Enolic Schiff base Aluminum Complexes and Their Catalytic Stereoselective Polymerization of Racemic Lactide

Xuan Pang,[a],[b] Hongzhi Du,[a],[b] Xuesi Chen*,[a] Xianhong Wang,[a] and Xiabin Jing[a]

[a] State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022;

[b] Graduate School of Chinese Academy of Sciences, Chinese Academy of Sciences, Beijing 100039, P. R. China
Legends

Table S1. Selected Bond Distances (Å) and Angles (deg) for complex 2a.
Table S2. Selected Bond Distances (Å) and Angles (deg) for complex 3a.
Table S3. Selected Bond Distances (Å) and Angles (deg) for complex 4a.
Table S4. Selected Bond Distances (Å) and Angles (deg) for complex 2b.
Table S5. Selected Bond Distances (Å) and Angles (deg) for complex 4b.

Checkcif Reports

Checkcif Report of complex 3a.
Checkcif Report of complex 4a.
Checkcif Report of complex 2b.
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Table S1. Selected Bond Distances (Å) and Angles (deg) for complex 2a.

<table>
<thead>
<tr>
<th>Bond/Distance</th>
<th>Value 1 (Å)</th>
<th>Value 2 (Å)</th>
<th>Value 3 (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al–N(1)</td>
<td>1.982(5)</td>
<td></td>
<td>1.999(5)</td>
</tr>
<tr>
<td>Al–N(2)</td>
<td>1.999(5)</td>
<td>2.000(5)</td>
<td></td>
</tr>
<tr>
<td>Al–O(1)</td>
<td>1.831(3)</td>
<td>1.831(3)</td>
<td>1.835(3)</td>
</tr>
<tr>
<td>Al–O(2)</td>
<td>1.835(3)</td>
<td>1.831(3)</td>
<td></td>
</tr>
<tr>
<td>Al–C(23)</td>
<td>1.970(4)</td>
<td>1.970(4)</td>
<td></td>
</tr>
<tr>
<td>O(2)–Al–O(1)</td>
<td>84.77(12)</td>
<td>84.77(12)</td>
<td>104.72(16)</td>
</tr>
<tr>
<td>O(1)–Al–C(23)</td>
<td>105.93(15)</td>
<td>105.93(15)</td>
<td>144.91(15)</td>
</tr>
<tr>
<td>O(1)–Al–N(1)</td>
<td>88.47(17)</td>
<td>88.47(17)</td>
<td>110.24(18)</td>
</tr>
<tr>
<td>O(2)–Al–N(2)</td>
<td>87.33(18)</td>
<td>87.33(18)</td>
<td>150.34(15)</td>
</tr>
<tr>
<td>C(23)–Al–N(1)</td>
<td>103.73(16)</td>
<td>103.73(16)</td>
<td>81.8(2)</td>
</tr>
</tbody>
</table>

Table S2. Selected Bond Distances (Å) and Angles (deg) for complex 3a.

<table>
<thead>
<tr>
<th>Bond/Distance</th>
<th>Value 1 (Å)</th>
<th>Value 2 (Å)</th>
<th>Value 3 (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al–N(1)</td>
<td>1.961(2)</td>
<td></td>
<td>2.081(2)</td>
</tr>
<tr>
<td>Al–N(2)</td>
<td>2.081(2)</td>
<td>2.081(2)</td>
<td></td>
</tr>
<tr>
<td>Al–O(1)</td>
<td>1.8881(18)</td>
<td></td>
<td>1.8108(19)</td>
</tr>
<tr>
<td>Al–O(2)</td>
<td>1.8108(19)</td>
<td>1.8108(19)</td>
<td></td>
</tr>
<tr>
<td>Al–C(1)</td>
<td>1.949(3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O(2)–Al–O(1)</td>
<td>84.94(8)</td>
<td></td>
<td>118.96(11)</td>
</tr>
<tr>
<td>O(1)–Al–C(1)</td>
<td>94.14(10)</td>
<td></td>
<td>120.41(9)</td>
</tr>
<tr>
<td>O(1)–Al–N(1)</td>
<td>88.32(8)</td>
<td></td>
<td>120.56(11)</td>
</tr>
<tr>
<td>O(2)–Al–N(2)</td>
<td>87.79(9)</td>
<td></td>
<td>167.88(9)</td>
</tr>
<tr>
<td>C(1)–Al–N(1)</td>
<td>97.87(10)</td>
<td></td>
<td>87.02(8)</td>
</tr>
</tbody>
</table>

Table S3. Selected Bond Distances (Å) and Angles (deg) for complex 4a.

