Angewandte Chemie
Eine Zeitschrift der Gesellschaft Deutscher Chemiker

Supporting Information

Crystal Structure of the Isopropylzinc Alkoxide of Pyrimidyl Alkanol: Mechanistic Insights for Asymmetric Autocatalysis with Amplification of Enantiomeric Excess

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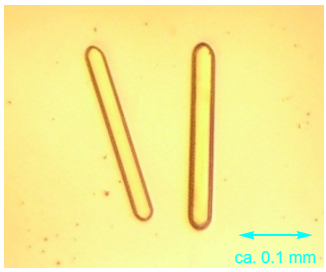
Supporting Information

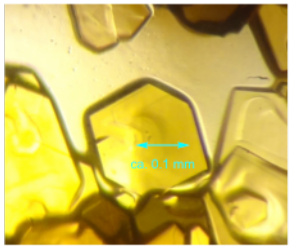
Preparation of single crystal for X-ray analysis

Enantiopure Tetramer (Crystal A)



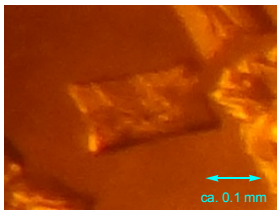
Single crystal of the enantiopure zinc alkoxide was made by the reaction with excess neat *i*-Pr_2Zn (0.726 mmol, 8.4 equiv.) with enantiopure (*S*)-pyrimidylalkanol **2** (0.086 mmol) at room temperature, the alkanol was dissolved by heating at 80 °C and became a deep yellow viscous oil. The yellow single crystal was obtained after keeping the oil at room temperature for the 1-2 weeks.

Racemic Tetramer (Crystal B)



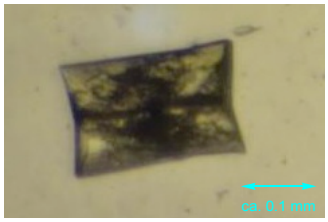
The zinc alkoxide of racemic alkanol was obtained by mixing a excess amount (0.726 mmol, 8.4 equiv.) of neat *i*-Pr_2Zn with racemic 5-pyrimidyl alkanol **2** (0.086 mmol) in the presence of a small amount of toluene (0.1 mL) and keep the vial for one week in refrigerator. The yellow single crystals were appeared, after the slow evaporation of the solvent for 1–2 weeks.

Enantiopure Oligomer (Crystal C)



(*R*)-5-Pyrimidyl alkanol **2** (0.086 mmol) was dissolved in *i*-Pr_2Zn (0.26 mmol, 3 equiv.) solution in toluene (0.2 mL) at room temperature. The single crystals were appeared after the slow evaporation of the solvent at room temperature without stirring for 1 month.

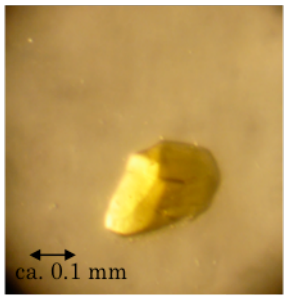
Racemic Oligomer (Crystal D)



Racemic 5-pyrimidyl alkanol **2** (0.086 mmol) was dissolved in *i*-Pr_2Zn (0.26 mmol, 3 equiv.) in the presence of THF (0.2 mL) at room temperature. The single crystals were appeared, after the slow evaporation of the solvent at room temperature without stirring for 2 weeks.

Enantiopure Tetramer with THF (Crystal E)

Enantiopure (*R*)-5-pyrimidylalkanol (0.086 mmol) was mixed with neat *i*-Pr_2Zn (0.726 mmol, 8.4 equiv.) and THF (0.2 mL) at room temperature, After keeping the oil at room temperature for the 1-2 weeks, the single crystal was obtained as yellow plates.



Details of Single Crystal X-ray Diffraction Analysis

The crystal was covered by Nujol and immediately mounted on X-ray diffractometer and cooled to 100 K by nitrogen gas flow. The X-ray single crystal diffraction was recorded by Rigaku R-axis Rapid II imaging plate diffractometer equipped with Cu Kα rotating anode X-ray tube (Crystal **A**) or Bruker Apex2 CCD diffractometer equipped with Mo Kα rotating anode X-ray tube (Crystal **B**, **C**, **D**, **E**) . Data collection, integration, and scaling, were carried out using the Rigaku RAPID AUTO or Bruker APEX II software. The diffraction was recorded at 100 K. Space groups were determined on the basis of systematic absences and intensity statistics, and the structures were solved by direct methods (*SHELXS*[1] or *SIR2011*[2]) and refined by full-matrix least-squares on F^2 using *SHELXL-2014*[1] program. All nonhydrogen atoms were refined using anisotropic displacement parameters otherwise noted. Hydrogen atoms were placed in idealized positions and refined using a riding model.

It should be noted that the alkoxide crystal are air and moisture sensitive. In addition, due to a tendency to disorder in the weekly coordinated diisopropyl zinc, we cannot obtained the high-angle data ideally in some crystals.

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1 G. M. Sheldrick, *Acta Crystallogr. A.* **2008**, *64*, 112–122.

