: structure analyses temperature; HS: high-spin; LS: low-spin

L = *N*,*N*'-di-tert-butyl-2,11-diaza[3,3](2,6)pyridinophane, L1= Hexachlorine tris-dioximate Butyl capped boron derivative; L2= Hexathiol tris-dioximate phenyl capped boron derivative; L3= Hexachlorine tris-dioximate methyl capped boron derivative; dpzca = dipyrazine–imide analogue; L4= 2,5-bis[1-[2-nitro-2-(pyridin-2-yl)-hydrazono]ethyl]pyrazine; L5 = 3,5-di-tert-butylcatechol; L6= 3,5-di-tert-butylsemiquinol; L7= 4,4-dimethyl-2,2-bis(2-pyridyl)oxazolidine N-oxide; papl= 1-(2-pyridylazo)-2-phenanthrol; tppz= 2,3,5,6-tetrakis(2-pyridyl)pyrazine ; L8= 4′-(4-bromophenyl)-2,2′:6′,2″-terpyridine ; terpy = 2,2':6',2''-terpyridine; 4-terpyridone = 2,6-bis(2-pyridyl)-4(1H)-pyridone; C5C12C10-terpy = 4'-5'''-decyl-1'''-heptadecyloxy-2,2':6',2''-terpyridine; C16-terpy= 4'-hexadecyloxy-2,2':6',2''-terpyridine; C14-terpy= 4'-tetradecyloxy-2,2':6',2''-terpyridine; C12-terpy= 4'-dodecyloxy-2,2':6',2''-terpyridine; Ar = C_6H_3-2,6-(C_6H_3-2,6-^{i}Pr$_2$)$_2$; NHAr'= NHC_6H_3-2,6-(C_6H_2-2,4,6-Me$_3$)$_2$; 3,4-lut = 3,4-dimethylpyridine;

Appendix: Checkcif

Complex **1**

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Complex1_296K

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Complex1_296K

```
Bond precision: C-C = 0.0032 A           Wavelength=0.71073

Cell:            a=11.801(3)     b=14.041(3)          c=15.332(4)
                 alpha=90        beta=90.076(10)      gamma=90
Temperature:     296 K

                Calculated                Reported
Volume          2540.5(11)                2540.5(10)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula C24 H32 Co N6 S2           ?
Sum formula     C24 H32 Co N6 S2          C24 H32 Co N6 S2
Mr              527.61                    527.60
Dx,g cm-3       1.379                     1.379
Z               4                         4
Mu (mm-1)       0.864                     0.864
F000            1108.0                    1108.0
F000'           1110.61
h,k,lmax        17,20,22                  16,20,22
Nref            8227                      7983
Tmin,Tmax       0.667,0.772               0.845,0.943
Tmin'           0.590
Correction method= # Reported T Limits: Tmin=0.845 Tmax=0.943
AbsCorr = MULTI-SCAN

Data completeness= 0.970          Theta(max)= 31.196

R(reflections)= 0.0462( 4665)     wR2(reflections)= 0.1218( 7983)

S = 1.017                 Npar= 298
```

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

Alert level C

PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low ’MainMol’ Ueq as Compared to Neighbors of C2 Check
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H9B ..H24A . 1.81 Ang.
x,y,z = 1_555 Check PLAT412_ALERT_2_C Short Intra XH3 .. XHn H16B ..H20A
. 1.89 Ang. x,y,z =
1_555 Check PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -
1.087 Report

Alert level G

PLAT230_ALERT_2_G Hirshfeld Test Diff for S2 --C2 . 5.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 --N5 . 9.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 --N6 . 7.5 s.u.
PLAT793_ALERT_4_G Model has Chirality at N1 (Centro SPGR) R Verify
PLAT793_ALERT_4_G Model has Chirality at N3 (Centro SPGR) R Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (II) . 2.01 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 228 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ..... 4.9 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
5 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
8 ALERT type 2 Indicator that the structure model may be wrong or deficient
2 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

