Supplementary material

N-Benzoylbenzamidinate Complexes of Aluminium: Highly Efficient Initiators for the Ring-Opening Polymerization of ε-Caprolactone

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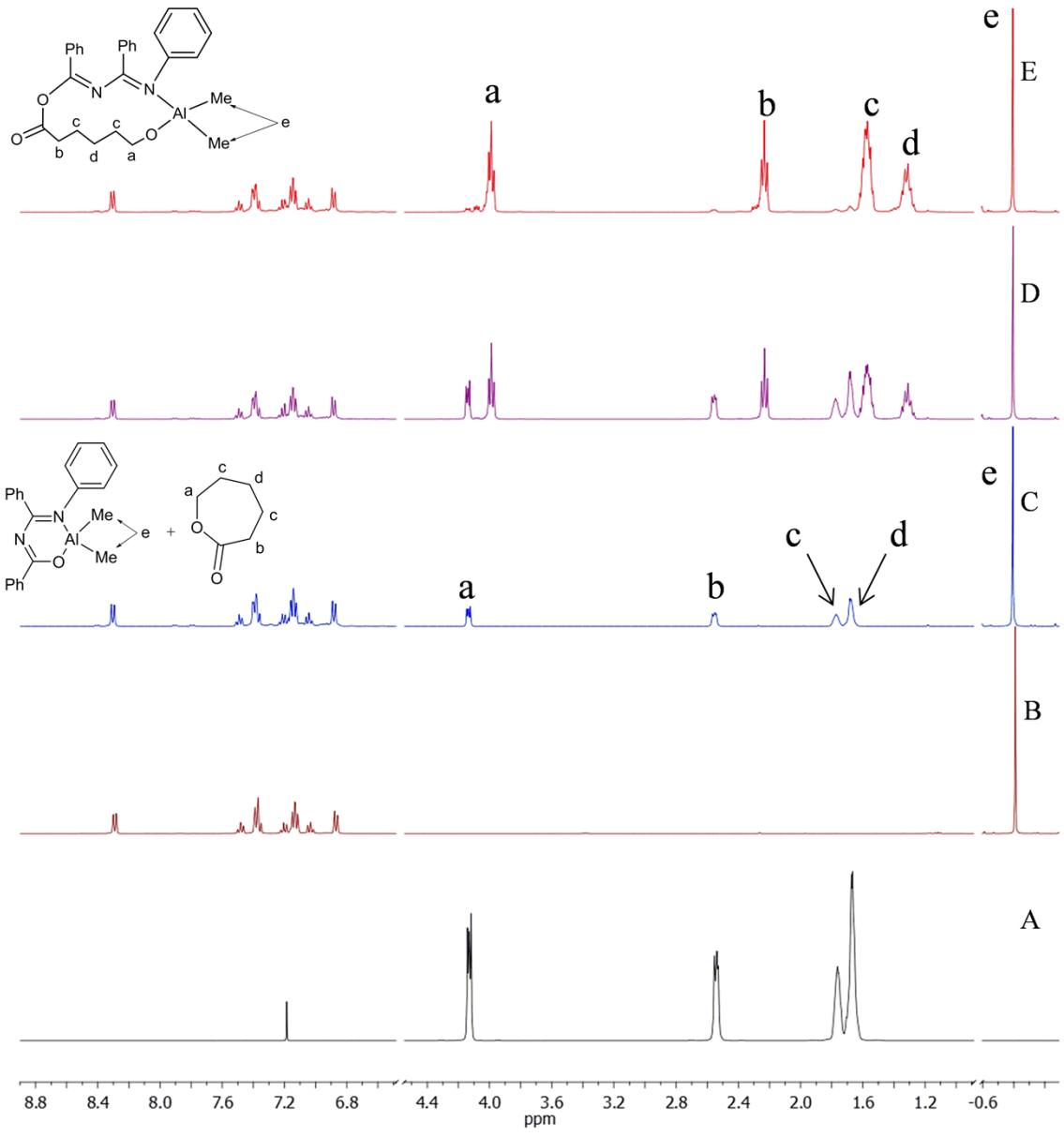

Figure S1. . ^{1}H NMR spectra of a reaction between **1** and ε-CL in 1:1 ratio in $CDCl_3$: A: ε-CL at room temperature. B: Complex **2** at room temperature. C: ε-CL and **2** at room temperature. D and E: ε-CL and **2** at 80 °C after 15 and 30 minutes respectively.