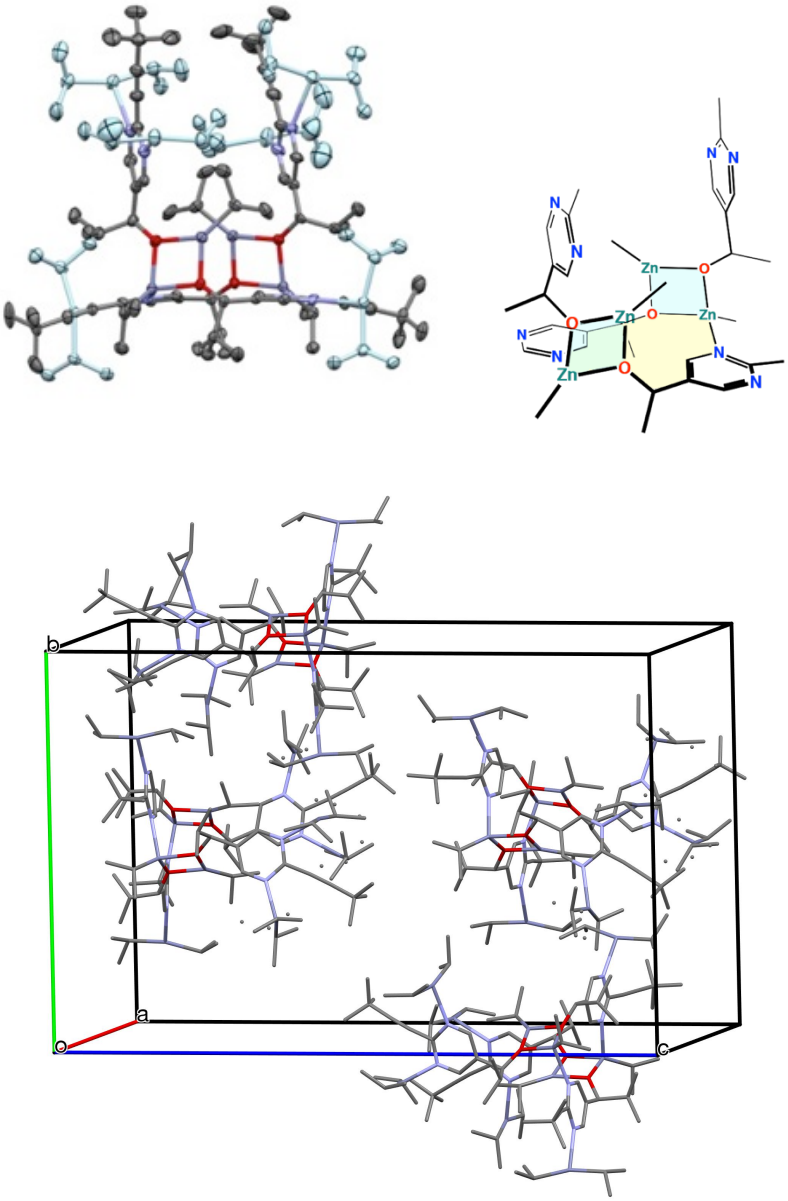
2 M. C. Burla, R. Caliandro, M. Camalli, B. Carrozzini, G. L. Cascarano, C. Giacovazzo, M. Mallamo, A. Mazzone, G. Polidori, R. Spagna, *J. Appl. Crystallogr.* **2012**, *45*, 357–361.

Table S1: Crystal and refinement data for **A**–**E**

	Crystal **A**	Crystal **B**	Crystal **C**	Crystal **D**	Crystal **E**
	CCDC 1420664	CCDC 1420666	CCDC 1420663	CCDC 1420665	CCDC 1420667
Formula	$C_{104}H_{188}N_8O_4Zn_{10}$	$C_{92}H_{160}N_8O_4Zn_8$	$C_{34}H_{52}N_4O_2Zn_2$	$C_{34}H_{52}N_4O_2Zn_2$	$C_{112}H_{204}N_8O_6Zn_{10}$
Configuration	only *S*	racemic (*meso*)	only *R*	racemic (*meso*)	only *R*
Z	4	4	2	4	2
Space group	$P2_12_12_1$	$C2/c$	$P2_1$	$P2_1/c$	$P2_1$
a (Å)	16.8592(3)	29.93(2)	6.2846 (4)	6.3721 (9)	11.4499 (7)
b (Å)	21.3576(4)	10.151 (8)	10.9782 (8)	10.7370 (15)	25.1924(15)
c (Å)	33.1066(6)	34.38 (3)	25.3989(19)	25.601 (4)	22.7023 (14)
α (deg.)	90	90	90	90	90
β (deg.)	90	104.154 (10)	95.355 (3)	96.730(2)	103.4220(10)
γ (deg.)	90	90	90	90	90
Radiation	Cu Kα	Mo Kα	Mo Kα	Mo Kα	Mo Kα
Temp. (K)	100	100	100	100	100
R_1	0.0416	0.0533	0.0655	0.0527	0.0340
$wR2$	0.1110	0.1469	0.2147	0.1409	0.0810
Flack parameter	0.022 (19)	–	0.12(4)	–	0.005(4)

Enantiopure Tetramer (Crystal A)

The coordinated diisopropyl zinc molecules have disordered structure in the direction of isopropyl group. Disordered isopropyl group was refined with restrictions (SADI, ISOR, DELU). The details were embedded in CIF as a SHELXL res file. The checkCIF result contain only C level alert. The responses to the checkCIF results were shown bellow.



Checkcif Result and Responcse

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) ..... 9.72 Note

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 5.7 Ratio

PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) ... 6.9 Ratio

PLAT234_ALERT_4_C Large Hirshfeld Difference Zn9 -- C93_A .. 0.20 Ang.

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds .... 0.0098 Ang.

Author Response: These alerts were probably caused by disorder of diisopropylzinc coordinated on pyrimidine ring. Although we try to model the disorder around diisopropylzinc, it was not possible to model all disorder.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C25 Check

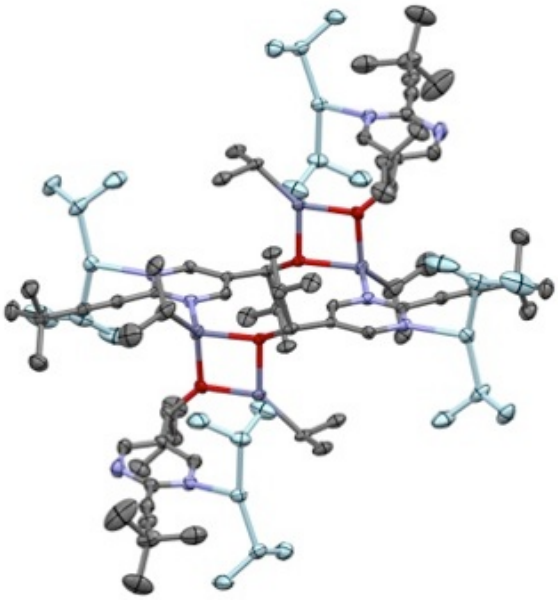
Author Response: C25 is a center carbon of *tert*-butyl group.

