Supporting Information

Synthesis of binuclear phenoxyimino organoaluminum complexes and their use as the catalyst precursors for efficient ring-opening polymerisation of ε-caprolactone

Hong-Ling Han, Yan Liu, Jing-Yu Liu, Kotohiro Nomura, Yue-Sheng Li

State Key Laboratory of Polymer Physics and Chemistry, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, China

College of Environment & Chemical Engineering, Yanshan University, Qinhuangdao 066004, China

Department of Chemistry, Graduate School of Science and Engineering, Tokyo Metropolitan University

CONTENTS

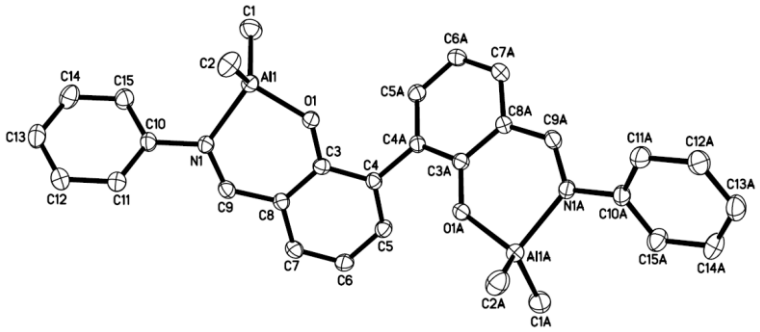

Figure S1. Molecular structure of complex **2a** with thermal ellipsoids at 30% probability level. Hydrogen atoms are omitted for clarity.

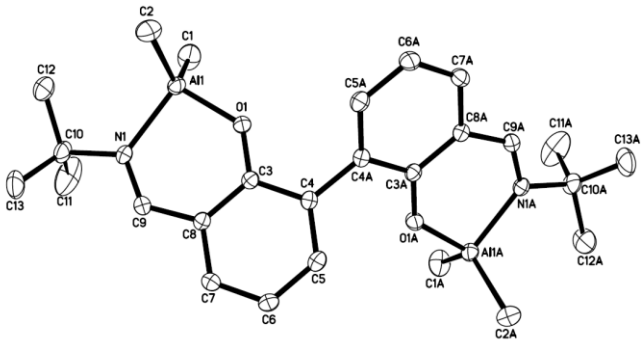

Figure S2. Molecular structure of complex **2e** with thermal ellipsoids at 30% probability level. Hydrogen atoms are omitted for clarity.

Table 1. Crystal data and structure refinements of complexes **2a-e**.

	2a	**2b**	**2c**	**2d**	**2e**
Empirical formula	$C_{30}H_{30}Al_2N_2O_2$	$C_{42}H_{54}Al_2N_2O_2+CH_2Cl_2$	$C_{54}H_{46}Al_2N_2O_2+CH_2Cl_2$	$C_{38}H_{50}Al_2N_2O_2$	$C_{26}H_{38}Al_2N_2O_2+CH_2Cl_2$
Formula weight	504.52	757.76	928.26	620.76	549.47
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic	monoclinic
Space group	Pccn	Pbcn	P2(1)/n	C2/c	C2/c
a (Å)	10.4697(7)	16.7382(6)	13.0666(6)	15.8192(9)	17.697(2)
b (Å)	18.1726(12)	17.1151(6)	13.3996(6)	13.1067(8)	12.5736(14)
c (Å)	14.8982(10)	15.2211(5)	28.7365(13)	18.7852(11)	16.2599(19)
α (°)	90.00	90.00	90.00	90.00	90.00
β (°)	90.00	90.00	102.3870(10)	104.5450(10)	121.377(2)
γ (°)	90.00	90.00	90.00	90.00	90.00
V (Å^3), Z	2834.6(3), 4	4360.5(3), 4	4914.3(4), 4	3770.0(4), 4	3089.0(6), 4
$Density_{calcd}$ (Mg/m^3)	1.182	1.154	1.255	1.094	1.182
Absorption coefficient (mm^{-1})	0.131	0.225	0.265	0.109	0.292
F(000)	1064	1616	1936	1336	1168
Crystal size/mm	0.30×0.24×0.13	0.42×0.36×0.28	0.38×0.20×0.20	0.30×0.23×0.15	0.32×0.25×0.19
θ range for data collection (°)	2.24 to 26.04	1.70 to 26.07	1.45 to 25.14	2.05 to 26.09	2.11 to 26.22
Reflections collected	14713	22905	24881	10305	8379
Independent reflections	2797 (R_{int}= 0.0620)	4319 (R_{int}= 0.0332)	8774 (R_{int}= 0.0488)	3735 (R_{int}= 0.0315)	3100 (R_{int}= 0.0297)
Data/restraints/ parameters	2797/0/163	4319/0/237	8774/0/581	3735/0/201	3100/0/164
Goodness-of-fit on F^2	1.058	1.052	1.032	1.090	1.037
Final R indices [I>2σ (I)]: R1, wR2	0.0463, 0.1188	0.0479, 0.1229	0.0902, 0.2687	0.0450, 0.1262	0.0421, 0.0970
Largest diff. Peak and hole (e Å^{-3})	0.284 and -0.236	0.818 and -0.713	2.435 and -0.946	0.231 and -0.225	0.285 and -0.312