Bimetallic bis(benzotriazole iminophenolate) cobalt, nickel and zinc complexes as versatile catalysts for coupling of carbon dioxide with epoxides and copolymerization of phthalic anhydride with cyclohexene oxide

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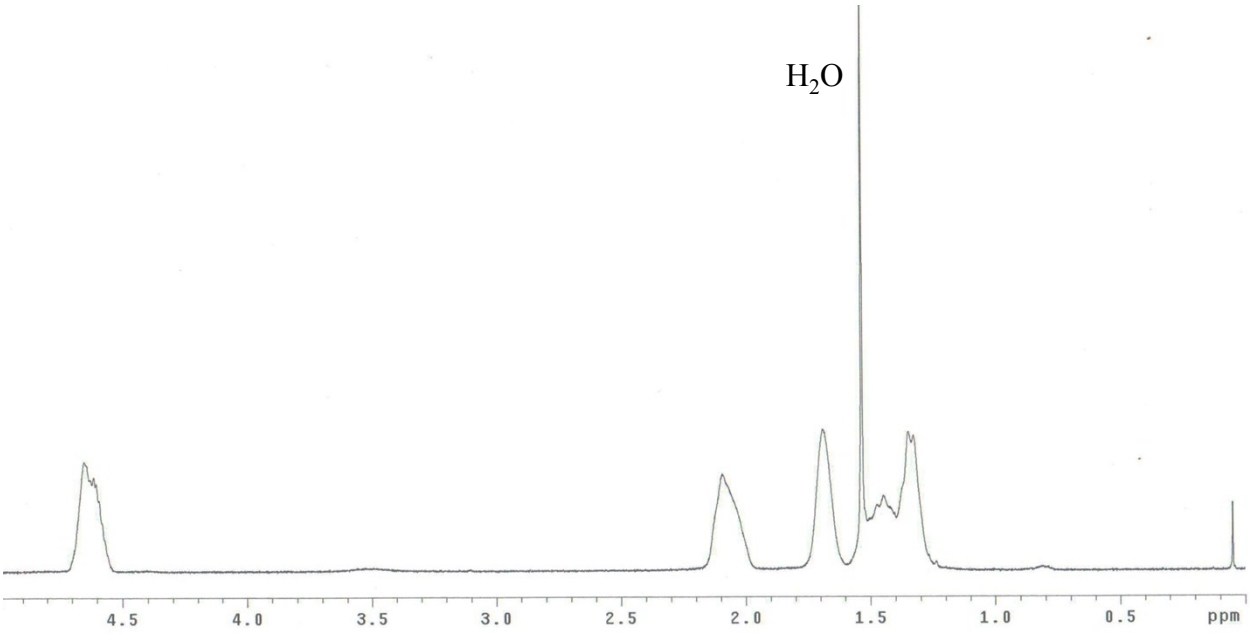
Fig. S1 ^{1}H NMR spectrum of the purified copolymer produced by using di-nickel acetate complex **2** (Table 2, entry 8) in $CDCl_3$. Peak at δ 4.65 ppm is assigned to the methine protons in PCHC, and no significant signals at 3.2-3.6 ppm confirms >99% carbonate linkages in PCHC.

Fig. S2 ^{1}H NMR spectra of the methine region of crude sample produced by coupling of CO_2 and cyclohexene oxide using di-zinc acetate complex **3** (Table 3, entry 8) in the presence of *n*-Bu_4NBr (0.0625 mol%) at 120 ^{o}C and 300 psi CO_2 (400 MHz, $CDCl_3$).

Fig. S3 GPC traces for the produced poly(PA-*alt*-CHO) with a bimodal molecular weight distribution catalysed by di-Co complex **1** (Table 4, entry 1).

Fig. S4 Copolymerization of PA and CHO catalysed by di-Co complex **1** at 110 ^{o}C. The relationship between M_n(■)/(PDI(▲) of polymer and the initial molar ratio $[PA]_0/[\mathbf{Cat.}]_0$ is shown.