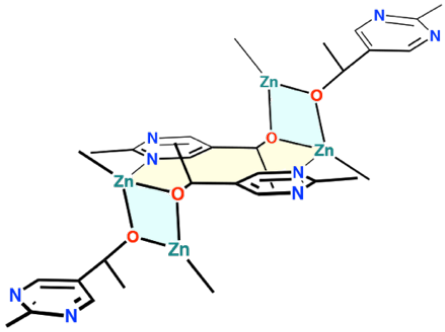
PLAT410_ALERT_2_C Short Intra H...H Contact H7.. H21 .. 1.97 Ang.

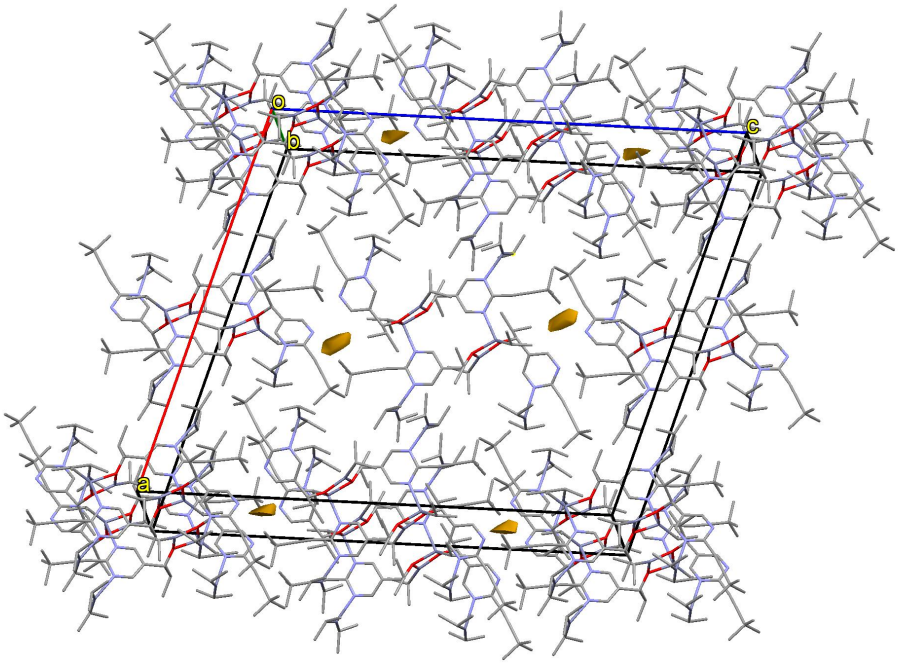
Author Response: These short contact hydrogen atoms are placed on the inside of the 12-membered ring by Zn-N coordination.

Racemic Tetramer (Crystal B)

The Crystal can be solved and refined without disorder structure nor restrictions.







Checkcif Result and Responcse

PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) Range 5.7 Ratio

PLAT222_ALERT_3_C Large Non-Solvent H Uiso(max)/Uiso(min) 6.2 Ratio

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds 0.0061 Ang.

PLAT601_ALERT_2_C Structure Contains Solvent Accessible VOIDS of 38 Ang3

Author Response: these alert probably caused by the unsolved disordered structure of *i*-Pr_2Zn.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C7 Check

Author Response: C7 is a center carbon of *tert*-butyl group.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for C34 Check

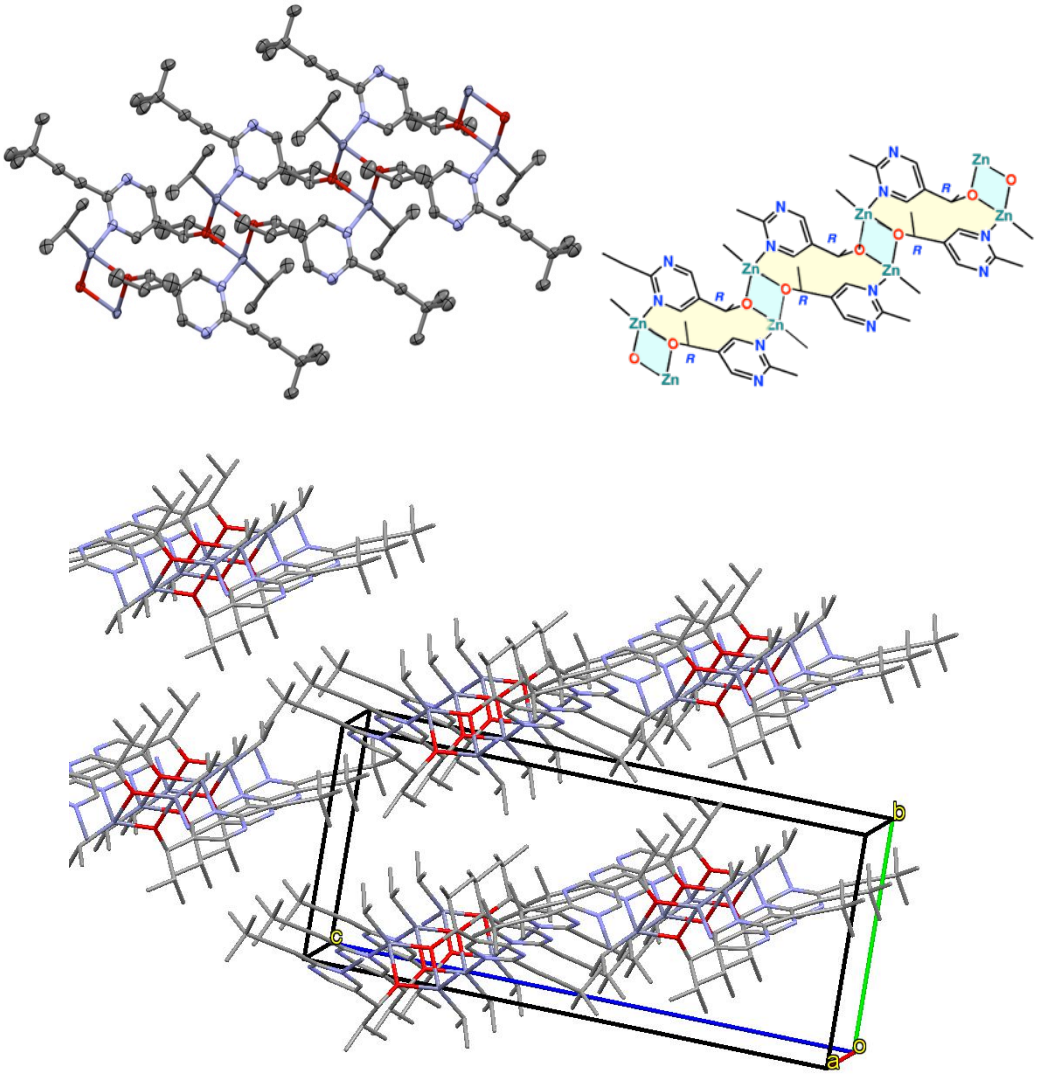
Author Response: C34 is a center carbon of *i*-propyl group.

