Supporting Information

for

Exploring Long Range para-Phenyl Effects in Unsymmetrically Fused bis(imino)pyridine-Cobalt Ethylene Polymerization Catalysts

Table of Contents

1. ^{1}H and ^{13}C NMR spectra of intermediate 2 and diketone 3

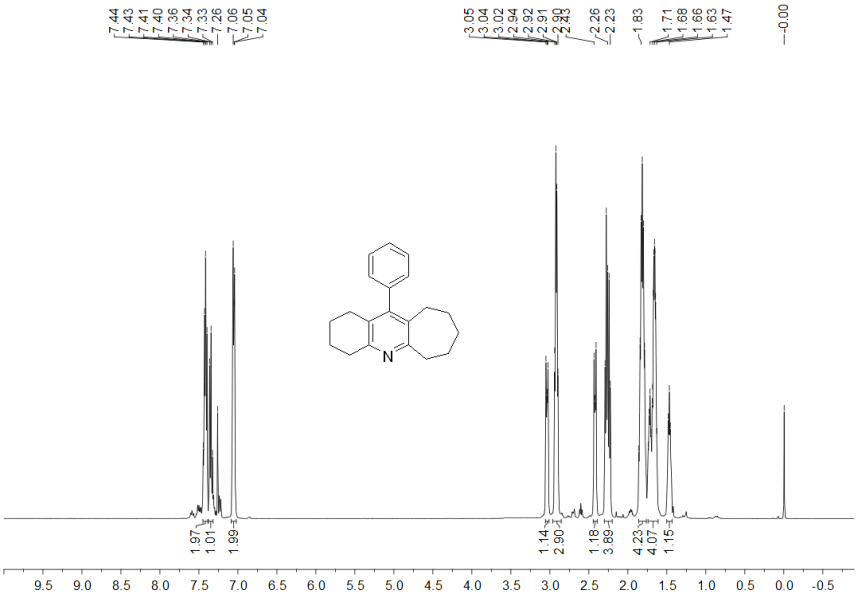


Figure S1. ^{1}H NMR spectrum of 11-phenyl-1,2,3,4,6,7,8,9,10-nonahydrocyclohepta[*b*]quinoline (**2**); recorded in $CDCl_3$ (400 MHz).

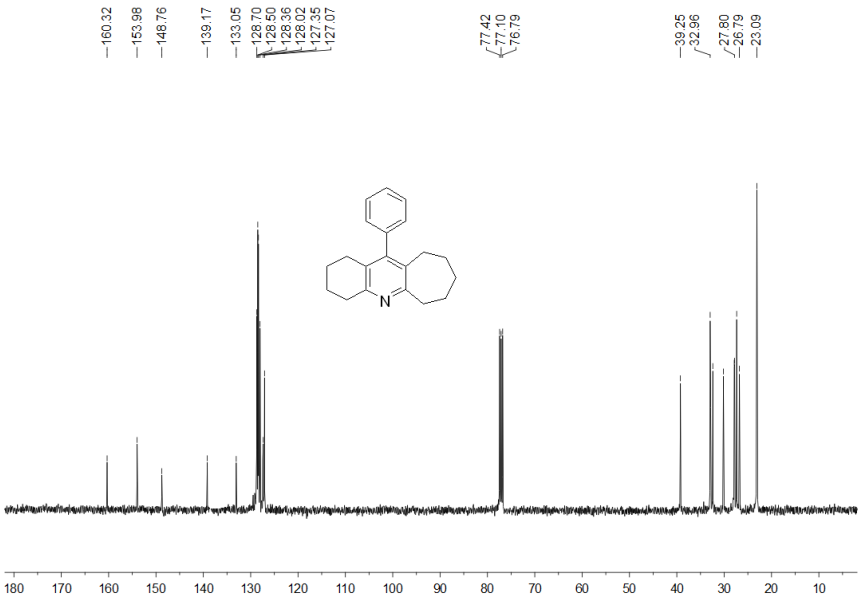


Figure S2. ^{13}C NMR spectrum of 11-phenyl-1,2,3,4,6,7,8,9,10-nonahydrocyclohepta[*b*]quinoline (**2**); recorded in $CDCl_3$ (400 MHz).

