Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supplementary Information

Synthetic Strategy for Switching the Single Ion Anisotropy in Tetrahedral Co(II) Complexes

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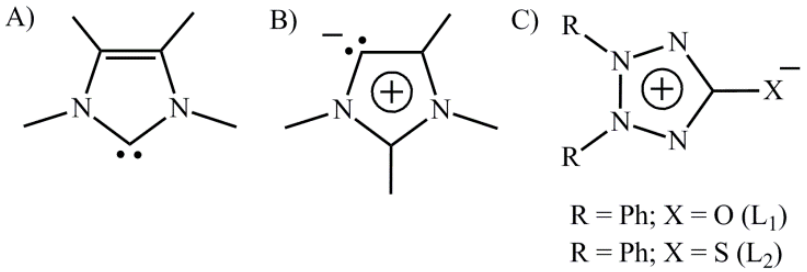
Scheme S1. Representative example of A) N-heterocyclic carbine; B) Diazomesoionic carbene and C) Exocyclic mesoionic 2,3-substituted-tetrazolium-5-(thi)olate.



Experimental:

Unless otherwise stated all the reactions (ligand and complex synthesis) were carried out under aerobic conditions.Infrared spectra werecollected for the solid samples using KBr pellets on a Perkin-ElmerFT-IR spectrometer in 400 to 4000 cm^{-1}range. NMR data was collected for the pure ligand using a Bruker Avance III 400 MHz instrument. Magnetic susceptibility measurements were performed using MPMS SQUID Magnetometer equipped with a 7 Tesla magnet in 300–2.0K.The elemental analysis (CHN) were carried out on a Elementar analysensysteme GmbH VarioEL.ESI-Mass spectrometry was performed using a Q-TOF micromass (YA-105) spectrometer. The chosen crystal was mounted on a Goniometer using mineral oil and the crystal is cooled down in stream of liquid nitrogen to 100 K using Oxford cryosystems cooler device. The data collection was done on Rigaku Saturn CCD diffractometer using a graphite monochromator (λ = 0.71073°). The unit cell determination and data reduction were performed using Rigaku CrystalClear-SM Expert 2.1 software. The structures were solved by direct methods and the refined by least-squares procedures on F^2 with SHELXTL package. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed based on the geometry and refined with a riding model.

Synthesis of 2,3-diphenyl-1,2,3,4-tetrazolium-5-olate (L_1):

The synthesis of L_1 has previously been reported elsewhere.[1] An alternative procedure has been developed in this work via a simple two step method in good yield, which is detailed below.

Step 1: Synthesis of 1,5-diphenylcarbonohydrazide

A solution of triphosgene (5g, 0.0169mol) in 40mL benzene was added to a solution of phenylhydrazine (21.86g, 0.2022mol) in 100mL DCM at -42°C (dry ice/acetonitrile bath) under nitrogen atmosphere. The reaction mixture was stirred for 48 hours. After that the precipitated phenylhydrazine hydrochloride was filtered under vacuum. The solvents were removed under reduced pressure and the product of interest was extracted with hexane. The hexane was removed under vacuum to obtain pure yellow coloured product of 1,5-diphenylcarbonohydrazide. Yield : 4.5 g (73.6%). ^{1}H-NMR ($CDCl_3$, 400MHz): δ 7.2 ppm (m,10H) and δ 4.43 ppm (s,4H) (Figure S1) . IR (KBr):- 3333 cm^{-1} ($-\nu_{NH}$), 2963 cm^{-1} ($\nu_{-C-H(aromatic)}$) and 1667 cm^{-1} ($\nu_{-C=O}$). Elemental analysis: Calc: C, 64.44%; H, 5.82%; N, 23.12% Found: C, 63.99%; H, 6.07%; N, 23.12%. ESI-MS: m/z = 243.12 (M+H), m/z 265.10 (M+Na)

Step 2: Synthesis of 2,3-diphenyl-1,2,3,4-tetrazolium-5-olate (L_1)

Into the hot (~80°C) benzene solvent (20 mL), 1,5-diphenylcarbonohydrazide (2g, 8.26mmol) was added followed by solid p-benzoquinone (2.2g, 20.66mmol). Upon addition of p-benzoquinone blue black precipitate begins to form. Then the reaction mixture was cooled to room temperature which was stirred further for another 24 hour. After completion of reaction, the blue black precipitate was collected and washed with diethyl ether (4-5 times). To ensure the complete removal of reduced product of p-benzoquinone the precipitate washed again withTHF (4-5 times). Thus obtained compound is pure and the purity of the ligand (L_1) was confirmed by NMR and mass spectrometry. Yield = 700 mg (35.7%). ^{1}H-NMR (CD_3OD, 400MHz) δ7.8 ppm (m,10H). ^{13}C-NMR (CD_3OD):-δ 127 ppm, 131 ppm , 133 ppm, 135 ppm and 173 ppm. IR (KBr pellet): 1667 cm^{-1} ($\nu_{C=O}$),1634 cm^{-1}($\nu_{C=N}$) and 1589 cm^{-1} ($\nu_{N=N}$). Elemental analysis: Calc: C, 65.26%; H, 4.63%; N, 23.41% Found: C, 64.52%; H, 3.6%; N, 23.07%. ESI-MS: m/z = 239.09 (M+H), m/z = 261.07 (M+Na).

Synthesis of **1**:

The ligand L_1 (0.5 g, 2.1 mmol) was dissolved in methanol (20 mL). Into this solution, methanolic solution of (0.5 g in 10 ml of MeOH, 2.1 mmol) $CoCl_2.6H_2O$ was added. The resultant reaction mixture was heated under reflux for 24 hours. After completion of reaction, the reaction mixture was cooled to room temperature before the solvent was stripped off using rotovap. The resultant residue was washed with DCM and diethyl ether several times to remove unreacted ligands and other impurities. This residue was recrystallized from acetonitrile. Blue coloured needle shaped crystals which are suitable for x-ray diffraction

were grown by diffusion of diethylether in acetonitrile solution of the complex after one week. Elemental analysis: Cal: C, 44.04%; H, 3.20%; N, 17.12%. Found: C, 43.7%; H, 2.94%; N, 17.57%. IR (KBr pellet): 2924 cm^{-1} ($\upsilon_{C-H(aromatic)}$) 1601 cm^{-1} ($\upsilon_{(C=O)}$).

Synthesis of **2**:

Same procedure was followed as in **1**, but $CoBr_2$ was used in place of $CoCl_2$. $6H_2O$. Elemental analysis: Cal: C, 36.18%; H, 2.63%; N, 14.06%. Found: C, 35.3%; H, 2.74%; N, 13.26%. IR (KBr Pellet): 2929 cm^{-1} ($\upsilon_{C-H(aromatic)}$) 1596 cm^{-1} ($\upsilon_{(C=O)}$).

Synthesis of **3**:

Same procedure has been followed as in **1**, but L_2 was used in place of L_1. Elemental analysis: Cal: C, 42.37%; H, 3.08 %; N, 16.47%; S, 7.54%. Found: C, 42.23%; H, 2.92%; N, 16.66%; S, 6.99%. IR (KBr pellet): 2944 cm^{-1} ($\upsilon_{C-H(aromatic)}$) 1348 cm^{-1} ($\upsilon_{(C=S)}$).

Synthesis of **4**:

Same procedure was followed as in **3**, but single crystal growth was effected by diffusing DCM into the acetonitrile solution. . Elemental analysis: Calc: C, 35.04%; H, 2.55%; N, 13.6%; S, 6.24%; Found: C, 34.7%; H, 2.25%; N 13.58%; S, 5.94%. IR (KBr pellet): 2923cm^{-1} ($\upsilon_{C-H(aromatic)}$) 1341 cm^{-1} ($\upsilon_{(C=S)}$).

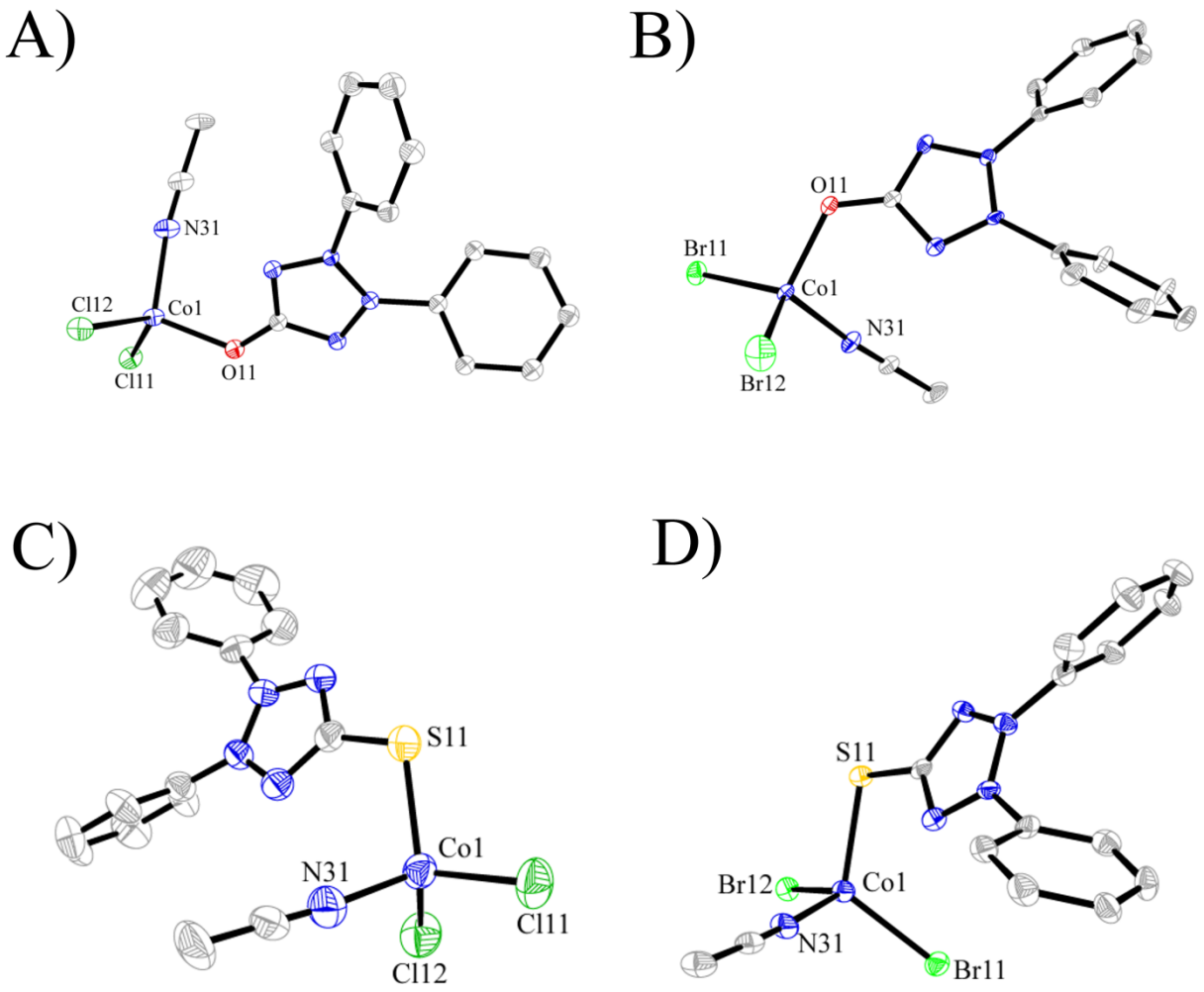


Figure S1. Molecular Structure of complexes A) **1**, B) **2**, C) **3** and D) **4**

Structural description:

Compounds **1** - **4** are isostructural and crystallize in the triclinic space group *P-1* (see Table S1 of ESI for crystallographic information). The asymmetric unit for both **1** and **2** reveal two crystallographically distinct molecules, however there is not much significant changes in the crystallographic parameters between two distinct molecules (Table S2 of ESI). On the contrary, the asymmetric unit of **3** and **4** contains only one unique molecule, with the Co(II) ions exhibiting distorted tetrahedral geometries. In all four complexes, two of the coordination sites are occupied by halide ions, while the third is taken by an acetonitrile molecule. The fourth coordination site is provided by the exocyclic oxygen (for **1** and **2**)/sulfur (for **3** and **4**) atom of the mesoionic ligand. Selected bond lengths and angles for **1**-**4**are given in TableS3. The packing diagrams of all four complexes reveal intermolecular hydrogen bonding interactions facilitated by the halide ions, the interactions being listed in Table S4.

Table S1. Crystallographic parameters for **1**-**4**

	1	**2**	**3**	**4**
Formula	$CoC_{16}H_{14.5}N_{5.5}O_1Cl_2$	$CoC_{16}H_{14.5}N_{5.5}O_1Br_2$	$CoC_{15}H_{13}N_5S_1Cl_2$	$Co_1C_{15}H_{13}Br_2N_5S$
Size [mm]	0.15 x 0.11 x 0.07	0.21 x 0.16 x 0.11	0.15 × 0.11 × 0.07	0.2 × 0.16 × 0.11
System	Triclinic	Triclinic	Triclinic	Triclinic
Space group	*P-1*	*P-1*	*P-1*	*P-1*
a [Å]	9.611(2)	9.832(2)	8.479(17)	8.441(7)
b [Å]	13.180(3)	13.304(3)	9.071(18)	9.015(8)
c [Å]	15.861(4)	15.925(3)	13.536(3)	13.725(13)
α [°]	75.031(8)	105.240(4)	77.03(3)	77.19(4)
β [°]	76.859(7)	103.610(5)	80.74(3)	80.64(5)
γ [°]	89.895(9)	90.386(3)	67.56(3)	68.94(4)
V [Å^3]	1886.7(8)	1948.2(6)	934.4(3)	946.4(15)
Z	4	4	2	2
ρ_{calcd}[g/cm^{-3}]	1.513	1.768	1.511	1.804
$2\Theta_{max}$	50.68	58.28	50.0	55.0
radiation	Mo K_α	Mo K_α	Mo K_α	Mo K_α
λ [Å]	0.71073	0.71073	0.71073	0.71073
T [K]	100	100	298	100
reflns	14756	33380	12443	14665
Ind. reflns	6751	10000	3248	4220
reflns with *I>2σ(I)*	3432	8832	2564	3290
R1	0.0843	0.0726	0.0782	0.0741
wR2	0.2251	0.2127	0.1126	0.1626

Table S2. Comparison of selected structural parameters of the two distinct molecules found in the unit cell of complexes**1** and **2**.

Complex **1**:

Label	Molecule 1 (Å)	Molecule 2 (Å)	Difference (Å)
Co-Cl1	2.228	2.250	0.022
Co-Cl2	2.252	2.239	0.013
Co-O11	2.010	2.015	0.005
Co-N31	1.957	1.958	0.001
Bond Angle (°)			
Cl2-Co-Cl1	117.0	115.6	1.4°
O11-Co-Cl1	113.0	114.0	1°
O11-Co-Cl2	105.8	104.8	1°
N31-Co-Cl1	108.4	106.5	1.9°
N31-Co-Cl2	109.2	110.8	1.6°
N31-Co-O11	102.4	104.6	2.2°

Complex **2**:

Label	Molecule 1 (Å)	Molecule 2 (Å)	Difference (Å)
Co-Br1	2.371	2.375	0.004
Co-Br2	2.312	2.345	0.033
Co-O11	1.957	1.948	0.009
Co-N31	2.004	2.012	0.008
Bond Angle (°)			
Br2-Co-Br1	115.6	114.7	0.9
O11-Co-Br1	105.7	104.4	1.3
O11-Co-Br2	114.3	114.5	0.2
N31-Co-Cl1	108.7	111.2	2.5
N31-Co-Cl2	108.7	106.8	1.9
N31-Co-O11	103.0	104.9	1.9

Table S3. Selected bond lengths and angles for **1**-**4**.