Table S1 Crystallographic data of complexes **1-6**



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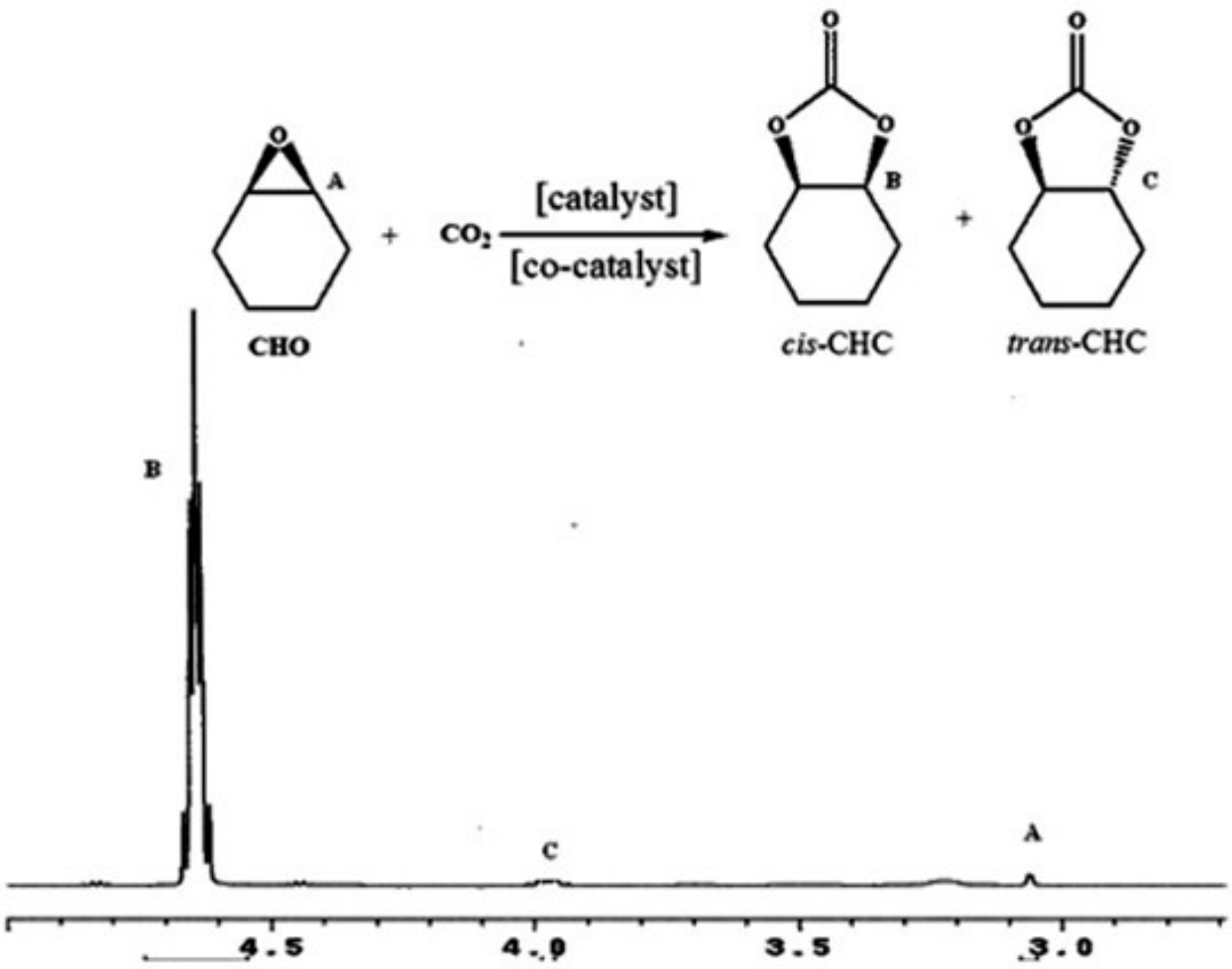

