SUPPORTING INFORMATION

Synthesis and Crystal Structures of Zn(II)- and Mn(II)- Diphenyldicarboxylate Complexes with N-Donor Ligand

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checkCIF/PLATON report

Structure factors have been supplied for datablock(s) S78-a

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: S78-a

Bond precision:	C-C=0.0058 A	Wavelength=0.71073	
Cell:	a=17.8013(15)	b=21.5491(18)	c=7.2749(6)
	alpha=90	beta=92.798(2)	gamma=90
Temperature:	200 K		
	Calculated Reported Volume		
	2787.3(4)	2787.3(4)	
Space group	C 2/c	C2/c	
Hall group	-C 2yc	-C 2yc	
Moiety formula	C16 H10 N O4 Zn	$C_{16}H_{10}NO_4Zn$	
Sum formula	C16 H10 N O4 Zn	$C_{16}H_{10}NO_4Zn$	
Mr	345.64	345.62	
Dx, g cm^{-3}	1.647	1.647	
Z	8	8	
Mu (mm^{-1})	1.779	1.779	
F000	1400.0	1400.0	
F000'	1402.85		
h, k, l$_{max}$	21, 26, 8	21, 26, 8	
Nref	2759	2713	
T$_{min}$, T$_{max}$	0.791,0.948	0.717,0.949	
T$_{min}$,	0.701		

Correction method = MULTI-SCAN

Data completeness = 0.983	Theta (max) = 26.040
R(reflections) = 0.0352 (2349)	wR2(reflections) = 0.1206 (2713)
S = 1.193	Npar = Npar = 199

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**
PLAT241_ALERT_2_C High   Ueq as Compared to Neighbors for .....   C15 Check
PLAT242_ALERT_2_C Low   Ueq as Compared to Neighbors for .....   N1 Check

⬤ **Alert level G**
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension ....   2 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_detailsin the CIF   Please Do !
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large.   22.09 Why ?
PLAT764_ALERT_4_G Overcomplete CIF Bond List Detected (Rep/Expd) .   1.14 Ratio
PLAT804_ALERT_5_G Number of ARU-Code Packing Problem(s) in PLATON   1 Info

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

0 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
0 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
3 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*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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CIF submission.

PLATON version of 05/02/2014; check.def file version of 05/02/2014

Datablock S78-a - ellipsoid plot
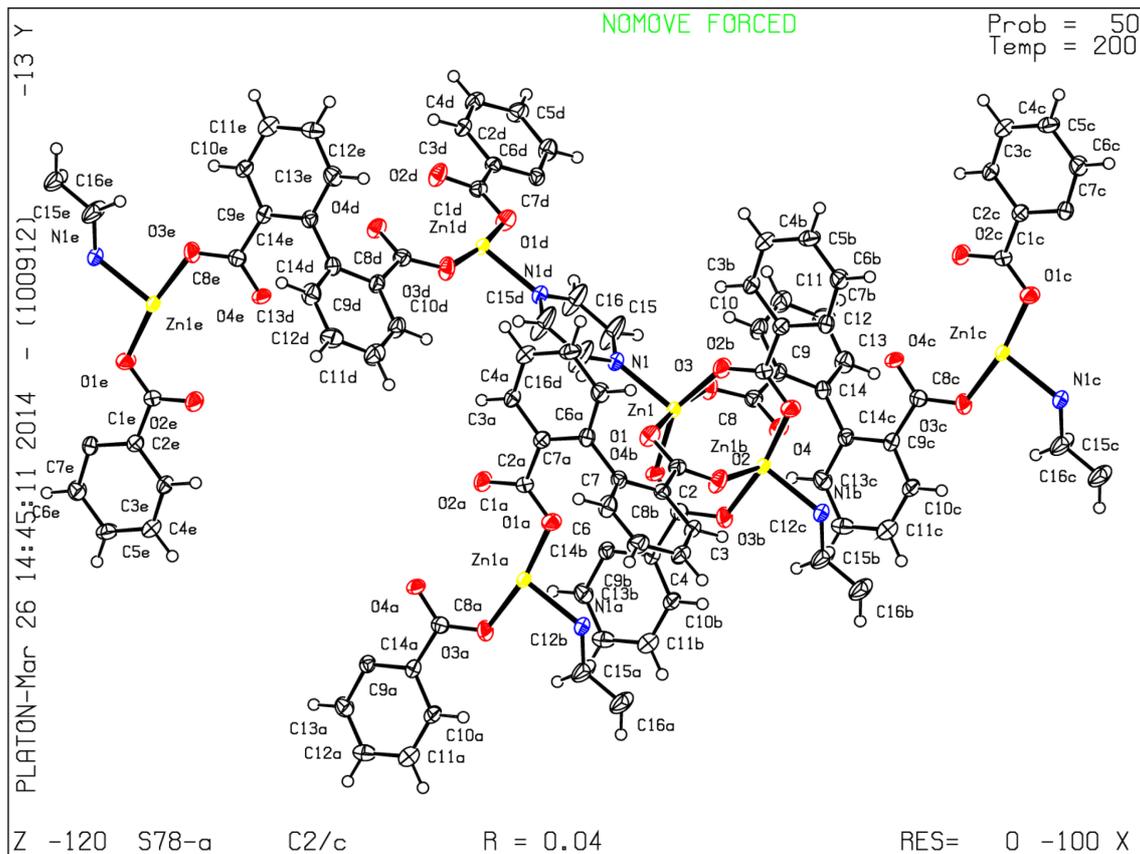
checkCIF/PLATON report