PLAT410_ALERT_2_C Short Intra H...H Contact H40.. H40 1.91 Ang.

Author Response: These short contact hydrogen atoms are placed on the inside of the 12-membered ring by Zn-N coordination.

Chiral Oligomer (Crystal C)

The structure was refined without disorder nor restriction.



Checkcif Result and Responcse

PLAT341_ALERT_3_B Low Bond Precision on C-C Bonds. 0.0172 Ang.

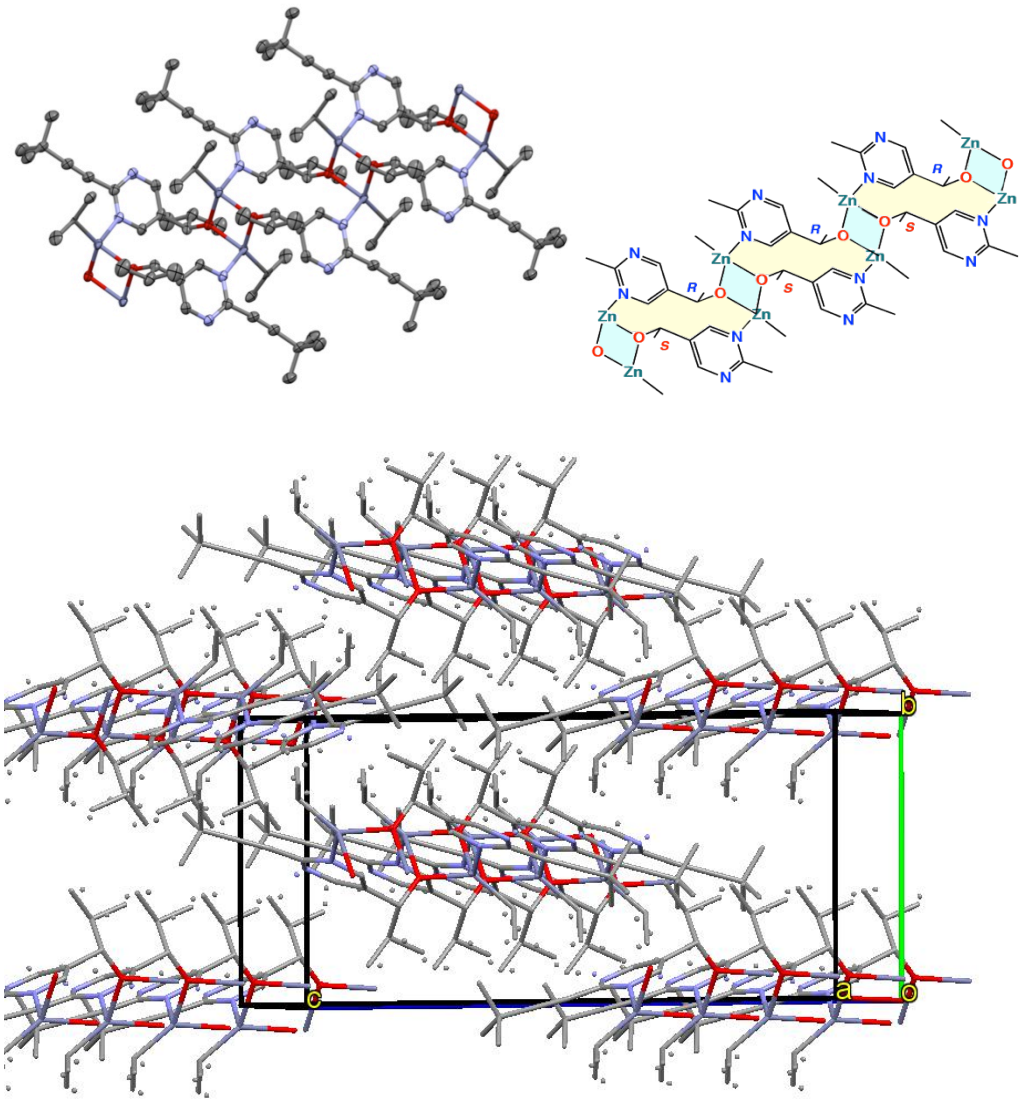
PLAT029_ALERT_3_C _diffrn_measured_fraction_theta_full Low.. 0.976 Note

PLAT090_ALERT_3_C Poor Data / Parameter Ratio (Zmax > 18) .... 8.60 Note

Author Response: These Alerts are due to the small crystal size and the quality of the measured crystal. Because of the instability of the alkoxide crystal and the high reactivity of diisopropyl zinc, we cannot obtain enough reflections from high 2theata region.

