Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Synthesis of Nitrogen Mustards on Cobalt(III)

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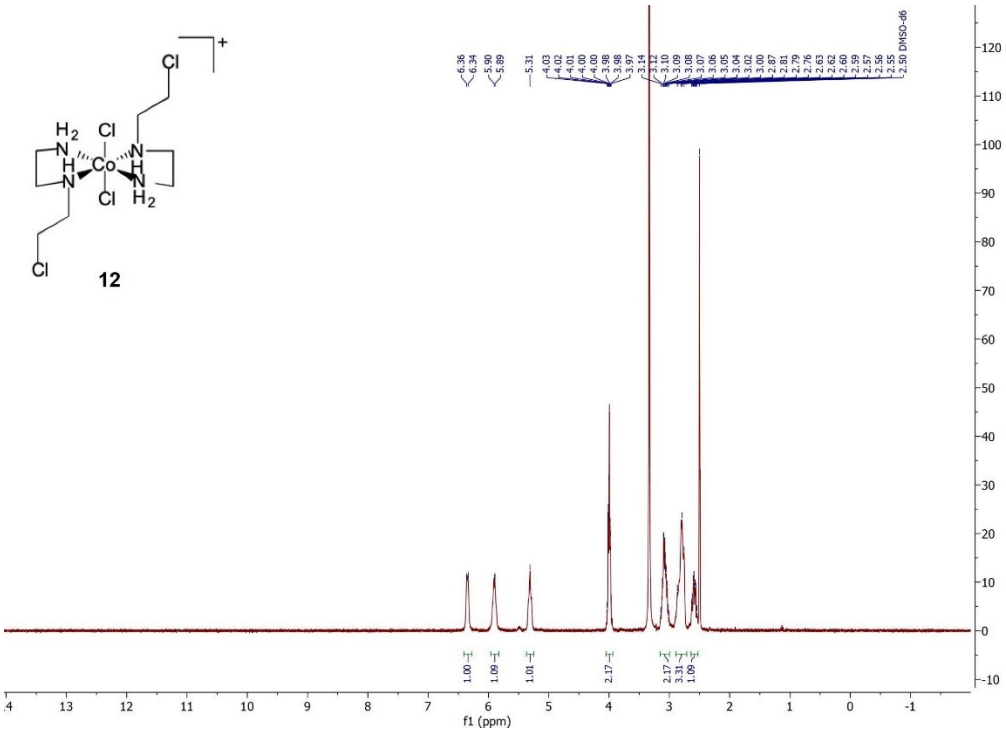
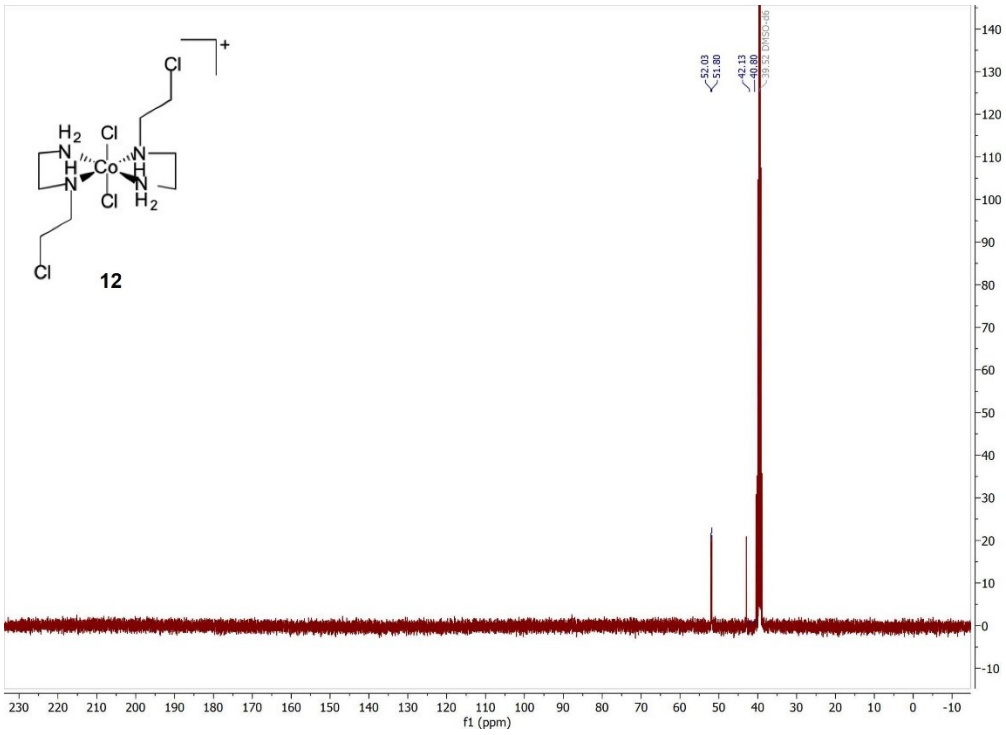
1.1 ^{1}H and ^{13}C NMR spectra of compounds that were able to be isolated in pure form from the complex isomeric mixtures

^{1}H NMR and ^{13}C NMR spectra of (OC-6-12')-[Co(ceen)$_2$(Cl)$_2$]Cl (**12**)

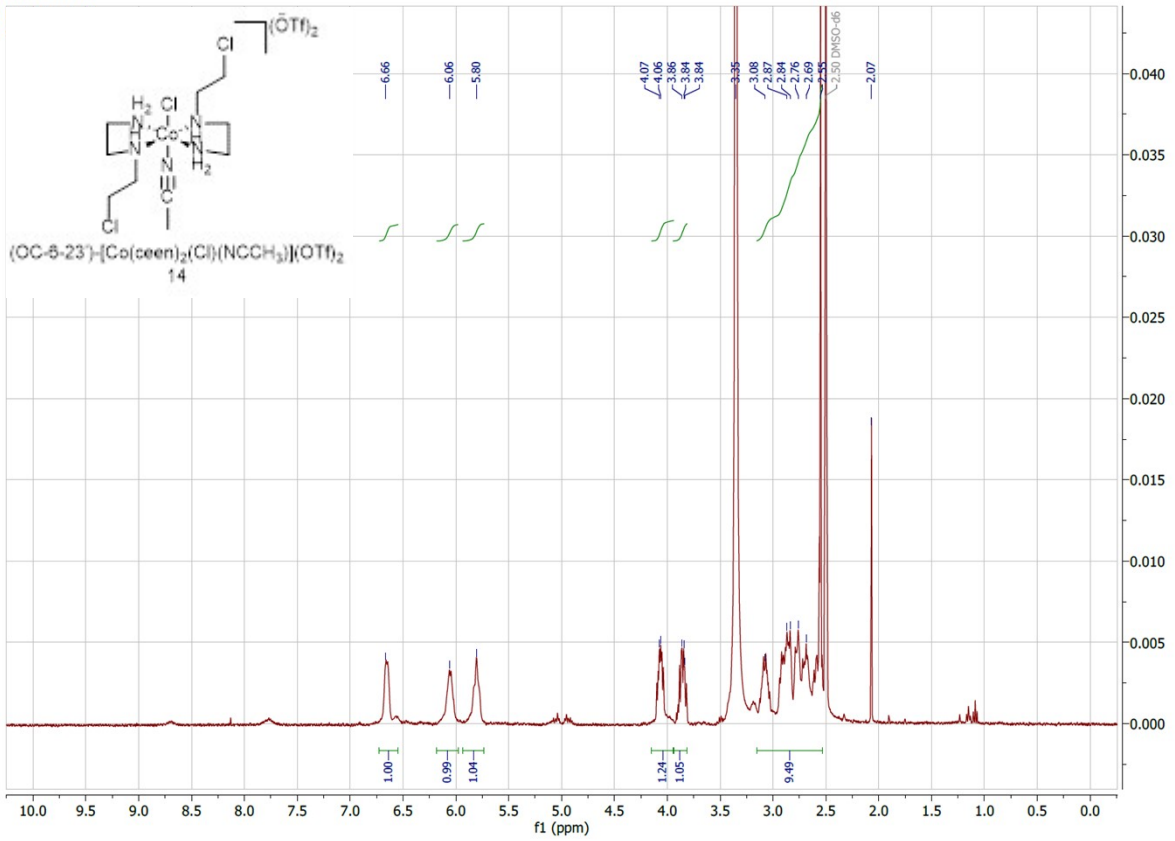


^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K).