Label	**1***	**2***	**3**	**4**
Co-X11 (Å)	2.239 (18)	2.373 (4)	2.222 (2)	2.369 (2)
Co-X12 (Å)	2.246 (17)	2.329 (3)	2.238 (17)	2.412 (3)
Co-Y11 (Å)	2.013 (5)	1.953 (4)	2.318 (18)	2.316 (3)
Co-N31 (Å)	1.958 (6)	2.008 (4)	2.013 (5)	2.017 (7)
Bond Angle (°)				
X12-Co- X11 (°)	116.3 (7)	115.2 (11)	110.2 (8)	109.2 (7)
Y11-Co- X11 (°)	113.5 (14)	105.1 (15)	103.2 (7)	119.30 (9)
Y11-Co- X12 (°)	105.3 (15)	114.4 (15)	118.1 (7)	101.24 (8)
N31-Co- X11 (°)	107.5 (18)	110.0 (14)	114.6 (15)	107.1 (2)
N31-Co- X12 (°)	110.0 (16)	107.8 (12)	106.5 (16)	114.5 (2)
N31-Co-Y11 (°)	103.5 (2)	104.0 (14)	104.4 (15)	105.7 (19)

Note:- X = Cl and Y = O for **1**, X = Br and Y = O for **2**, X = Cl and Y = S for **3** and X = Br and Y = S for **4**.

* Average bond length and bond angle of the two distinct molecules in the unit cell.

Table S4. Atoms involved in intermolecular hydrogen bondingand the corresponding bond distances.

Hydrogen bonding in "**1**"

Hydrogenbond donor (D)…acceptor(A)	D… A (Å)
C21-H21...Cl1_$1	3.628(7)
C52-H52...O11_$1	3.329(9)
C53-H53...Cl1_$2	3.519(7)
C62-H62A...Cl1_$2	3.798(8)
C17-H17...Cl3_$2	3.712(7)
C32-H32B...Cl3_$2	3.696(9)
C2S-H2S2...Cl4_$2	3.820(10)
C32-H32A...Cl2_$3	3.656(8)
C49-H49...Cl2_$4	3.538(7)
C19-H19...Cl4_$4	3.484(7)
C51-H51...Cl4_$5	3.826(8)
C32-H32C...O41_$6	3.293(9)

$1 = +X, Y-1, +Z; $2 = 2-X, 2-Y, -Z; $3 = 2-X, 3-Y, -Z-1; $4 = 1-X, 2-Y, -Z; $5 = 1-X, 1-Y, -Z; $6 = X+1, Y+1, Z-1

Hydrogen bonding in "**2**"

Hydrogen bond donor (D)…acceptor(A)	D… A (Å)
C15-H15A...Br1_$1	3.710(5)
C53-H53A...Br1_$2	3.599(5)
C62-H62C...Br1_$2	3.868(6)
C62-H62A...Br1_$3	3.647(5)
C32-H32A...Br2_$4	3.675(6)
C43-H43A...Br2_$1	3.509(4)
C49-H49A...Br2_$1	3.644(5)
C19-H19A...Br3_$5	3.801(5)
C32-H32B...Br3_$5	3.786(6)
C17-H17A...Br4_$6	3.578(5)
C51-H51A...Br4_$7	3.879(5)
C2S-H2S1...Br4_$8	3.837(7)
C2S-H2S3...Br4_$9	4.005(8)

$1 = +X, 1+Y, +Z; $2 = 1+X, 1+Y, +Z; $3 = 1-X, 1-Y, 2-Z; $4 = -X, -Y, 1-Z; $5 = X-1, Y-1, +Z; $6 = +X, Y-1, +Z; $7 = 1-X, 2-Y, 2-Z; $8 = 1-X, 2-Y, 1-Z; $9 = +X, Y-1, Z-1

Hydrogen bonding in "**3**"

Hydrogen bond donor (D)…acceptor(A)	D… A (Å)
C(21)-H(21)...Cl(11)_$1	3.651(8)
C(23)-H(23)...Cl(12)_$2	3.584(7)
C(25)-H(25B)...Cl(12)_$3	3.457(9)

$1 = x,y,z-1 $2 = -x+1,-y+1,-z+1 $3 = -x,-y+1,-z+1

Hydrogen bonding in "**4**"

Hydrogen bond donor (D)…acceptor(A)	D… A (Å)
C(13)-H(13)...Br(11)_$1	3.802(9)
C(19)-H(19)...Br(11)_$1	3.697(8)
C(32)-H(32B)...Br(11)_$2	3.575(10)
C(15)-H(15)...Br(12)_$3	3.689(8)

$1 = -x,-y+1,-z $2 = -x+1,-y+1,-z; $3 = x,y,z+1

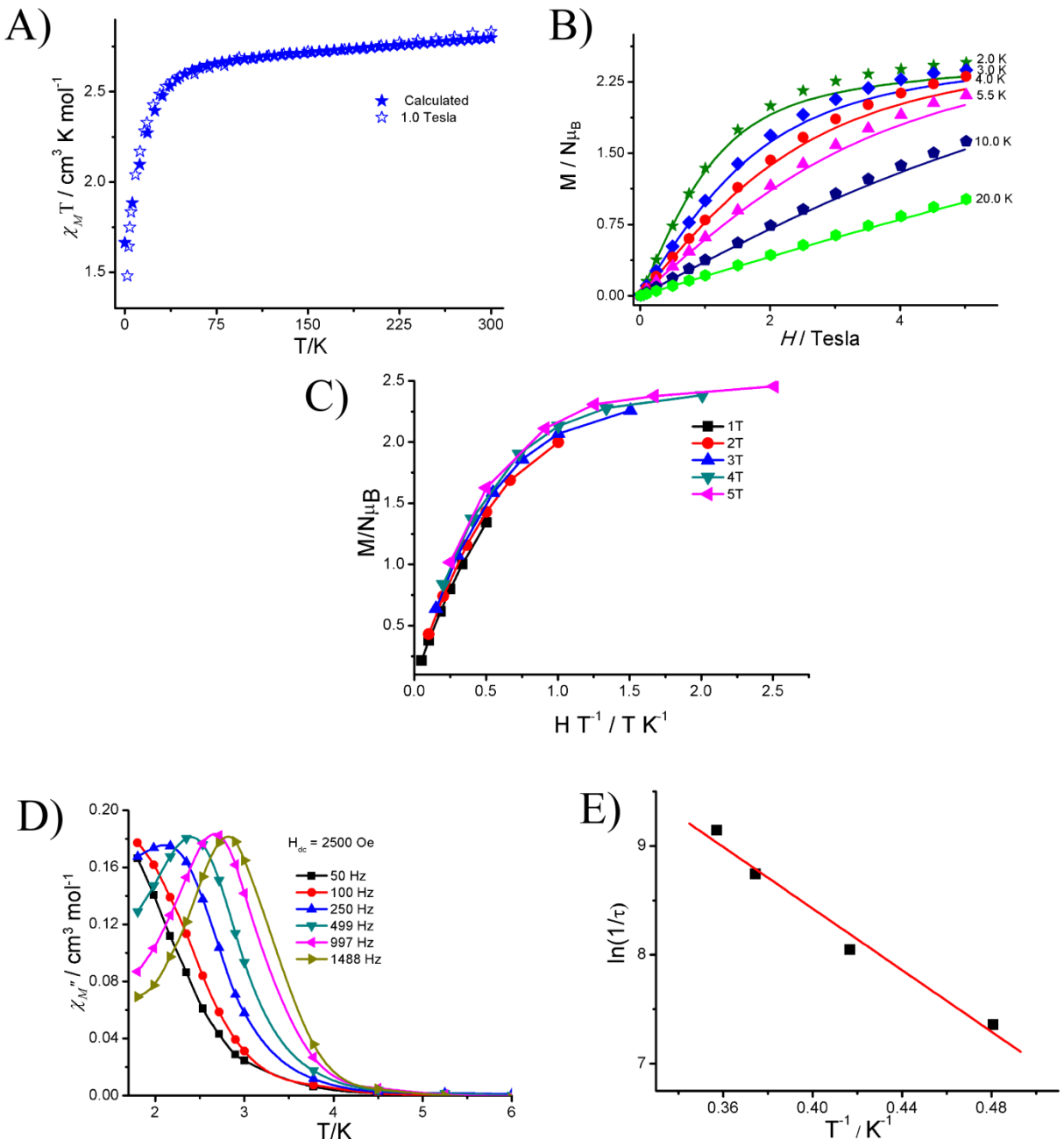


Figure S2. A) Temperature dependent $\chi_M T$ data recorded on a polycrystalline sample of **1**. Open stars represent the experimental data and the filled star represent the $\chi_M T$ computed values using CASSCF results; B) Field dependent magnetization data of **1** measured at the indicated temperatures. Symbols represent the experimental data, with the solid lines representing the computed magnetization data using CASSCF results. C) Reduced magnetization plot of **1.** D) Temperature dependence of the out-of-phase component of the alternating current (ac) susceptibility measured at the indicated optimum external dc-field of **1**. E) Arrhenius plot constructed from the ac susceptibility measurement of **1**.

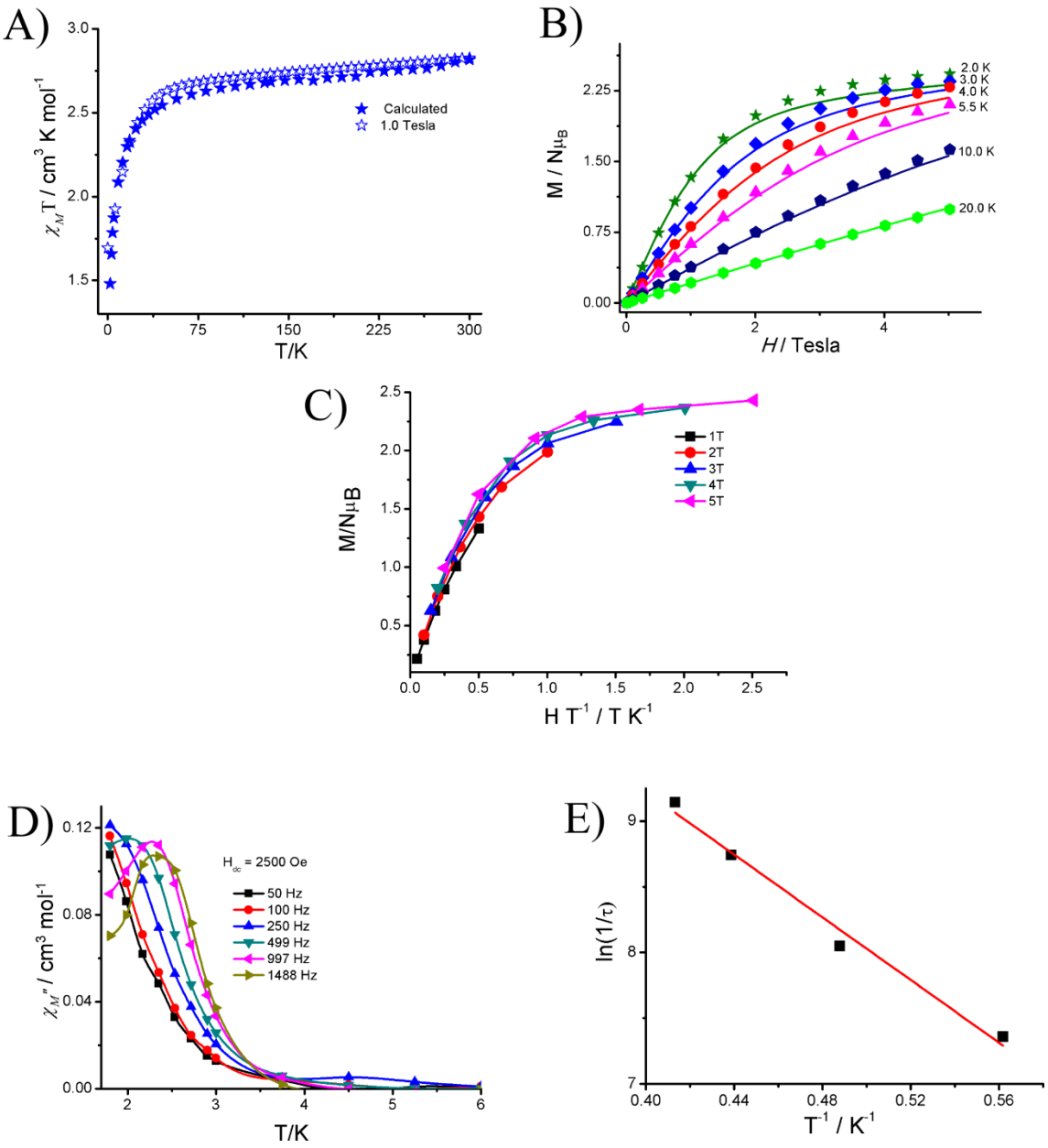


Figure S3. A) Temperature dependent $\chi_M T$ data recorded on a polycrystalline sample of **2**. Open stars represent the experimental data and the filled star represent the $\chi_M T$ computed values using CASSCF results; B) Field dependent magnetization data of **2** measured at the indicated temperatures. Symbols represent the experimental data, with the solid lines representing the computed magnetization data using CASSCF results. C) Reduced magnetization plot of **2.** D) Temperature dependence of the out-of-phase component of the alternating current (ac) susceptibility measured at the indicated optimum external dc-field of **2**. E) Arrhenius plot constructed from the ac susceptibility measurement of **2.**

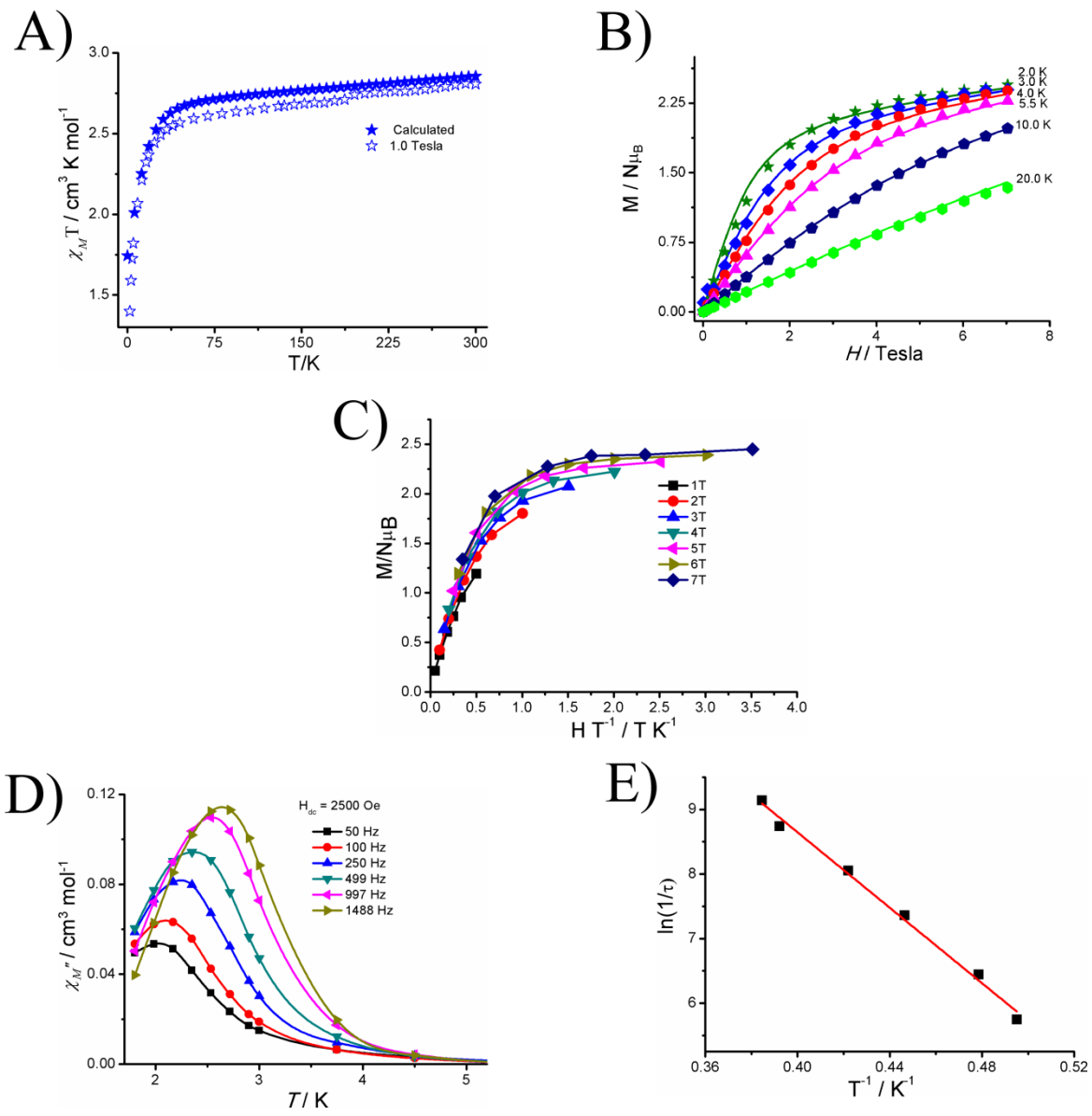


Figure S4. A) Temperature dependent $\chi_M T$ data recorded on a polycrystalline sample of **3**. Open stars represent the experimental data and the filled star represent the $\chi_M T$ computed values using CASSCF results; B) Field dependent magnetization data of **3** measured at the indicated temperatures. Symbols represent the experimental data, with the solid lines representing the computed magnetization data using CASSCF results. C) Reduced magnetization plot of **3**. D) Temperature dependence of the out-of-phase component of the alternating current (ac) susceptibility measured at the indicated optimum external dc-field of **3**. E) Arrhenius plot constructed from the ac susceptibility measurement of **3**.