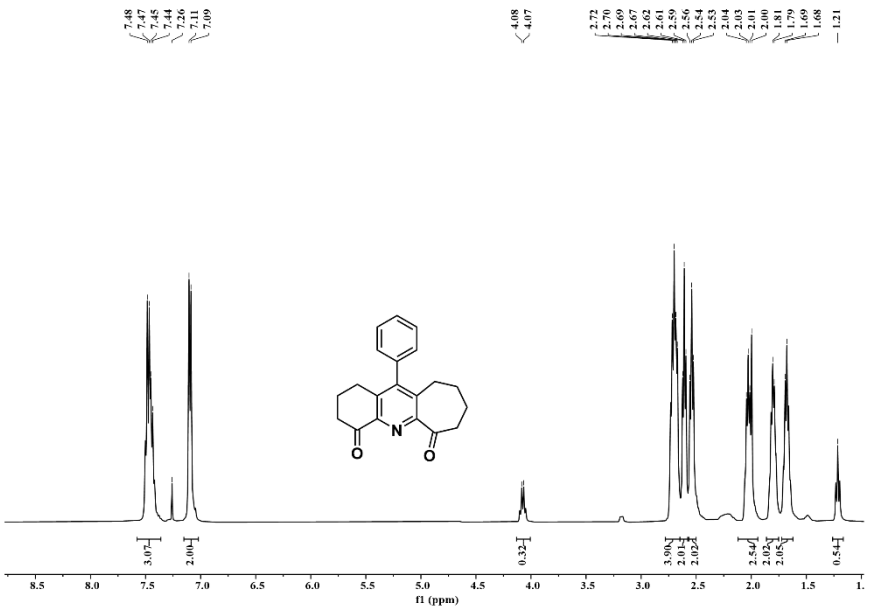


Figure S3. [1]H NMR spectrum of 11-phenyl-1,2,3,7,8,9,10-heptahydrocyclohepta[*b*]quinoline-4,6-dione (**3**); recorded in $CDCl_3$ (400 MHz).

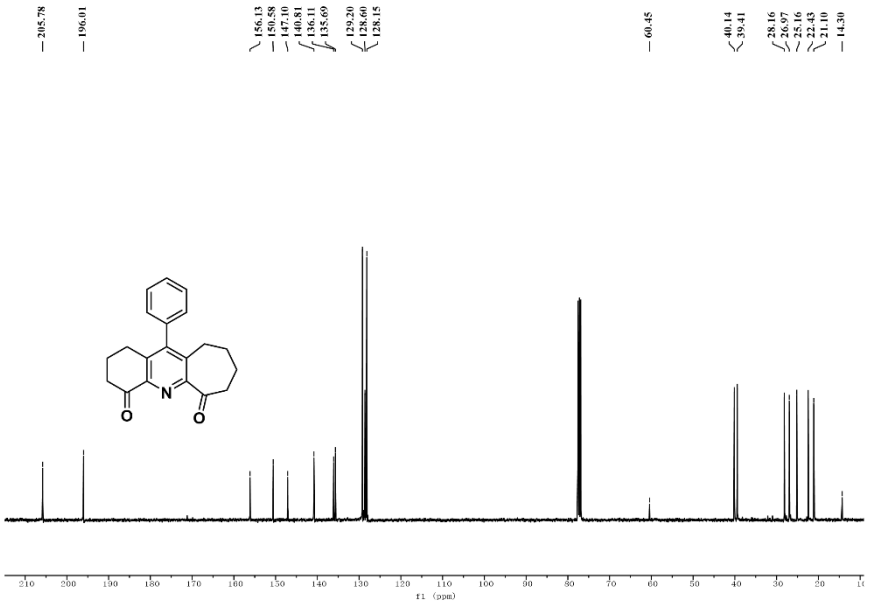
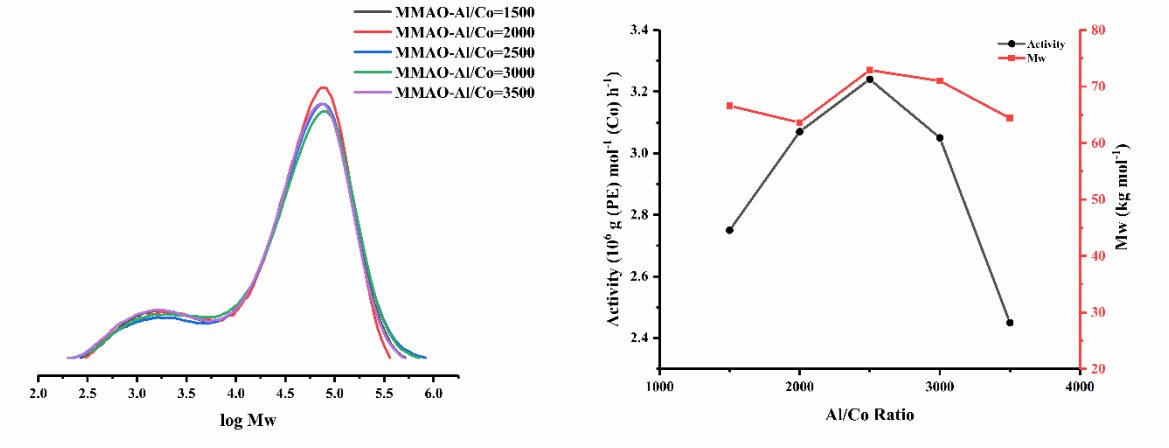