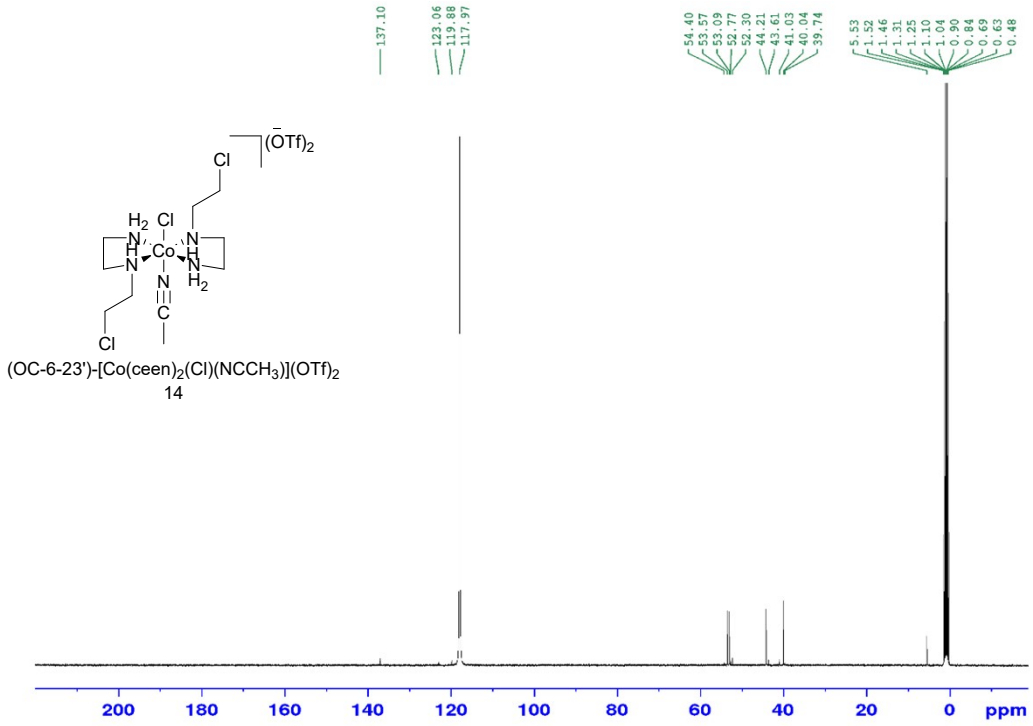


^{13}C NMR spectrum (101 MHz, DMSO-d_6, 298 K).

^{1}H NMR and ^{13}C NMR spectra of (OC-6-23')-[Co(ceen)$_2$(Cl)(NCCH$_3$)](OTf)$_2$ (**14**)

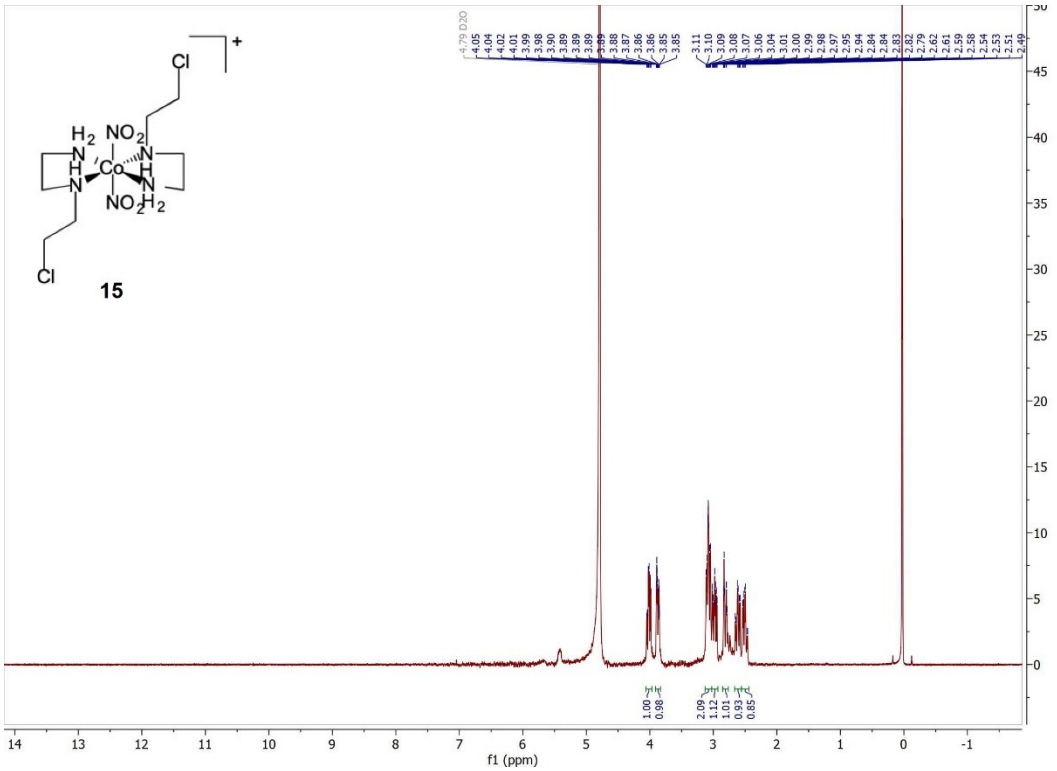


^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K).

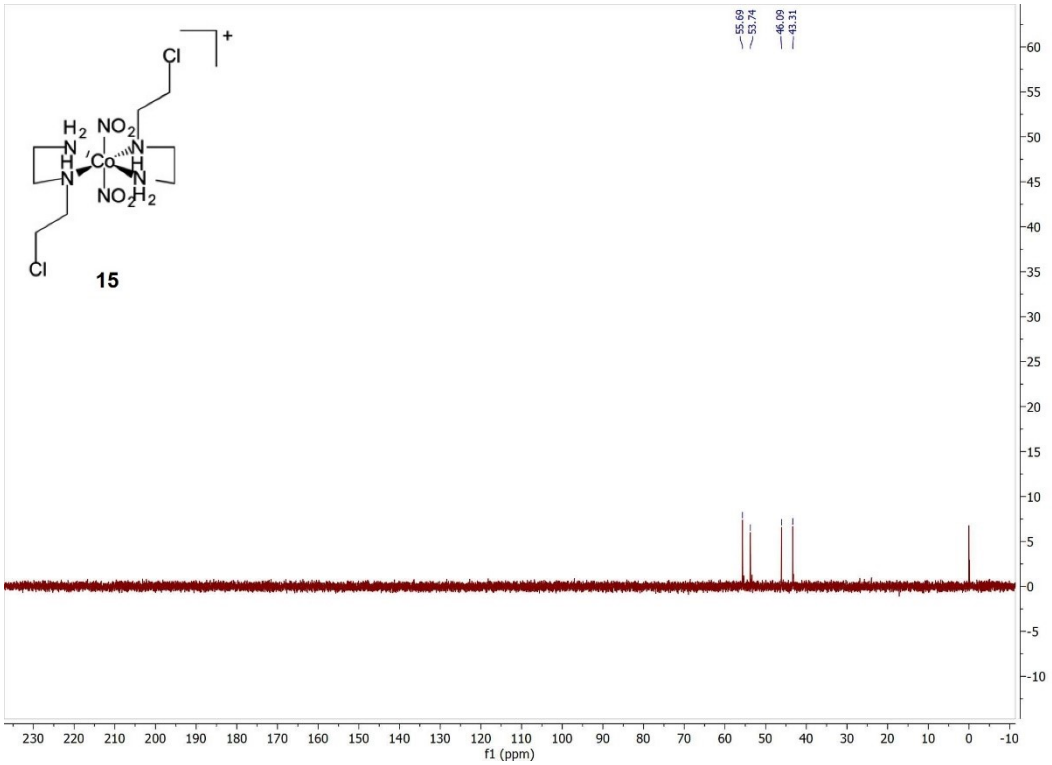


^{13}C NMR spectrum (101 MHz, CD3CN, 298 K).