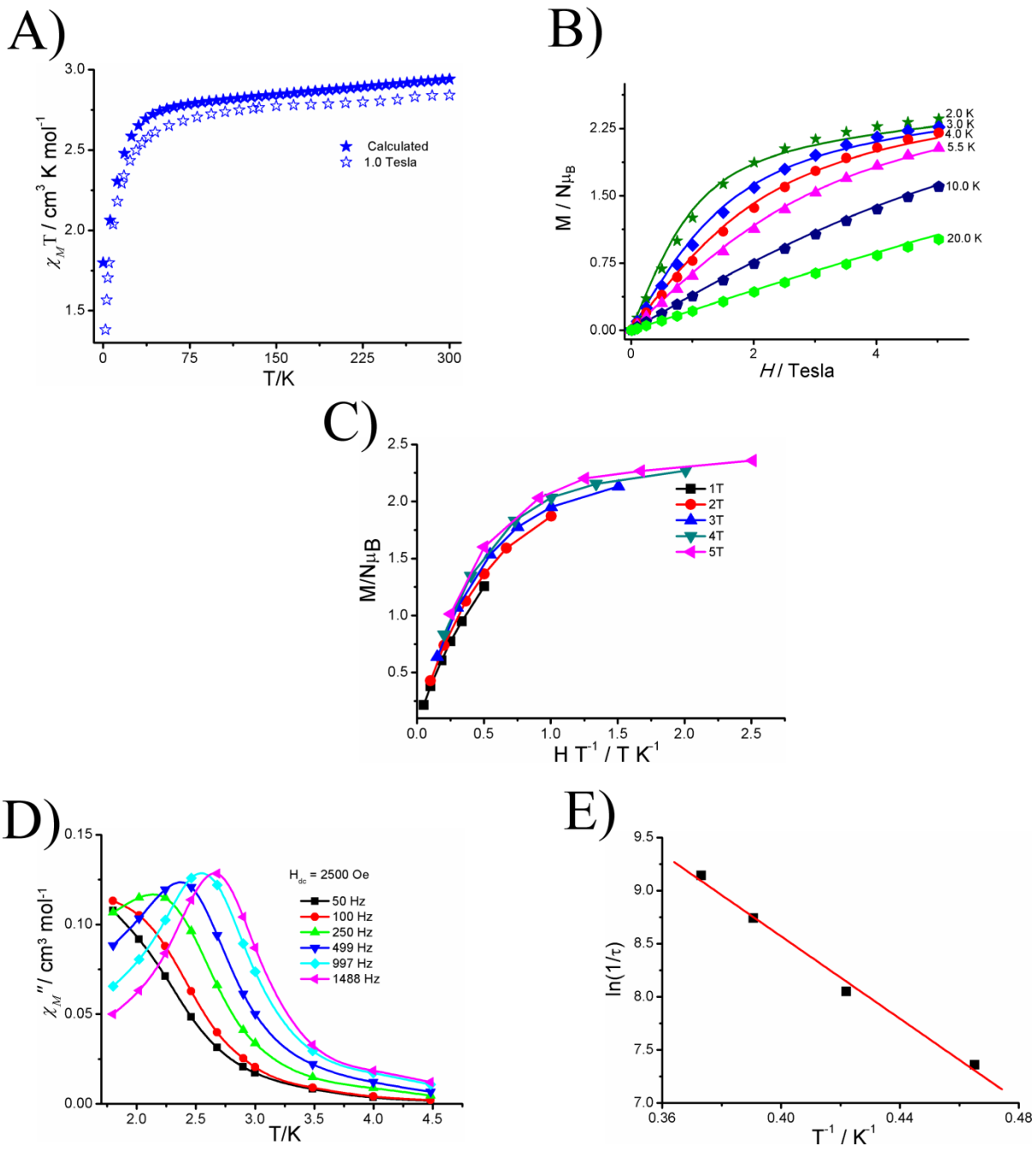


Figure S5. A) Temperature dependent $\chi_M T$ data recorded on a polycrystalline sample of **4**. Open stars represent the experimental data and the filled star represent the $\chi_M T$ computed values using CASSCF results; B) Field dependent magnetization data of **4** measured at the indicated temperatures. Symbols represent the experimental data, with the solid lines representing the computed magnetization data using CASSCF results. C) Reduced magnetization plot of **4**. D) Temperature dependence of the out-of-phase component of the alternating current (ac) susceptibility measured at the indicated optimum external dc-field of **4**. E) Arrhenius plot constructed from the ac susceptibility measurement of **4**.

Table S5. Comparison of the SH parameters of **1**-**4**extracted from *ab initio*[#] calculations and fitting of the experimental data ($\chi_M T(T)$ and $M(H)$) using PHI[*].

Complex	[#]D_{cal} (cm^{-1})	[#]$\lvert E/D\rvert_{cal}$	[#]g_{cal} (g_{xx},g_{yy},g_{zz})	[*]D_{fit} (cm^{-1})	[*]D_{fit} (cm^{-1})	*g-value
1	20.35	0.18	2.47, 2.39, 2.21	+15.61	-7.96	2.34
2	18.54	0.24	2.49, 2.38, 2.23	+11.16	-5.84	2.34
3	-15.90	0.21	2.28, 2.36, 2.50	+11.15	-11.3	2.34
4	-16.61	0.16	2.31, 2.38, 2.54	+11.6	-10.32	2.34

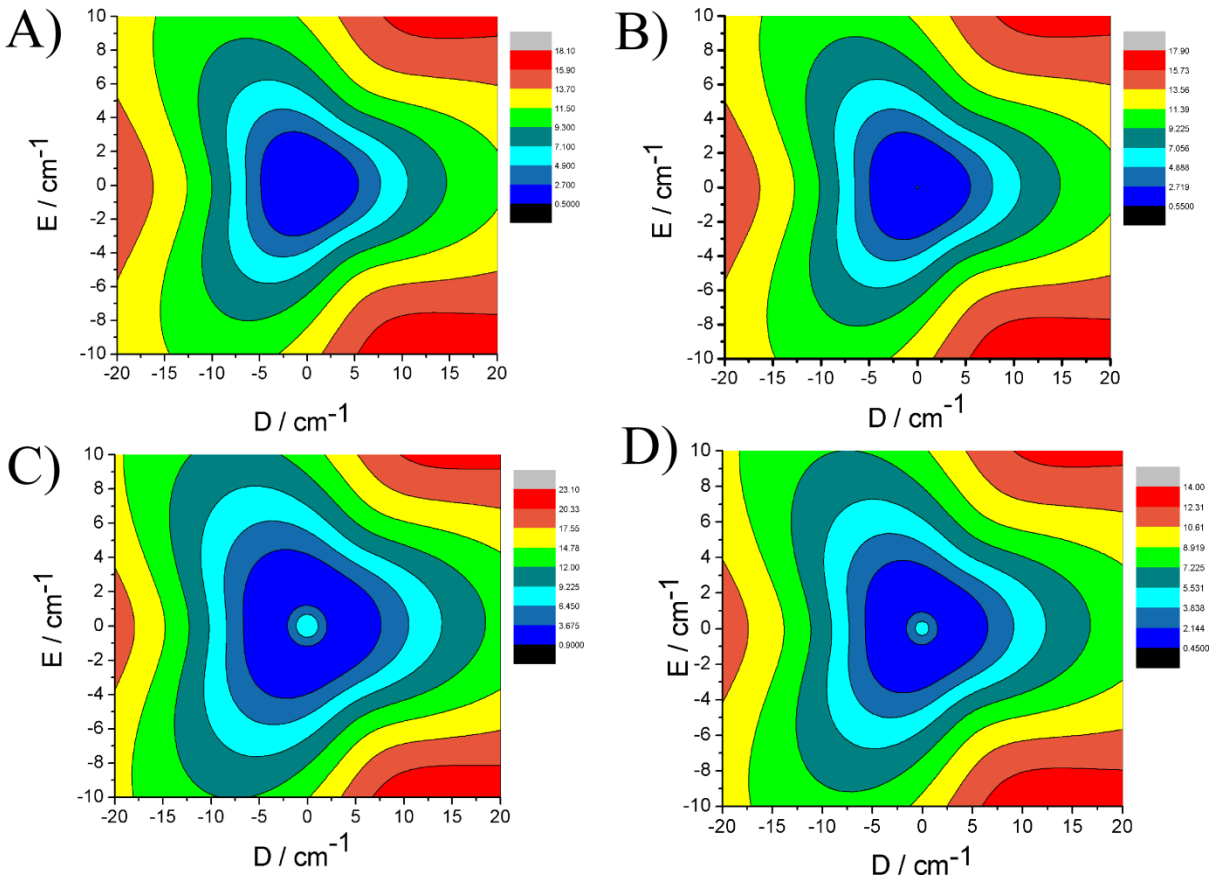


Figure S6. The magnetic data can be fitted using multiple parameters using PHI software which is represented in the 2-dimentional plot for A) **1** B) **2** c) **3** d) **4**. This clearly shows a range of parameters can yield a good fit to the magnetic data.

It was found that fits (phi) of the magnetic data were insensitive to sign of the *D* value which is clearly reflected in Table S5 and Figure S6 (see above). Although good fits for each were obtained yielding different parameters listed above in Table S5, much better fitting was obtained when using positive *D* values for complex **1** and **2,** and negative *D* values for **3** and **4**. This trend is consistent with the computed SH parameters from *ab initio* calculations and EPR spectroscopic measurements.

Computation details:

Here we have performed all the *ab initio* calculations using MOLCAS 7.8 [2] suite. We have employed [ANO-RCC...6s5p3d2f1g.] basis set for Co, [ANO-RCC...4s3p2d.] basis set for C, [ANO-RCC...4s3p2d.] basis set for O, [ANO-RCC...2s1p.] basis set for H, [ANO-RCC...4s3p2d.] basis set for N, [ANO-RCC...5s4p2d.] basis set for S, [ANO-RCC...5s4p2d1f..] basis set for Cl, [ANO-RCC…6s5p3d1f.] basis set for Br, and [ANO-RCC....6s5p3d1f.] basis set for Se atoms. The ground state d- electron configuration for Co(II) is $3d^7$ and in all four complexes the Co(II) ion is tetrahedral, possessing an orbitally non-degenerate $^4A_2$ ground state. Any unsymmetrical coordination environment or symmetry lowering causes mixing of the ground and excited states via spin-orbit interaction. The spin-orbit coupling constant λ for the free Co(II) ion is estimated to be ~450 cm^{-1} and as we can see from the Table S6, S7, S11, S12 and S16 that $^4T_2$ state is almost 2000 cm^{-1} far from the $^4A_2$ ground state for all the complexes.This will result in a weak zfs in these complexes via second-order spin-orbit interactions. First we have performed CASSCF (Multi configurational complete active space self-consistent field (CASSCF) calculations)_calculations with an active space of seven active electrons in five 3d orbitals (7,5). With this active space, we have computed 10 quartets as well 40 doublets states in the CI procedure. After computing these excited states, we have mixed all these 35 quartets and 40 doublets using RASSI-SO (Restricted Active Space State Interaction) module to compute the spin-orbit coupled states. Due to hardware limitations we have not performed second order CASPT2 calculations. Further on, we have taken these computed SO states into the SINGLE_ANISO [3] program to compute the D-tensors. The Cholesky decomposition for two electron integrals is employed throughout. Using SINGLE_ANISO code we have also extracted the crystal field parameters as implemented in MOLCAS 7.8.Structural optimization, Mulliken charges and the spin densities have been computed using DFT calculations employing Gaussian 09 [4] suite. Here we have employed the B3LYP [5] functional, Ahlrichs triple ζ basis set [4] for all the atoms.

The sign as well as the magnitude of the zfs parameters are also reproducible using CASSCF/NEVPT2 methodology implemented in ORCA 3.0. The details of these calculations along with in depth bonding analysis will be published elsewhere.

Table S6. CASSCF+RASSI computed spin-free and spin-orbit state energies for complex **1**

Spin-free Energies (cm^{-1})	Spin-Orbit states (cm^{-1})	CASSCF+RASSI computed results					
0	0	g_X	2.475	X_M	0.402318	-0.676216	-0.617148
2769.545	42.593	g_Y	2.392	Y_M	0.670903	0.676445	-0.303828
3332.815	2711.211	g_z	2.218	Z_M	0.622920	-0.291811	0.725822
3450.773	2881.927						
4859.425	3178.274	D_X	-10.404	X_A	0.999961	-0.008617	0.001940
6293.926	3399.97	D_Y	-3.165	Y_A	0.008671	0.999517	-0.029858
7685.765	3647.166	D_Z	13.569	Z_A	-0.001682	0.029874	0.999552
21128.786	3890.029	D	20.3531				
21624.628	5017.824	|E|	3.6195				
23180.537	5180.626						
19374.4	6357.098	*D and E values are given in cm^{-1}*					
19651.344	6553.855						
19885.516	7975.806						
20301.314	8046.886						
20580.299	19398.42						
20969.324	19649.521						
21861.8	19849.621						
22145.234	20578.039						
22281.828	20766.072						
25644.273	21160.027						
26155.405	21198.083						
26221.125	21365.093						
26601.827	21691.752						
26847.738	21805.905						
27063.268	21919.499						
27569.51	22197.958						
27895.588	22622.29						
28174.59	23223.78						
28725.905	23356.967						
28850.158	25782.187						
29245.167	26144.195						
29712.701	26495.802						
30492.376	26852.993						
30694.714	27025.344						
31272.975	27324.682						
31532.468	27829.772						
32481.762	……						
32836.962							
44234.263							
44626.081							
45216.318							
45335.135							
45868.934							
45925.524							
67784.297							
67961.483							
69029.896							
69385.091							
70161.971							

Table S7. CASSCF+RASSI computed spin-free and spin-orbit state energies for complex **2**

Spin-free Energies (cm^{-1})	Spin-Orbit states (cm^{-1})	CASSCF+RASSI computed results					
0	0	g_X	2.492	X_M	0.295075	-0.778587	-0.553835
2644.261	40.120	g_Y	2.383	Y_M	0.789142	0.525388	-0.318153
3142.821	2574.946	g_z	2.239	Z_M	0.538688	-0.343176	0.769445
3201.462	2749.829						
4683.806	2961.292	D_X	-10.599	X_A	0.999828	-0.017896	-0.004961
6169.94	3186.840	D_Y	-1.763	Y_A	0.017808	0.999690	-0.017385
7579.047	3444.270	D_Z	12.362	Z_A	0.005271	0.017294	0.999837
20916.758	3722.232	D	18.543				
21721.02	4839.889	|E|	4.418				
22689.072	4985.060						
19179.84	6234.521	*D and E values are given in cm^{-1}*					
19556.759	6426.856						
19693.899	7863.801						
20063.817	7929.608						
20381.326	19202.430						
20782.547	19525.263						
21607.562	19695.827						
21975.282	20345.167						
22050.827	20579.026						
25407.384	20974.880						
25968.595	20998.611						
26079.279	21174.282						
26571.603	21661.414						
26611.166	21784.704						
26963.2	21857.721						
27381.884	22015.606						
27661.213	22399.552						
27927.787	22748.412						
28449.866	22890.989						
28685.012	25545.832						
29143.79	26051.554						
29565.749	26297.578						
30306.714	26735.364						
30400.823	26908.309						
31005.079	27120.012						
31270.054	27595.064						
32240.356	……						
32441.465							
43996.565							
44406.293							
44900.297							
45024.603							
45486.748							
45535.227							
45664.36							
67590.254							
67652.741							
68380.691							
69083.543							
69550.495							

Table S8. Angle between the g-tensors and*D*-Tensors for complexes **1**-**4**.