Publication of your CIF in IUCr journals

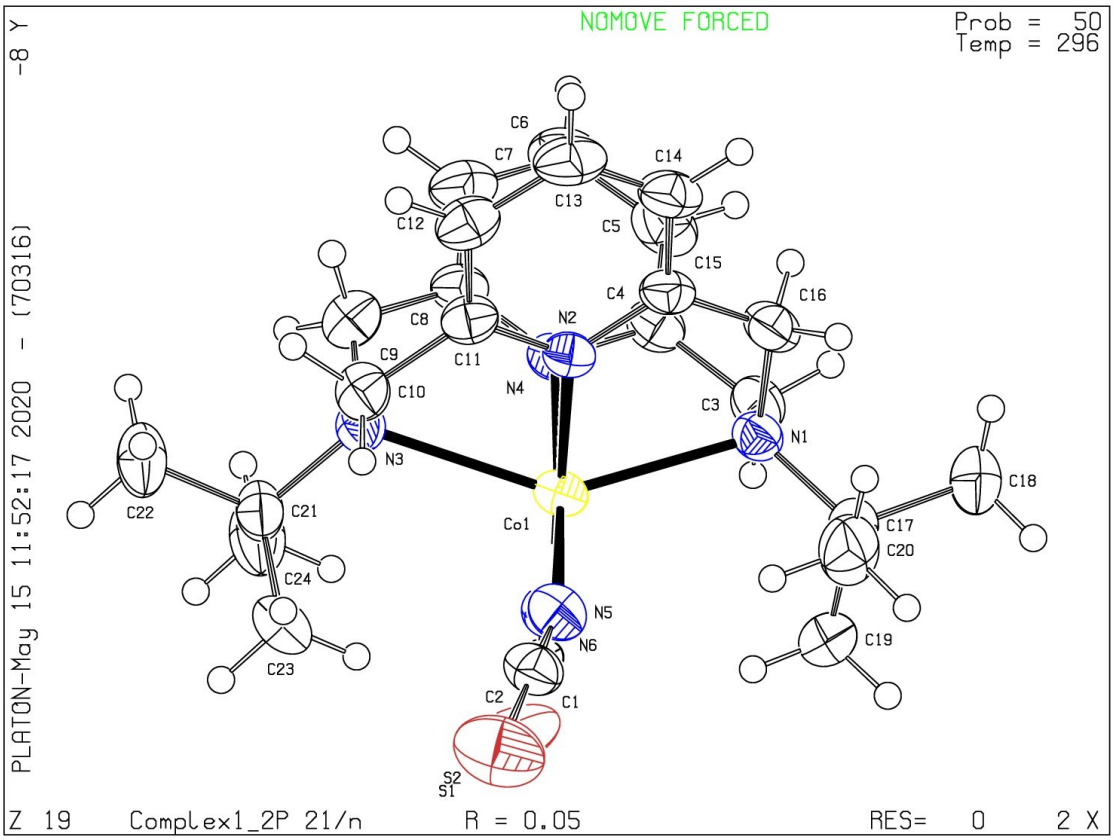
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

PLATON version of 22/04/2020; check.def file version of 09/03/2020

Datablock Complex1_296K - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Complex1_100K

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: Complex1_100K

```
Bond precision: C-C = 0.0030 A           Wavelength=0.71073
Cell:           a=11.6028(9)    b=13.9245(11)     c=15.2779(12)
                alpha=90        beta=90.056(4)    gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          2468.4(3)                 2468.3(3)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula C24 H32 Co N6 S2           ?
Sum formula     C24 H32 Co N6 S2          C24 H32 Co N6 S2
Mr              527.61                    527.60
Dx,g cm-3       1.420                     1.420
Z               4                         4
Mu (mm-1)       0.889                     0.889
F000            1108.0                    1108.0
F000'           1110.61
h,k,lmax        16,19,21                  16,19,21
Nref            7612                      7597
Tmin,Tmax       0.659,0.766               0.845,0.943
Tmin'           0.581
Correction method= # Reported T Limits: Tmin=0.845 Tmax=0.943
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 30.634

R(reflections)= 0.0419( 5246)     wR2(reflections)= 0.1026( 7597)

S = 1.009                 Npar= 426
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The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level**.