^{1}H NMR and ^{13}C NMR spectra of (OC-6-12')-[Co(ceen)$_2$(NO$_2$)$_2$]Cl (**15**)

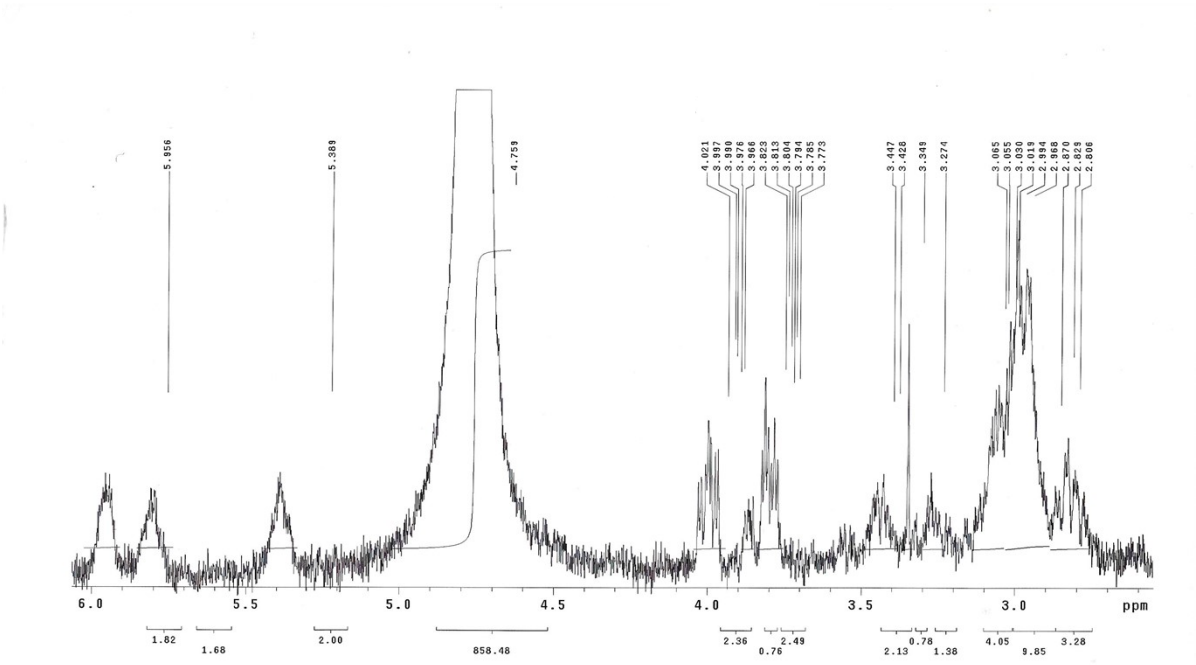


^{1}H NMR spectrum (400 MHz, D_2O, 298 K).

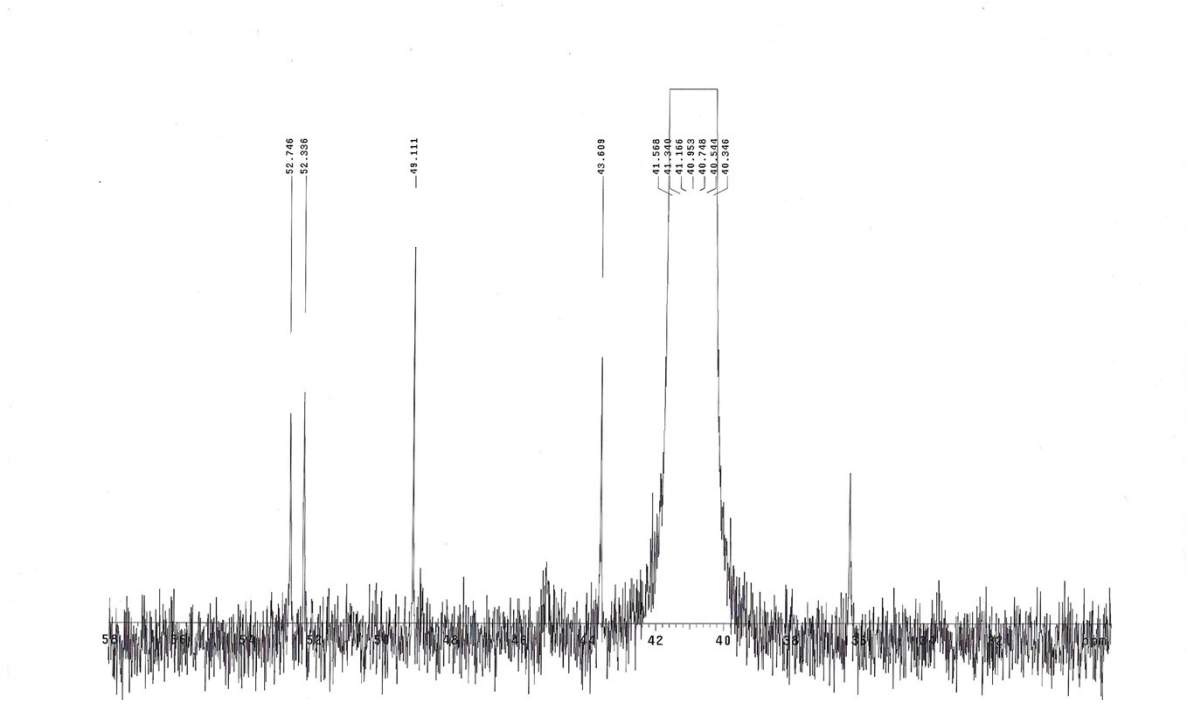


^{13}C NMR spectrum (101 MHz, D_2O, 298 K). Referenced to 3-(Trimethylsilyl)propionic-2,2,3,3-d4 acid sodium salt (TMSP) at 0 ppm.

^{1}H NMR and ^{13}C NMR spectra of the bulk material from which *trans* chlorido (OC-6-12')-[Co(Cl)$_2$(heen)$_2$]Cl (**16**) and *cis* amine *trans* chlorido (OC-6-13')-[Co(Cl)$_2$(heen)$_2$]Cl (**17**) were crystallised.



^{1}H NMR spectrum (400 MHz, DMSO-d_6, 298 K).



^{13}C NMR spectrum (101 MHz, DMSO-d_6, 298 K).

1.2 Crystallographic Summary Tables (CSD 2163481-2163482 and 2163484-2163491)

Structure	***6***	***9***	***10***	***11***	***12***
Formula	$C_8H_{22}CoF_6N_4O_2P$	$C_8H_{23}CoI_2N_4O_2$	$C_8H_{22}Cl_5CoN_4O_2Zn_2$	$C_8H_{22}Cl_4CoN_4O_3Zn_2$	$C_{12}H_{34}Cl_5N_4O_2$
Formula weight	410.19	520.03	573.21	553.76	502.61
Crystal system	orthorhombic	monoclinic	triclinic	orthorhombic	orthorhombic
Space group	*Pbcn*	$P2_1/c$	*P*-1	*Aea*2	*Pbcn*
a/Å	10.0855(6)	14.0248(3)	8.0188(6)	25.8579(7)	19.2961(3)
b/Å	18.6517(10)	9.5014(2)	9.4646(6)	11.1659(3)	8.06940(10)
c/Å	7.9440(4)	11.3201(2)	13.1434(8)	13.2095(3)	27.6193(5)
α/°	90	90	76.033(5)	90	90
β/°	90	102.667(2)	79.660(5)	90	90
γ/°	90	90	74.106(6)	90	90
V/Å³	1494.36(14)	1471.75(5)	924.12(11)	3813.94(17)	4300.54(12)
Z	4	4	2	8	8
T/K	120.01(10)	120.01(10)	202(110)	120.00(10)	120.01 (10)
μ/mm⁻¹	10.788	5.360	16.711	14.951	1.433
Total reflections	6525	37075	16321	35287	244629
Unique reflections (R_{int})	1384 (0.0377)	4076 (0.0461)	3394 (0.0624)	3509 (0.0652)	11529 (0.0523)
R_1 indices [I>2σ(I)]	0.0350	0.0196	0.0765	0.0341	0.0327
ωR2 (all data)	0.0973	0.0467	0.2492	0.0886	0.0793
Flack	n/a	n/a	n/a	0.049(7)	n/a