Racemic Oligomer (Crystal D)

The structure seems contain disorder on the chiral center of the alkoxide such as (*R*)-alkoxid incorporate to the position which should be occupied by (*S*)-alkoxid. The disordered structure refined with restrictions (SADI, ISOR, DELU) and constrictions (EADP). The two B level alert in the checkCIF were probably caused by this disordered structure.



Checkcif Result and Responcse

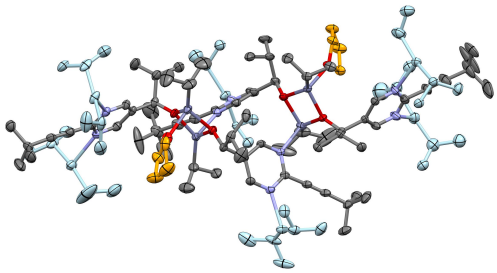
PLAT213_ALERT_2_B Atom C11_A has ADP max/min Ratio ..... 4.6 prolat

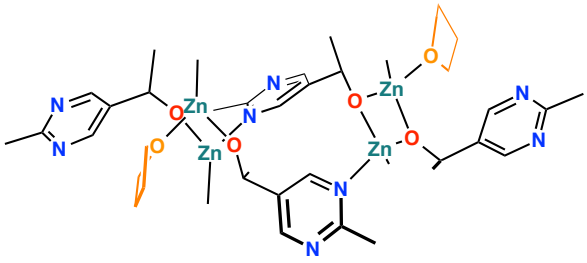
PLAT213_ALERT_2_B Atom C11A_B has ADP max/min Ratio .... 4.6 prolat

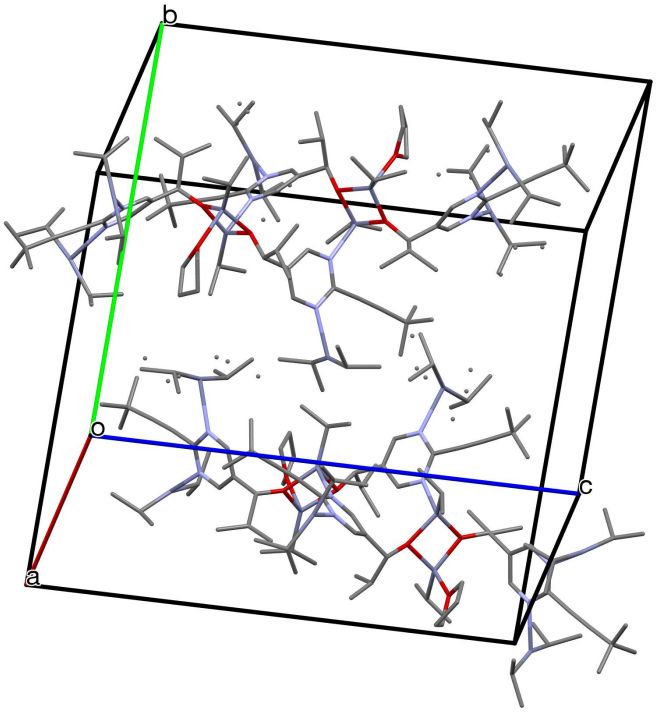
Author Response: C11 is a center carbon atom in *i*-Pr group, which have a disordered structure.

Enantiopure Tetramer with THF (Crystal E)

The structure contains disorder in coordinating diisopropylzinc. The disordered structure refined with restrictions (ISOR).







Checkcif Result and Responcse

PLAT213_ALERT_2_B Atom C14 has ADP max/min Ratio ... 4.1 prolat

Author Response: C14 is a terminal carbon of *t*-Bu group. This alert might be caused by unsolved disorder of *t*-Bu group.

PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) Range =6.7 Ratio

PLAT222_ALERT_3_B Large Non-Solvent H Uiso(max)/Uiso(min) ... 8.3 Ratio

Author Response: these alert probably caused by the unsolved disordered structure of *i*-Pr_2Zn.

PLAT213_ALERT_2_C Atom C11 has ADP max/min Ratio ..... 3.1 prolat

Author Response: C11 is placed at the *t*-Bu at the terminal of tetramer structure.

PLAT213_ALERT_2_C Atom C56 has ADP max/min Ratio ..... 3.3 prolat

PLAT213_ALERT_2_C Atom C70 has ADP max/min Ratio ..... 3.6 prolat

Author Response: C56 is placed at the terminal of *i*-Pr group and C70 is placed at terminal of *t*-Bu group. Relatively large ADP max/min ratio might be caused by the rotation of *i*-Pr or *t*-Bu group.

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C11 Check

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for .... C54 Check

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C67 Check

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ... C100 Check

PLAT242_ALERT_2_C Low Ueq as Compared to Neighbors for ..... C103 Check

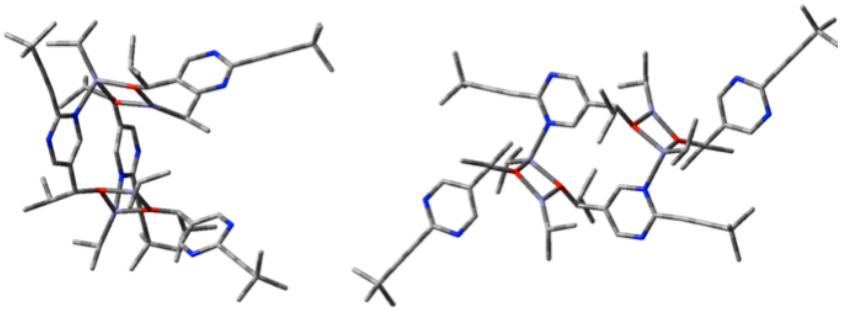
Author Response: C11 and C67 are center carbon atoms in *t*-Bu group. C54, C100, and C103 are center carbon atoms in *i*-Pr group.

PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0075 Ang.

Author Response: these alert probably caused by the unsolved disordered structure of *i*-Pr_2Zn.