<table>
<thead>
<tr>
<th>Bond/Distance</th>
<th>Value 1 (Å)</th>
<th>Value 2 (Å)</th>
<th>Value 3 (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al–N(1)</td>
<td>2.0639(14)</td>
<td></td>
<td>1.9674(15)</td>
</tr>
<tr>
<td>Al–N(2)</td>
<td>1.9674(15)</td>
<td>1.9674(15)</td>
<td></td>
</tr>
<tr>
<td>Al–O(1)</td>
<td>1.8151(12)</td>
<td></td>
<td>1.8724(12)</td>
</tr>
<tr>
<td>Al–O(2)</td>
<td>1.8724(12)</td>
<td>1.8724(12)</td>
<td></td>
</tr>
<tr>
<td>Al–C(15)</td>
<td>1.9885(18)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O(2)–Al–O(1)</td>
<td>86.02(5)</td>
<td></td>
<td>96.53(7)</td>
</tr>
<tr>
<td>O(1)–Al–C(15)</td>
<td>119.25(7)</td>
<td></td>
<td>167.78(6)</td>
</tr>
<tr>
<td>O(1)–Al–N(1)</td>
<td>88.18(5)</td>
<td></td>
<td>95.69(7)</td>
</tr>
<tr>
<td>O(2)–Al–N(2)</td>
<td>87.58(6)</td>
<td></td>
<td>120.60(6)</td>
</tr>
<tr>
<td>C(15)–Al–N(2)</td>
<td>120.15(7)</td>
<td></td>
<td>86.13(6)</td>
</tr>
</tbody>
</table>
Table S4. Selected Bond Distances (Å) and Angles (deg) for complex 2b.

<table>
<thead>
<tr>
<th>Bond</th>
<th>Distance</th>
<th>Bond</th>
<th>Distance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al–N(1)</td>
<td>1.9897(16)</td>
<td>Al–N(2)</td>
<td>1.9827(16)</td>
</tr>
<tr>
<td>Al–O(1)</td>
<td>1.8217(13)</td>
<td>Al–O(2)</td>
<td>1.8389(13)</td>
</tr>
<tr>
<td>Al–O(3)</td>
<td>1.7443(14)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O(2)–Al–O(1)</td>
<td>89.65(6)</td>
<td>O(2)–Al–O(3)</td>
<td>100.30(6)</td>
</tr>
<tr>
<td>O(1)–Al–O(3)</td>
<td>113.05(7)</td>
<td>O(2)–Al–N(1)</td>
<td>165.50(7)</td>
</tr>
<tr>
<td>O(1)–Al–N(1)</td>
<td>89.03(6)</td>
<td>O(3)–Al–N(1)</td>
<td>93.49(7)</td>
</tr>
<tr>
<td>O(2)–Al–N(2)</td>
<td>89.83(6)</td>
<td>O(1)–Al–N(2)</td>
<td>133.27(6)</td>
</tr>
<tr>
<td>O(3)–Al–N(2)</td>
<td>112.98(7)</td>
<td>N(1)–Al–N(2)</td>
<td>80.62(7)</td>
</tr>
</tbody>
</table>

Table S5. Selected Bond Distances (Å) and Angles (deg) for complex 4b.