Structure	***13***	***14***	***15***	***16***	***17***
Formula	$C_{10}H_{24}Cl_3CoF_6N_4O_7S_2$	$C_{12}H_{25}Cl_3CoF_6N_5O_6S_2$	$C_8H_{22}Cl_3CoN_6O_4$	$C_8H_{26}Cl_3CoN_4O_3$	$C_8H_{24}Cl_3CoN_4O_2$
Formula weight	655.73	678.77	431.59	391.61	373.59
Crystal system	monoclinic	monoclinic	triclinic	triclinic	monoclinic
Space group	$P2_1/n$	$P2_1/n$	*P*-1	*P*-1	$P2_1/n$
a/Å	10.2797(2)	15.5162(3)	13.5798(13)	9.7046(5)	11.5210(7)
b/Å	19.2548(4)	10.8096(2)	14.7189(12)	10.3901(5)	10.6094(6)
c/Å	12.9988(3)	16.1940(3)	15.3910(13)	10.4141(6)	12.7807(8)
α/°	90	90	77.760(7)	62.180(5)	90
β/°	109.284(2)	111.555(2)	78.576(7)	63.266(5)	98.647(6)
γ/°	90	90	83.603(7)	88.467(4)	90
V/Å³	2428.54(9)	2526.17(9)	2939.1(5)	806.81(9)	1544.44(16)
Z	4	4	6	2	4
T/K	120.00 (10)	120.00(10)	120.01(10)	120.01(10)	120.01(10)
μ/mm⁻¹	11.000	10.582	10.842	13.004	13.508
Total reflections	13412	13382	42568	14650	11198
Unique reflections (R_{int})	5040 (0.0383)	5254 (0.0394)	12250 (0.0826)	3000 (0.0473)	2814 (0.0607)
R_1 indices [I>2σ(I)]	0.0336	0.0487	0.0803	0.0365	0.0426
ωR2 (all data)	0.0862	0.1329	0.3186	0.1034	0.1081

X-ray crystal structures with complete asymmetric unit

1.2.1 Asymmetric unit of complex p_1p_3-*f,f*-[Co(heen-H)$_2$]PF$_6$, **[6]PF$_6$**

The slow diffusion of diethyl ether into a methanolic solution of bulk material of **[6]PF$_6$** provided red block-like X-ray quality crystals. The asymmetric unit comprised of half a [Co(heen-H)$_2$]$^+$ cation and half a hexafluoridophosphate counter ion.

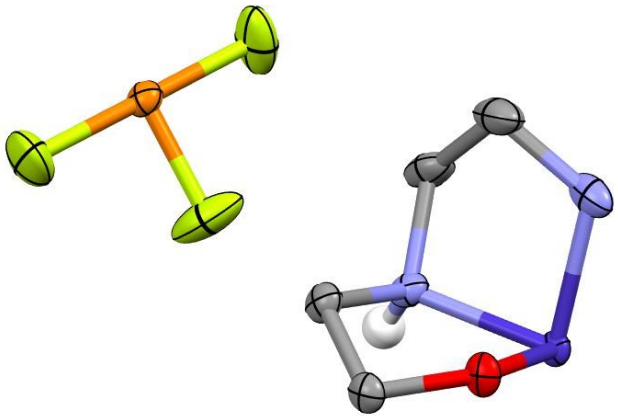


Fig. 7 View of the contents of the asymmetric unit, comprising of one half of a [Co(heen-H)$_2$]$^+$cation and one half of a hexafluorophosphate counter ion. Hydrogens were omitted for clarity, except for the secondary nitrogen hydrogen atom. Colour coding: carbon (grey), nitrogen (light purple), oxygen (red), fluoride (yellow), phosphate (orange) and cobalt (dark purple).

1.2.2 Asymmetric unit of complex p_1s-*f,f*-[Co(heen)(heen-H)](I$^-$)$_2$, **9**

The bulk material of p_1s-*f,f*-[Co(heen)(heen-H)](I$^-$)$_2$ **9** was dissolved in water and the slow evaporation of the solution provided red plate-like X-ray quality crystals. The asymmetric unit comprised of complete [Co(heen)(heen-H)]$^{2+}$ cation and two iodide counter ions.

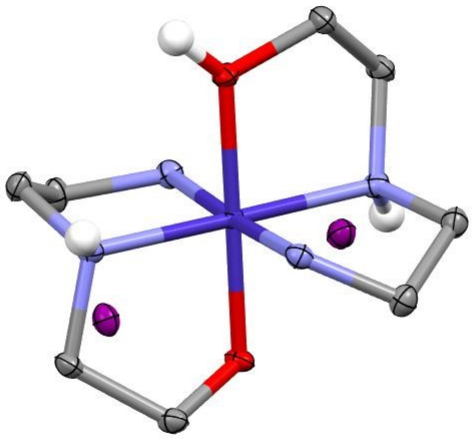


Fig. 8 View of the contents of the asymmetric unit, comprising of one complete [Co(heen)(heen-H)]$^{2+}$ cation and two iodide counter ions. Hydrogens were omitted for clarity, except for the secondary nitrogen and heen oxygen hydrogen atoms. Colour coding: carbon (grey), nitrogen (light purple), oxygen (red), iodide (fuchsia) and cobalt (dark purple).

1.2.3 Asymmetric unit of complexes {(OC-6-13')-[Co(heen-H)$_2$ZnCl$_2$ZnCl$_3$]}$_n$, **10**, and (OC-6-2'3)-[Co(heen-H)$_2$Cl$_2$ZnOZnCl$_2$], **11**.

The slow evaporation of the pink solution obtained from the reaction of [Co(heen)(heen-H)](I$^-$)$_2$ **9** with ZnCl$_2$ provided pink plate X-ray quality crystals of **10** and **11**.

1.2.3.1 The asymmetric unit consisted of one complete [Co(heen-H)$_2$ZnCl$_2$ZnCl$_3$] neutral complex, **10**.

Attempts to collect data at the standard temperature of 120K gave poor data due to what appeared to be a phase transition at about 160K. Data collected at 200K gave the best results, but still has high residual electron density in the vicinity of the chloride atoms of the ZnCl$_2$ moiety. Attempts to model this as disorder rapidly lead to instability in the model.

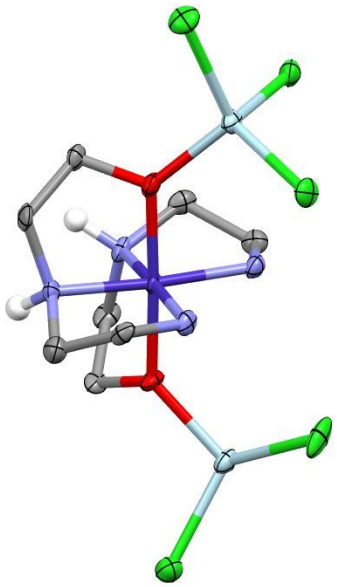


Fig. 9 View of the contents of the asymmetric unit comprising of one complete [Co(heen-H)$_2$ZnCl$_2$ZnCl$_3$] neutral complex. Hydrogens were omitted for clarity, except for the secondary nitrogen hydrogen atoms. Colour coding: carbon (light grey), nitrogen (light purple), oxygen (red), chloride (green), zinc (light blue) and cobalt (dark purple).

1.2.3.2 The asymmetric unit consisted of one complete $[Co(heen\text{-}H)_2Cl_2ZnOZnCl_2]$ neutral complex.

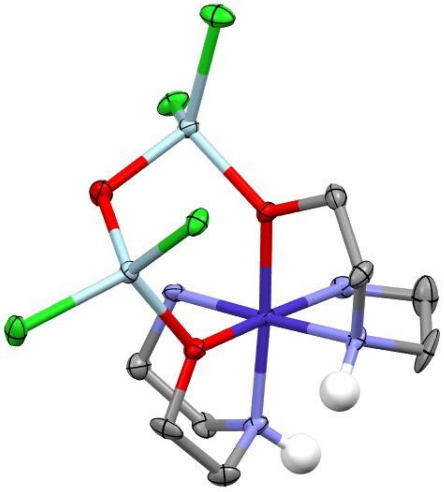


Fig. 10 View of the contents of the asymmetric unit comprising of one complete $[Co(heen\text{-}H)_2Cl_2ZnOZnCl_2]$ neutral complex. Hydrogens were omitted for clarity, except for the secondary nitrogen hydrogen atoms. Colour coding: carbon (light grey), nitrogen (light purple), oxygen (red), chloride (green), zinc (light blue) and cobalt (dark purple).

1.2.4 Asymmetric unit of complex (OC-6-12')-$[Co(ceen)_2(Cl)_2]Cl$, **[12]Cl**

The slow evaporation of a dilute solution of the bulk material of **[12]Cl** in ethanol, provided green block-like X-ray quality crystals. The asymmetric unit comprised of one complete $[Co(ceen)_2(Cl)_2]^+$ cation, two uncoordinated ethanol solvent molecules and two half chloride counter ions.