```
Click on the hyperlinks for more details of the test.
```

Alert level C

```
RINTA01_ALERT_3_C  The value of Rint is greater than 0.12
           Rint given   0.133
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        4.2 Ratio
```

Alert level G

```
PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 .........      0.133 Report
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         32 Note
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S1       --C1       .         7.6 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    S2       --C2       .         7.5 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    N5       --C1       .         5.7 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N4       .         5.3 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N5       .        16.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N6       .        14.3 s.u.
PLAT793_ALERT_4_G Model has Chirality at N1          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N3          (Centro SPGR)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       2.34 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         15 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         11 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   2 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  14 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   7 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
4 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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Publication of your CIF in IUCr journals

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Crystallographica Section C or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

Publication of your CIF in other journals

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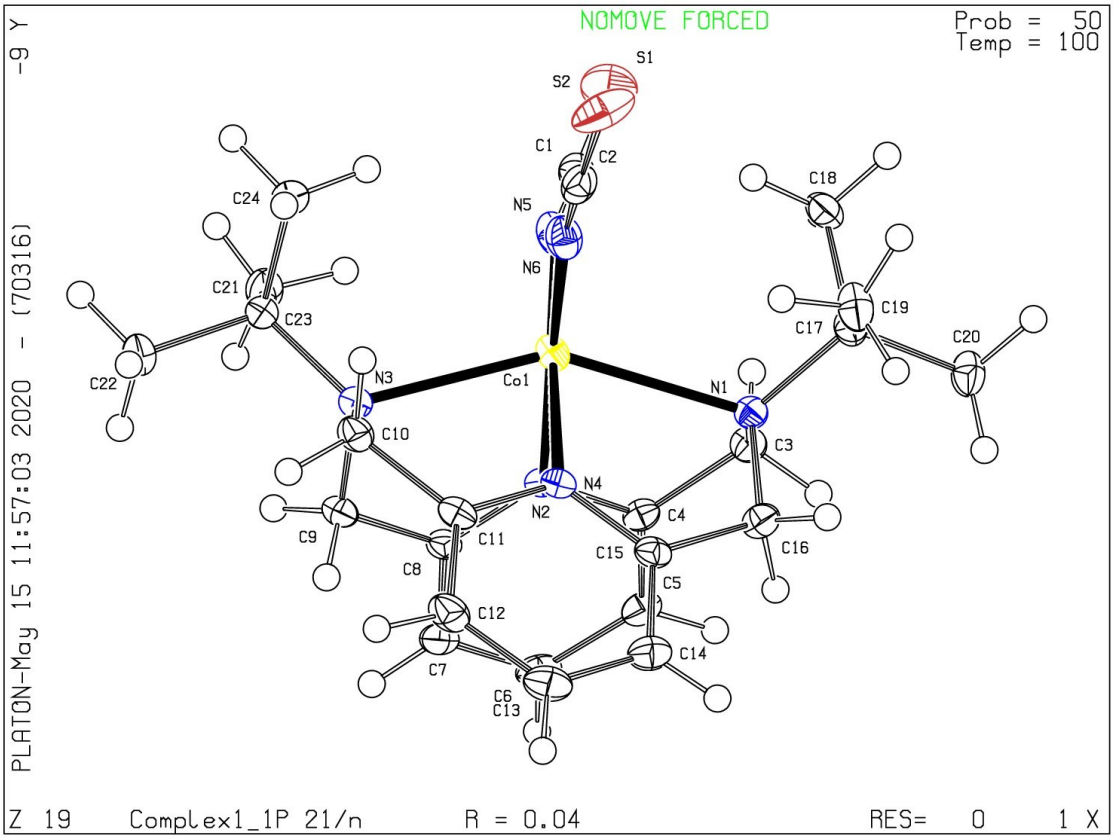
PLATON version of 22/04/2020; check.def file version of 09/03/2020

Datablock Complex1_100K - ellipsoid plot



Complex 2

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Complex2_296K

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Complex2_296K

```
Bond precision: C-C = 0.0069 A            Wavelength=0.71073

Cell:     a=11.725(4)     b=14.041(4)     c=15.673(4)     alpha=90
                beta=90.133(14) gamma=90
Temperature:     296 K

                Calculated                Reported
Volume          2580.3(13)                2580.3(12)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula C24 H32 Co N6 Se2          ?
Sum formula     C24 H32 Co N6 Se2         C24 H32 Co N6 Se2
Mr              621.41                    621.40
Dx,g cm-3       1.600                     1.600
Z               4                         4
Mu (mm-1)       3.510                     3.510
F000            1252.0                    1252.0
F000'           1252.96
h,k,lmax        16,20,22                  16,20,22
Nref            8008                      7940
Tmin,Tmax       0.186,0.361               0.763,0.821
Tmin'           0.133
Correction method= # Reported T Limits: Tmin=0.763 Tmax=0.821
AbsCorr = MULTI-SCAN

Data completeness= 0.992          Theta(max)= 30.681

R(reflections)= 0.0559( 3235)     wR2(reflections)= 0.1559( 7940)

S = 0.982                 Npar= 298
```

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

Alert level B

RINTA01_ALERT_3_B The value of Rint is greater than 0.18
Rint given 0.198

Response: This alert is generated might be due to thermal disorder in the molecule at high temperature.