Angle (°)	**1**	**2**	**3**	**4**
g_{zz}-Co-D_{zz}	3.429	2.072	3.813	3.940
g_{yy}-Co-D_{yy}	3.563	2.852	4.256	2.423
g_{xx}-Co-D_{xx}	1.012	2.128	3.849	3.362

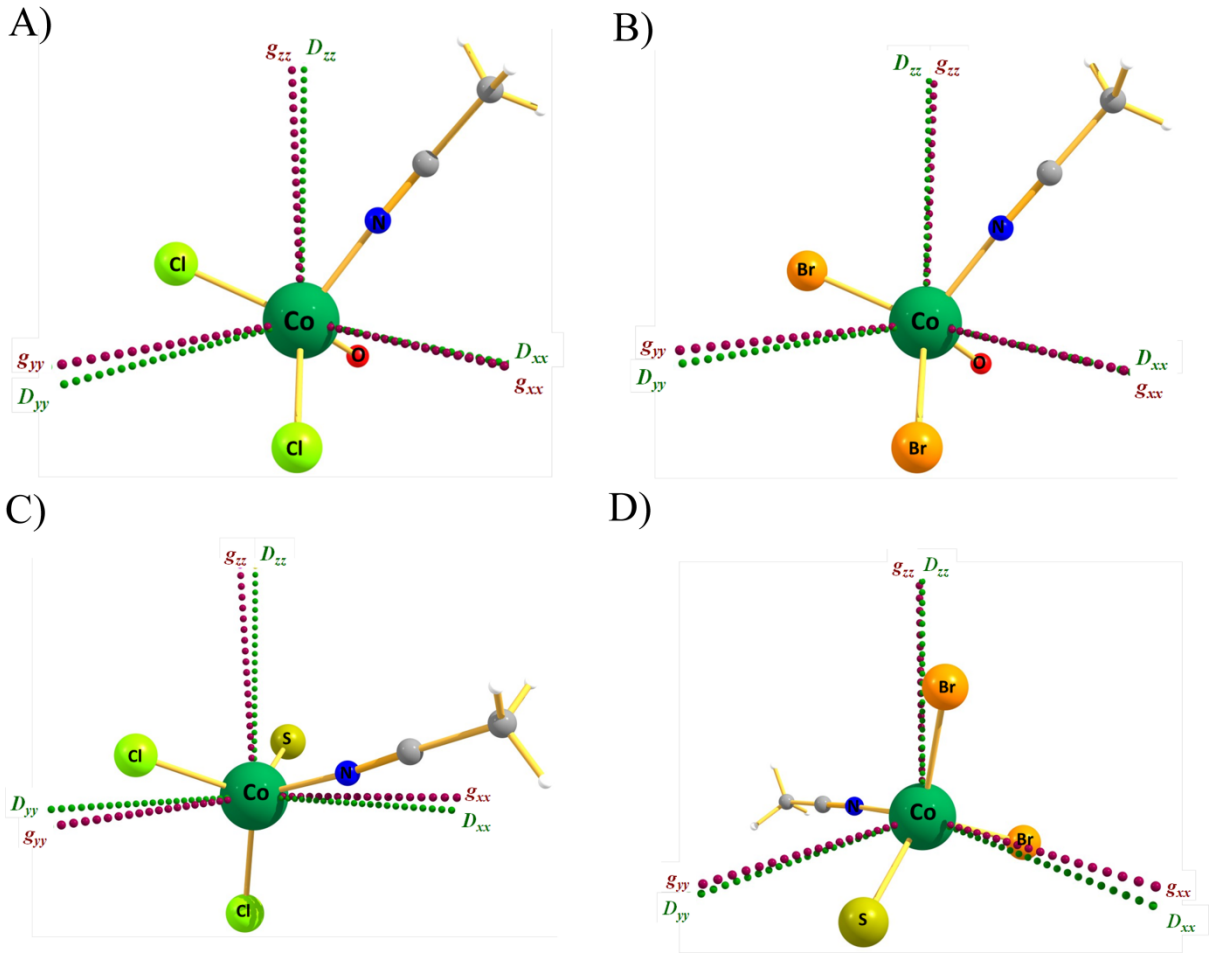


Figure S7.Orientation of the *g*-tensors and *D*-Tensors for complexes **1**-**4** **(**A-D**)** respectively.

Table S9. CSD survey of Cobalt(II) tetrahedral complexes for complexes with D and U_{eff}values reported in literature.

S.No	Complex	D (cm^{-1})	U_{eff}(cm^{-1}) (applied field, Tesla)	references
1	$(Ph_4P)_2[Co(4,5\text{-dimercapto-1,3-di-thiole-2-thione})_2]\cdot(MeCN)$	-161	33.9	[6]
1	$[Co(SePh)_4]^{2-}$	-83	19	[7]
2	$[Co(AsPh_3)_2I_2]$	-74.7	32.6 (0.1)	[8]
3	$[Co(SPh)_4]^{2-}$	-70	21	[9]
5	[Co(2-(4,5-diphenyl-1H-imidazol-2-yl)phenol)$_2$]	-41	61.9 (0.04)	[10]
6	$[Co(PPh_3)_2I_2]$	-36.9	30.6 (0.1)	[8]
7	[Co(2-(4,5-diphenyl-1H-imidazol-2-yl)-6-methoxyphenol)$_2$]	-35	43.8 (0.04)	[10]
8	$Co(PPh_3)_2Cl_2$	-16.2	25.8 (0.1)	[11]
9	[Co(Xantphos)Cl_2] (Xantphos = 9,9-dimethyl-4,5-bis(diphenyl-phosphino) xanthenes)	-15.4	20.8 (0.1)	[11]
10	Co(DPEphos)Cl_2 (DPEphos = 2,2'-bis(diphenyl-phosphino) diphenyl ether)	-14.4	24.3 (0.1)	[11]
11	$[Co(PPh_3)_2Br_2]$	-13	25.7 (0.2)	[12]
12	Complex **4**	-12.91	13.8 (0.25)	In this paper
13	$(Ph_4P)_2[Co(OPh)_4](CH_3CN)$	-11.1	21 (0.14)	[7]
14	Complex **3**	-10.19	20.2 (0.25)	In this paper
15	[Co(dmph)Br] (dmph = 2,9-dimethyl-1,10-phenanthroline)	11.68	22.8 (0.1)	[11]
16	[Co(1,1,1-tris-[2N-(1,1,3,3-tetramethylguanidino)methyl]ethane) Cl](CF_3SO_3)	12.7	24 (0.15)	[13]
17	Complex **1**	16.33	10.3 (0.25)	In this paper
18	Complex **2**	18.66	8.3 (0.25)	In this paper

Table S10. Coordinates for the optimized structure of **1** and **3**and model complex $[Co(Cl)_2(MeCN)L_{Se}]$analogousto complex **1**or**3**.Comparison of selected structural parameters of the optimized structure and its corresponding crystal structure of complexes **1** and **3**

Complex **1**

Co	2.916700	0.244800	0.362400
Cl	1.839200	0.031700	-1.725900
Cl	4.018500	2.216400	0.489100
N	-0.560500	-1.321400	1.356400
N	-1.686600	-0.816100	0.826300
N	-1.618200	0.556400	0.836100
N	-0.455300	0.940000	1.369700
N	4.346800	-1.155600	0.253100
O	1.769400	-0.289400	2.038200
C	0.218700	-0.229000	1.648600
C	-2.555500	1.462600	0.229600
C	-3.880600	1.492400	0.660100
H	-4.218100	0.835400	1.447800
C	-4.753400	2.400600	0.066300
H	-5.783600	2.441500	0.389800
C	-4.293400	3.265700	-0.928700
H	-4.973900	3.972900	-1.381900
C	-2.959700	3.223700	-1.338700
H	-2.604400	3.894100	-2.107700
C	-2.073900	2.317700	-0.760600
H	-1.041200	2.249900	-1.070300
C	-2.691400	-1.600200	0.149400
C	-3.691300	-2.220000	0.893100
H	-3.719500	-2.107800	1.967500
C	-4.635800	-2.995100	0.223600
H	-5.418300	-3.488000	0.782600
C	-4.563500	-3.140200	-1.163600
H	-5.298100	-3.743400	-1.678700
C	-3.543100	-2.520400	-1.886800
H	-3.480500	-2.647600	-2.958000
C	-2.587300	-1.745300	-1.232300
H	-1.763400	-1.281400	-1.758500
C	5.218500	-1.905500	0.141600
C	6.319200	-2.838500	-0.002700
H	6.235600	-3.642400	0.728900
H	7.269100	-2.325400	0.149700
H	6.315800	-3.274500	-1.002000

Complex **3**

Co	2.735189000	0.353682000	0.020524000
Cl	0.975685000	-0.103787000	-1.484591000
Cl	3.633680000	2.446341000	-0.045274000
N	-0.523542000	-1.417774000	1.467937000
N	-1.614155000	-0.851820000	0.930403000
N	-1.460926000	0.514593000	0.915967000
N	-0.284946000	0.836736000	1.447945000
N	4.313532000	-0.895419000	-0.500924000
S	2.010336000	-0.526871000	2.224429000
C	0.320113000	-0.369332000	1.747107000
C	-2.333697000	1.461796000	0.280143000
C	-3.668845000	1.568446000	0.683019000
H	-4.059318000	0.938383000	1.473127000
C	-4.478320000	2.519644000	0.057607000
H	-5.515093000	2.621412000	0.358013000
C	-3.948071000	3.347814000	-0.940545000
H	-4.580805000	4.088803000	-1.417307000
C	-2.606030000	3.226783000	-1.322990000
H	-2.197188000	3.867208000	-2.096002000
C	-1.781421000	2.276621000	-0.714893000
H	-0.746031000	2.139864000	-1.007188000
C	-2.644110000	-1.581439000	0.234557000
C	-3.712276000	-2.120478000	0.955140000
H	-3.771201000	-1.983289000	2.028999000
C	-4.683102000	-2.849678000	0.262621000
H	-5.519065000	-3.279675000	0.802796000
C	-4.570582000	-3.028198000	-1.122450000
H	-5.326725000	-3.595161000	-1.655013000
C	-3.483371000	-2.488857000	-1.821934000
H	-3.392372000	-2.641205000	-2.891424000
C	-2.500108000	-1.760999000	-1.144990000
H	-1.631727000	-1.353941000	-1.654140000
C	5.237291000	-1.516912000	-0.841939000
C	6.395883000	-2.284761000	-1.270467000
H	6.641280000	-3.051070000	-0.528613000
H	7.260959000	-1.625354000	-1.392445000
H	6.192756000	-2.775766000	-2.227316000

Coordinates of optimized model complex $[Co(Cl)_2(MeCN)L_{Se}]$ analogousto**1**or**3**

Cl	0.702991000	-0.077453000	-1.636276000
Cl	3.436224000	2.497075000	-0.532762000
N	-0.560517000	-1.321362000	1.356367000
N	-1.686633000	-0.816100000	0.826318000
N	-1.618189000	0.556427000	0.836115000
N	-0.455347000	0.940008000	1.369733000
N	4.011647000	-0.830987000	-0.888231000
Se	2.038459000	-0.299867000	2.105798000
C	0.218651000	-0.229022000	1.648625000
C	-2.555470000	1.462603000	0.229603000
C	-3.880612000	1.492399000	0.660123000
H	-4.218053000	0.835399000	1.447794000
C	-4.753369000	2.400580000	0.066309000
H	-5.783589000	2.441533000	0.389808000
C	-4.293399000	3.265703000	-0.928661000
H	-4.973904000	3.972881000	-1.381899000
C	-2.959684000	3.223706000	-1.338720000
H	-2.604380000	3.894114000	-2.107684000
C	-2.073947000	2.317654000	-0.760637000
H	-1.041208000	2.249865000	-1.070298000
C	-2.691354000	-1.600247000	0.149350000
C	-3.691260000	-2.220002000	0.893105000
H	-3.719477000	-2.107843000	1.967513000
C	-4.635761000	-2.995101000	0.223556000
H	-5.418259000	-3.488028000	0.782559000
C	-4.563543000	-3.140186000	-1.163573000
H	-5.298122000	-3.743435000	-1.678654000
C	-3.543079000	-2.520373000	-1.886765000
H	-3.480499000	-2.647551000	-2.957960000
C	-2.587257000	-1.745311000	-1.232289000
H	-1.763401000	-1.281388000	-1.758496000
C	4.864446000	-1.493307000	-1.298958000
C	5.938536000	-2.315976000	-1.820859000
H	6.196266000	-3.101682000	-1.110375000
H	6.823916000	-1.706384000	-2.003351000
H	5.636181000	-2.780182000	-2.759887000

Comparison of selected structural parameters between the optimized models compared to its corresponding crystal structure:

Complex **1**

	Optimized Structure	Crystal Structure
Co-O11 (Å)	2.100	1.957
Co-Cl11 (Å)	2.360	2.228
Co-Cl12 (Å)	2.262	2.252
Co-N31 (Å)	2.005	2.010
Cl11-Co-Cl12 (°)	110.53	115.640
Cl11-Co-N31 (°)	102.38	106.473
Cl11-Co-O11 (°)	115.71	114.004
Cl12-Co-N31 (°)	105.33	110.794
Cl12-Co-O11 (°)	116.30	104.813
O11-Co-N31 (°)	104.80	104.637

Complex **3**

	Optimized Structure	Crystal Structure
Co-S11 (Å)	2.482	2.319
Co-Cl11 (Å)	2.360	2.222
Co-Cl12 (Å)	2.278	2.242
Co-N31 (Å)	2.079	2.015
Cl11-Co-Cl12 (°)	116.98	110.228
Cl11-Co-N31 (°)	106.83	114.653
Cl11-Co-S11 (°)	106.25	103.165
Cl12-Co-N31 (°)	104.19	106.535
Cl12-Co-S11 (°)	117.82	118.042
S11-Co-N31 (°)	103.37	104.430

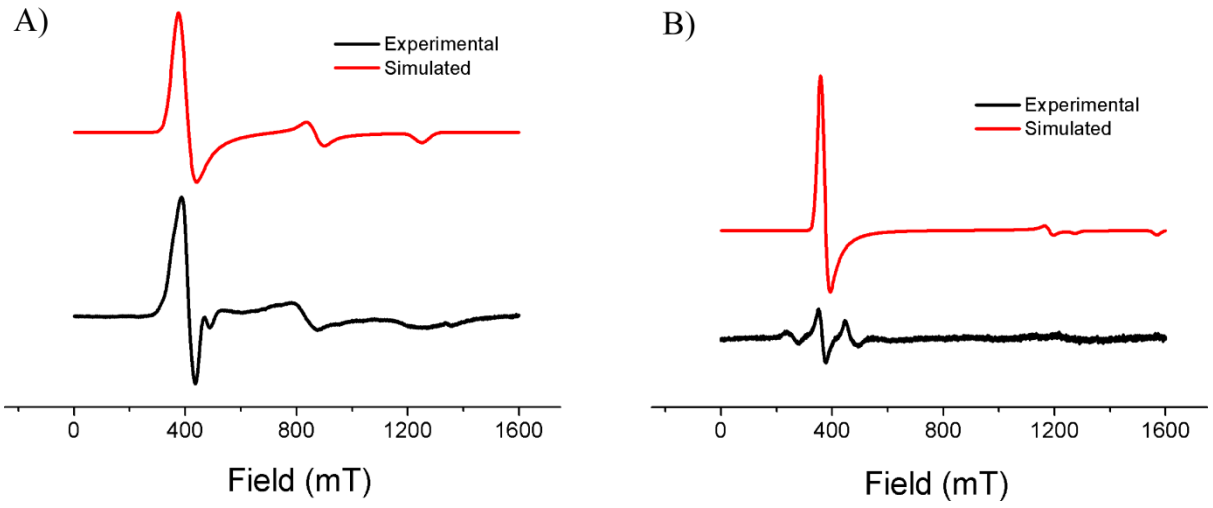


Figure S8. Q-band EPR spectra of polycrystalline samples of **2** and **4** recorded at 5.0 K. Frequency: 34 GHz .