Details of DFT Calculation

The DFT calculation was performed start from the obtained structure in the X-ray diffraction analysis using Gaussian 09 (Revision C)[3]. The coordinated diisopropyl zinc was removed to simplify the calculation. The structure optimization and frequency analysis performed in B3LYP/6-31G(d) level and single point energy was calculated under B3LYP/6-311+G(d,p) level.



Enantiopure Tetramer (Tetramer A')

[3] Gaussian 09, Revision **C.01**, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

C	4.806000	-3.488800	0.652000	C	-3.421900	8.171200	-4.341800	H	6.094700	0.948600	-2.912300
C	5.316500	-3.261200	2.084000	C	-4.509400	9.135900	-3.810300	H	4.420100	1.515900	-2.976200
C	4.683900	-4.991000	0.356200	C	-2.035800	8.853600	-4.259600	H	-1.940800	-2.156100	-3.436800
C	0.566200	1.002000	2.688200	C	-3.733600	7.790100	-5.807900	H	-2.374100	-5.870000	-1.322500
C	1.204100	1.052900	4.088500	C	4.511300	5.222300	2.857500	H	-0.721600	-5.274900	-1.514200
C	0.323000	2.422100	2.159100	N	2.150100	-2.743100	-1.684500	H	-1.838100	-4.462500	-0.400600
C	-5.398100	-2.586400	-0.639000	N	1.921000	-3.010800	-4.041200	H	-3.302900	-3.830600	-2.335800
C	-5.566300	-4.079500	-0.319700	N	-2.635800	-2.288500	1.695500	H	-2.489800	-4.145800	-4.688900
C	-5.838600	-2.298300	-2.084000	N	-2.456400	-2.569700	4.055100	H	-1.114300	-5.091300	-4.082500
C	-0.366000	1.013900	-2.687200	N	4.532200	2.866200	2.557500	H	-2.761100	-5.682200	-3.856800
C	0.087300	2.392900	-2.188300	N	3.802300	4.308100	0.785000	H	-2.707000	1.452100	1.206700
C	-0.948000	1.123000	-4.108400	N	-3.870300	3.643200	-2.569400	H	-4.754300	0.170000	1.641800
C	1.039200	-2.811900	2.544700	N	-2.916100	4.894200	-0.758900	H	-6.214000	2.088400	-0.260800
C	1.473800	-4.307300	2.559400	O	1.503900	-2.149300	1.384900	H	-5.896600	0.376400	-0.603600
C	1.300900	-4.959100	3.938700	O	3.089900	-0.368300	0.312300	H	-6.936600	0.832500	0.749300
C	0.810100	-5.152500	1.467000	O	-1.908900	-1.896400	-1.386000	H	-4.176600	2.220900	2.940600
C	3.616100	0.714700	-0.444100	O	-3.135000	0.160000	-0.345900	H	-5.113700	3.213800	1.807500
C	4.894200	0.289800	-1.220800	Zn	3.197000	-2.407300	0.200600	H	-5.928300	2.007200	2.807600
C	6.096200	-0.011000	-0.317300	Zn	1.608400	-0.169400	1.511400	H	0.028700	-2.923000	-4.837200
C	5.262000	1.316700	-2.302200	Zn	-3.619200	-1.815200	-0.194400	H	0.450800	-2.480300	-0.586100
C	-1.564000	-2.657300	-2.527400	Zn	-1.625000	0.061800	-1.524500	H	6.167200	-4.193200	-5.712300
C	-1.762900	-4.962000	-1.370700	H	5.584800	-3.102900	-0.023200	H	7.763000	-4.712000	-5.126600
C	-2.244500	-4.058200	-2.510400	H	6.257000	-3.804800	2.276700	H	6.292100	-5.504700	-4.524700
C	-2.142300	-4.778100	-3.862500	H	5.509400	-2.200700	2.293800	H	8.483800	-4.215800	-2.735900
C	-3.460700	1.317500	0.413000	H	4.600600	-3.607800	2.842900	H	7.412000	-3.325900	-1.633300
C	-4.824700	1.146400	1.141900	H	4.415600	-5.181400	-0.690700	H	7.013900	-4.986300	-2.102200
C	-6.031800	1.109200	0.196600	H	5.628500	-5.526800	0.553900	H	8.320400	-2.330600	-4.446100
C	-5.015800	2.208500	2.234700	H	3.919700	-5.478100	0.977900	H	6.735500	-1.774900	-5.026000