Structure factors have been supplied for datablock(s) K13619-a

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No syntax errors found. CIF dictionary Interpreting this report

Datablock: K13619-a

Bond precision:	C-C = 0.0102 A	Wavelength = 0.71073	
Cell:	a = 25.495(2)	b = 17.9875(17)	c = 12.3012(11)
	alpha = 90	beta = 90.845(2)	gamma = 90
Temperature:	200 K		
	Calculated	Reported Volume	
Volume	5640.6(9)	5640.5(9)	
Space group	C 2/c	C2/c	
Hall group	-C 2yc	-C 2yc	
Moiety formula	$C_{62}H_{44}Mn_3N_4O_{12}$	$C_{62}H_{44}Mn_3N_4O_{12}$	
Sum formula	$C_{62}H_{44}Mn_3N_4O_{12}$	$C_{62}H_{44}Mn_3N_4O_{12}$	
Mr	1201.83	1201.83	
Dx, g cm^{-3}	1.415	1.415	
Z	4	4	
Mu (mm^{-1})	0.728	0.728	
F000	2460.0	2460.0	
F000'	2465.07		
h, k, l$_{max}$	31,22,15	31,22,15	
Nref	5564	5555	
T$_{min}$, T$_{max}$	0.924,0.950	0.924,0.951	
T$_{min}$'	0.923		

Correction method = MULTI-SCAN

Data completeness = 0.998	Theta(max) = 26.020
R(reflections) = 0.0749(3580)	wR2(reflections) = 0.2486(5555)
S = 1.118	Npar= Npar = 367

The following ALERTS were generated. Each ALERT has the format

test-name_ALERT_alert-type_alert-level.

Click on the hyperlinks for more details of the test.

🔘 **Alert level B**

PLAT230_ALERT_2_B Hirshfeld Test Diff for	C2	--	C7	..	10.0 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for	C9	--	C14	..	9.5 su
PLAT230_ALERT_2_B Hirshfeld Test Diff for	C12	--	C13	..	9.0su

🔘 **Alert level C**

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range	3.1 Ratio
PLAT230_ALERT_2_C Hirshfeld Test Diff for C5 -- C6 ...	6.8 su
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for	C6 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for	C7 Check

PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C13 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C14 Check
PLAT241_ALERT_2_C High Ueq as Compared to Neighbors for ..... C23 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... N1 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C2 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C5 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C9 Check
PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C12 Check
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C2 -C7 1.37 Ang.
PLAT334_ALERT_2_C Small Average Benzene C-C Dist. C9 -C14 1.37 Ang.
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.0102 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H4 .. H6 .. 1.97 Ang.
PLAT411_ALERT_2_C Short Inter H...H Contact H13 .. H13 .. 2.07 Ang.