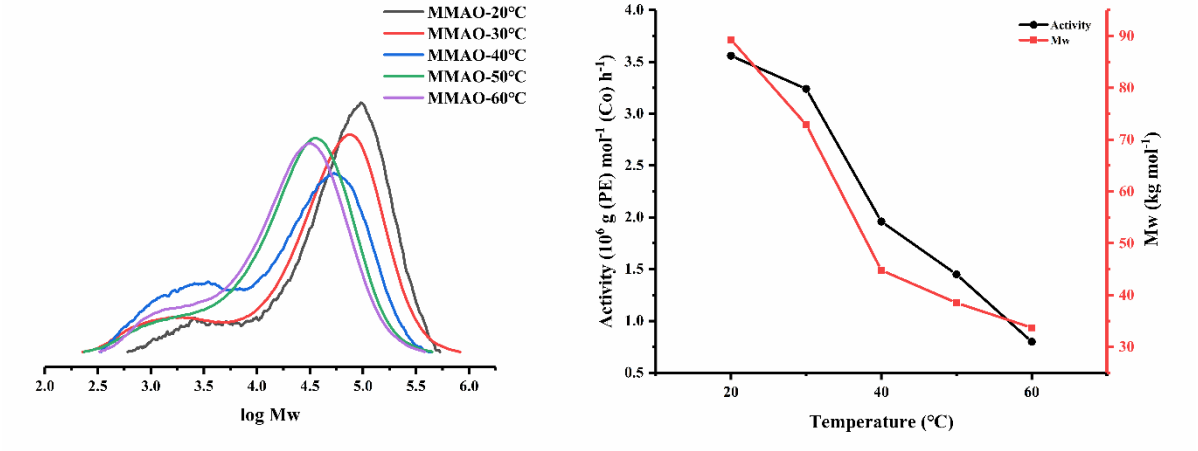
Figure S4. [13]C NMR spectrum of 11-phenyl-1,2,3,7,8,9,10-heptahydrocyclohepta[*b*]quinoline-4,6-dione (**3**); recorded in $CDCl_3$ (400 MHz).

2. GPC traces of selected polyethylenes along with plots of activity and polymer molecular weight as a function of various parameters



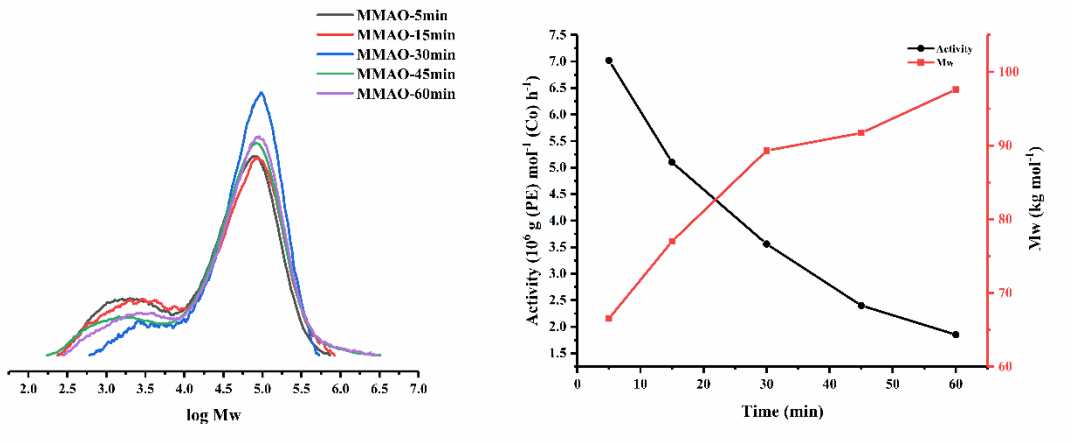
(**a**) (**b**)