C	2.662500	-2.949300	-2.923100	H	-0.420500	0.524700	2.796200	H	7.246800	-1.420900	-3.363900
C	0.598400	-2.897500	-3.909500	H	1.324000	0.055800	4.534100	H	-0.912800	-2.305300	0.601300
C	-0.047700	-2.742900	-2.677100	H	2.195100	1.524200	4.068400	H	-0.575400	-2.776400	4.856100
C	0.815000	-2.648700	-1.588300	H	0.588600	1.644000	4.785600	H	-7.599500	-4.140000	2.288700
C	4.073300	-3.112100	-3.080800	H	1.257300	2.977700	2.016600	H	-7.202400	-4.614900	3.952000
C	5.247500	-3.288600	-3.331600	H	-0.201300	2.424800	1.195100	H	-8.803300	-3.940600	3.581100
C	6.658800	-3.511000	-3.685200	H	-0.287200	3.010600	2.864500	H	-6.884400	-2.818500	5.765800
C	6.719300	-4.546000	-4.835500	H	-6.098800	-2.046700	0.017200	H	-7.063200	-1.101800	5.358600
C	7.437100	-4.042600	-2.459800	H	-4.891900	-4.711500	-0.914200	H	-8.489400	-2.160600	5.379900
C	7.274400	-2.172000	-4.159800	H	-5.364400	-4.299900	0.736000	H	-7.656500	-0.406400	2.951000
C	-3.177000	-2.405700	2.933700	H	-6.589500	-4.432300	-0.538400	H	-7.861200	-1.642200	1.693300
C	-1.302600	-2.408400	1.602800	H	-5.828100	-1.226000	-2.320100	H	-9.066500	-1.483900	2.989900
C	-0.468800	-2.636800	2.694100	H	-5.187800	-2.789400	-2.821200	H	4.519400	0.838400	2.197100
C	-1.132500	-2.671100	3.926400	H	-6.860700	-2.663400	-2.282600	H	3.193300	3.420600	-0.971100
C	-4.596900	-2.362800	3.083400	H	0.532900	0.380800	-2.750000	H	2.882200	7.431000	5.159100
C	-5.787400	-2.384600	3.317700	H	0.578000	2.343700	-1.207900	H	3.753200	8.975300	5.279200
C	-7.224000	-2.444500	3.631400	H	0.803400	2.853800	-2.889100	H	3.145000	8.412700	3.706100
C	-7.735200	-3.877800	3.342400	H	-0.750300	3.093600	-2.092300	H	6.098000	9.214500	4.307700
C	-7.423500	-2.109800	5.129000	H	-0.228300	1.589700	-4.800100	H	6.882300	7.839000	3.501700
C	-7.996600	-1.429200	2.758200	H	-1.210400	0.144100	-4.532700	H	5.512200	8.654400	2.725600
C	4.272900	4.079100	2.026300	H	-1.852700	1.744300	-4.132000	H	6.502000	6.409500	5.610600
C	4.314900	1.815800	1.764900	H	1.498600	-2.359700	3.441600	H	5.718100	7.795800	6.399800
C	3.840800	1.921900	0.451200	H	2.548000	-4.263500	2.344900	H	4.871100	6.237800	6.283000
C	3.592300	3.231000	0.025500	H	1.761800	-5.953100	3.946300	H	-2.525000	3.882900	0.992200
C	4.708700	6.190200	3.559700	H	1.776900	-4.368600	4.731100	H	-4.253200	1.646300	-2.244600
C	4.941600	7.369900	4.408300	H	0.244000	-5.091700	4.200800	H	-4.309200	9.418500	-2.771700
C	3.593600	8.090500	4.651300	H	0.940600	-4.707800	0.476200	H	-4.528100	10.047200	-4.419900
C	5.920300	8.327800	3.687500	H	1.254700	-6.153700	1.439900	H	-5.500300	8.672000	-3.853200
C	5.546300	6.922400	5.759400	H	-0.264800	-5.275100	1.646200	H	-1.794300	9.127100	-3.227400
C	-3.397500	4.777200	-2.011400	H	2.880000	1.011000	-1.209800	H	-1.248600	8.187800	-4.628300
C	-2.931200	3.786200	-0.014700	H	4.612500	-0.640700	-1.733200	H	-2.031300	9.764700	-4.869900
C	-3.417100	2.555100	-0.467300	H	6.912300	-0.447800	-0.905200	H	-3.750100	8.690500	-6.433600
C	-3.873900	2.559900	-1.791600	H	6.484200	0.900400	0.152100	H	-2.975200	7.107600	-6.205100
C	-3.404400	5.957800	-2.824300	H	5.840200	-0.722500	0.472400	H	-4.708300	7.297400	-5.885900
C	-3.412100	6.956000	-3.511700	H	5.575900	2.271000	-1.862300				