⚫ **Alert level G**
PLAT003_ALERT_2_G Number of Uiso or Uij Restrained non-H Atoms ... 4 Why ?
PLAT004_ALERT_5_G Polymeric Structure Found with Dimension .... 3 Info
PLAT005_ALERT_5_G No _iucr_refine_instructions_details in the CIF Please Do !
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT072_ALERT_2_G SHELXL First Parameter in WGHT Unusually Large. 0.13 Why ?
PLAT083_ALERT_2_G SHELXL Second Parameter in WGHT Unusually Large. 10.97 Why ?
PLAT860_ALERT_3_G Number of Least-Squares Restraints .... 24 Note

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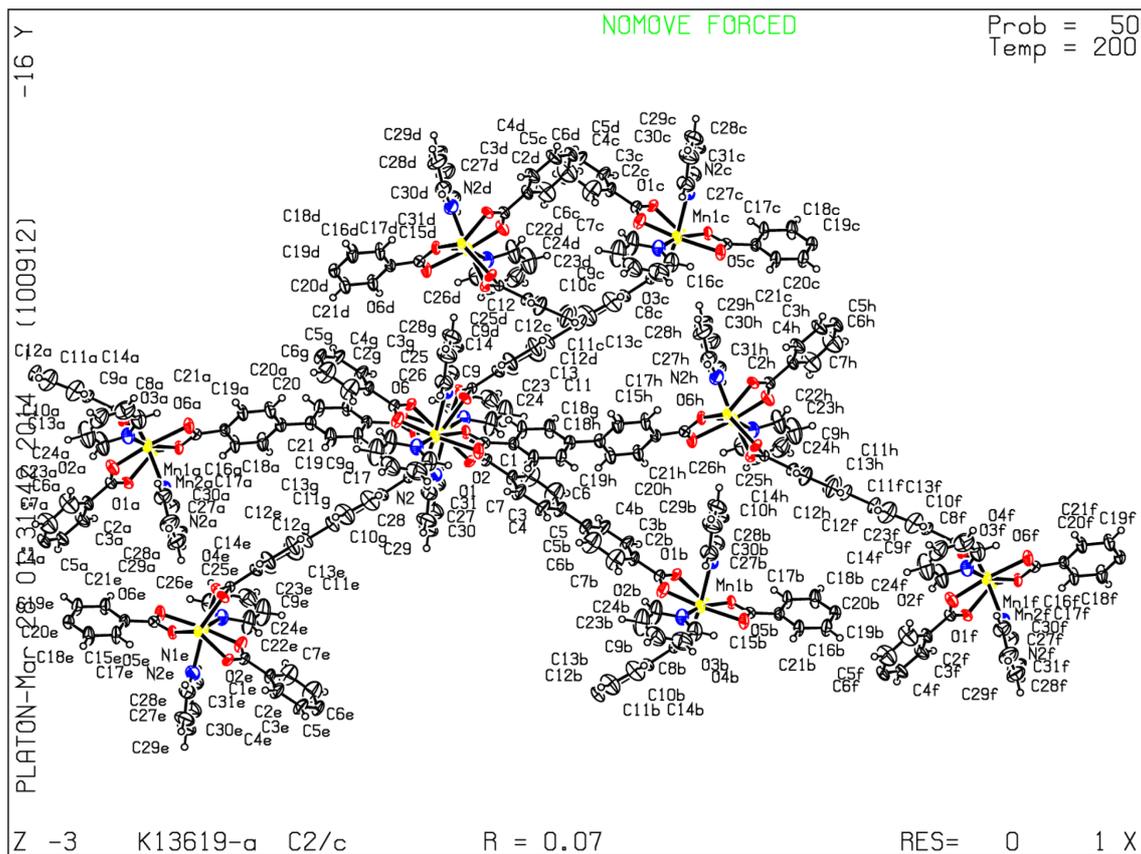**PLATON version of 05/02/2014; check.def file version of 05/02/2014**