Figure S5. (**a**) GPC traces for the polymers produced using **Co3**/MMAO at various Al:Co molar ratios and (**b**) plots of catalytic activity and M_w of the polymers as a function of the Al:Co molar ratio.



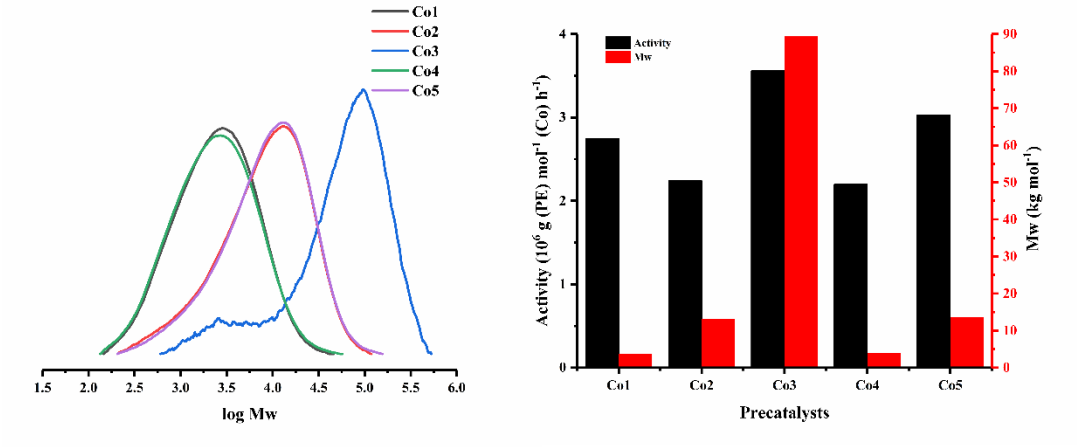
(**a**) (**b**)

Figure S6. (**a**) GPC traces for the polymers produced using **Co3**/MMAO at various temperatures and (**b**) plots of catalytic activity and M_w of the polymers as a function of reaction temperature.



(**a**) (**b**)

Figure S7. (**a**) GPC traces for the polymers produced using **Co3**/MMAO at various reaction times and (**b**) plots of catalytic activity and M_w of the polymers as a function of the reaction time.



(**a**) (**b**)

Figure S8. (**a**) GPC traces for the polymers produced using **Co1** – **Co5** with MMAO as activator and (**b**) a bar chart comparing their catalytic activities and polyethylene molecular weight.

3.1. H and ^{13}C NMR spectra of selected polyethylenes

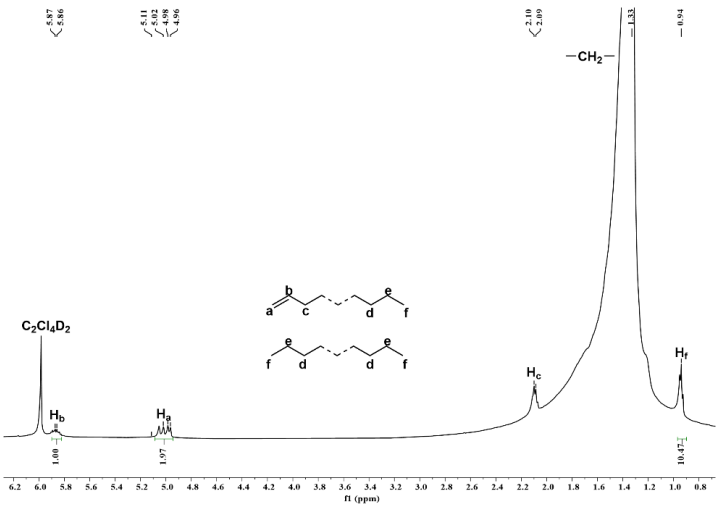


Figure S9. ^{1}H NMR spectrum of the polyethylene produced using **Co3**/MMAO at a run temperature of 20 °C (entry 6, Table 3); recorded in 1,1,2,2-tetrachloroethane-d_2 at 100 °C.