Alert level C

PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low .. 41% Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C1 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C2 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00689 Ang.
PLAT412_ALERT_2_C Short Intra XH3 .. XHn H3B ..H20C . 1.83 Ang.
x,y,z = 1_555 Check PLAT412_ALERT_2_C Short Intra XH3 .. XHn H10B ..H22A
. 1.89 Ang. x,y,z =
1_555 Check PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -
2.585 Report

Alert level G

PLAT020_ALERT_3_G The Value of Rint is Greater Than 0.12 ..... 0.198 Report
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 --N5 . 6.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X) Co1 --N6 . 7.5 s.u.
PLAT793_ALERT_4_G Model has Chirality at N1 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at N3 (Centro SPGR) S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (II) . 2.15 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 71 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 0 Info

---

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7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
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1 ALERT type 5 Informative message, check

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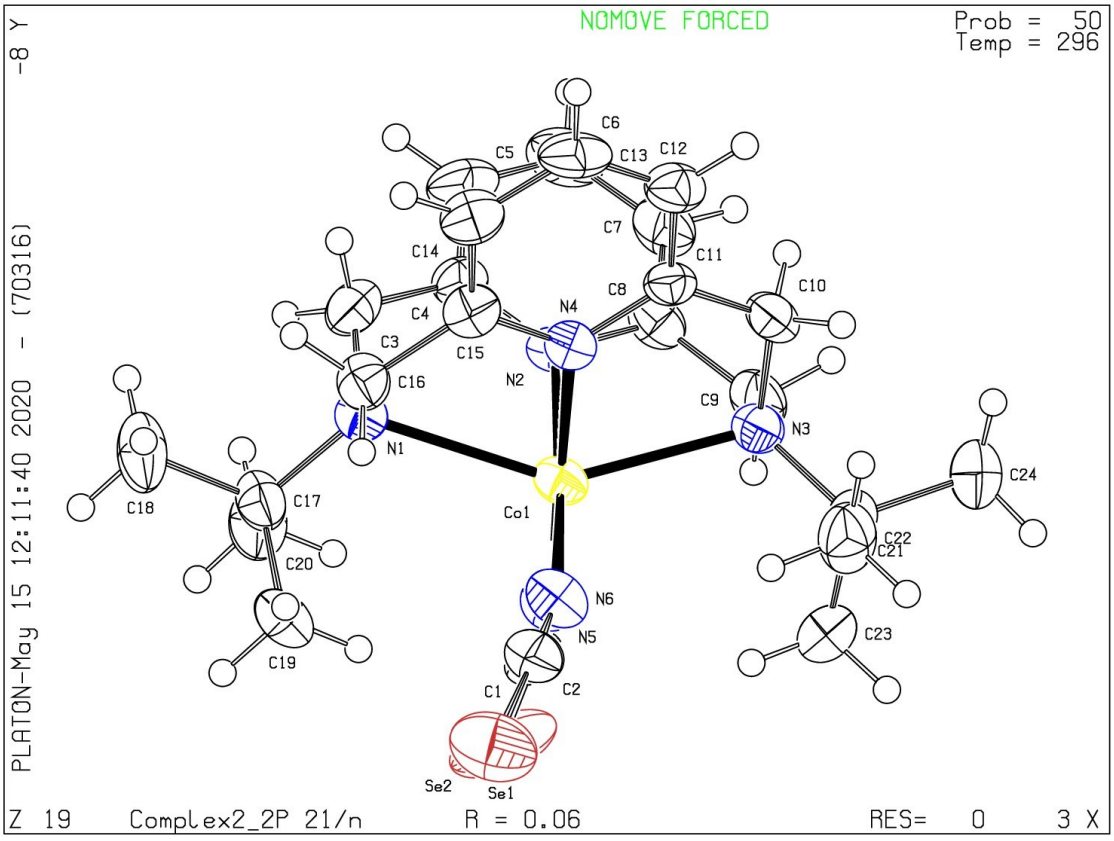
PLATON version of 22/04/2020; check.def file version of 09/03/2020

Datablock Complex2_296K - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Complex2_240K