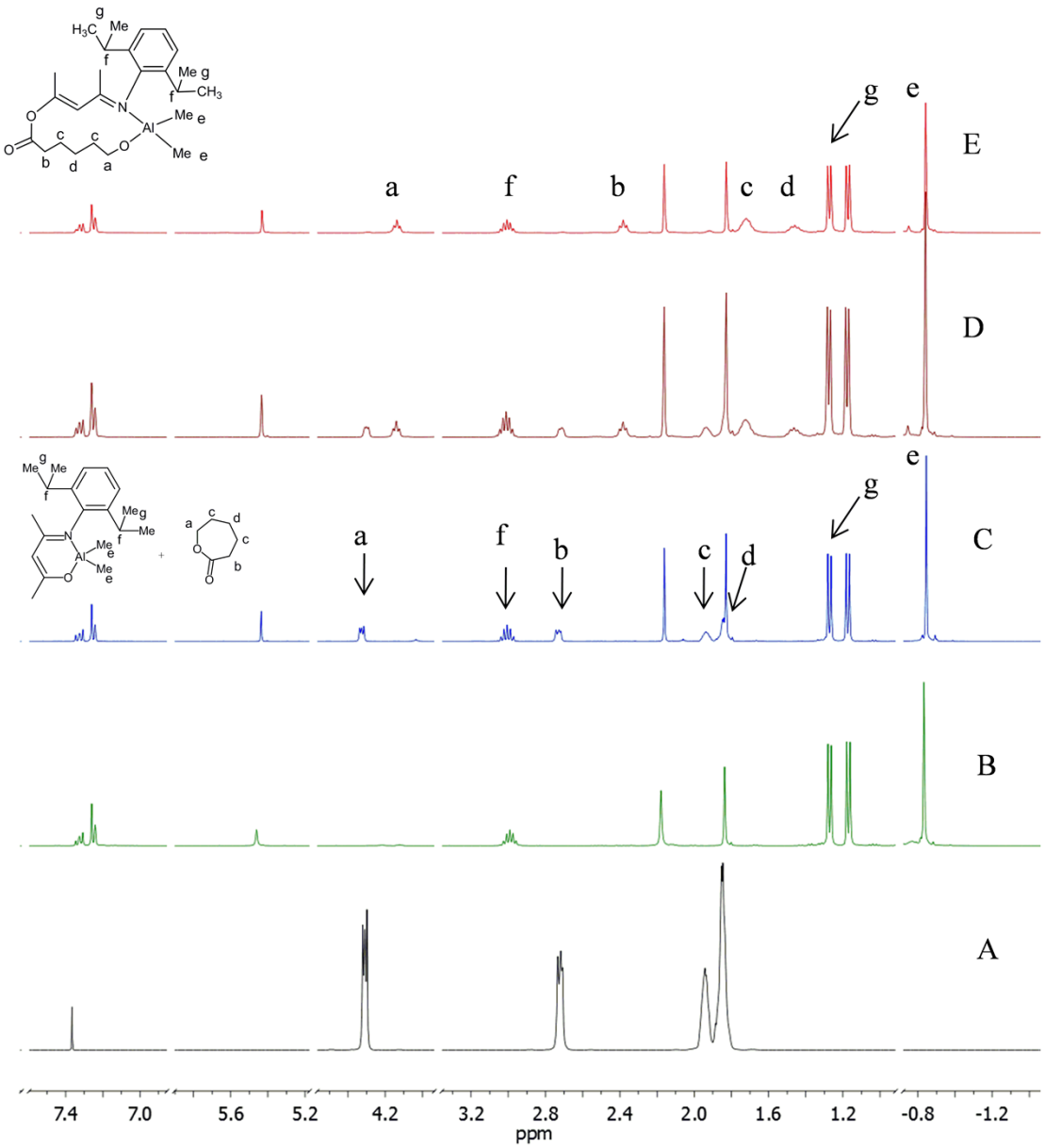

Figure S2. ^{1}H NMR spectra of a reaction between ketiminate-Al complex and ε-CL in 1:1 ratio in $CDCl_3$: A: ε-CL at room temperature. B: Ketiminate-Al complex at room temperature. C: ε-CL and ketiminate-Al complex at room temperature. D and E: ε-CL and ketiminate-Al complex at 80 °C after 1 and 2 h respectively.