Table S11. CASSCF+RASSI computed spin-free and spin-orbit state energies for complex **3**

Spin-free Energies (cm^{-1})	Spin-Orbit states (cm^{-1})	CASSCF+RASSI computed results					
0	0	g_X	2.283	X_M	-0.775676	-0.174963	0.606395
2342.588	33.621	g_Y	2.362	Y_M	0.587089	-0.552653	0.591524
3155.256	2327.533	g_z	2.504	Z_M	0.231631	0.814839	0.531399
3694.984	2497.421						
4485.831	3103.316	D_X	-8.441	X_A	0.999436	0.026725	0.026725
5881.02	3303.912	D_Y	2.163	Y_A	-0.026185	0.999310	0.026331
7024.682	3744.684	D_Z	-10.605	Z_A	0.021029	-0.025784	0.999446
20885.819	3744.684	D	-15.907				
21391.565	3947.948	|E|	3.138				
22421.444	4698.599						
19313.604	4810.408	*D and E values are given in cm^{-1}*					
19522.537	5949.505						
19762.363	6157.947						
19886.987	7333.397						
20164.016	7420.579						
20497.992	19255.534						
21460.062	19484.891						
21964.52	19729.654						
22014.925	20209.679						
25074.002	20411.996						
25532.181	20885.054						
25882.183	21965.762						
26313.159	22379.466						
26491.257	22484.587						
26563.843	22628.673						
26883.458	25167.003						
27618.524	25751.369						
27889.849	26070.353						
28246.047	26375.619						
28400.95	26686.661						
29066.917	26893.416						
29120.314	27262.056						
29858.486	27734.744						
30109.906	28107.216						
30495.01	28488.600						
31073.827	28725.865						
31916.72	……						
32111.127							
43621.186							
44162.287							
44356.582							
44761.856							
45097.798							
45195.989							
45377.974							
66673.519							
67558.053							
67767.149							
68818.64							
68997.799							

Table S12. CASSCF+RASSI computed spin-free and spin-orbit state energies for complex **4**

Spin-free Energies (cm^{-1})	Spin-Orbit states (cm^{-1})	CASSCF+RASSI computed results					
0	0	g_X	2.310	X_M	-0.499559	-0.102104	0.860241
1966.356	34.527	g_Y	2.386	Y_M	0.695306	-0.639573	0.327866
2949.575	1977.112	g_z	2.543	Z_M	0.516710	0.761920	0.390498
3314.767	2154.240						
4161.181	2830.906	D_X	8.244	X_A	0.999436	0.026725	0.026725
5350.563	3080.781	D_Y	2.833	Y_A	-0.026185	0.999310	0.026331
6640.002	3429.478	D_Z	-11.077	Z_A	0.021029	-0.025784	0.999446
20846.422	3671.148	D	-16.6155				
21057.365	4375.882	|E|	2.7056				
21866.165	4461.162						
19020.668	5455.241	*D and E values are given in cm^{-1}*					
19466.443	5654.542						
19693.173	6961.327						
19763.033	7027.352						
19953.608	19002.581						
20267.63	19405.699						
21096.177	19673.645						
21715.042	20050.329						
21781.111	20274.296						
24873.949	20698.639						
25133.888	20843.072						
25755.91	20915.342						
26141.16	21131.216						
26243.113	21199.758						
26548.654	21292.982						
26712.701	21741.945						
27259.375	21955.540						
27692.29	22112.171						
27985.509	22145.978						
28057.401	24938.140						
28781.745	25463.951						
28838.724	25924.309						
29334.546	26236.000						
29845.25	26454.879						
29967.225	26809.437						
30599.069	27111.745						
31307.626	……						
31495.167							
43444.295							
43985.236							
44039.181							
44442.808							
44781.124							
44829.908							
45050.956							
66535.963							
67356.226							
67657.178							
68308.117							

Table S13. DFT computed spin densities of complex **1**-**4.** The bold fonts represent the computed spin densities on the metal ion and atoms attached in the first coordination sphere.

Complex **1**	Complex **2**	Complex **3**	Complex **4**
1 Co 2.624422	**1 Co 2.590176**	**1 Co 2.558237**	**1 Co 2.535982**
2 Cl 0.141803	**2 Br 0.163610**	**2 Cl 0.161403**	**2 Br 0.155234**
3 Cl 0.149555	**3 Br 0.157562**	**3 Cl 0.150315**	**3 Br 0.171715**
4 N 0.005154	**4 O 0.049631**	**4 S 0.073747**	**4 S 0.077762**
5 N -0.001879	5 N 0.005628	5 N -0.001751	5 N 0.011568
6 N 0.000786	6 N 0.000781	6 N 0.000231	6 N 0.000497
7 N 0.005768	7 N -0.002011	7 N 0.009664	7 N -0.002534
8 N 0.032285	8 N 0.005022	8 N -0.000430	8 N -0.001108
9 O 0.046386	9 C 0.001154	**9 N 0.032624**	9 C 0.012901
10 C 0.000976	10 C 0.000113	10 C 0.012296	10 C 0.000202
11 C 0.000067	11 C 0.000030	11 C 0.000382	11 C 0.000831
12 C 0.000224	12 H 0.000008	12 C -0.000128	12 H -0.000007
13 H -0.000012	13 C -0.000060	13 H 0.000014	13 C -0.000261
14 C -0.000055	14 H 0.000003	14 C 0.000062	14 H 0.000009
15 H 0.000009	15 C 0.000113	15 H -0.000006	15 C 0.000436
16 C 0.000135	16 H -0.000007	16 C -0.000067	16 H -0.000023
17 H -0.000009	17 C -0.000042	17 H 0.000004	17 C -0.000195
18 C -0.000076	18 H 0.000011	18 C 0.000047	18 H 0.000002
19 H 0.000003	19 C 0.000194	19 H 0.000000	19 C -0.000101
20 C 0.000075	20 H -0.000008	20 C 0.000083	20 H 0.000048
21 H 0.000006	21 C -0.000008	21 H -0.000007	21 C 0.000460
22 C -0.000025	22 C -0.000077	22 C 0.000200	22 C -0.000235
23 C -0.000020	23 H -0.000002	23 C -0.000040	23 H 0.000013
24 H 0.000048	24 C 0.000056	24 H 0.000078	24 C 0.000131
25 C 0.000058	25 H -0.000001	25 C -0.000147	25 H -0.000011
26 H -0.000005	26 C -0.000096	26 H 0.000000	26 C -0.000216
27 C -0.000076	27 H 0.000007	27 C 0.000320	27 H 0.000013
28 H 0.000005	28 C 0.000048	28 H -0.000018	28 C 0.000113
29 C 0.000057	29 H -0.000005	29 C -0.000188	29 H -0.000006
30 H 0.000001	30 C -0.000025	30 H 0.000008	30 C -0.000061
31 C -0.000095	31 H 0.000037	31 C 0.000604	31 H -0.000004
32 H -0.000004	32 N 0.031775	32 H -0.000018	32 N 0.031021
33 C -0.006242	33 C -0.004408	33 C 0.001724	33 C 0.005182
34 C 0.001553	34 C 0.001585	34 C 0.000944	34 C 0.000634
35 H -0.000474	35 H 0.000001	35 H 0.000045	35 H -0.000191
36 H -0.000331	36 H -0.000369	36 H 0.000032	36 H 0.000145
37 H -0.000072	37 H -0.000425	37 H -0.000264	37 H 0.000057

Table S14. CASSCF+RASSI[b] computed *D* and *E* values, along with the *g*-values for [$CoCl_2$(phenanthroline)] and [$CoCl_2(PPh_3)_2$]. The ΔE indicates the first excitation energy computed at spin-free state of Co^{II} complexes.

Complex : **[$CoCl_2$(phenanthroline)]**								
Crystal structure[12]					**Optimised structure**			
D_{exp} (cm^{-1})	D_{cal}[b] (cm^{-1})	$\|E\|_{cal}$[b (cm^{-1})	ΔE[b] (cm^{-1})	g_{xx}, g_{yy}, g_{zz}[b]	D_{cal}[b] (cm^{-1})	$\|E\|_{cal}$[b] (cm^{-1})	ΔE[b] (cm^{-1})	g_{xx}, g_{yy}, g_{zz}[b]
11.7	16.28	4.50	1953.87	2.27,2.41,2.56	19.20	-1.98	2365.56	2.47,2.39,2.20
Complex : [$CoCl_2(PPh_3)_2$]								
Crystal structure[11]					**Optimised structure**			
D_{exp} (cm^{-1})	D_{cal}[b] (cm^{-1})	$\|E\|_{cal}$[b(cm^{-1})	ΔE[b](cm^{-1})	g_{xx}, g_{yy}, g_{zz}[b]	D_{cal}[b](cm^{-1})	$\|E\|_{cal}$[b](cm^{-1})	ΔE[b](cm^{-1})	g_{xx}, g_{yy}, g_{zz}[b]
-16.2	-21.38	0.82	2819.10	2.27,2.29,2.50	-33.83	1.84	2133.13	2.29,2.32 ,2.68

Table S15. **CASSCF+RASSI[b] computed *D* and *E* values, along with the *g*-values for**[$CoCl_2(PPh_3)(MeCN)$] and[$CoCl_2$(Pyridine)(MeCN)]**.**The ΔE indicates the first excitation energy computed at spin-free state of Co^{II} complexes..

The computed Spin Hamiltonian parameters for the model complex [$CoCl_2(PPh_3)(MeCN)$]:

Optimized Structure			
D_{cal}[b](cm^{-1})	$\|E\|_{cal}$[b](cm^{-1})	△E[b](cm^{-1})	g_{xx}, g_{yy}, g_{zz}[b]
-41.13	7.67	1525.90	2.20,2.36,2.74

The computed Spin Hamiltonian parameters for the model complex [$CoCl_2$(Pyridine)(MeCN)]

Optimized Structure			
D_{cal}[b](cm^{-1})	$\|E\|_{cal}$[b](cm^{-1})	△E[b](cm^{-1})	g_{xx}, g_{yy}, g_{zz}[b]
22.13	5.24	2178.38	2.52,2.42,2.22

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 F^2^ >2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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C47 0.0161(16) 0.0177(16) 0.0166(17) -0.0044(10) -0.0052(10) -0.0001(10)
C48 0.0164(16) 0.0170(17) 0.0165(17) -0.0048(10) -0.0053(10) 0.0003(10)
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C50 0.0221(17) 0.0227(18) 0.0219(18) -0.0059(10) -0.0068(10) 0.0003(10)
C51 0.0282(19) 0.0283(19) 0.027(2) -0.0079(11) -0.0079(10) 0.0019(10)
C52 0.0246(18) 0.0251(18) 0.0236(19) -0.0065(10) -0.0061(10) 0.0023(10)
C53 0.0202(17) 0.0218(17) 0.0206(18) -0.0056(10) -0.0055(10) 0.0009(10)
N61 0.011(3) 0.033(4) 0.021(4) -0.009(3) -0.003(3) -0.007(2)
C61 0.014(3) 0.035(4) 0.019(4) -0.008(3) -0.008(3) -0.003(3)
C62 0.015(3) 0.048(5) 0.017(4) -0.010(4) 0.000(3) 0.000(3)
N1S 0.054(5) 0.085(7) 0.029(5) -0.012(5) -0.020(4) -0.017(4)
C1S 0.038(5) 0.047(5) 0.022(5) -0.001(4) -0.014(4) -0.001(4)
C2S 0.053(6) 0.055(6) 0.045(7) -0.016(5) -0.013(5) -0.004(5)

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All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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N11 C11 N15 111.6(6) . . ?
C13 C12 C17 123.2(7) . . ?
C13 C12 N12 117.0(6) . . ?
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C22 C23 C18 117.4(6) . . ?
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C47 C42 N42 121.6(6) . . ?
C43 C42 N42 116.7(6) . . ?
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Rigaku Saturn724+ (4x4 bin mode)
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
 not relevant to the choice of reflections for refinement.  R-factors based
 on F^2^ are statistically about twice as large as those based on F, and R-
 factors based on ALL data will be even larger.
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N13 N 0.1119(4) 0.2683(3) 0.6649(2) 0.0122(7) Uani 1 1 d . . .
N14 N 0.1101(4) 0.1727(3) 0.6747(3) 0.0151(7) Uani 1 1 d . . .
C11 C 0.0906(5) 0.1885(4) 0.7596(3) 0.0133(8) Uani 1 1 d . . .
C12 C 0.0991(4) 0.4483(3) 0.7516(3) 0.0117(7) Uani 1 1 d . . .
C13 C -0.0066(5) 0.5008(4) 0.7858(3) 0.0165(8) Uani 1 1 d . . .
H13A H -0.0786 0.4639 0.7987 0.020 Uiso 1 1 calc R . .
C14 C -0.0040(5) 0.6082(4) 0.8004(3) 0.0176(8) Uani 1 1 d . . .
H14B H -0.0733 0.6460 0.8254 0.021 Uiso 1 1 calc R . .
C15 C 0.1001(5) 0.6612(4) 0.7785(3) 0.0178(8) Uani 1 1 d . . .
H15A H 0.0997 0.7346 0.7867 0.021 Uiso 1 1 calc R . .
C16 C 0.2044(5) 0.6065(4) 0.7448(3) 0.0178(8) Uani 1 1 d . . .
H16A H 0.2758 0.6431 0.7309 0.021 Uiso 1 1 calc R . .
C17 C 0.2057(5) 0.4993(4) 0.7311(3) 0.0155(8) Uani 1 1 d . . .
H17A H 0.2773 0.4619 0.7085 0.019 Uiso 1 1 calc R . .
C18 C 0.1307(5) 0.2907(4) 0.5836(3) 0.0152(8) Uani 1 1 d . . .
C19 C 0.0276(6) 0.3405(4) 0.5377(3) 0.0241(10) Uani 1 1 d . . .
H19A H -0.0539 0.3602 0.5585 0.029 Uiso 1 1 calc R . .
C20 C 0.0484(7) 0.3604(5) 0.4598(3) 0.0298(12) Uani 1 1 d . . .
H20A H -0.0187 0.3958 0.4269 0.036 Uiso 1 1 calc R . .
C21 C 0.1683(7) 0.3282(5) 0.4299(4) 0.0337(13) Uani 1 1 d . . .
H21A H 0.1809 0.3406 0.3761 0.040 Uiso 1 1 calc R . .
C22 C 0.2671(6) 0.2790(5) 0.4773(4) 0.0293(12) Uani 1 1 d . . .
H22A H 0.3479 0.2579 0.4561 0.035 Uiso 1 1 calc R . .
C23 C 0.2508(5) 0.2594(4) 0.5566(3) 0.0223(10) Uani 1 1 d . . .
H23A H 0.3195 0.2260 0.5904 0.027 Uiso 1 1 calc R . .
N31 N -0.1241(4) -0.0153(3) 0.6220(3) 0.0185(8) Uani 1 1 d . . .
C31 C -0.2036(5) 0.0003(4) 0.5630(3) 0.0183(9) Uani 1 1 d . . .
C32 C -0.3032(6) 0.0202(5) 0.4879(3) 0.0279(11) Uani 1 1 d . . .
H32A H -0.2555 0.0239 0.4412 0.042 Uiso 1 1 calc R . .
H32B H -0.3440 0.0867 0.5078 0.042 Uiso 1 1 calc R . .
H32C H -0.3778 -0.0363 0.4637 0.042 Uiso 1 1 calc R . .
Co2 Co 0.63387(6) 1.22846(5) 0.73959(4) 0.01181(15) Uani 1 1 d . . .
Br3 Br 0.72605(5) 1.29592(4) 0.63868(3) 0.02175(14) Uani 1 1 d . . .
Br4 Br 0.45968(6) 1.32462(5) 0.79517(4) 0.02733(15) Uani 1 1 d . . .
O41 O 0.5739(3) 1.0835(2) 0.6742(2) 0.0145(6) Uani 1 1 d . . .
N41 N 0.5483(4) 0.9059(3) 0.6587(2) 0.0118(6) Uani 1 1 d . . .
N42 N 0.5409(4) 0.8541(3) 0.7176(2) 0.0095(6) Uani 1 1 d . . .
N43 N 0.5512(4) 0.9195(3) 0.7989(2) 0.0106(6) Uani 1 1 d . . .
N44 N 0.5676(4) 1.0164(3) 0.7960(2) 0.0132(7) Uani 1 1 d . . .
C41 C 0.5642(4) 1.0080(3) 0.7088(3) 0.0117(7) Uani 1 1 d . . .
C42 C 0.5245(4) 0.7417(3) 0.6923(3) 0.0121(7) Uani 1 1 d . . .
C43 C 0.4314(5) 0.6935(4) 0.6108(3) 0.0151(8) Uani 1 1 d . . .
H43A H 0.3783 0.7338 0.5754 0.018 Uiso 1 1 calc R . .
C44 C 0.4179(5) 0.5863(4) 0.5824(3) 0.0190(9) Uani 1 1 d . . .
H44B H 0.3551 0.5522 0.5266 0.023 Uiso 1 1 calc R . .
C45 C 0.4950(5) 0.5269(4) 0.6343(3) 0.0196(9) Uani 1 1 d . . .
H45A H 0.4849 0.4528 0.6141 0.024 Uiso 1 1 calc R . .