<table>
<thead>
<tr>
<th>Bond</th>
<th>Distance</th>
<th>Bond</th>
<th>Distance</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al–N(1)</td>
<td>1.967(3)</td>
<td>Al–N(2)</td>
<td>2.011(4)</td>
</tr>
<tr>
<td>Al–O(1)</td>
<td>1.861(3)</td>
<td>Al–O(2)</td>
<td>1.802(3)</td>
</tr>
<tr>
<td>Al–O(3)</td>
<td>1.740(3)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>O(2)–Al–O(1)</td>
<td>86.74(12)</td>
<td>O(2)–Al–O(3)</td>
<td>121.83(14)</td>
</tr>
<tr>
<td>O(1)–Al–O(3)</td>
<td>98.49(13)</td>
<td>O(2)–Al–N(1)</td>
<td>120.31(14)</td>
</tr>
<tr>
<td>O(1)–Al–N(1)</td>
<td>89.21(14)</td>
<td>O(3)–Al–N(1)</td>
<td>117.67(14)</td>
</tr>
<tr>
<td>O(2)–Al–N(2)</td>
<td>89.07(13)</td>
<td>O(1)–Al–N(2)</td>
<td>172.87(14)</td>
</tr>
<tr>
<td>O(3)–Al–N(2)</td>
<td>88.62(14)</td>
<td>N(1)–Al–N(2)</td>
<td>87.94(14)</td>
</tr>
</tbody>
</table>
Complex 2a

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: p385

Bond precision: C-C = 0.0074 Å Wavelength=0.71073

Cell: a=7.4501(6) b=18.6477(16) c=15.5635(14)
alpha=90 beta=98.717(2) gamma=90

Calculated Reported

Volume 2137.2(3) 2137.2(3)

Space group P 21/n P2(1)/n

Hall group -P 2yn ?

Moiety formula C24 H27 Al N2 O2 ?

Sum formula C24 H27 Al N2 O2 C24 H27 Al N2 O2

Mr 402.46 402.46

Dx,g cm⁻³ 1.251 1.251

Z 4 4

Mu (mm⁻¹) 0.117 0.117

F000 856.0 856.0

F000’ 856.55

h,k,lmax 8,22,18 8,22,18

Nref 3865 3855

Tmin,Tmax 0.985,0.988 0.959,0.988

Tmin’ 0.959

Correction method= AbsCorr=MULTI-SCAN

Data completeness= Ratio = 0.997 Theta(max)= 25.250

R(reflections)= 0.0825( 2572) wR2(reflections)= 0.1932( 3855)

S = 1.015 Npar= 265

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

PLAT213_ALERT_2_B Atom C11 has ADP max/min Ratio ............. 4.20 prola
PLAT241_ALERT_2_B Check High Ueq as Compared to Neighbors for C12
Alert level C

ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as Multi-scan

PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical . ?

PLAT213_ALERT_2_C Atom C9 has ADP max/min Ratio ............ 3.10 prola
PLAT213_ALERT_2_C Atom C10 has ADP max/min Ratio ............ 3.50 prola
PLAT213_ALERT_2_C Atom C12 has ADP max/min Ratio ............ 3.10 prola
PLAT213_ALERT_2_C Atom C13 has ADP max/min Ratio ............ 3.60 prola
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.01 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.34 Ratio

PLAT230_ALERT_2_C Hirshfeld Test Diff for C8 - C9 ... 5.11 su
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C4
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C11
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for N1
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for N2
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ... 7
PLAT360_ALERT_2_C Short C(sp3)-C(sp3) Bond C11 - C12 ... 1.43 Ang.
PLAT380_ALERT_4_C Check Incorrectly? Oriented X(sp2)-Methyl Moiety C13

0 ALERT level A = In general: serious problem
2 ALERT level B = Potentially serious problem
16 ALERT level C = Check and explain
0 ALERT level G = General alerts; check

2 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
2 ALERT type 3 Indicator that the structure quality may be low
1 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Complex 3a