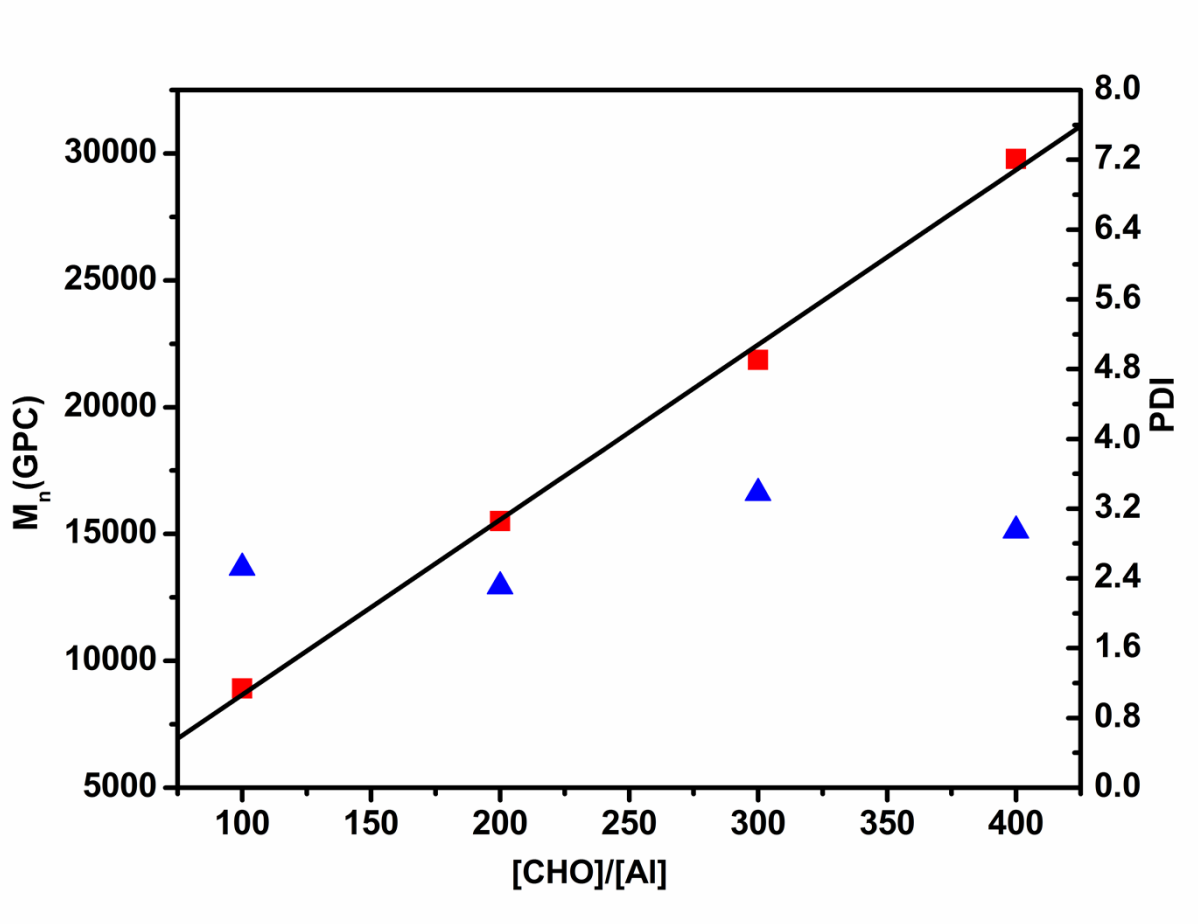

Figure S3. Plot of number-averaged molecular weight (M_n) and polydispersity index, (PDI) *vs* [CHO]/[Al] for the polymerization of cyclohexene oxide using complex **1** at room temperature (entries 1 – 4, Table 2). Red squares (■) represent M_n (uncorrected) values and bule triangles (▲) represent PDI values.