C46 C 0.5872(5) 0.5770(4) 0.7163(3) 0.0188(9) Uani 1 1 d . . .
H46A H 0.6393 0.5365 0.7519 0.023 Uiso 1 1 calc R . .
C47 C 0.6040(5) 0.6846(4) 0.7465(3) 0.0148(8) Uani 1 1 d . . .
H47A H 0.6671 0.7188 0.8022 0.018 Uiso 1 1 calc R . .
C48 C 0.5468(5) 0.8905(3) 0.8796(3) 0.0140(8) Uani 1 1 d . . .
C49 C 0.4326(6) 0.8282(4) 0.8784(3) 0.0212(9) Uani 1 1 d . . .
H49A H 0.3573 0.8061 0.8263 0.025 Uiso 1 1 calc R . .
C50 C 0.4319(7) 0.7991(4) 0.9559(4) 0.0281(12) Uani 1 1 d . . .
H50A H 0.3558 0.7554 0.9569 0.034 Uiso 1 1 calc R . .
C51 C 0.5420(7) 0.8336(5) 1.0322(3) 0.0299(12) Uani 1 1 d . . .
H51A H 0.5418 0.8125 1.0847 0.036 Uiso 1 1 calc R . .
C52 C 0.6520(6) 0.8988(5) 1.0314(3) 0.0272(11) Uani 1 1 d . . .
H52A H 0.7256 0.9240 1.0841 0.033 Uiso 1 1 calc R . .
C53 C 0.6553(5) 0.9276(4) 0.9543(3) 0.0203(9) Uani 1 1 d . . .
H53A H 0.7307 0.9719 0.9532 0.024 Uiso 1 1 calc R . .
N61 N 0.7860(4) 1.2211(3) 0.8468(3) 0.0175(7) Uani 1 1 d . . .
C61 C 0.8706(5) 1.2049(4) 0.9037(3) 0.0172(8) Uani 1 1 d . . .
C62 C 0.9761(6) 1.1833(5) 0.9758(3) 0.0251(10) Uani 1 1 d . . .
H62A H 0.9367 1.1883 1.0277 0.038 Uiso 1 1 calc R . .
H62B H 1.0570 1.2342 0.9927 0.038 Uiso 1 1 calc R . .
H62C H 1.0059 1.1127 0.9557 0.038 Uiso 1 1 calc R . .
N1S N 0.2252(8) 0.3957(7) 0.0673(4) 0.059(2) Uani 1 1 d . . .
C1S C 0.2575(7) 0.4489(6) 0.0284(4) 0.0383(14) Uani 1 1 d . . .
C2S C 0.3005(8) 0.5180(6) -0.0192(4) 0.0420(15) Uani 1 1 d . . .
H2S1 H 0.3762 0.5682 0.0215 0.063 Uiso 1 1 calc R . .
H2S2 H 0.2204 0.5556 -0.0412 0.063 Uiso 1 1 calc R . .
H2S3 H 0.3338 0.4768 -0.0702 0.063 Uiso 1 1 calc R . .

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Br1 0.0218(2) 0.0243(3) 0.0213(2) 0.01011(19) 0.01166(19) 0.00539(18)
Br2 0.0305(3) 0.0404(4) 0.0445(4) 0.0176(3) 0.0201(3) 0.0131(2)
O11 0.0213(16) 0.0167(15) 0.0110(14) 0.0055(12) 0.0018(12) -0.0009(12)
N11 0.0140(16) 0.0178(18) 0.0099(15) 0.0053(14) 0.0065(13) 0.0011(13)
N12 0.0135(16) 0.0139(17) 0.0089(15) 0.0022(13) 0.0073(13) 0.0002(13)
N13 0.0162(16) 0.0135(17) 0.0066(15) 0.0000(13) 0.0053(13) -0.0024(13)
N14 0.0191(18) 0.0163(18) 0.0107(16) 0.0033(14) 0.0053(14) 0.0008(14)
C11 0.0140(18) 0.016(2) 0.0094(18) 0.0030(15) 0.0021(15) 0.0007(15)
C12 0.0127(18) 0.0134(18) 0.0091(17) 0.0019(14) 0.0043(14) 0.0014(14)
C13 0.0153(19) 0.021(2) 0.0145(19) 0.0034(16) 0.0076(16) 0.0020(16)
C14 0.0158(19) 0.019(2) 0.017(2) 0.0001(16) 0.0056(16) 0.0057(16)
C15 0.020(2) 0.016(2) 0.018(2) 0.0059(17) 0.0047(17) 0.0045(17)
C16 0.022(2) 0.016(2) 0.017(2) 0.0042(16) 0.0093(17) -0.0009(17)
C17 0.0169(19) 0.019(2) 0.0124(18) 0.0032(16) 0.0082(16) 0.0010(16)
C18 0.022(2) 0.018(2) 0.0065(17) 0.0014(15) 0.0077(16) -0.0031(16)
C19 0.027(2) 0.035(3) 0.015(2) 0.014(2) 0.0071(19) 0.003(2)
C20 0.043(3) 0.038(3) 0.013(2) 0.012(2) 0.010(2) 0.001(2)
C21 0.052(4) 0.036(3) 0.016(2) 0.005(2) 0.017(2) -0.013(3)

C22 0.035(3) 0.034(3) 0.022(2) -0.001(2) 0.024(2) -0.002(2)
C23 0.026(2) 0.025(2) 0.018(2) 0.0019(18) 0.0134(19) 0.0026(19)
N31 0.0169(18) 0.026(2) 0.0132(17) 0.0080(16) 0.0015(15) 0.0014(15)
C31 0.019(2) 0.023(2) 0.0120(19) 0.0036(17) 0.0040(17) 0.0005(17)
C32 0.029(3) 0.037(3) 0.013(2) 0.006(2) -0.0033(19) 0.005(2)
Co2 0.0117(3) 0.0149(3) 0.0089(3) 0.0036(2) 0.0023(2) 0.0013(2)
Br3 0.0248(3) 0.0242(3) 0.0192(2) 0.00794(19) 0.00890(19) -0.00028(19)
Br4 0.0249(3) 0.0344(3) 0.0249(3) 0.0083(2) 0.0100(2) 0.0101(2)
O41 0.0199(15) 0.0137(14) 0.0116(14) 0.0050(11) 0.0056(12) -0.0001(12)
N41 0.0150(16) 0.0148(17) 0.0080(15) 0.0051(13) 0.0049(13) 0.0020(13)
N42 0.0098(15) 0.0142(16) 0.0050(14) 0.0019(13) 0.0035(12) 0.0027(12)
N43 0.0134(16) 0.0145(16) 0.0045(14) 0.0020(13) 0.0042(12) 0.0012(13)
N44 0.0164(17) 0.0139(17) 0.0096(16) 0.0026(13) 0.0044(13) 0.0010(13)
C41 0.0133(18) 0.0141(19) 0.0080(17) 0.0034(14) 0.0031(14) 0.0013(14)
C42 0.0150(18) 0.0141(19) 0.0091(17) 0.0033(15) 0.0065(15) 0.0024(15)
C43 0.0165(19) 0.020(2) 0.0096(18) 0.0031(16) 0.0068(16) 0.0024(16)
C44 0.022(2) 0.022(2) 0.0137(19) 0.0016(17) 0.0096(17) 0.0012(17)
C45 0.025(2) 0.014(2) 0.023(2) 0.0012(17) 0.0151(19) 0.0005(17)
C46 0.022(2) 0.018(2) 0.020(2) 0.0074(17) 0.0089(18) 0.0070(17)
C47 0.0182(19) 0.016(2) 0.0125(18) 0.0055(16) 0.0060(16) 0.0041(16)
C48 0.022(2) 0.017(2) 0.0065(17) 0.0062(15) 0.0055(16) 0.0081(16)
C49 0.031(2) 0.021(2) 0.016(2) 0.0060(18) 0.0154(19) 0.0018(19)
C50 0.051(3) 0.021(2) 0.021(2) 0.0075(19) 0.025(2) 0.005(2)
C51 0.054(3) 0.032(3) 0.016(2) 0.014(2) 0.023(2) 0.020(3)
C52 0.034(3) 0.041(3) 0.0085(19) 0.008(2) 0.0087(19) 0.019(2)
C53 0.019(2) 0.030(3) 0.0095(19) 0.0008(17) 0.0036(17) 0.0064(18)
N61 0.0140(17) 0.024(2) 0.0135(17) 0.0054(15) 0.0005(14) 0.0030(15)
C61 0.018(2) 0.020(2) 0.0115(19) 0.0015(16) 0.0031(16) 0.0028(17)
C62 0.025(2) 0.033(3) 0.013(2) 0.0050(19) -0.0032(18) 0.009(2)
N1S 0.056(4) 0.087(6) 0.031(3) 0.009(3) 0.014(3) -0.021(4)
C1S 0.035(3) 0.055(4) 0.019(3) -0.001(3) 0.008(2) -0.005(3)
C2S 0.044(4) 0.054(4) 0.024(3) 0.010(3) 0.002(3) 0.001(3)

_geom_special_details
;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
;

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Co1 N31 2.004(4) . ?
Co1 Br2 2.3125(9) . ?
Co1 Br1 2.3713(8) . ?
O11 C11 1.276(5) . ?
N11 N12 1.319(5) . ?

N11 C11 1.357(6) . ?
N12 N13 1.327(5) . ?
N12 C12 1.425(5) . ?
N13 N14 1.322(5) . ?
N13 C18 1.453(5) . ?
N14 C11 1.372(5) . ?
C12 C17 1.391(6) . ?
C12 C13 1.393(6) . ?
C13 C14 1.385(7) . ?
C13 H13A 0.9500 . ?
C14 C15 1.398(6) . ?
C14 H14B 0.9500 . ?
C15 C16 1.391(6) . ?
C15 H15A 0.9500 . ?
C16 C17 1.385(6) . ?
C16 H16A 0.9500 . ?
C17 H17A 0.9500 . ?
C18 C23 1.380(6) . ?
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C19 C20 1.395(6) . ?
C19 H19A 0.9500 . ?
C20 C21 1.401(9) . ?
C20 H20A 0.9500 . ?
C21 C22 1.366(9) . ?
C21 H21A 0.9500 . ?
C22 C23 1.399(7) . ?
C22 H22A 0.9500 . ?
C23 H23A 0.9500 . ?
N31 C31 1.139(6) . ?
C31 C32 1.442(7) . ?
C32 H32A 0.9800 . ?
C32 H32B 0.9800 . ?
C32 H32C 0.9800 . ?
Co2 O41 1.948(3) . ?
Co2 N61 2.012(4) . ?
Co2 Br4 2.3455(8) . ?
Co2 Br3 2.3753(8) . ?
O41 C41 1.279(5) . ?
N41 N42 1.316(5) . ?
N41 C41 1.369(6) . ?
N42 N43 1.338(5) . ?
N42 C42 1.440(5) . ?
N43 N44 1.312(5) . ?
N43 C48 1.445(5) . ?
N44 C41 1.356(5) . ?
C42 C43 1.389(6) . ?
C42 C47 1.403(6) . ?
C43 C44 1.374(7) . ?
C43 H43A 0.9500 . ?
C44 C45 1.392(7) . ?
C44 H44B 0.9500 . ?
C45 C46 1.397(7) . ?
C45 H45A 0.9500 . ?
C46 C47 1.380(6) . ?
C46 H46A 0.9500 . ?

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C48 C53 1.372(7) . ?
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C49 C50 1.389(6) . ?
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C61 C62 1.447(6) . ?
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C62 H62B 0.9800 . ?
C62 H62C 0.9800 . ?
N1S C1S 1.142(10) . ?
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O11 Co1 Br2 114.27(10) . . ?
N31 Co1 Br2 108.68(12) . . ?
O11 Co1 Br1 105.69(10) . . ?
N31 Co1 Br1 108.75(12) . . ?
Br2 Co1 Br1 115.58(3) . . ?
C11 O11 Co1 123.1(3) . . ?
N12 N11 C11 103.9(3) . . ?
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N12 N13 C18 126.1(4) . . ?
N13 N14 C11 102.8(4) . . ?
O11 C11 N11 123.5(4) . . ?
O11 C11 N14 124.6(4) . . ?
N11 C11 N14 111.9(4) . . ?
C17 C12 C13 122.6(4) . . ?
C17 C12 N12 119.3(4) . . ?
C13 C12 N12 118.1(4) . . ?
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C13 C14 C15 120.3(4) . . ?
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C14 C15 H15A 120.1 . . ?
C17 C16 C15 120.9(4) . . ?
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C16 C17 C12 117.9(4) . . ?
C16 C17 H17A 121.0 . . ?
C12 C17 H17A 121.0 . . ?
C23 C18 C19 124.1(4) . . ?
C23 C18 N13 117.3(4) . . ?
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C22 C21 H21A 119.6 . . ?
C20 C21 H21A 119.6 . . ?
C21 C22 C23 120.8(5) . . ?
C21 C22 H22A 119.6 . . ?
C23 C22 H22A 119.6 . . ?
C18 C23 C22 117.2(5) . . ?
C18 C23 H23A 121.4 . . ?
C22 C23 H23A 121.4 . . ?
C31 N31 Co1 174.9(4) . . ?
N31 C31 C32 179.5(5) . . ?
C31 C32 H32A 109.5 . . ?
C31 C32 H32B 109.5 . . ?
H32A C32 H32B 109.5 . . ?
C31 C32 H32C 109.5 . . ?
H32A C32 H32C 109.5 . . ?
H32B C32 H32C 109.5 . . ?
O41 Co2 N61 104.94(16) . . ?
O41 Co2 Br4 114.50(10) . . ?
N61 Co2 Br4 106.81(12) . . ?
O41 Co2 Br3 104.36(9) . . ?
N61 Co2 Br3 111.17(12) . . ?
Br4 Co2 Br3 114.71(3) . . ?
C41 O41 Co2 126.2(3) . . ?
N42 N41 C41 103.1(3) . . ?
N41 N42 N43 110.9(3) . . ?
N41 N42 C42 121.4(3) . . ?
N43 N42 C42 127.7(3) . . ?
N44 N43 N42 110.0(3) . . ?
N44 N43 C48 123.7(3) . . ?
N42 N43 C48 126.3(4) . . ?
N43 N44 C41 104.2(3) . . ?
O41 C41 N44 126.3(4) . . ?
O41 C41 N41 122.0(4) . . ?