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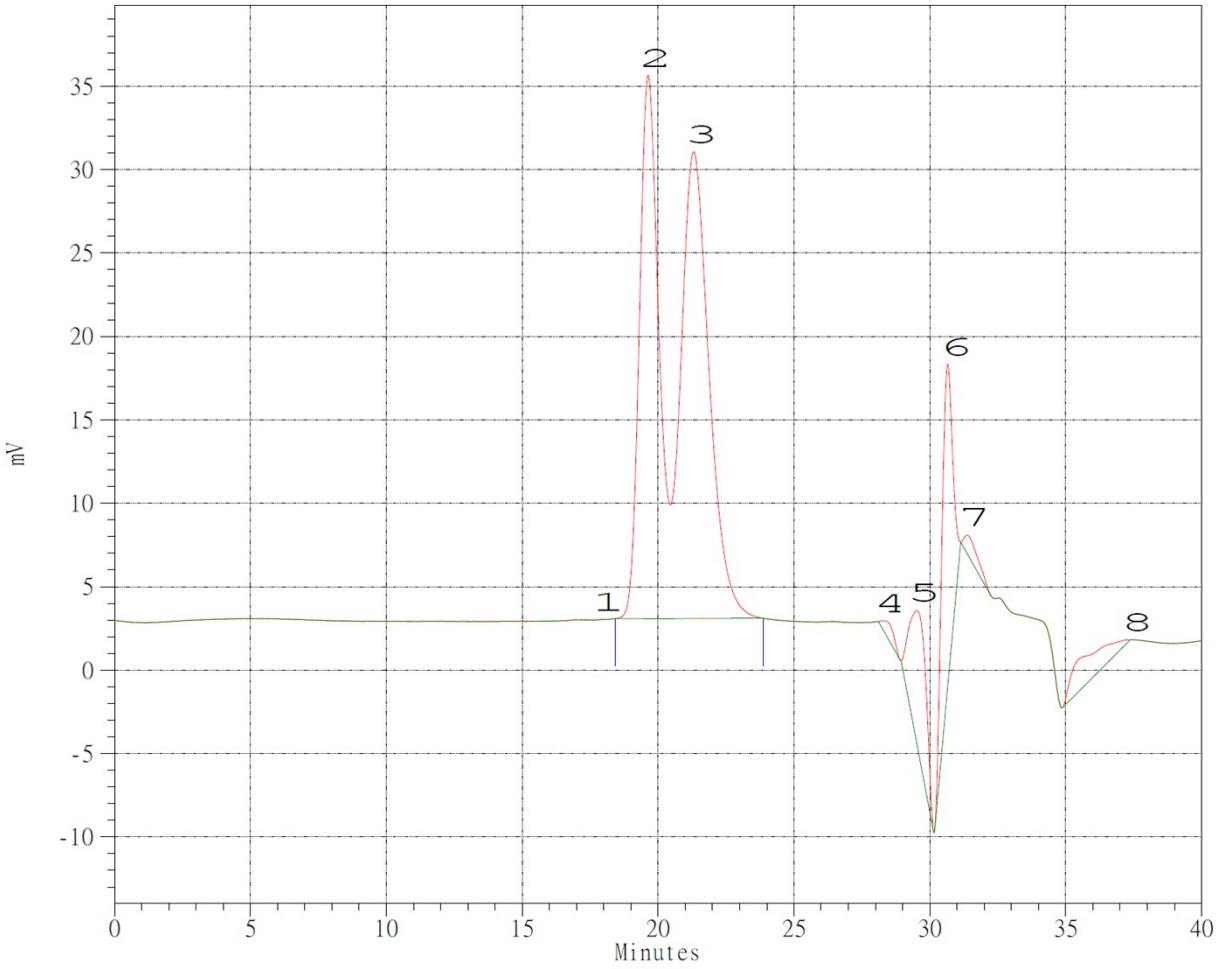