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Complex2_240K

```
Bond precision: C-C = 0.0052 A           Wavelength=0.71073
Cell:           a=11.6923(6)     b=13.9860(7)       c=15.6498(8)
                alpha=90         beta=90.018(2)     gamma=90
Temperature:    240 K

                Calculated                Reported
Volume          2559.2(2)                 2559.2(2)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula C24 H32 Co N6 Se2          ?
Sum formula     C24 H32 Co N6 Se2         C24 H32 Co N6 Se2
Mr              621.41                    621.40
Dx,g cm-3       1.613                     1.613
Z               4                         4
Mu (mm-1)       3.539                     3.539
F000            1252.0                    1252.0
F000'           1252.96
h,k,lmax        16,19,22                  16,19,22
Nref            7814                      7040
Tmin,Tmax       0.183,0.358               0.751,0.810
Tmin'           0.131
Correction method= # Reported T Limits: Tmin=0.751 Tmax=0.810
AbsCorr = MULTI-SCAN

Data completeness= 0.901          Theta(max)= 30.541

R(reflections)= 0.0568( 3272)     wR2(reflections)= 0.1126( 7040)

S = 1.002                 Npar= 304
```

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level.**

Click on the hyperlinks for more details of the test.

Alert level C

```
PLAT026_ALERT_3_C Ratio Observed / Unique Reflections (too) Low ..        46% Check
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C1 Check
PLAT480_ALERT_4_C Long H...A H-Bond Reported H23A     ..N6       .       2.90 Ang.
PLAT480_ALERT_4_C Long H...A H-Bond Reported H23A     ..N6       .       2.90 Ang.
PLAT906_ALERT_3_C Large K Value in the Analysis of Variance ......     3.485 Check
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L=    0.600        85 Report
```

Alert level G

```
PLAT230_ALERT_2_G Hirshfeld Test Diff for    Se1      --C1       .        6.5 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N5       .        8.0 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N6       .        8.5 s.u.
PLAT793_ALERT_4_G Model has Chirality at N1          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N3          (Centro SPGR)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (II)      .       2.32 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        690 Note
PLAT941_ALERT_3_G Average HKL Measurement Multiplicity ...........        3.5 Low
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
```

```
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   0 ALERT level B = A potentially serious problem, consider carefully
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  10 ALERT level G = General information/check it is not something unexpected

   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
4 ALERT type 3 Indicator that the structure quality may be low
5 ALERT type 4 Improvement, methodology, query or suggestion
   1 ALERT type 5 Informative message, check
```

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Publication of your CIF in other journals

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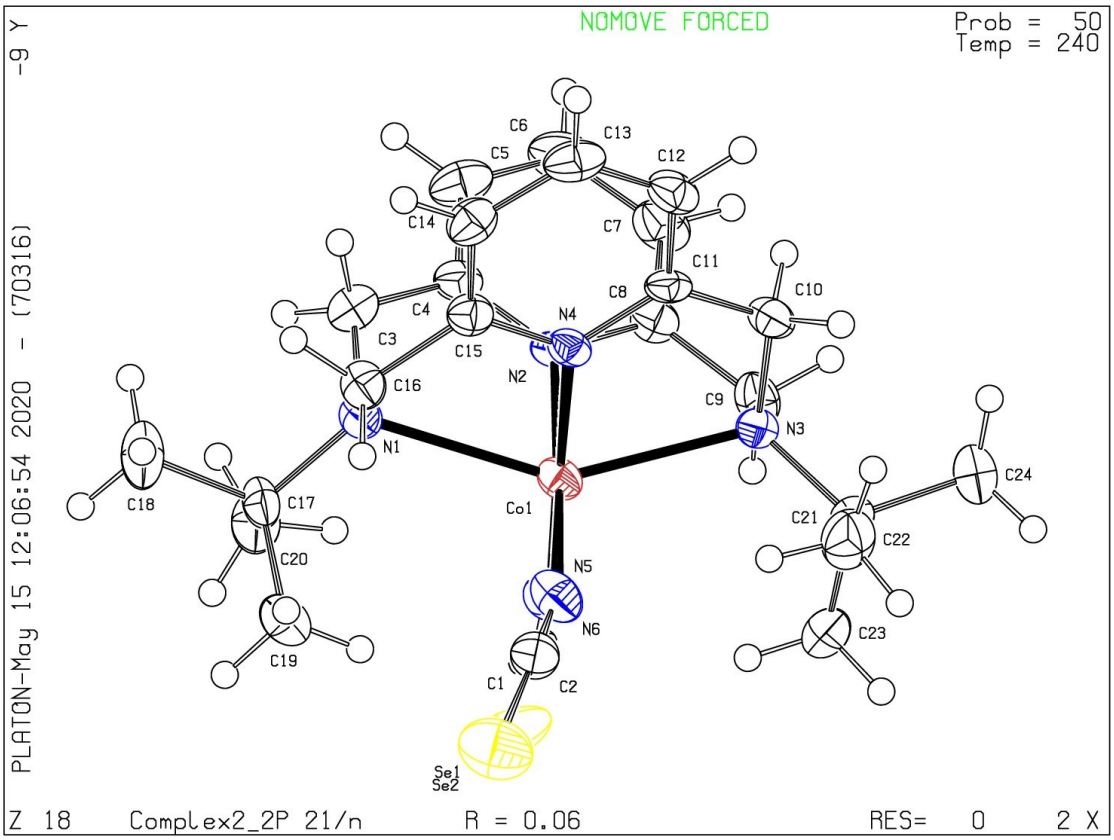
PLATON version of 22/04/2020; check.def file version of 09/03/2020