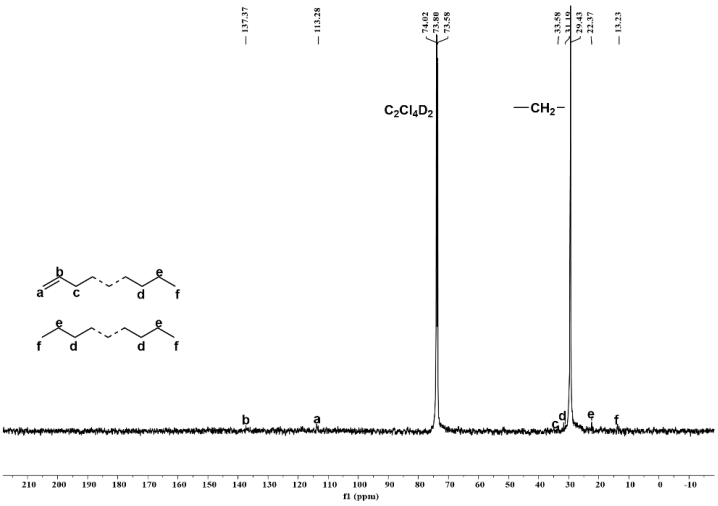


Figure S10. ^{13}C NMR spectrum of the polyethylene produced using **Co3**/MMAO at a run temperature of 20 °C (entry 6, Table 3); recorded in 1,1,2,2-tetrachloroethane-d_2 at 100 °C.

4. Method used to calculate the end-group ratios

From previous studies, it was ascertained that there could be two different end-groups for the linear polyethylene, one involves a vinyl group and the other a saturated n-propyl group. Therefore, there should be two different polymer chains, one chain (chain A, the amount is set as x) has a vinyl and a saturated n-propyl chain end. The other chain (chain B, the amount is set as y) has both saturated n-propyl end-groups. By recording the ^{1}H NMR spectra, the integral for the vinyl hydrogen and the n-propyl protons can be directly obtained. As seen in Figure S9, the integral of the vinyl hydrogen H_b can be set as a, and the integral of the methyl hydrogen H_f in the n-propyl group can be set as b. Then from the equation $x / (3x + 6y) = a / b$, the ratio of $x / y = 6 / (b / a - 3)$. Therefore, the ratio of the different end-groups can be calculated from the ratio of the integral of the corresponding proton signals.

5. X-ray crystallographic studies

Table S1. Crystal data and structure refinement for **Co1**, **Co2** and **Co3**.

	Co1	**Co2·CH_2Cl_2**	**Co3**
CCDC number	2266582	2266583	2266584
Empirical formula	$C_{36}H_{37}Cl_2CoN_3$	$C_{41}H_{47}Cl_4CoN_3$	$C_{44}H_{53}Cl_2CoN_3$
Formula weight	641.51	782.54	753.72
Temperature/K	170.00(10)	169.98(10)	170(2)
Crystal system	orthorhombic	orthorhombic	monoclinic
Space group	Pbca	Pbca	$P2_1/n$
a/Å	15.3184(2)	19.7057(2)	12.5080(3)
b/Å	20.2922(2)	19.1429(2)	17.3199(4)
c/Å	22.2570(2)	20.5944(2)	18.4354(4)
α/°	90	90	90
β/°	90	90	103.464(2)
γ/°	90	90	90
Volume/Å^3	6918.46(13)	7768.71(14)	3884.03(16)
Z	8	8	4
ρ_{calc}g/cm^3	1.232	1.338	1.289
μ/mm^{-1}	5.511	6.240	4.984
F(000)	2680.0	3272.0	1596.0
Crystal size/mm^3	0.25 × 0.2 × 0.15	0.25 × 0.2 × 0.18	0.32 × 0.28 × 0.2
Radiation	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	7.944 to 155.194	7.738 to 155.524	7.096 to 154.566
Index ranges	-19 ≤ h ≤ 17, -21 ≤ k ≤ 25, -28 ≤ l ≤ 28	-22 ≤ h ≤ 24, -23 ≤ k ≤ 24, -22 ≤ l ≤ 25	-15 ≤ h ≤ 15, -17 ≤ k ≤ 21, -23 ≤ l ≤ 20
Reflections collected	50936	62152	29223
Independent reflections	7233 [R_{int} = 0.0523, R_{sigma} = 0.0310]	8112 [R_{int} = 0.0440, R_{sigma} = 0.0245]	7898 [R_{int} = 0.0406, R_{sigma} = 0.0363]
Data/restraints/parameters	7233/229/447	8112/45/466	7898/224/523
Goodness-of-fit on F^2	1.054	1.006	1.066
Final R indexes [I>=2σ (I)]	R_1 = 0.0485, wR_2 = 0.1265	R_1 = 0.0579, wR_2 = 0.1697	R_1 = 0.0464, wR_2 = 0.1265
Final R indexes [all data]	R_1 = 0.0546, wR_2 = 0.1309	R_1 = 0.0670, wR_2 = 0.1796	R_1 = 0.0526, wR_2 = 0.1329
Largest diff. peak/hole / e Å^{-3}	0.49/-0.39	1.84/-0.85	1.05/-0.41