N44 C41 N41 111.7(4) . . ?
C43 C42 C47 122.2(4) . . ?
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C44 C43 C42 118.6(4) . . ?
C44 C43 H43A 120.7 . . ?
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C43 C44 C45 120.9(5) . . ?
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C42 C47 H47A 121.1 . . ?
C53 C48 C49 123.1(4) . . ?
C53 C48 N43 118.3(4) . . ?
C49 C48 N43 118.6(4) . . ?
C48 C49 C50 117.7(5) . . ?
C48 C49 H49A 121.1 . . ?
C50 C49 H49A 121.1 . . ?
C49 C50 C51 120.4(5) . . ?
C49 C50 H50A 119.8 . . ?
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C52 C51 C50 119.9(4) . . ?
C52 C51 H51A 120.1 . . ?
C50 C51 H51A 120.1 . . ?
C53 C52 C51 120.5(5) . . ?
C53 C52 H52A 119.8 . . ?
C51 C52 H52A 119.8 . . ?
C48 C53 C52 118.3(5) . . ?
C48 C53 H53A 120.9 . . ?
C52 C53 H53A 120.8 . . ?
C61 N61 Co2 172.2(4) . . ?
N61 C61 C62 179.1(5) . . ?
C61 C62 H62A 109.5 . . ?
C61 C62 H62B 109.5 . . ?
H62A C62 H62B 109.5 . . ?
C61 C62 H62C 109.5 . . ?
H62A C62 H62C 109.5 . . ?
H62B C62 H62C 109.5 . . ?
N1S C1S C2S 178.8(8) . . ?
C1S C2S H2S1 109.5 . . ?
C1S C2S H2S2 109.5 . . ?
H2S1 C2S H2S2 109.5 . . ?
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C11 N11 N12 N13 0.7(5) . . . . ?
C11 N11 N12 C12 -178.7(4) . . . . ?
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C12 N12 N13 N14 178.1(4) . . . . ?
N11 N12 N13 C18 -179.8(4) . . . . ?
C12 N12 N13 C18 -0.4(7) . . . . ?
N12 N13 N14 C11 1.2(5) . . . . ?
C18 N13 N14 C11 179.9(4) . . . . ?
Co1 O11 C11 N11 156.2(3) . . . . ?
Co1 O11 C11 N14 -23.4(6) . . . . ?
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N12 N11 C11 N14 0.1(5) . . . . ?
N13 N14 C11 O11 178.8(4) . . . . ?
N13 N14 C11 N11 -0.8(5) . . . . ?
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N13 N12 C12 C17 -48.7(6) . . . . ?
N11 N12 C12 C13 -48.6(6) . . . . ?
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C17 C12 C13 C14 -0.5(7) . . . . ?
N12 C12 C13 C14 178.7(4) . . . . ?
C12 C13 C14 C15 1.9(7) . . . . ?
C13 C14 C15 C16 -2.2(7) . . . . ?
C14 C15 C16 C17 1.0(7) . . . . ?
C15 C16 C17 C12 0.5(7) . . . . ?
C13 C12 C17 C16 -0.7(7) . . . . ?
N12 C12 C17 C16 -179.9(4) . . . . ?
N14 N13 C18 C23 -57.5(6) . . . . ?
N12 N13 C18 C23 120.9(5) . . . . ?
N14 N13 C18 C19 121.8(5) . . . . ?
N12 N13 C18 C19 -59.8(6) . . . . ?
C23 C18 C19 C20 -0.5(8) . . . . ?
N13 C18 C19 C20 -179.7(5) . . . . ?
C18 C19 C20 C21 1.4(9) . . . . ?
C19 C20 C21 C22 -1.3(9) . . . . ?
C20 C21 C22 C23 0.2(9) . . . . ?
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N13 C18 C23 C22 178.6(4) . . . . ?
C21 C22 C23 C18 0.7(8) . . . . ?
O11 Co1 N31 C31 7(4) . . . . ?
Br2 Co1 N31 C31 -114(4) . . . . ?
Br1 Co1 N31 C31 119(4) . . . . ?
Co1 N31 C31 C32 70(71) . . . . ?
N61 Co2 O41 C41 36.7(4) . . . . ?
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Br4 Co2 O41 C41 -80.1(4) . . . . ?
Br3 Co2 O41 C41 153.7(3) . . . . ?
C41 N41 N42 N43 0.2(4) . . . . ?
C41 N41 N42 C42 -179.6(3) . . . . ?
N41 N42 N43 N44 -0.9(5) . . . . ?
C42 N42 N43 N44 178.9(4) . . . . ?
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C42 N42 N43 C48 -0.5(6) . . . . ?
N42 N43 N44 C41 1.2(4) . . . . ?
C48 N43 N44 C41 -179.4(4) . . . . ?
Co2 O41 C41 N44 13.4(6) . . . . ?
Co2 O41 C41 N41 -166.8(3) . . . . ?
N43 N44 C41 O41 178.7(4) . . . . ?
N43 N44 C41 N41 -1.1(5) . . . . ?
N42 N41 C41 O41 -179.2(4) . . . . ?
N42 N41 C41 N44 0.6(5) . . . . ?
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C47 C42 C43 C44 -0.4(6) . . . . ?
N42 C42 C43 C44 177.0(4) . . . . ?
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C43 C44 C45 C46 0.0(7) . . . . ?
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N44 N43 C48 C53 -53.4(6) . . . . ?
N42 N43 C48 C53 125.8(5) . . . . ?
N44 N43 C48 C49 125.5(5) . . . . ?
N42 N43 C48 C49 -55.2(6) . . . . ?
C53 C48 C49 C50 -2.6(7) . . . . ?
N43 C48 C49 C50 178.5(4) . . . . ?
C48 C49 C50 C51 1.1(8) . . . . ?
C49 C50 C51 C52 1.1(8) . . . . ?
C50 C51 C52 C53 -1.9(8) . . . . ?
C49 C48 C53 C52 1.8(7) . . . . ?
N43 C48 C53 C52 -179.3(4) . . . . ?
C51 C52 C53 C48 0.5(7) . . . . ?
O41 Co2 N61 C61 4(3) . . . . ?
Br4 Co2 N61 C61 126(3) . . . . ?
Br3 Co2 N61 C61 -109(3) . . . . ?
Co2 N61 C61 C62 -54(40) . . . . ?

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C53 H53A Br1  0.95 3.02 3.599(5) 120.9 1_665
C62 H62C Br1  0.98 3.05 3.868(6) 142.0 1_665
C62 H62A Br1  0.98 3.07 3.647(5) 119.1 2_667
C32 H32A Br2  0.98 2.79 3.675(6) 150.7 2_556
C43 H43A Br2  0.95 3.06 3.509(4) 110.6 1_565
C49 H49A Br2  0.95 2.85 3.644(5) 141.7 1_565
C19 H19A Br3  0.95 2.98 3.801(5) 145.1 1_445
C32 H32B Br3  0.98 2.97 3.786(6) 141.5 1_445
C17 H17A Br4  0.95 2.94 3.578(5) 125.4 1_545
C51 H51A Br4  0.95 2.97 3.879(5) 160.3 2_677
C2S H2S1 Br4  0.98 2.95 3.837(7) 150.6 2_676
C2S H2S3 Br4  0.98 3.04 4.005(8) 169.4 1_544

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 'H'  'H'   0.0000   0.0000
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 'N'  'N'   0.0061   0.0033
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 'Cl'  'Cl'   0.1484   0.1585
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 'x, y, z'
 '-x, -y, -z'

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_cell_angle_beta                  80.74(3)
_cell_angle_gamma                 67.56(3)
_cell_volume                      934.4(3)
_cell_formula_units_Z             2
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
wR and
```

```
 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

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 'calc w=1/[\s^2^(Fo^2^)+(0.0148P)^2^+1.4120P] where
P=(Fo^2^+2Fc^2^)/3'
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S11 S 0.28608(18) 0.64865(18) 0.38125(11) 0.0447(4) Uani 1 1 d . . .
Cl1 Cl 0.11173(19) 1.1160(2) 0.36928(13) 0.0647(5) Uani 1 1 d . . .
Cl2 Cl 0.2758(2) 0.9227(2) 0.14523(11) 0.0628(5) Uani 1 1 d . . .
N11 N 0.3364(5) 0.7182(5) 0.5587(3) 0.0361(11) Uani 1 1 d . . .
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N12 N 0.3031(5) 0.6672(5) 0.6555(3) 0.0352(11) Uani 1 1 d . . .
N13 N 0.2317(5) 0.5555(5) 0.6672(3) 0.0360(11) Uani 1 1 d . . .
N14 N 0.2142(5) 0.5330(5) 0.5776(3) 0.0373(11) Uani 1 1 d . . .
C11 C 0.2791(6) 0.6346(6) 0.5102(4) 0.0359(13) Uani 1 1 d . . .
C12 C 0.1772(7) 0.4716(6) 0.7621(4) 0.0404(14) Uani 1 1 d . . .
C13 C 0.0156(7) 0.4676(8) 0.7729(5) 0.0598(18) Uani 1 1 d . . .
H13 H -0.0586 0.5221 0.7220 0.072 Uiso 1 1 calc R . .
C14 C -0.0341(9) 0.3809(9) 0.8610(6) 0.080(2) Uani 1 1 d . . .
H14 H -0.1428 0.3753 0.8699 0.096 Uiso 1 1 calc R . .
C15 C 0.0760(10) 0.3030(9) 0.9353(5) 0.078(2) Uani 1 1 d . . .
H15 H 0.0406 0.2471 0.9956 0.094 Uiso 1 1 calc R . .
C16 C 0.2365(9) 0.3064(9) 0.9217(5) 0.075(2) Uani 1 1 d . . .
H16 H 0.3113 0.2504 0.9722 0.090 Uiso 1 1 calc R . .
C17 C 0.2901(8) 0.3917(7) 0.8343(4) 0.0550(17) Uani 1 1 d . . .
H17 H 0.4000 0.3946 0.8248 0.066 Uiso 1 1 calc R . .
C18 C 0.3383(6) 0.7268(7) 0.7367(4) 0.0379(13) Uani 1 1 d . . .
C19 C 0.2050(7) 0.8031(7) 0.8011(4) 0.0491(16) Uani 1 1 d . . .
H19 H 0.0934 0.8145 0.7939 0.059 Uiso 1 1 calc R . .
C20 C 0.2403(8) 0.8626(8) 0.8769(4) 0.0618(19) Uani 1 1 d . . .
H20 H 0.1520 0.9143 0.9218 0.074 Uiso 1 1 calc R . .
C21 C 0.4051(8) 0.8456(8) 0.8861(4) 0.0591(18) Uani 1 1 d . . .
H21 H 0.4281 0.8853 0.9376 0.071 Uiso 1 1 calc R . .
C22 C 0.5369(7) 0.7702(8) 0.8197(5) 0.0575(18) Uani 1 1 d . . .
H22 H 0.6484 0.7597 0.8264 0.069 Uiso 1 1 calc R . .
C23 C 0.5043(7) 0.7101(7) 0.7433(4) 0.0466(15) Uani 1 1 d . . .
H23 H 0.5922 0.6598 0.6976 0.056 Uiso 1 1 calc R . .
N31 N 0.5335(6) 0.8835(6) 0.3413(4) 0.0531(14) Uani 1 1 d . . .
C31 C 0.6610(8) 0.8660(7) 0.3660(5) 0.0486(15) Uani 1 1 d . . .
C32 C 0.8266(8) 0.8422(8) 0.3940(6) 0.084(2) Uani 1 1 d . . .
H32A H 0.8713 0.7379 0.4364 0.126 Uiso 1 1 calc R . .
H32B H 0.8163 0.9252 0.4306 0.126 Uiso 1 1 calc R . .
H32C H 0.9029 0.8478 0.3338 0.126 Uiso 1 1 calc R . .