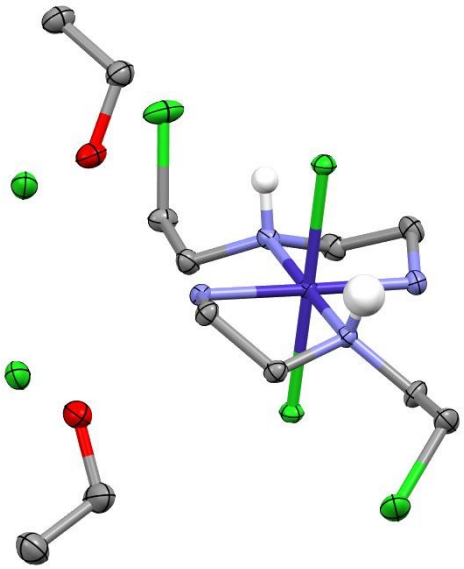


Fig. 1 View of the contents of the asymmetric unit, comprising of one complete $[Co(ceen)_2(Cl)_2]^+$ cation, two chloride counter ions and two uncoordinated ethanol solvent molecules. Hydrogens were omitted for clarity, except for the secondary nitrogen hydrogen atoms. Colour coding: carbon (grey), nitrogen (light purple), oxygen (red), chloride (green) and cobalt (dark purple).

1.2.5 Asymmetric unit of complex (OC-6-23')-$[Co(ceen)_2(Cl)(OH_2)](OTf)_2$, **13**

The slow evaporation of the purple filtrate obtained during the synthesis of complex **3** yielded purple prismatic X-ray quality crystals of $[Co(ceen)_2(Cl)(OH_2)](OTf)_2$ **13**. The asymmetric unit consisted of one complete $[Co(ceen)_2(Cl)(OH_2)]^{2+}$ cation and two triflate counter ions.

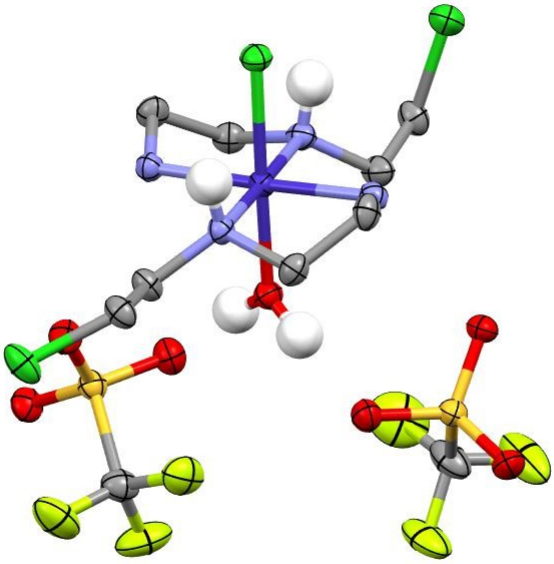


Fig. 2 View of the contents of the asymmetric unit, comprising of one complete $[Co(ceen)_2(Cl)(OH_2)]^{2+}$ cation and two triflate counter ions. Hydrogens were omitted for clarity, except for the secondary nitrogen and OH_2 hydrogen atoms. Colour coding: carbon (grey), nitrogen (light purple), oxygen (red), chloride (fluorescent green), fluoride (green/yellow), sulfur (yellow) and cobalt (dark purple).

1.2.6 Asymmetric unit of complex (OC-6-23')-$[Co(ceen)_2(Cl)(NCCH_3)](OTf)_2$, **14**

The slow vapour diffusion of diethyl ether into a solution of complex **3** in acetonitrile at -4 °C provided red block-like X-ray quality crystals of $[Co(ceen)_2(Cl)(NCCH_3)](OTf)_2$ **14**. The asymmetric unit consisted of one complete $[Co(ceen)_2(Cl)(NCCH_3)]^{2+}$ cation and two triflate counter ions.

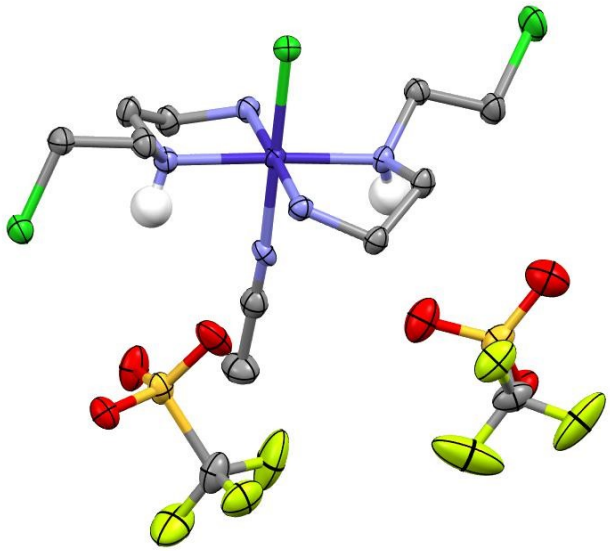


Fig. 3 View of the contents of the asymmetric unit, comprising of one complete $[Co(ceen)_2(Cl)(NCCH_3)]^{2+}$ cation and two triflate counter ions. Hydrogens were omitted for clarity, except for the secondary nitrogen hydrogen atoms. Colour coding: carbon (grey), nitrogen (light purple), oxygen (red), chloride (fluorescent green), fluoride (green/yellow), sulfur (yellow) and cobalt (dark purple).

1.2.7 Asymmetric unit of complex (OC-6-12')-[$Co(ceen)_2(NO_2)_2$]Cl, **15**

The reaction of complex **2** with sodium nitrite ($NaNO_2$) and ammonium hydroxide (NH_4OH) provided access to [$Co(ceen)_2(NO_2)_2$]Cl **15**, and upon neutralization of the resultant solution and leaving it to stand in the fridge for one week orange block X-ray quality crystals were obtained. The asymmetric unit consisted of three complete $[Co(ceen)_2(NO_2)_2]^+$ cations and six half occupancy chloride counter ions. The model originally included a large number of partial occupancy water molecules. The chloride counterions were allowed to refine in occupancy, before being fixed at 0.5. The water molecules were then removed from the final model and their electron density was incorporated using the SQUEEZE algorithm. Although not included in the model, it is expected that some Cl/H_2O disorder exists in the structure.

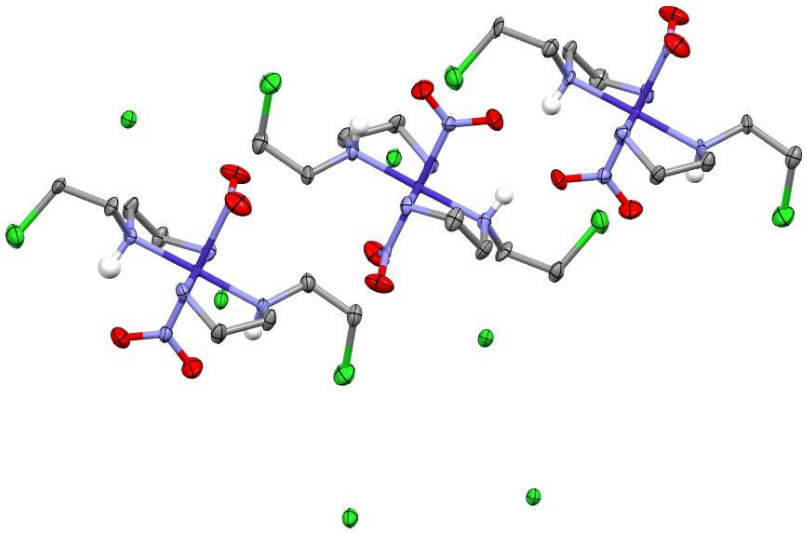


Fig. 4 View of the contents of the asymmetric unit, comprising of three complete $[Co(ceen)_2(NO_2)_2]^+$ cations and six half occupancy chloride counter ions. Hydrogens were omitted for clarity, except for the secondary nitrogen hydrogen atoms. Colour coding: carbon (grey), nitrogen (light purple), oxygen (red), chloride (green) and cobalt (dark purple).