Racemic Tetramer (Tetramer B')

C	-4.487200	-1.693600	-2.021200	C	9.893500	-1.332300	0.067300	H	-4.477900	-6.525100	-2.140800
C	-3.800500	-2.460800	-3.160700	C	12.215900	-2.313700	0.986900	H	-6.244700	-6.596300	-1.971900
C	-5.403300	-0.597000	-2.587900	C	11.940100	-3.180900	2.238200	H	-5.442500	-5.044900	-2.303600
C	-3.175100	3.303000	1.847600	C	13.161700	-1.147000	1.355500	H	-7.391800	-5.604300	0.072800
C	-3.665300	4.412000	0.902100	C	4.057200	4.963200	-0.040300	H	-6.438600	-4.818400	1.347400
C	-1.777800	1.636900	-1.573200	C	5.370500	6.016400	1.752300	H	-6.613500	-4.039700	-0.241100
C	-1.700500	0.920900	-2.951800	C	6.511600	5.009400	-0.270800	H	-14.023900	3.138500	-0.187000
C	-1.555000	1.921900	-4.107200	C	12.864800	-3.183600	-0.116800	H	-13.248700	2.009100	0.944900
C	-0.626600	-0.170400	-3.035400	C	10.943100	-1.772800	0.483500	H	-12.517100	3.595400	0.637400
C	-0.482000	2.348700	-1.201300	C	5.133200	7.119600	-0.515700	H	-5.996800	-7.722300	0.301400
C	-4.987800	-0.665900	1.956300	C	4.791200	0.309000	-3.432800	H	-4.227000	-7.655500	0.158000
C	-3.454400	-0.830600	3.969800	C	-0.279400	3.715700	-1.420200	H	-5.027000	-6.962600	1.581200
C	-5.944800	-0.713800	4.338600	C	1.836500	3.635400	-0.562300	H	-4.727200	0.833600	3.469800
C	-6.309300	-0.162900	1.399100	C	5.259100	5.768400	0.228000	H	1.077100	-4.300700	1.860000
C	-7.435100	-0.976100	1.247400	C	3.055600	4.315100	-0.261600	H	-1.902800	4.665900	3.001500
C	-6.489300	1.160900	0.987300	C	1.804100	-3.646600	-2.492000	H	-1.500900	2.959300	3.237700
C	-8.657200	0.760400	0.425100	C	0.598100	1.695300	-0.609500	H	-1.032300	3.784100	1.746200
C	-9.906400	1.252600	-0.076400	N	1.741500	2.311900	-0.278200	H	-0.574100	-0.613000	0.387200
C	-12.254000	2.164200	-1.003600	N	0.852100	4.356800	-1.119900	H	5.149900	2.440800	1.512000
C	-11.998000	3.256300	-2.068600	N	7.618200	-1.675200	-0.520400	H	3.127200	1.849600	3.744000
C	-13.045700	0.993700	-1.632700	N	8.617900	0.492700	-0.756900	H	4.540900	2.888300	3.890300
C	-4.044100	-4.944100	0.036200	O	2.183900	-0.722200	0.545600	H	3.220100	3.337200	2.798000
C	-5.355200	-5.991200	-1.761600	O	3.917000	0.244600	-1.149000	H	4.845500	-0.158300	3.121400
C	-6.497900	-5.001300	0.268900	Zn	3.285300	1.068500	0.587800	H	5.992200	0.120500	1.811000
C	-13.058900	2.764000	0.174800	Zn	3.123100	-1.501900	-1.003800	H	6.131800	1.028000	3.323600
C	-10.965600	1.664600	-0.497400	H	-5.142700	-2.415300	-1.507300	H	3.881800	-3.191400	-2.682800
C	-5.111200	-7.107600	0.499200	H	-3.210800	-3.309500	-2.792200	H	2.972100	-4.534100	-0.072900
C	-4.780200	-0.266000	3.442900	H	-4.531000	-2.860800	-3.885300	H	3.703000	-5.351800	-1.452500
C	0.287800	-3.689500	1.423700	H	-3.118200	-1.821000	-3.737000	H	4.647100	-4.184900	-0.518600
C	-1.827600	-3.611700	0.564400	H	-6.123200	-1.001800	-3.319200	H	2.543300	-2.399500	1.703000
C	-5.243100	-5.752400	-0.236000	H	-5.986200	-0.095300	-1.805800	H	2.685500	-0.407500	3.054800
C	-3.044800	-4.293500	0.260600	H	-4.837900	0.185200	-3.114500	H	0.589300	-2.402500	4.088200
C	-1.834000	3.691700	2.491200	H	-3.911300	3.227000	2.663000	H	2.345500	-2.659100	4.086900
C	-0.592900	-1.669300	0.616000	H	-2.980700	4.560100	0.055600	H	1.634600	-1.376200	5.074800
N	-1.734900	-2.287500	0.282900	H	-4.658500	4.203200	0.484400	H	-0.376700	-0.226100	3.027400
N	-0.842500	-4.332100	1.121900	H	-3.731900	5.380900	1.422400	H	0.738400	0.759800	3.975100
N	-7.636100	1.639200	0.507500	H	-2.536800	2.427900	-1.698600	H	0.715400	0.918400	2.218600
N	-8.602500	-0.540900	0.769500	H	-2.678700	0.435000	-3.050400	H	5.044500	1.787400	-1.893500
O	-2.179700	0.750300	-0.541200	H	-0.584100	2.432000	-4.083100	H	3.282500	0.579900	-4.982400
O	-3.906400	-0.220000	1.158100	H	-1.628200	1.404800	-5.070100	H	2.627400	0.592900	-3.333200
Zn	-3.278600	-1.043400	-0.580800	H	-2.340500	2.686800	-4.082200	H	3.512800	1.998200	-3.945700
Zn	-3.126300	1.531700	1.002500	H	-0.707100	-0.889200	-2.214100	H	6.905000	0.273700	-4.037300
C	4.494500	1.719800	2.027100	H	-0.731600	-0.731300	-3.970600	H	5.762800	0.495300	-5.369500
C	3.809500	2.488400	3.166700	H	0.383600	0.255800	-3.024200	H	6.106500	1.838200	-4.272800
C	5.410600	0.623100	2.593600	H	-5.012600	-1.768100	1.923200	H	7.431500	2.010500	-1.488500
C	3.153800	-3.268400	-1.860200	H	-3.268200	-0.494500	4.996100	H	5.637400	-1.862900	-1.049900
C	3.648000	-4.385400	-0.926300	H	-3.475900	-1.928600	3.976300	H	11.267700	-4.011200	1.999500
C	1.783500	-1.609100	1.578000	H	-2.612300	-0.516800	3.347400	H	12.880900	-3.595500	2.619700
C	1.706900	-0.892700	2.956400	H	-6.072400	-1.803900	4.302500	H	11.478200	-2.586200	3.033000
C	1.560700	-1.893300	4.111900	H	-5.748900	-0.442100	5.381900	H	12.720000	-0.515500	2.133100
C	0.633800	0.199400	3.039700	H	-6.894300	-0.254700	4.047200	H	14.113900	-1.541300	1.729900
C	0.488300	-2.321900	1.206600	H	-7.393200	-2.031300	1.519500	H	13.366900	-0.518400	0.483000
C	5.004700	0.686200	-1.941000	H	-5.658300	1.863600	1.035500	H	5.453800	5.073200	2.300200
C	3.474100	0.900700	-3.952100	H	-11.434500	4.093600	-1.644300	H	6.261800	6.619700	1.959800
C	5.962500	0.750600	-4.322800	H	-11.427200	2.854700	-2.912300	H	4.494600	6.555600	2.127200
C	6.319000	0.157500	-1.390400	H	-12.953300	3.638000	-2.448400	H	6.622800	4.050700	0.245600
C	7.457100	0.951400	-1.229300	H	-12.493500	0.551900	-2.468600	H	6.452600	4.819800	-1.348100
C	6.478900	-1.173600	-0.994100	H	-13.233900	0.206700	-0.895400	H	7.407500	5.610200	-0.077700
C	8.652700	-0.813300	-0.428100	H	-14.010700	1.354500	-2.008400	H	13.813500	-3.597400	0.245600

H	12.209800	-4.014900	-0.397100	H	4.250900	7.673100	-0.178900	H	1.009800	-3.739400	-1.739200
H	13.067700	-2.591000	-1.014800	H	4.721200	-0.789200	-3.474200	H	1.467200	-2.908000	-3.230600
H	6.021100	7.732100	-0.320700	H	-1.068000	4.327600	-1.856900	H	0.577400	0.639600	-0.378600
H	5.049600	6.968200	-1.596800	H	1.862600	-4.618000	-3.008800				