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report
Datablock: p083
Bond precision: C-C = 0.0044 Å Wavelength=0.71073 Å
Cell: a=29.660(3) b=7.5901(6) c=22.3793(19) Å
alpha=90 beta=116.486(2) gamma=90
Calculated Reported
Volume 4509.3(7) 4509.4(7) Å³
Space group C 2/c C2/c
Hall group -C 2yc
Moiety formula C25 H29 Al N2 O2
Sum formula C25 H29 Al N2 O2 C25 H29 Al N2 O2
Mr 416.48 416.48
Dx,g cm⁻³ 1.227 1.227
Z 8 8
Mu (mm⁻¹) 0.113 0.113
F000 1776.0 1776.0
F000’ 1777.13
h,k,lmax 36,9,27 36,9,27
Nref 4467 4434
Tmin,Tmax 0.980,0.993 0.955,0.994
Tmin’ 0.955
Correction method= AbsCorr=MULTI-SCAN
Data completeness= Ratio = 0.993 Theta(max)= 26.050°
R(reflections)= 0.0613( 2996) wR2(reflections)= 0.1489( 4434)
S = 1.037 Npar= 274
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 A
PLAT093_ALERT_1_A No su’s on H-atoms, but refinement reported as . mixed
Alert level C
ABSTY02_ALERT_1_C An _exptl_absorp_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorp_process_details field.
Absorption correction given as Multi-scan
PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical . ?
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 2.83 Ratio
PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.05 Ratio
PLAT232_ALERT_2_C Hirshfeld Test Diff (M-X) Al - C1 .. 9.74 su
1 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
5 ALERT level C = Check and explain
0 ALERT level G = General alerts; check
3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Complex 4a
checkCIF/PLATON report
No syntax errors found. CIF dictionary Interpreting this report
Datablock: q458
Bond precision: C-C = 0.0024 A Wavelength=0.71073
Cell: a=9.9827(7) b=11.1884(8) c=21.7980(16)
alpha=90 beta=96.119(1) gamma=90
Calculated Reported
Volume 2420.8(3) 2420.8(3)
Space group P 21/c P2(1)/c
Hall group -P 2ybc ?
Moiety formula C27 H33 Al N2 O2 ?
Sum formula C27 H33 Al N2 O2 C27 H33 Al N2 O2
Mr 444.53 444.53
Dx,g cm-3 1.220 1.220
Z 4 4
Mu (mm-1) 0.110 0.110
F000 952.0 952.0
F000’ 952.58
h,k,lmax 12,13,26 12,13,26
Nref 4774 4766
Tmin, Tmax 0.973, 0.984 0.947, 0.984
Tmin’ 0.946
Correction method = AbsCorr = MULTI-SCAN
Data completeness = Ratio = 0.998 Theta(max) = 26.000
R(reflections) = 0.0438 (3926) wR2(reflections) = 0.1214 (4766)
S = 1.036 Npar = 294

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
ABSTY02_ALERT_1_C An _exptl_absorp_correction_type has been given without a literature citation. This should be contained in the _exptl_absorp_process_details field.
Absorption correction given as Multi-scan
PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical. ?
0 ALERT level A = In general: serious problem
0 ALERT level B = Potentially serious problem
2 ALERT level C = Check and explain
0 ALERT level G = General alerts; check
2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
0 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
0 ALERT type 4 Improvement, methodology, query or suggestion
0 ALERT type 5 Informative message, check

Complex 2b

checkCIF/PLATON report
No syntax errors found. CIF dictionary Interpreting this report
Datablock: q470
Bond precision: C-C = 0.0033 A Wavelength=0.71073
Cell: a=10.4661(11) b=10.6923(11) c=12.2855(13)
alpha=86.341(2) beta=66.205(1) gamma=64.024(1)
Calculated Reported
Volume 1120.2(2) 1120.2(2)
Space group P -1 P-1
Hall group -P 1

Moiety formula C25 H29 Al N2 O3
Sum formula C25 H29 Al N2 O3 C25 H29 Al N2 O3
Mr 432.48 432.48
Dx,g cm-3 1.282 1.282
Z 2 2
Mu (mm-1) 0.120 0.120
F000 460.0 460.0
F000’ 460.30
h,k,lmax 12,12,14 12,12,14
Nref 4177 4093
Tmin,Tmax 0.981,0.996 0.939,0.996
Tmin’ 0.938
Correction method= AbsCorr=MULTI-SCAN
Data completeness= Ratio = 0.980 Theta(max)= 25.500
R(reflections)= 0.0431( 3288) wR2(reflections)= 0.1151( 4093)
S = 1.017 Npar= 284