1.2.8 Asymmetric unit of complex *trans* amine *trans* chlorido (OC-6-12')-[$Co(Cl)_2(heen)_2$]Cl, **16**

The slow evaporation of the bulk material of complex **16/17** in a 1:1 mixture of ethanol:water, provided green block-like X-ray quality crystals of *trans* amine *trans* chlorido [$Co(Cl)_2(heen)_2$]Cl **16**. The asymmetric unit consisted of one complete $[Co(Cl)_2(heen)_2]^+$ cation, one chloride counter ion and one uncoordinated ethanol solvent molecule.

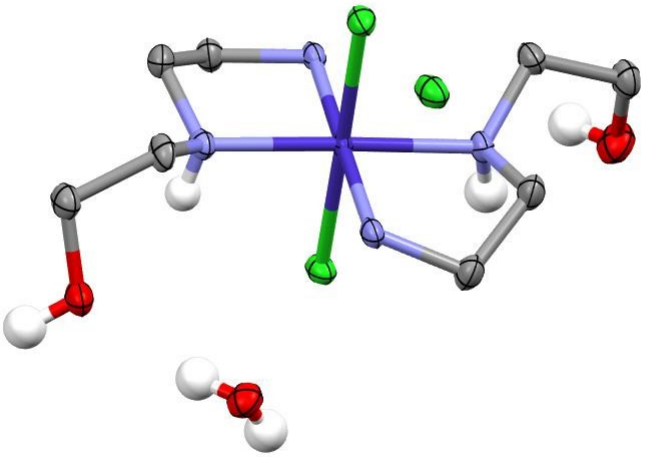


Fig. 5 View of the contents of the asymmetric unit, comprising of one complete [$[Co(Cl)_2(heen)_2]^+$ cation one chloride counter ion and one uncoordinated water molecule. Hydrogens were omitted for clarity, except for the secondary nitrogen, oxygen of the heen ligands and uncoordinated water molecule hydrogen atoms. Colour coding: carbon (grey), nitrogen (light purple), oxygen (red), chloride (green) and cobalt (dark purple).

1.2.9 Asymmetric unit of complex *cis* amine *trans* chlorido (OC-6-13')-$[Co(Cl)_2(heen)_2]Cl$, **17**

The slow diffusion of diethyl ether into a methanolic solution of the bulk material of complex **16/17** provided blue fine needle shaped X-ray quality crystals of *cis* amine *trans* chlorido $[Co(Cl)_2(heen)_2]Cl$ **17**. The asymmetric unit consisted of one complete $[Co(Cl)_2(heen)_2]^+$ cation and one chloride counter ion.

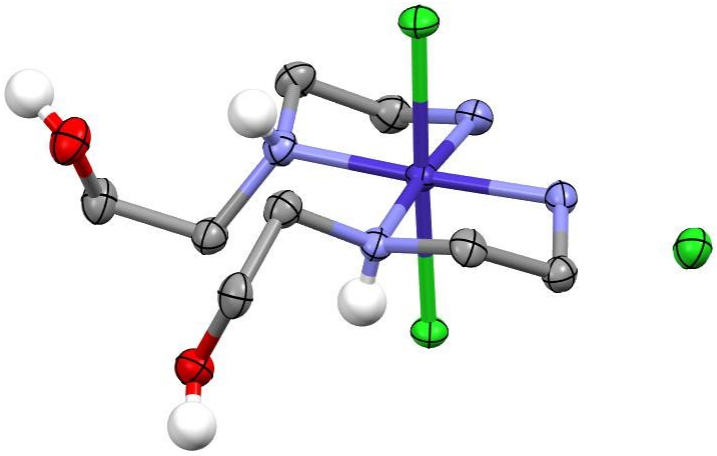


Fig. 6 View of the contents of the asymmetric unit, comprising of one complete $[Co(Cl)_2(heen)_2]^+$ cation and one chloride counter ion. Hydrogens were omitted Hydrogens were omitted for clarity, except for the secondary nitrogen and oxygen of the heen ligand hydrogen atoms. Colour coding: carbon (grey), nitrogen (light purple), oxygen (red), chloride (green) and cobalt (dark purple).

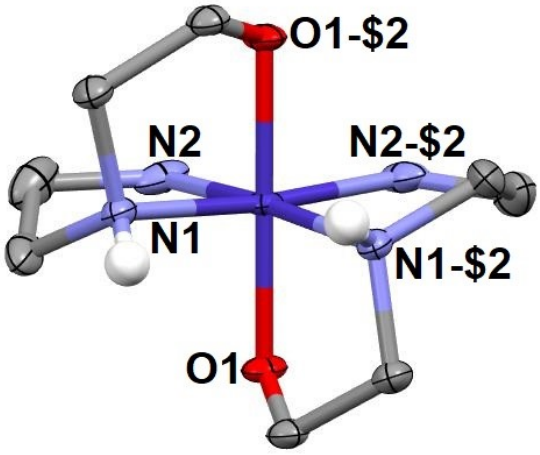
1.3 X-ray Crystal Structure Solution Details for $[Co(ceen)_2(NO_2)_2]Cl$ **(15)**

Multiple $Co(ceen)_2(NO_2)_2]Cl$ (**15**) data sets were collected, however, the quality of the data was consistently very poor. There is also unaccounted for disorder associated with the NO_2 groups of each of the three molecules in the asymmetric unit. The disorder arises from impurity of the

complex mixture, with $[Co(ceen)_2(NO_2)Cl]Cl$ precursor still remaining. Attempts to account for the disordered counter parts (Cl) resulted in numerous NPD atoms and/or bond length and angles resistant to constraints. The SQUEEZE routine resulted in a decrease of the R_1 value from 15.23 to 8.03%.

1.4 Bond distances and angles around the Co(III) metal centre

1.4.1 Complex p_1p_3-*f*,*f*-$[Co(heen\text{-}H)_2]PF_6$, **[6]$PF_6$**



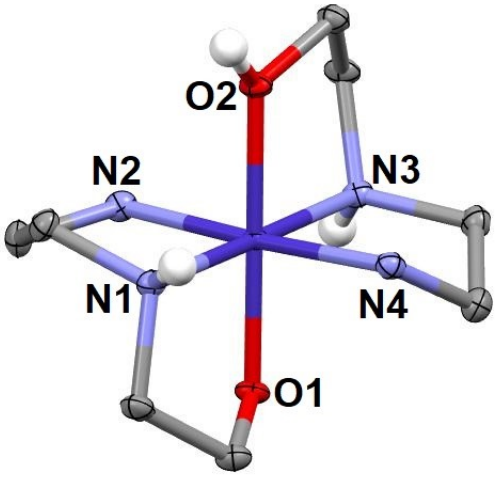
Co1	Distance	Angles				

O1	1.9065 (0.0017)					
O1-$2	1.9065 (0.0017)	179.59 (0.09)				
N1-$2	1.9300 (0.0022)	88.42 (0.08)	91.29 (0.08)			
N1	1.9301 (0.0022)	91.29 (0.08)	88.42 (0.08)	91.04 (0.15)		
N2-$2	1.9628 (0.0021)	94.07 (0.07)	86.21 (0.07)	86.75 (0.10)	174.14 (0.08)	
N2	1.9628 (0.0021)	86.21 (0.07)	94.07 (0.07)	174.14 (0.08)	86.75 (0.10)	95.96 (0.12)
	Co1	**O1**	**O1-$2**	**N1-$2**	**N1**	**N2-$2**

-The "$" represents the atoms generation through the 2-fold symmetry axis.