***Table* S1.** Selected bond lengths (Å) and angles (°) for the Complexes **1** and **2**

Complex **1**			
Zn1-O1	2.075(3)	Zn1-O2^{i}	2.002(3)
Zn1-O3	2.068(3)	Zn1-O4^{i}	1.989(3)
Zn1-N1	2.068(3)	Zn1^{i}-O2	2.002(3)
Zn1^{i}-O4	1.989(3)	C1-O1	1.252(5)
C1-O2	1.261(5)	C8-O3	1.264(5)
C8-O4	1.252(5)	Zn1-Zn1^{i}	2.894(1)
O4^{i}-Zn1-O2^{i}	150.42(12)	O4^{i}-Zn1-O3	91.58(13)
O2^{i}-Zn1-O3	86.93(13)	O4^{i}-Zn1-N1	108.11(12)
O2^{i}-Zn1-N1	101.47(12)	O3-Zn1-N1	93.50(12)
O4^{i}-Zn1- O1	88.97(13)	O2^{i}-Zn1-O1	87.83(13)
O3-Zn1-O1	170.33(12)	N1-Zn1-O1	95.50(12)
O2- C1- O1	124.3(4)	O4-C8-O3	125.5(4)
Symmetry transformations used to generate equivalent atoms: (i) 1–x, y, 1/2-z.			
Complex 2			
Mn1-O1	2.154(3)	Mn1-O1^{i}	2.154(3)
Mn1-O3	2.154(3)	Mn1-O3^{i}	2.154(3)
Mn1-O5	2.249(5)	Mn1-O5i	2.249(4)
Mn2-O2	2.092(4)	Mn2-O4	2.126(4)
Mn2-N1	2.220(5)	Mn2-O6	2.235(4)
Mn2-O5	2.268(4)	Mn2-N2	2.305(5)
C1-O1	1.257(7)	C1-O2	1.256(7)
C15-O5	1.272(7)	C15-O6	1.254(6)
O1-Mn1-O1^{i}	180.00(14)	O1-Mn1-O3	91.00(15)
O1^{i}-Mn1-O3	89.00(15)	O1-Mn1-O3^{i}	89.00(15)
O1^{i}-Mn1-O3^{i}	91.00(15)	O3-Mn1-O3^{i}	180.00(18)
O1-Mn1- O5	92.17(15)	O1^{i}-Mn1-O5	87.83(15)
O3-Mn1-O5	94.38(14)	O3^{i}-Mn1-O5	85.62(14)
O1-Mn1-O5^{i}	87.83(15)	O1^{i}-Mn1-O5^{i}	92.17(15)
O3-Mn1-O5^{i}	85.62(14)	O3^{i}-Mn1-O5^{i}	94.38(14)
O5-Mn1-O5^{i}	180.0	O2-Mn2-O4	87.02(17)
O2-Mn2-N1	93.79(19)	O4-Mn2-N1	89.28(18)
O2-Mn2-O6	163.91(16)	O4-Mn2-O6	92.64(16)
N1-Mn2-O6	102.30(17)	O2-Mn2-O5	105.67(15)
O4-Mn2-O5	91.44(14)	N1-Mn2-O5	160.54(17)
O6-Mn2-O5	58.25(14)	O2-Mn2-N2	85.1(2)
O4-Mn2-N2	170.64(18)	N1-Mn2-N2	96.2(2)
O6-Mn2-N2	93.60(18)	O5-Mn2-N2	85.94(16)
O2- C1- O1	125.7(5)	O6-C15- O5	120.4(5)

Symmetry transformations used to generate equivalent atoms: (i) 1/2-x, 1/2-y, 1-z