CheckCIF/PLATON report for Co1:

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tx11698a_auto_sq

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: tx11698a_auto_sq

Bond precision: C-C = 0.0042 A Wavelength=1.54184

Cell: a=15.3184(2) b=20.2922(2) c=22.2570(2)
alpha=90 beta=90 gamma=90
Temperature: 170 K

	Calculated	Reported
Volume	6918.46(13)	6918.46(13)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C36 H37 Cl2 Co N3 [+ solvent]	C36 H37 Cl2 Co N3
Sum formula	C36 H37 Cl2 Co N3 [+ solvent]	C36 H37 Cl2 Co N3
Mr	641.52	641.51
Dx,g cm-3	1.232	1.232
Z	8	8
Mu (mm-1)	5.511	5.511
F000	2680.0	2680.0
F000'	2672.75	
h,k,lmax	19,25,28	19,25,28
Nref	7365	7233
Tmin,Tmax	0.306,0.438	0.546,1.000
Tmin'	0.219	

Correction method= # Reported T Limits: Tmin=0.546 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max)= 77.597

R(reflections)= 0.0485(6406) wR2(reflections)= 0.1309(7233)

S = 1.054 Npar= 447

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

Alert level C

PLAT220_ALERT_2_C	NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range	3.5 Ratio
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C19 Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C20 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C15 Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C18 Check
PLAT331_ALERT_2_C	Small Aver Phenyl C-C Dist C15 --C20 .	1.37 Ang.
PLAT911_ALERT_3_C	Missing FCF Refl Between Thmin & STh/L= 0.600	4 Report

Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	2 Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	14 Report
PLAT083_ALERT_2_G	SHELXL Second Parameter in WGHT Unusually Large	6.28 Why ?
PLAT142_ALERT_4_G	s.u. on b - Axis Small or Missing	0.00020 Ang.
PLAT143_ALERT_4_G	s.u. on c - Axis Small or Missing	0.00020 Ang.
PLAT172_ALERT_4_G	The CIF-Embedded .res File Contains DFIX Records	1 Report
PLAT178_ALERT_4_G	The CIF-Embedded .res File Contains SIMU Records	1 Report
PLAT186_ALERT_4_G	The CIF-Embedded .res File Contains ISOR Records	1 Report
PLAT188_ALERT_3_G	A Non-default SIMU Restraint Value has been used	0.0200 Report
PLAT230_ALERT_2_G	Hirshfeld Test Diff for C4 --C5 .	5.2 s.u.
PLAT301_ALERT_3_G	Main Residue Disorder .....(Resd 1)	17% Note
PLAT411_ALERT_2_G	Short Inter H...H Contact H19 ..H12C . 1-x,1-y,1-z =	2.00 Ang. 5_666 Check
PLAT605_ALERT_4_G	Largest Solvent Accessible VOID in the Structure	101 A**3
PLAT794_ALERT_5_G	Tentative Bond Valency for Co1 (II) .	2.02 Info
PLAT860_ALERT_3_G	Number of Least-Squares Restraints	229 Note
PLAT869_ALERT_4_G	ALERTS Related to the Use of SQUEEZE Suppressed	1 Info
PLAT912_ALERT_4_G	Missing # of FCF Reflections Above STh/L= 0.600	129 Note
PLAT933_ALERT_2_G	Number of HKL-OMIT Records in Embedded .res File	3 Note
PLAT978_ALERT_2_G	Number C-C Bonds with Positive Residual Density.	2 Info