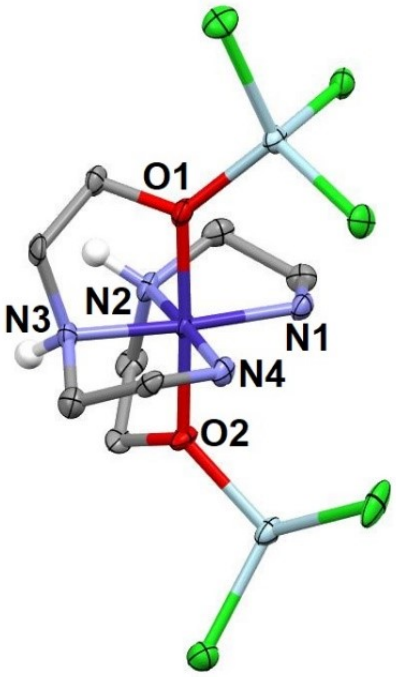
1.4.2 Complex *p*$_1$*s*-*f*,*f*-[Co(heen)(heen-H)](I$^-$)$_2$, **9**

Co1	**Distance**	**Angles**				
O1	1.8920 (0.0015)					
O2	1.9176 (0.0015)	179.73 (0.07)				
N4	1.9469 (0.0018)	89.73 (0.08)	90.48 (0.07)			
N2	1.9509 (0.0019)	92.65 (0.08)	87.14 (0.08)	177.14 (0.09)		
N1	1.9544 (0.0018)	85.69 (0.07)	94.12 (0.07)	96.24 (0.08)	85.53 (0.08)	
N3	1.9618 (0.0018)	94.87 (0.07)	85.32 (0.07)	83.96 (0.08)	94.24 (0.08)	179.40 (0.08)
	Co1	**O1**	**O2**	**N4**	**N2**	**N1**



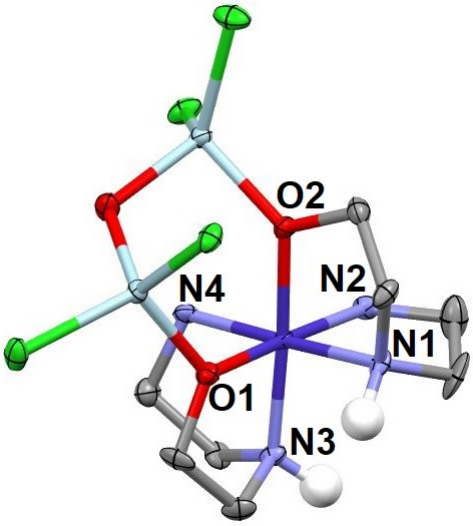
1.4.3 Complex $\{(OC\text{-}6\text{-}13')\text{-}[Co(heen\text{-}H)_2ZnCl_2ZnCl_3]\}_n$, **10**

Co1	**Distance**	**Angles**				
O2	1.9181 (0.0085)					
O1	1.9212 (0.0091)	177.70 (0.37)				
N1	1.9539 (0.0106)	91.22 (0.43)	90.81 (0.42)			
N4	1.9598 (0.0103)	91.01 (0.42)	89.94 (0.42)	93.62 (0.44)		
N3	1.9726 (0.0105)	93.25 (0.42)	84.72 (0.41)	175.53 (0.46)	86.24 (0.45)	
N2	1.9734 (0.0105)	85.19 (0.41)	93.88 (0.41)	85.98 (0.44)	176.16 (0.45)	94.45 (0.44)
	Co1	**O2**	**O1**	**N1**	**N4**	**N3**



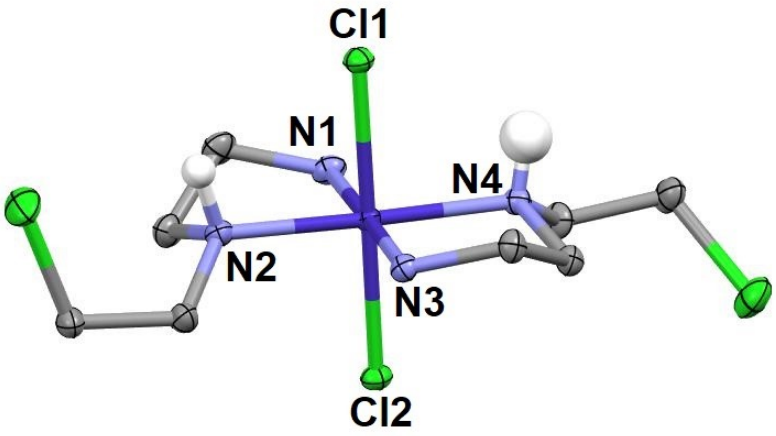
Co1	Distance	Angles				
O1	1.9142 (0.0049)					
O2	1.9220 (0.0049)	89.50 (0.22)				
N3	1.9342 (0.0060)	86.42 (0.24)	175.67 (0.24)			
N1	1.9591 (0.0058)	90.32 (0.23)	86.46 (0.22)	95.01 (0.25)		
N4	1.9608 (0.0061)	90.61 (0.23)	92.17 (0.22)	86.42 (0.25)	178.34 (0.26)	
N2	1.9611 (0.0055)	176.09 (0.24)	90.42 (0.24)	93.75 (0.26)	85.78 (0.25)	93.30 (0.25)
	Co1	**O1**	**O2**	**N3**	**N1**	**N4**

1.4.4 Complex (OC-6-2'3)-[Co(heen-H)$_2$Cl$_2$ZnOZnCl$_2$], **11**

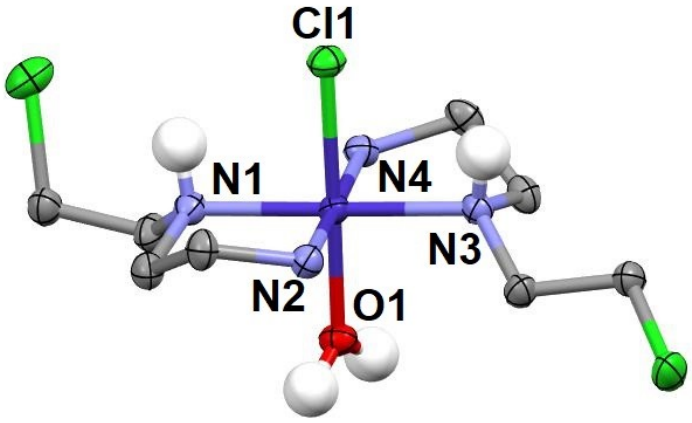


Co1	Distance	Angles				
N3	1.9481 (0.0009)					
N1	1.9668 (0.0009)	178.79 (0.04)				
N4	1.9937 (0.0009)	86.15 (0.04)	95.04 (0.04)			
N2	1.9993 (0.0009)	93.31 (0.04)	85.49 (0.04)	177.92 (0.04)		
Cl2	2.2292 (0.0003)	90.14 (0.03)	90.03 (0.03)	90.96 (0.03)	91.05 (0.03)	
Cl1	2.2495 (0.0003)	89.68 (0.03)	90.13 (0.03)	89.56 (0.03)	88.43 (0.03)	179.44 (0.01)
	Co1	**N3**	**N1**	**N4**	**N2**	**Cl2**