Datablock Complex2_240K - ellipsoid plot



checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Complex2_100K

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Complex2_100K

```
Bond precision: C-C = 0.0030 A           Wavelength=0.71073
Cell:           a=11.6185(15)     b=13.8515(19)      c=15.550(2)
                alpha=90          beta=90.276(7)     gamma=90
Temperature:    100 K

                Calculated                Reported
Volume          2502.5(6)                 2502.5(6)
Space group     P 21/n                    P 21/n
Hall group      -P 2yn                    -P 2yn
Moiety formula C24 H32 Co N6 Se2          ?
Sum formula     C24 H32 Co N6 Se2         C24 H32 Co N6 Se2
Mr              621.41                    621.40
Dx,g cm-3       1.649                     1.649
Z               4                         4
Mu (mm-1)       3.619                     3.619
F000            1252.0                    1252.0
F000'           1252.96
h,k,lmax        16,19,22                  16,19,22
Nref            7743                      7730
Tmin,Tmax       0.176,0.350               0.801,0.920
Tmin'           0.125
Correction method= # Reported T Limits: Tmin=0.801 Tmax=0.920
AbsCorr = MULTI-SCAN

Data completeness= 0.998          Theta(max)= 30.672

R(reflections)= 0.0335( 5904)     wR2(reflections)= 0.0756( 7730)

S = 1.014                 Npar= 426
```

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level.**

```
Click on the hyperlinks for more details of the test.
```

Alert level C

```
PLAT222_ALERT_3_C NonSolvent Resd 1  H   Uiso(max)/Uiso(min) Range        6.8 Ratio
```

Alert level G

```
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         32 Note
PLAT230_ALERT_2_G Hirshfeld Test Diff for    Se1      --C1       .        6.0 s.u.
PLAT230_ALERT_2_G Hirshfeld Test Diff for    Se2      --C2       .        6.2 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N5       .        6.6 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N6       .        5.8 s.u.
PLAT793_ALERT_4_G Model has Chirality at N1          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N3          (Centro SPGR)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (III)     .       2.91 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600         15 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.         11 Info
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
0 ALERT level B = A potentially serious problem, consider carefully
1 ALERT level C = Check. Ensure it is not caused by an omission or oversight
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   1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   5 ALERT type 2 Indicator that the structure model may be wrong or deficient
   1 ALERT type 3 Indicator that the structure quality may be low
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   1 ALERT type 5 Informative message, check
```