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Co1 0.0385(4) 0.0427(5) 0.0419(5) -0.0076(4) -0.0067(3) -0.0111(4)
S11 0.0556(9) 0.0444(10) 0.0362(8) -0.0094(7) -0.0081(7) -0.0174(8)
Cl1 0.0556(10) 0.0568(12) 0.0698(12) -0.0239(9) -0.0085(8) 0.0012(8)
Cl2 0.0703(10) 0.0810(13) 0.0382(9) -0.0121(8) -0.0084(7) -0.0262(9)
N11 0.040(3) 0.035(3) 0.033(3) -0.008(2) -0.001(2) -0.014(2)
N12 0.036(2) 0.034(3) 0.037(3) -0.011(2) -0.004(2) -0.012(2)
N13 0.041(3) 0.034(3) 0.036(3) -0.007(2) -0.005(2) -0.016(2)
N14 0.046(3) 0.032(3) 0.036(3) -0.008(2) -0.007(2) -0.013(2)
C11 0.037(3) 0.029(3) 0.039(3) -0.006(3) -0.008(2) -0.007(3)
C12 0.050(3) 0.029(3) 0.039(3) -0.003(3) -0.002(3) -0.013(3)
C13 0.051(4) 0.063(5) 0.070(5) -0.001(4) -0.008(3) -0.031(4)
C14 0.075(5) 0.088(6) 0.085(6) 0.004(5) 0.012(4) -0.057(5)
C15 0.103(6) 0.080(6) 0.049(5) 0.005(4) 0.008(4) -0.045(5)
C16 0.084(5) 0.068(5) 0.058(5) 0.005(4) -0.015(4) -0.017(4)
C17 0.059(4) 0.055(4) 0.048(4) 0.000(3) -0.005(3) -0.023(3)
```

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C18 0.044(3) 0.041(4) 0.033(3) -0.013(3) -0.001(2) -0.018(3)
C19 0.046(3) 0.068(5) 0.046(4) -0.026(3) 0.002(3) -0.029(3)
C20 0.065(4) 0.088(6) 0.048(4) -0.042(4) 0.019(3) -0.038(4)
C21 0.076(5) 0.080(5) 0.044(4) -0.026(4) -0.009(3) -0.043(4)
C22 0.046(4) 0.076(5) 0.060(4) -0.023(4) -0.013(3) -0.022(3)
C23 0.042(3) 0.052(4) 0.054(4) -0.022(3) 0.001(3) -0.022(3)
N31 0.048(3) 0.050(4) 0.064(4) -0.013(3) -0.012(3) -0.015(3)
C31 0.051(4) 0.042(4) 0.059(4) -0.012(3) -0.008(3) -0.020(3)
C32 0.063(4) 0.067(5) 0.140(7) -0.027(5) -0.050(4) -0.021(4)

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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters
are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Co1 Cl1 2.222(2) . ?
Co1 Cl2 2.2376(17) . ?
Co1 S11 2.3182(18) . ?
S11 C11 1.715(5) . ?
N11 N12 1.312(5) . ?
N11 C11 1.359(6) . ?
N12 N13 1.335(5) . ?
N12 C18 1.443(6) . ?
N13 N14 1.313(5) . ?
N13 C12 1.443(6) . ?
N14 C11 1.354(6) . ?
C12 C17 1.360(7) . ?
C12 C13 1.368(7) . ?
C13 C14 1.374(8) . ?
C14 C15 1.364(9) . ?
C15 C16 1.355(9) . ?
C16 C17 1.375(8) . ?
C18 C19 1.368(7) . ?
C18 C23 1.372(7) . ?
C19 C20 1.380(7) . ?
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C21 C22 1.376(8) . ?
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N11 N12 N13 110.5(4) . . ?
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N11 N12 N13 N14 -1.0(5) . . . . ?
C18 N12 N13 N14 178.4(4) . . . . ?
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C18 N12 N13 C12 -0.6(8) . . . . ?
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Co1 S11 C11 N14 157.7(4) . . . . ?
Co1 S11 C11 N11 -23.0(5) . . . . ?
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C17 C12 C13 C14 0.9(10) . . . . ?
N13 C12 C13 C14 176.7(6) . . . . ?
C12 C13 C14 C15 0.6(11) . . . . ?
C13 C14 C15 C16 -1.9(13) . . . . ?
C14 C15 C16 C17 1.7(12) . . . . ?
C13 C12 C17 C16 -1.1(10) . . . . ?
N13 C12 C17 C16 -176.8(6) . . . . ?
C15 C16 C17 C12 -0.2(11) . . . . ?
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N12 C18 C19 C20 -178.6(5) . . . . ?
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C21 C22 C23 C18 -0.6(9) . . . . ?
Cl1 Co1 N31 C31 92(5) . . . . ?
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S11 Co1 N31 C31 -34(5) . . . . ?
Co1 N31 C31 C32 131(18) . . . . ?

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 'H'  'H'   0.0000   0.0000
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Br'  'Br'  -0.2901   2.4595
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 'Co'  'Co'   0.3494   0.9721
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 '-x, -y, -z'

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_cell_angle_beta                  80.64(5)
_cell_angle_gamma                 68.94(4)
_cell_volume                      946.4(15)
_cell_formula_units_Z             2
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Rigaku Saturn724+ (4x4 bin mode)
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor
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 goodness of fit S are based on F^2^, conventional R-factors R are
based
 on F, with F set to zero for negative F^2^. The threshold
expression of
 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc.
and is
 not relevant to the choice of reflections for refinement.  R-
factors based
 on F^2^ are statistically about twice as large as those based on F,
and R-
 factors based on ALL data will be even larger.
;

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P=(Fo^2^+2Fc^2^)/3'
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.
Br12 Br 0.26361(10) 0.42043(9) -0.35561(6) 0.0236(2) Uani 1 1 d . .
.
Co1 Co 0.31286(13) 0.39526(11) -0.18353(8) 0.0202(3) Uani 1 1 d . .
.
S11 S 0.2962(2) 0.1415(2) -0.11584(14) 0.0191(4) Uani 1 1 d . . .
N11 N 0.3448(8) 0.2162(7) 0.0589(4) 0.0176(13) Uani 1 1 d . . .
N12 N 0.3102(7) 0.1658(6) 0.1557(5) 0.0166(13) Uani 1 1 d . . .
N13 N 0.2368(8) 0.0518(7) 0.1673(5) 0.0176(13) Uani 1 1 d . . .
N14 N 0.2209(7) 0.0264(6) 0.0799(5) 0.0167(13) Uani 1 1 d . . .
C11 C 0.2864(9) 0.1290(7) 0.0122(6) 0.0166(15) Uani 1 1 d . . .
C12 C 0.3443(10) 0.2273(8) 0.2359(5) 0.0174(15) Uani 1 1 d . . .
C13 C 0.2059(10) 0.3032(8) 0.3007(6) 0.0237(17) Uani 1 1 d . . .
H13 H 0.0924 0.3124 0.2938 0.028 Uiso 1 1 calc R . .
C14 C 0.2440(10) 0.3639(9) 0.3751(6) 0.0241(17) Uani 1 1 d . . .
H14 H 0.1542 0.4175 0.4199 0.029 Uiso 1 1 calc R . .
C15 C 0.4121(10) 0.3479(9) 0.3856(6) 0.0245(17) Uani 1 1 d . . .
H15 H 0.4360 0.3883 0.4378 0.029 Uiso 1 1 calc R . .
C16 C 0.5436(11) 0.2724(9) 0.3190(6) 0.0276(18) Uani 1 1 d . . .
H16 H 0.6576 0.2614 0.3260 0.033 Uiso 1 1 calc R . .
C17 C 0.5101(10) 0.2133(8) 0.2427(6) 0.0214(16) Uani 1 1 d . . .
H17 H 0.5995 0.1642 0.1962 0.026 Uiso 1 1 calc R . .
C18 C 0.1800(10) -0.0292(8) 0.2625(6) 0.0203(16) Uani 1 1 d . . .
C19 C 0.0137(10) -0.0293(8) 0.2747(6) 0.0237(17) Uani 1 1 d . . .
H19 H -0.0605 0.0254 0.2232 0.028 Uiso 1 1 calc R . .
C20 C -0.0419(11) -0.1116(9) 0.3642(6) 0.0267(18) Uani 1 1 d . . .
H20 H -0.1550 -0.1142 0.3749 0.032 Uiso 1 1 calc R . .
C21 C 0.0716(12) -0.1907(9) 0.4384(6) 0.032(2) Uani 1 1 d . . .
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C22 C 0.2387(11) -0.1899(10) 0.4233(6) 0.033(2) Uani 1 1 d . . .
H22 H 0.3141 -0.2455 0.4741 0.039 Uiso 1 1 calc R . .
C23 C 0.2946(10) -0.1095(9) 0.3356(6) 0.0236(17) Uani 1 1 d . . .
H23 H 0.4081 -0.1081 0.3247 0.028 Uiso 1 1 calc R . .
N31 N 0.5495(8) 0.3823(7) -0.1641(6) 0.0268(16) Uani 1 1 d . . .
C31 C 0.6830(11) 0.3662(8) -0.1497(6) 0.0240(17) Uani 1 1 d . . .
C32 C 0.8590(10) 0.3397(9) -0.1330(7) 0.0294(19) Uani 1 1 d . . .
H32A H 0.9100 0.2293 -0.0973 0.044 Uiso 1 1 calc R . .
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H32C H 0.9251 0.3554 -0.1977 0.044 Uiso 1 1 calc R . .

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Br12 0.0236(5) 0.0257(4) 0.0225(4) -0.0046(3) -0.0031(3) -0.0090(3)
Co1 0.0161(6) 0.0190(5) 0.0253(6) -0.0026(4) -0.0037(4) -0.0057(4)
S11 0.0199(10) 0.0178(8) 0.0203(10) -0.0031(7) -0.0043(7) -0.0063(7)
N11 0.019(4) 0.019(3) 0.018(3) -0.005(2) -0.005(3) -0.007(2)
N12 0.013(3) 0.012(3) 0.025(3) -0.005(2) -0.001(3) -0.005(2)
N13 0.015(3) 0.018(3) 0.021(3) -0.002(2) -0.002(3) -0.007(2)
N14 0.010(3) 0.017(3) 0.022(3) 0.001(2) -0.003(2) -0.005(2)
C11 0.008(4) 0.012(3) 0.028(4) -0.006(3) -0.003(3) 0.000(3)
C12 0.023(4) 0.018(3) 0.015(4) -0.007(3) -0.004(3) -0.008(3)
C13 0.021(4) 0.021(3) 0.027(4) 0.001(3) -0.005(3) -0.007(3)
C14 0.021(4) 0.037(4) 0.018(4) -0.010(3) 0.001(3) -0.012(3)
C15 0.023(5) 0.030(4) 0.024(4) -0.004(3) 0.003(3) -0.014(3)
C16 0.026(5) 0.036(4) 0.028(5) -0.007(3) -0.002(4) -0.018(4)
C17 0.013(4) 0.023(3) 0.030(4) -0.005(3) -0.002(3) -0.008(3)
C18 0.022(4) 0.016(3) 0.021(4) -0.004(3) -0.002(3) -0.005(3)
C19 0.020(4) 0.021(3) 0.030(4) 0.000(3) -0.002(3) -0.009(3)
C20 0.023(5) 0.030(4) 0.030(5) -0.003(3) 0.004(4) -0.017(3)
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C22 0.033(5) 0.036(4) 0.026(5) 0.002(3) -0.002(4) -0.013(4)
C23 0.023(4) 0.026(4) 0.025(4) -0.003(3) -0.007(3) -0.010(3)
N31 0.012(4) 0.024(3) 0.045(5) -0.004(3) -0.006(3) -0.007(3)
C31 0.031(5) 0.016(3) 0.025(4) -0.001(3) -0.006(4) -0.008(3)
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 All esds (except the esd in the dihedral angle between two l.s.
planes)
 are estimated using the full covariance matrix.  The cell esds are
taken
 into account individually in the estimation of esds in distances,
angles
 and torsion angles; correlations between esds in cell parameters
are only
 used when they are defined by crystal symmetry.  An approximate
(isotropic)
 treatment of cell esds is used for estimating esds involving l.s.
planes.
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Br12 Co1 2.412(3) . ?
Co1 N31 2.017(7) . ?
Co1 S11 2.316(3) . ?
S11 C11 1.726(8) . ?
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N12 N13 1.348(8) . ?
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N13 N14 1.306(9) . ?
N13 C18 1.448(9) . ?
N14 C11 1.357(8) . ?
C12 C17 1.377(11) . ?
C12 C13 1.407(10) . ?
C13 C14 1.389(11) . ?
C13 H13 0.9500 . ?
C14 C15 1.401(11) . ?
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C15 H15 0.9500 . ?
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C18 C23 1.398(11) . ?
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C20 C21 1.403(12) . ?
C20 H20 0.9500 . ?
C21 C22 1.394(12) . ?
C21 H21 0.9500 . ?
C22 C23 1.368(10) . ?
C22 H22 0.9500 . ?
C23 H23 0.9500 . ?
N31 C31 1.128(10) . ?
C31 C32 1.466(12) . ?
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S11 Co1 Br12 101.24(8) . . ?
Br11 Co1 Br12 109.24(7) . . ?
C11 S11 Co1 104.6(2) . . ?
N12 N11 C11 103.7(6) . . ?
N11 N12 N13 109.8(6) . . ?
N11 N12 C12 124.4(6) . . ?
N13 N12 C12 125.7(6) . . ?
N14 N13 N12 110.3(5) . . ?
N14 N13 C18 124.4(6) . . ?
N12 N13 C18 125.3(6) . . ?
N13 N14 C11 104.8(6) . . ?
N14 C11 N11 111.4(6) . . ?
N14 C11 S11 123.1(6) . . ?
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N11 C11 S11 125.6(5) . . ?
C17 C12 C13 123.4(7) . . ?
C17 C12 N12 118.1(6) . . ?
C13 C12 N12 118.4(7) . . ?
C14 C13 C12 116.5(8) . . ?
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C13 C14 C15 121.4(7) . . ?
C13 C14 H14 119.3 . . ?
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C17 C16 C15 120.7(8) . . ?
C17 C16 H16 119.7 . . ?
C15 C16 H16 119.7 . . ?
C12 C17 C16 118.4(7) . . ?
C12 C17 H17 120.8 . . ?
C16 C17 H17 120.8 . . ?
C19 C18 C23 122.9(7) . . ?
C19 C18 N13 117.3(7) . . ?
C23 C18 N13 119.7(7) . . ?
C18 C19 C20 118.4(8) . . ?
C18 C19 H19 120.8 . . ?
C20 C19 H19 120.8 . . ?
C19 C20 C21 119.0(7) . . ?
C19 C20 H20 120.5 . . ?
C21 C20 H20 120.5 . . ?
C22 C21 C20 121.1(7) . . ?
C22 C21 H21 119.4 . . ?
C20 C21 H21 119.4 . . ?
C23 C22 C21 120.3(8) . . ?
C23 C22 H22 119.9 . . ?
C21 C22 H22 119.9 . . ?
C22 C23 C18 118.2(8) . . ?
C22 C23 H23 120.9 . . ?
C18 C23 H23 120.9 . . ?
C31 N31 Co1 175.8(6) . . ?
N31 C31 C32 177.7(8) . . ?
C31 C32 H32A 109.5 . . ?
C31 C32 H32B 109.5 . . ?
H32A C32 H32B 109.5 . . ?
C31 C32 H32C 109.5 . . ?
H32A C32 H32C 109.5 . . ?
H32B C32 H32C 109.5 . . ?

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Br11 Co1 S11 C11 -48.3(3) . . . . ?
Br12 Co1 S11 C11 -168.1(2) . . . . ?
C11 N11 N12 N13 0.9(7) . . . . ?
C11 N11 N12 C12 -178.1(6) . . . . ?
N11 N12 N13 N14 -0.4(7) . . . . ?
C12 N12 N13 N14 178.5(6) . . . . ?
N11 N12 N13 C18 -179.3(6) . . . . ?
C12 N12 N13 C18 -0.3(10) . . . . ?
N12 N13 N14 C11 -0.3(7) . . . . ?
C18 N13 N14 C11 178.6(6) . . . . ?
N13 N14 C11 N11 0.8(8) . . . . ?
N13 N14 C11 S11 179.7(5) . . . . ?
N12 N11 C11 N14 -1.0(7) . . . . ?
N12 N11 C11 S11 -179.9(5) . . . . ?
Co1 S11 C11 N14 157.7(5) . . . . ?
Co1 S11 C11 N11 -23.6(6) . . . . ?
N11 N12 C12 C17 -59.4(9) . . . . ?
N13 N12 C12 C17 121.8(7) . . . . ?
N11 N12 C12 C13 118.5(7) . . . . ?
N13 N12 C12 C13 -60.3(9) . . . . ?
C17 C12 C13 C14 -0.8(11) . . . . ?
N12 C12 C13 C14 -178.5(6) . . . . ?
C12 C13 C14 C15 -0.9(11) . . . . ?
C13 C14 C15 C16 1.3(11) . . . . ?
C14 C15 C16 C17 0.0(11) . . . . ?
C13 C12 C17 C16 2.0(11) . . . . ?
N12 C12 C17 C16 179.8(6) . . . . ?
C15 C16 C17 C12 -1.6(11) . . . . ?
N14 N13 C18 C19 -51.1(9) . . . . ?
N12 N13 C18 C19 127.7(7) . . . . ?
N14 N13 C18 C23 126.0(8) . . . . ?
N12 N13 C18 C23 -55.2(9) . . . . ?
C23 C18 C19 C20 0.7(11) . . . . ?
N13 C18 C19 C20 177.7(6) . . . . ?
C18 C19 C20 C21 0.1(11) . . . . ?
C19 C20 C21 C22 -0.9(12) . . . . ?
C20 C21 C22 C23 0.9(13) . . . . ?
C21 C22 C23 C18 -0.1(12) . . . . ?
C19 C18 C23 C22 -0.7(11) . . . . ?
N13 C18 C23 C22 -177.6(7) . . . . ?
S11 Co1 N31 C31 -9(10) . . . . ?
Br11 Co1 N31 C31 119(10) . . . . ?
Br12 Co1 N31 C31 -120(10) . . . . ?
Co1 N31 C31 C32 63(29) . . . . ?

loop_
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C13 H13 Br11  0.95 3.06 3.802(9) 135.6 2_565
C19 H19 Br11  0.95 3.08 3.697(8) 124.3 2_565
C32 H32B Br11  0.98 2.86 3.575(10) 130.3 2_665
C15 H15 Br12  0.95 2.99 3.689(8) 131.2 1_556

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_diffrn_reflns_theta_full              27.50
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_refine_diff_density_max    1.942
_refine_diff_density_min   -1.305
_refine_diff_density_rms    0.180
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