1.4.5 Complex (OC-6-12')-[Co(ceen)$_2$(Cl)$_2$]Cl, **[12]Cl**

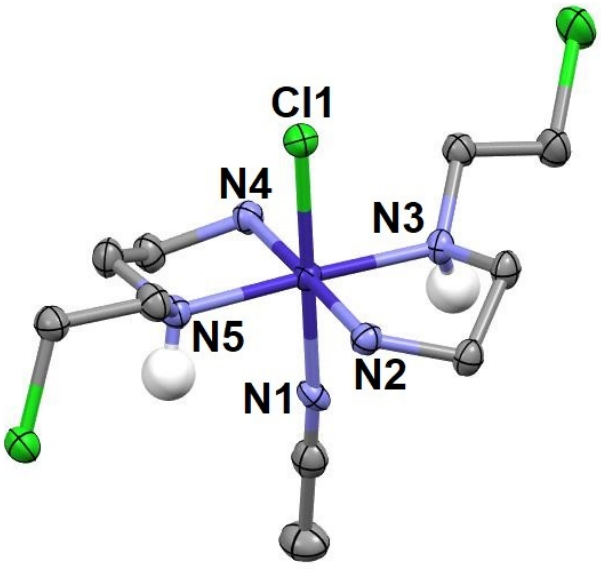


1.4.6 Complex (OC-6-23')-[Co(ceen)$_2$(Cl)(OH$_2$)](OTf)$_2$, **13**



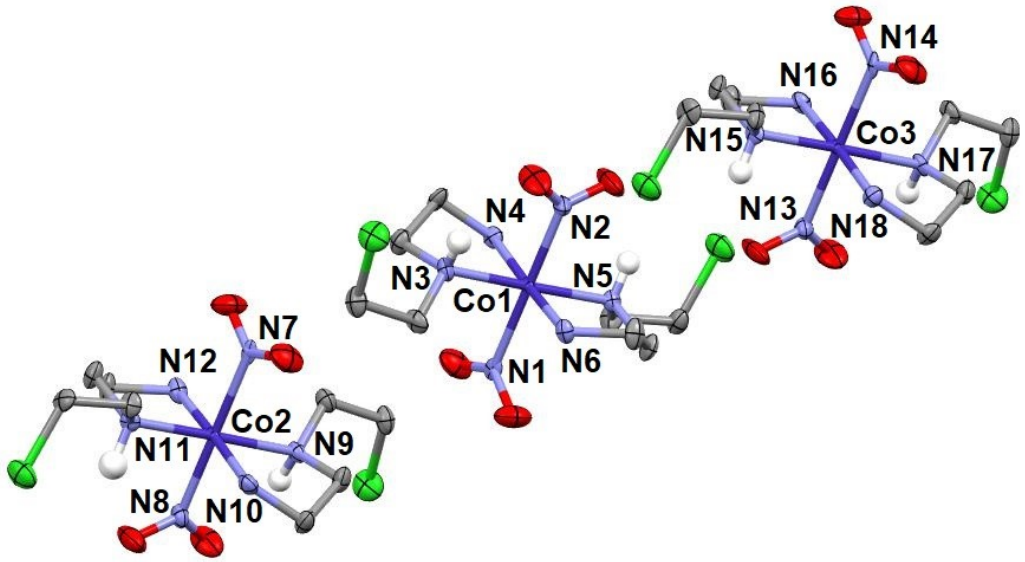
1.4.7 Complex (OC-6-23')-$[Co(ceen)_2(Cl)(NCCH_3)](OTf)_2$, **14**

Co1	**Distance**	**Angles**				
N2	1.9491 (0.0020)					
O1	1.9518 (0.0018)	91.95 (0.08)				
N4	1.9610 (0.0020)	177.44 (0.09)	90.59 (0.08)			
N3	1.9940 (0.0019)	93.68 (0.08)	91.74 (0.08)	85.89 (0.08)		
N1	1.9989 (0.0019)	86.10 (0.08)	89.12 (0.08)	94.30 (0.08)	179.12 (0.08)	
Cl1	2.2079 (0.0006)	88.63 (0.06)	178.83 (0.06)	88.84 (0.06)	89.24 (0.06)	89.90 (0.06)
	Co1	**N2**	**O1**	**N4**	**N3**	**N1**



Co1	**Distance**	**Angles**				
N2	1.9515 (0.0025)					
N4	1.9536 (0.0025)	178.48 (0.10)				
N1	1.9554 (0.0024)	90.39 (0.10)	88.16 (0.10)			
N3	2.0011 (0.0024)	86.53 (0.10)	93.90 (0.10)	89.10 (0.10)		
N5	2.0087 (0.0025)	93.49 (0.10)	86.02 (0.10)	88.43 (0.10)	177.53 (0.10)	
Cl1	2.2179 (0.0008)	90.54 (0.07)	90.92 (0.07)	179.03 (0.07)	90.68 (0.07)	91.79 (0.07)
	Co1	**N2**	**N4**	**N1**	**N3**	**N5**

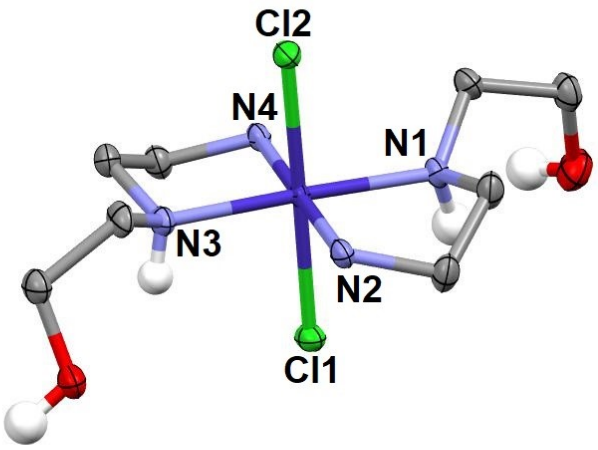
1.4.8 Complex (OC-6-12')-$[Co(ceen)_2(NO_2)_2]Cl$, **15**



Co1	Distance	Angles				

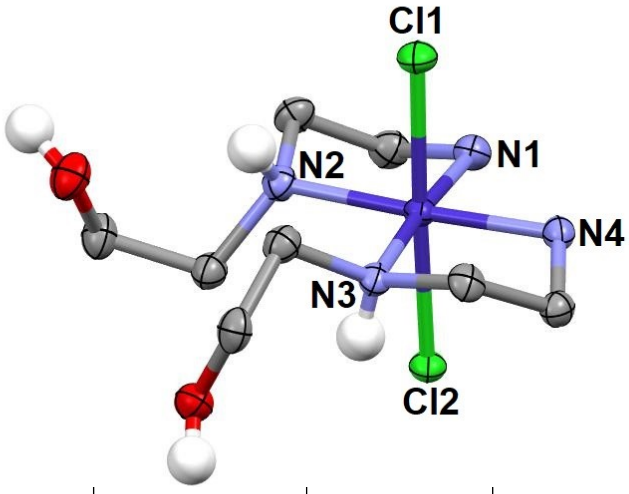
Co3	Distance	Angles				
N16	1.9423 (0.0043) 1.9460 (0.0043)					
N18	1.9509 (0.0042) 1.9483 (0.0046)	177.62 (0.18) 177.69 (0.20)				
N13	1.9746 (0.0046) 1.9799 (0.0046)	88.84 (0.20) 88.84 (0.20)	88.78 (0.20) 88.80 (0.20)			
N17	1.9850 (0.0045) 1.9859 (0.0044)	86.00 (0.19) 85.99 (0.19)	93.75 (0.18) 86.25 (0.19)	89.27 (0.19) 89.43 (0.19)		
N15	2.0000 (0.0046) 1.9990 (0.0043)	93.99 (0.18) 86.12 (0.20)	86.20 (0.19) 93.69 (0.19)	89.41 (0.19) 89.26 (0.19)	178.68 (0.18) 178.71 (0.18)	
N14	2.0418 (0.0046) 2.0397 (0.0045)	91.30 (0.18) 91.30 (0.18)	90.98 (0.18) 91.00 (0.18)	179.76 (0.18) 179.84 (0.20)	90.68 (0.18) 90.66 (0.18)	90.64 (0.18) 90.69 (0.18)
	Co3	N16	N18	N13	N17	N15

1.4.9 *trans* amine *trans* chlorido (OC-6-12')-$[Co(Cl)_2(heen)_2]Cl$ complex, **16**



Co2	Distance	Angles				
N12	1.9417 (0.0047)					
N10	1.9539 (0.0047)	177.72 (0.20)				
N8	1.9710 (0.0049)	88.85 (0.20)	88.88 (0.20)			
N11	1.9976 (0.0044)	86.37 (0.19)	93.47 (0.18)	89.18 (0.19)		
N9	2.0019 (0.0043)	93.50 (0.19)	86.61 (0.19)	89.50 (0.19)	178.68 (0.18)	
N7	2.0465 (0.0044)	91.23 (0.19)	91.05 (0.18)	179.87 (0.18)	90.72 (0.18)	90.60 (0.18)
	Co2	N12	N10	N8	N11	N9

1.4.10 *cis* amine *trans* chlorido (OC-6-13')-[$Co(Cl)_2(heen)_2$]Cl complex, **17**



N3	2.0058 (0.0033)	86.32 (0.14)	175.84 (0.14)			
N2	2.0077 (0.0034)	176.49 (0.14)	86.38 (0.14)	97.05 (0.13)		
Cl1	2.2479 (0.0011)	90.01 (0.11)	91.41 (0.11)	91.00 (0.10)	88.93 (0.10)	
Cl2	2.2528 (0.0011)	88.31 (0.11)	87.92 (0.11)	89.57 (0.10)	92.70 (0.10)	178.20 (0.04)
	Co1	**N4**	**N1**	**N3**	**N2**	**Cl1**

Co1	**Distance**	**Angles**				
N4	1.9548 (0.0023)					
N2	1.9562 (0.0024)	178.78 (0.10)				
N3	1.9884 (0.0023)	85.81 (0.10)	94.97 (0.10)			
N1	1.9965 (0.0023)	93.12 (0.10)	86.05 (0.10)	177.10 (0.10)		
Cl2	2.2358 (0.0007)	90.97 (0.08)	89.95 (0.08)	91.02 (0.07)	91.70 (0.07)	
Cl1	2.2659 (0.0007)	89.63 (0.08)	89.46 (0.08)	88.20 (0.08)	89.09 (0.07)	178.98 (0.03)
	Co1	**N4**	**N2**	**N3**	**N1**	**Cl2**