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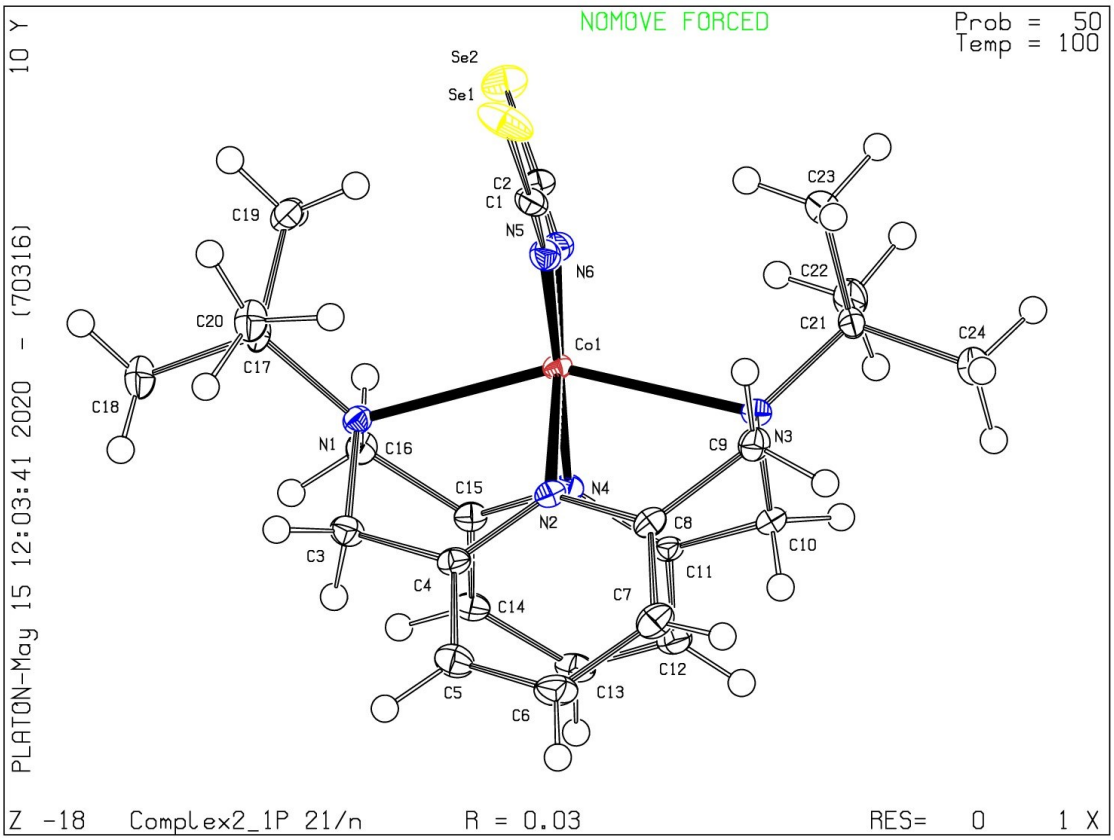
PLATON version of 22/04/2020; check.def file version of 09/03/2020

Datablock Complex2_100K - ellipsoid plot



Complex 3

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) Complex3

THIS REPORT IS FOR GUIDANCE ONLY. IF USED AS PART OF A REVIEW PROCEDURE FOR PUBLICATION, IT SHOULD NOT REPLACE THE EXPERTISE OF AN EXPERIENCED CRYSTALLOGRAPHIC REFEREE.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: Complex3

```
Bond precision: C-C = 0.0037 A           Wavelength=0.71073
Cell:           a=13.3379(2)    b=12.6230(2)        c=18.7965(4)
                alpha=90        beta=110.087(1)     gamma=90
Temperature:    296 K

                Calculated              Reported
Volume          2972.16(9)              2972.16(9)
Space group     P 21/c                  P 21/c
Hall group      -P 2ybc                 -P 2ybc
Moiety formula C30 H32 Co N10           ?
Sum formula     C30 H32 Co N10          C30 H32 Co N10
Mr              591.59                  591.58
Dx,g cm-3       1.322                   1.322
Z               4                       4
Mu (mm-1)       0.615                   0.615
F000            1236.0                  1236.0
F000'           1237.68
h,k,lmax        19,18,26                19,18,26
Nref            9147                    9010
Tmin,Tmax       0.741,0.814             0.875,0.943
Tmin'           0.644
Correction method= # Reported T Limits: Tmin=0.875 Tmax=0.943
AbsCorr = MULTI-SCAN

Data completeness= 0.985          Theta(max)= 30.599

R(reflections)= 0.0447( 5288)     wR2(reflections)= 0.1247( 9010)

S = 0.999                 Npar= 498
```

The following ALERTS were generated. Each ALERT has the format **test-name_ALERT_alert-type_alert-level.**
Click on the hyperlinks for more details of the test.