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

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

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

Publication of your CIF in IUCr journals

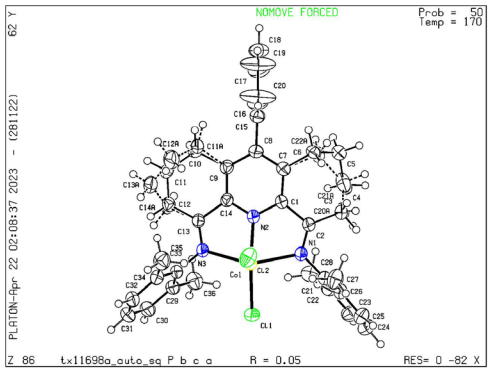
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

Publication of your CIF in other journals

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

PLATON version of 28/11/2022; check.def file version of 28/11/2022

Datablock tx11698a_auto_sq - ellipsoid plot



CheckCIF/PLATON report for Co2:

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tx11698a_auto_sq

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: tx11698a_auto_sq

Bond precision: C-C = 0.0042 A Wavelength=1.54184

Cell: a=15.3184(2) b=20.2922(2) c=22.2570(2)
alpha=90 beta=90 gamma=90

Temperature: 170 K

	Calculated	Reported
Volume	6918.46(13)	6918.46(13)
Space group	P b c a	P b c a
Hall group	-P 2ac 2ab	-P 2ac 2ab
Moiety formula	C36 H37 Cl2 Co N3 [+ solvent]	C36 H37 Cl2 Co N3
Sum formula	C36 H37 Cl2 Co N3 [+ solvent]	C36 H37 Cl2 Co N3
Mr	641.52	641.51
Dx,g cm-3	1.232	1.232
Z	8	8
Mu (mm-1)	5.511	5.511
F000	2680.0	2680.0
F000'	2672.75	
h,k,lmax	19,25,28	19,25,28
Nref	7365	7233
Tmin,Tmax	0.306,0.438	0.546,1.000
Tmin'	0.219	

Correction method= # Reported T Limits: Tmin=0.546 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.982 Theta(max)= 77.597

R(reflections)= 0.0485(6406) wR2(reflections)= 0.1309(7233)

S = 1.054 Npar= 447

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

Alert level C

PLAT220_ALERT_2_C NonSolvent Resd 1 C Ueq(max)/Ueq(min) Range 3.5 Ratio
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C19 Check
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C20 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C15 Check
PLAT242_ALERT_2_C Low 'MainMol' Ueq as Compared to Neighbors of C18 Check
PLAT331_ALERT_2_C Small Aver Phenyl C-C Dist C15 --C20 . 1.37 Ang.
PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 4 Report

Alert level G

PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite 2 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 14 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large 6.28 Why ?
PLAT142_ALERT_4_G s.u. on b - Axis Small or Missing ..... 0.00020 Ang.
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..... 0.00020 Ang.
PLAT172_ALERT_4_G The CIF-Embedded .res File Contains DFIX Records 1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records 1 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records 1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used 0.0200 Report
PLAT230_ALERT_2_G Hirshfeld Test Diff for C4 --C5 . 5.2 s.u.
PLAT301_ALERT_3_G Main Residue Disorder .....(Resd 1) 17% Note
PLAT411_ALERT_2_G Short Inter H...H Contact H19 ..H12C . 2.00 Ang.
1-x,1-y,1-z = 5_666 Check
PLAT605_ALERT_4_G Largest Solvent Accessible VOID in the Structure 103 A**3
PLAT794_ALERT_5_G Tentative Bond Valency for Co1 (II) . 2.02 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints ..... 229 Note
PLAT869_ALERT_4_G ALERTS Related to the Use of SQUEEZE Suppressed ! Info
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 129 Note
PLAT933_ALERT_2_G Number of HKL-OMIT Records in Embedded .res File 3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 2 Info