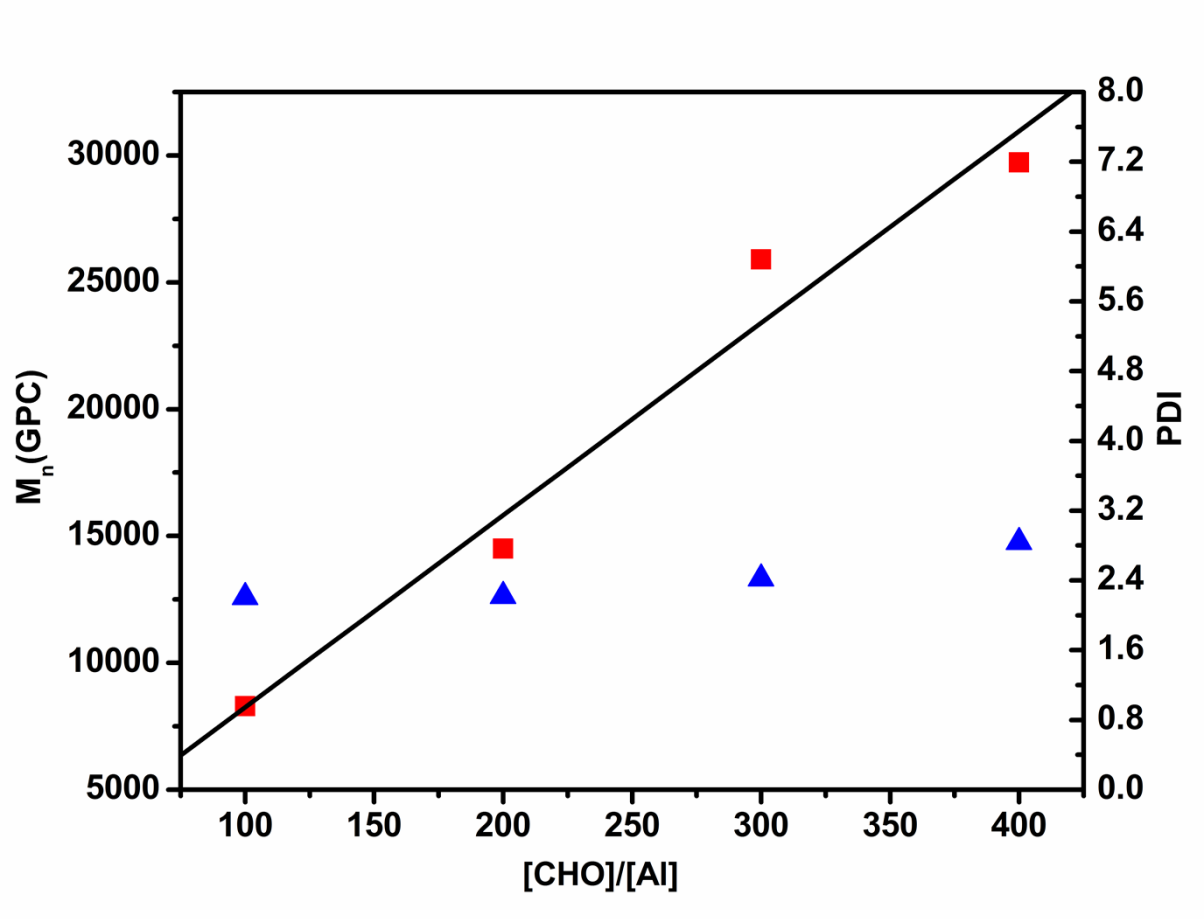

Figure S4. Plot of number-averaged molecular weight (M_n) and polydispersity index, (PDI) *vs* [CHO]/[Al] for the polymerization of cyclohexene oxide using complex **2** at room temperature (entries 4 – 8, Table 2). Red squares (■) represent M_n (uncorrected) values and bule triangles (▲) represent PDI values.

Table S1. Crystal Data for Compounds **1**, **3** and **4**

	1	**3**	**4**
empirical formula	$C_{28}H_{33}N_2OAl$	$C_{53}H_{57}N_4O_2Al$	$C_{60}H_{45}AlN_6O_3$
formula wt	440.54	809.01	925.00
temp (K)	150(2)	150(2)	150(2)
cryst syst	monoclinic	Orthorhombic	triclinic
space group	*I2/a*	$P2_12_12_1$	$P\bar{1}$
a (Å)	25.2618(13)	13.1875(5)	11.3761(4)
b (Å)	11.2363(7)	17.1684(9)	12.4523(5)
c (Å)	22.8425(16)	20.1357(10)	19.8133(7)
α (deg)	90.00	90.00	99.277(3)
β (deg)	106.040(7)	90.00	96.531(3)
γ (deg)	90.00	90.00	109.381(3)
V (Å^3)	4998.0(6)	4558.9(4)	2570.54(16)
Z	8	4	2
ρ_{calcd} (Mg m^{-3})	1.171	1.179	1.195
μ (mm^{-1})	0.103	0.089	0.090
F(000)	1888.0	1728.0	968.0
cryst size (mm)	0.3 × 0.3 × 0.1	0.42 × 0.21 × 0.2	0.35 × 0.31 × 0.3
θ range (deg)	2.73–29.22	2.55–25	2.96–25
no.of collected/unique rflns	17036 /5948 (*R*(int) = 0.0477)	14429 /7812 (*R*(int) = 0.0610)	23555/9060 [*R*(int) = 0.0584]
no.ofdata/restraints/ params	5948/0/295	7812/0/550	9060/0/631
*R*1, *wR*2 ($I > 2\sigma(I)$)[a]	0.0532, 0.1386	0.0632, 0.0784	0.0525, 0.11136
*R*1, *wR*2 (all data)[a]	0.0702, 0.1537	0.1186, 0.0952	0.0937, 0.1339
GOF	1.040	0.991	0.905
$\Delta\rho_{max}/\Delta\rho_{min}$ (e Å^{-3})	0.53/–0.47	0.24/–0.31	0.22/–0.32

[a] $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{0.5}$.