Alert level C

```
ABSTY02_ALERT_1_C  An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
           Absorption correction given as multi-scan
PLAT220_ALERT_2_C NonSolvent Resd 1  N   Ueq(max) / Ueq(min) Range        3.2 Ratio
PLAT242_ALERT_2_C Low    'MainMol' Ueq as Compared to Neighbors of         C8 Check
```

Alert level G

```
PLAT063_ALERT_4_G Crystal Size Possibly too Large for Beam Size ..       0.70 mm
PLAT164_ALERT_4_G Nr. of Refined C-H H-Atoms in Heavy-Atom Struct.         32 Note
PLAT230_ALERT_2_G Hirshfeld Test Diff for    C2       --C4       .        5.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N5       .        9.1 s.u.
PLAT232_ALERT_2_G Hirshfeld Test Diff (M-X)  Co1      --N6       .        9.0 s.u.
PLAT793_ALERT_4_G Model has Chirality at N1          (Centro SPGR)          S Verify
PLAT793_ALERT_4_G Model has Chirality at N3          (Centro SPGR)          S Verify
PLAT794_ALERT_5_G Tentative Bond Valency for Co1       (III)     .       2.90 Info
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary .     Please Do !
PLAT910_ALERT_3_G Missing # of FCF Reflection(s) Below Theta(Min).          2 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600        134 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.          1 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by          1 Check
```

```
   0 ALERT level A = Most likely a serious problem - resolve or explain
   0 ALERT level B = A potentially serious problem, consider carefully
   3 ALERT level C = Check. Ensure it is not caused by an omission or oversight
  13 ALERT level G = General information/check it is not something unexpected

   2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
   6 ALERT type 2 Indicator that the structure model may be wrong or deficient
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```

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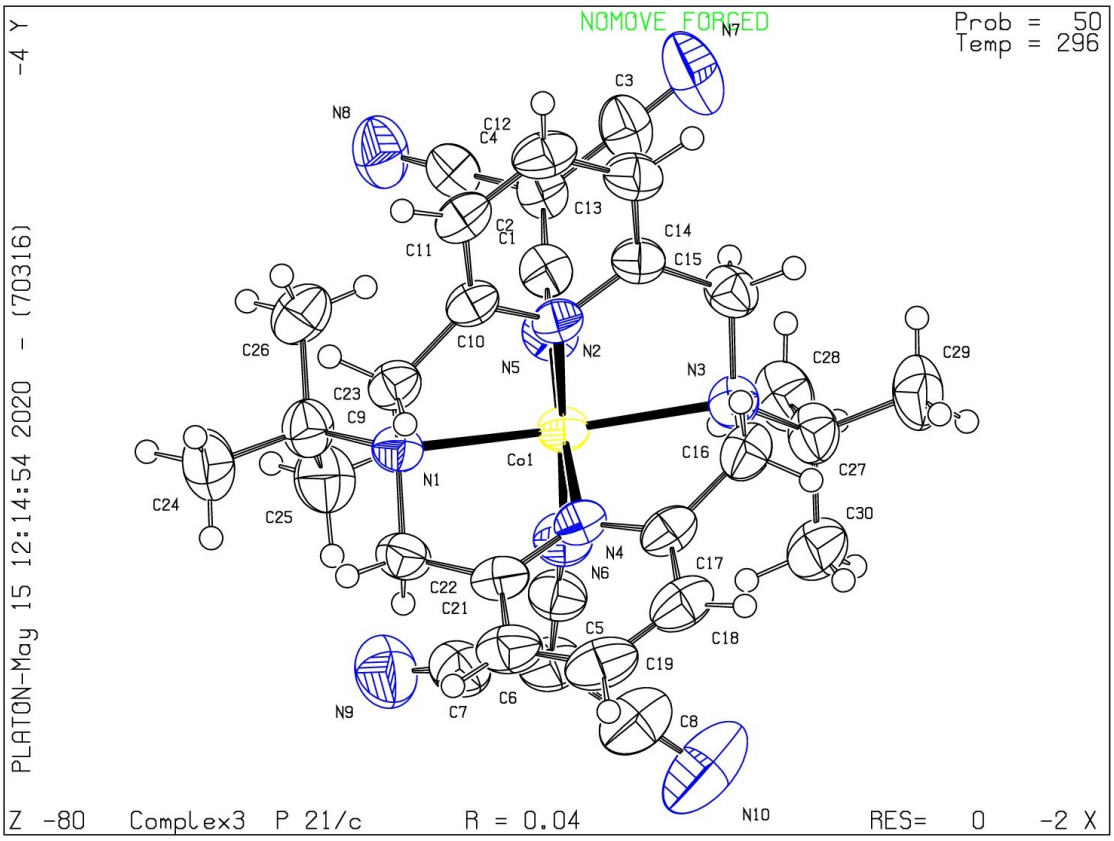

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