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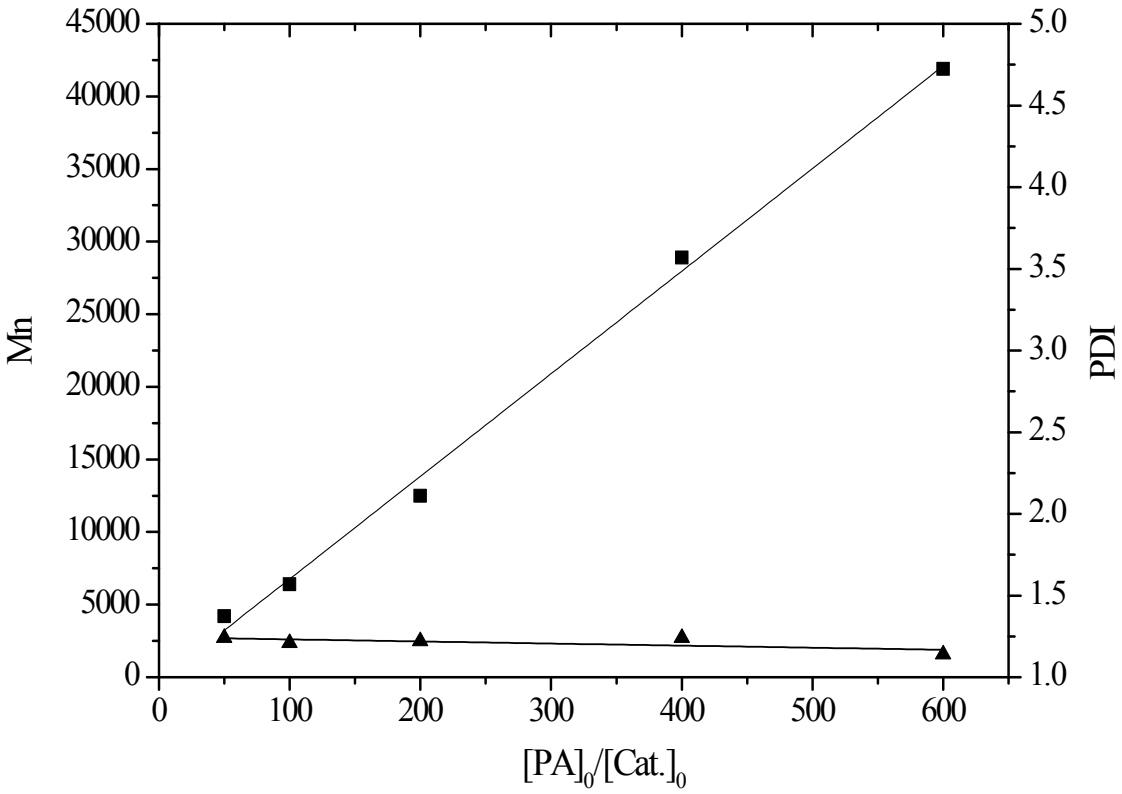

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	1·2CH_2Cl_2	**2**·2EtOH	**3**·CH_2Cl_2	**4**	**5**	**6**
Formula	$C_{53}H_{68}Cl_4Co_2N_8O_6$	$C_{55}H_{76}N_8Ni_2O_8$	$C_{52}H_{66}Cl_2N_8O_6Zn_2$	$C_{48}H_{60}N_8O_7Co_2$	$C_{44}H_{52}N_8O_2Ni$	$C_{44}H_{52}N_8O_2Zn$
Formula weight	1172.81	1094.66	1100.77	978.91	783.63	790.32
Temp (K)	120(2)	120(2)	120(2)	120(2)	150(2)	120(2)
Crystal system	Triclinic	Monoclinic	Triclinic	Triclinic	Monoclinic	Triclinic
Space group	*P*-1	*P*2(1)/n	*P*-1	*P*-1	*C*2/c	*P*-1
a (Å)	12.2124(6)	13.1227(6)	12.9858(11)	12.0764(3)	28.656(2)	12.6986(10)
b (Å)	12.9259(8)	12.4772(4)	14.1768(11)	13.8920(4)	11.8914(8)	12.8906(13)
c (Å)	18.2099(9)	34.7916(16)	16.4564(12)	19.0298(5)	28.057(2)	14.9043(16)
α (deg)	81.229(5)	90	66.927(7)	104.928(2)	90	90.191(9)
β (deg)	83.807(4)	100.473(4)	89.457(6)	100.071(2)	110.549(2)	108.659(8)
γ (deg)	78.292(5)	90	72.168(7)	90.969(2)	90	92.048(7)
V(Å^3)	2773.0(3)	5601.7(4)	2632.1(4)	3030.81(14)	8952.5(11)	2309.7(4)
Z	2	4	2	2	8	2
D_{calc}(Mg/m^3)	1.405	1.298	1.389	1.313	1.286	1.330
μ (Mo Kα)(mm^{-1})	0.846	0.731	1.069	0.612	0.486	2.230
F(000)	1224	2328	1152	1261	3672	972
Reflections collected	36981	31571	23383	33237	107795	20732
No. of parameters	672	670	653	739	550	560
Indep. reflns (R_{int})	13181(0.0540)	13249(0.0465)	12009(0.0519)	14087(0.0390)	9159(0.0823)	8741(0.0918)
$R1[I > 2\sigma(I)]$	0.0685	0.0694	0.0626	0.0777	0.0951	0.1020
w$R2$ $[I > 2\sigma(I)]$	0.1535	0.1491	0.1261	0.2171	0.2706	0.2717
Goodness-of-fit on F^2	1.035	1.029	1.012	1.025	1.002	1.009