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
PLAT220_ALERT_2_B Large Non-Solvent C Ueq(max)/Ueq(min) ... 3.56 Ratio
Alert level C
ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as multi-scan
PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical . ?
PLAT222_ALERT_3_C Large Non-Solvent H Ueq(max)/Ueq(min) ... 3.81 Ratio
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C23
Alert level G
PLAT794_ALERT_5_G Check Predicted Bond Valency for Al1 (3) 3.02

0 ALERT level A = In general: serious problem
1 ALERT level B = Potentially serious problem
4 ALERT level C = Check and explain
1 ALERT level G = General alerts; check
2 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
1 ALERT type 3 Indicator that the structure quality may be low
0 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

Complex 4b

checkCIF/PLATON report

No syntax errors found. CIF dictionary Interpreting this report

Datablock: q117s
Bond precision: C-C = 0.0070 Å Wavelength=0.71073
Cell: a=22.4239(14) b=13.4238(8) c=21.9046(14)
alpha=90 beta=102.749(1) gamma=90
Calculated Reported
Volume 6431.0(7) 6431.0(7)
Space group C c Cc
Hall group C -2yc ?
Moiety formula C28 H35 Al N2 O3, C7 H8 ?
Sum formula C35 H43 Al N2 O3 C70 H86 AL2 N4 O6
Mr 566.69 1133.39
Dx,g cm-3 1.171 1.171
Z 8 4
Mu (mm-1) 0.099 0.099
F000 2432.0 2432.0
F000’ 2433.40
h,k,lmax 27,16,27 27,16,27
Nref 6344(12680) 8412
Tmin,Tmax 0.974,0.981 0.974,0.982
Tmin’ 0.974
Correction method= AbsCorr=MULTI-SCAN
Data completeness= 1.33(0.66) Theta(max)= 26.040
R(reflections)= 0.0533( 6588) wR2(reflections)= 0.1483( 8412)
S = 1.009 Npar= 678

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
PLAT201_ALERT_2_B Isotropic non-H Atoms in Main Residue(s) ........ 1
Alert level C
ABSTY02_ALERT_1_C An _exptl_absorpt_correction_type has been given without
a literature citation. This should be contained in the
_exptl_absorpt_process_details field.
Absorption correction given as Multi-scan
PLAT041_ALERT_1_C Calc. and Rep. SumFormula Strings Differ ... ?
PLAT045_ALERT_1_C Calculated and Reported Z Differ by ............. 2.00 Ratio
PLAT066_ALERT_1_C Predicted and Reported Transmissions Identical . ?
PLAT202_ALERT_3_C Isotropic non-H Atoms in Anion/Solvent ........ 14
PLAT220_ALERT_2_C Large Non-Solvent C Ueq(max)/Ueq(min) ... 2.66 Ratio
PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for C3
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C54
PLAT244_ALERT_4_C Low 'Solvent' Ueq as Compared to Neighbors for C62
PLAT331_ALERT_2_C Small Average Phenyl C-C Dist. C57 -C62 1.37 Ang.
PLAT340_ALERT_3_C Low Bond Precision on C-C Bonds (x 1000) Ang ... 7
Alert level G
REFLT03_ALERT_4_G ALERT: MoKa measured Friedel data cannot be used to
determine absolute structure in a light-atom
study EXCEPT under VERY special conditions.
It is preferred that Friedel data is merged in such cases.
From the CIF: _diffrn_reflns_theta_max 26.04
From the CIF: _reflns_number_total 8412
Count of symmetry unique reflns 6344
Completeness (_total/calc) 132.60%
TEST3: Check Friedels for noncentro structure
Estimate of Friedel pairs measured 2068
Fraction of Friedel pairs measured 0.326
Are heavy atom types Z>Si present no
PLAT794_ALERT_5_G Check Predicted Bond Valency for Al1 (3) 3.03
PLAT794_ALERT_5_G Check Predicted Bond Valency for Al2 (3) 3.05
PLAT860_ALERT_3_G Note: Number of Least-Squares Restraints ........ 2
0 ALERT level A = In general: serious problem
1 ALERT level B = Potentially serious problem
11 ALERT level C = Check and explain
4 ALERT level G = General alerts; check
4 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
5 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
2 ALERT type 4 Improvement, methodology, query or suggestion
2 ALERT type 5 Informative message, check