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

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

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

Publication of your CIF in IUCr journals

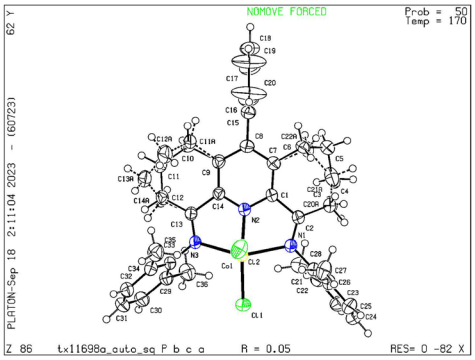
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section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

Publication of your CIF in other journals

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

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock tx11698a_auto_sq - ellipsoid plot



CheckCIF/PLATON report for Co3:

checkCIF/PLATON report

Structure factors have been supplied for datablock(s) tx11699

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

No syntax errors found. CIF dictionary Interpreting this report

Datablock: tx11699

```
Bond precision:   C-C = 0.0050 A          Wavelength=1.54184

Cell:             a=19.7057(2)     b=19.1429(2)     c=20.5944(2)
                  alpha=90         beta=90          gamma=90
Temperature:      170 K

                  Calculated                  Reported
Volume            7768.71(14)                 7768.71(14)
Space group       P b c a                     P b c a
Hall group        -P 2ac 2ab                  -P 2ac 2ab
Moiety formula    C40 H45 Cl2 Co N3, C H2 Cl2 C40 H45 Cl2 Co N3, C H2 Cl2
Sum formula       C41 H47 Cl4 Co N3           C41 H47 Cl4 Co N3
Mr                782.55                      782.54
Dx,g cm-3         1.338                       1.338
Z                 8                           8
Mu (mm-1)         6.240                       6.240
F000              3272.0                      3272.0
F000'             3271.38
h,k,lmax          24,24,26                    24,24,25
Nref              8292                        8112
Tmin,Tmax         0.257,0.325                 0.587,1.000
Tmin'             0.183

Correction method= # Reported T Limits: Tmin=0.587 Tmax=1.000
AbsCorr = MULTI-SCAN

Data completeness= 0.978          Theta(max)= 77.762

R(reflections)= 0.0577( 6857)                wR2(reflections)=
                                             0.1694( 8112)
S = 1.069                 Npar= 466
```

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

Alert level C

```
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ....      2.13 Report
PLAT220_ALERT_2_C NonSolvent   Resd 1  C    Ueq(max)/Ueq(min) Range    3.2 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for    Cl1      --Cl2     .      6.7 s.u.
PLAT241_ALERT_2_C High   'MainMol' Ueq as Compared to Neighbors of     Cl1 Check
PLAT244_ALERT_4_C Low    'Solvent' Ueq as Compared to Neighbors of     C41 Check
PLAT260_ALERT_2_C Large Average Ueq of Residue Including      Cl3     0.108 Check
PLAT971_ALERT_2_C Check Calcd Resid. Dens.  1.00Ang From Cl2           1.93 eA-3
```

Alert level G

```
PLAT002_ALERT_2_G Number of Distance or Angle Restraints on AtSite       5 Note
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ...       6 Report
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT  Unusually Large    8.57 Why ?
PLAT143_ALERT_4_G s.u. on c - Axis Small or Missing ..............  0.00020 Ang.
PLAT176_ALERT_4_G The CIF-Embedded .res File Contains SADI Records       2 Report
PLAT177_ALERT_4_G The CIF-Embedded .res File Contains DELU Records       1 Report
PLAT178_ALERT_4_G The CIF-Embedded .res File Contains SIMU Records       2 Report
PLAT186_ALERT_4_G The CIF-Embedded .res File Contains ISOR Records       1 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used  0.0200 Report
PLAT188_ALERT_3_G A Non-default SIMU Restraint Value has been used  0.0200 Report
PLAT302_ALERT_4_G Anion/Solvent/Minor-Residue Disorder (Resd  2  )      67% Note
PLAT432_ALERT_2_G Short Inter X...Y Contact  C16A      ..C9      .     3.15 Ang.
                                             x,y,z  =          1_555 Check
PLAT794_ALERT_5_G Tentative Bond Valency for Co1      (II)       .     2.02 Info
PLAT860_ALERT_3_G Number of Least-Squares Restraints .............      45 Note
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L=  0.600      174 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density.       2 Info
```

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

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

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

Publication of your CIF in IUCr journals

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

Publication of your CIF in other journals

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

PLATON version of 06/07/2023; check.def file version of 30/06/2023

Datablock tx11699 - ellipsoid plot