

Supplementary Materials: Pyrazole Supported Zinc(II) Benzoates as Catalysts for the Ring Opening Copolymerization of Cyclohexene Oxide and Carbon Dioxide

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Table S1. Crystallographic data for complex 2.

Empirical formula	C ₄₄ H ₃₀ N ₈ O ₁₂ Zn
Formula weight	928.13
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	
$a = 13.9192(8)$ Å	$\alpha = 90^\circ$
$b = 13.7516(7)$ Å	$\beta = 103.4660(10)^\circ$
$c = 21.5005(12)$ Å	$\gamma = 90^\circ$
Z	4
Density (calculated)	1.540 Mg/m ³
Absorption coefficient	0.693 mm ⁻¹
F(000)	1904
Crystal size	0.21 × 0.11 × 0.04 mm ³
Theta range for data collection	1.50 to 28.34°
Index ranges	-18 ≤ h ≤ 18, -17 ≤ k ≤ 18, -28 ≤ l ≤ 28
Reflections collected	77200
Independent reflections	9969 [R(int) = 0.0689]
Completeness to theta = 28.34°	99.7%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9728 and 0.8682
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	9969 / 7 / 586
Goodness-of-fit on F ²	1.030
Final R indices [I > 2sigma(I)]	R1 = 0.0402, wR2 = 0.0838
R indices (all data)	R1 = 0.0656, wR2 = 0.0947
Largest diff. peak and hole	0.529 and -0.582 e.Å ⁻³

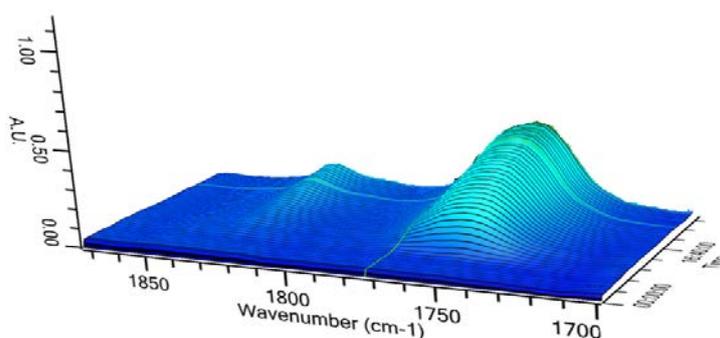


Figure S1. Three-dimensional stack plot of the IR data collected every minute with ReactIR during CHO/CO₂ copolymerisation using catalyst 1.

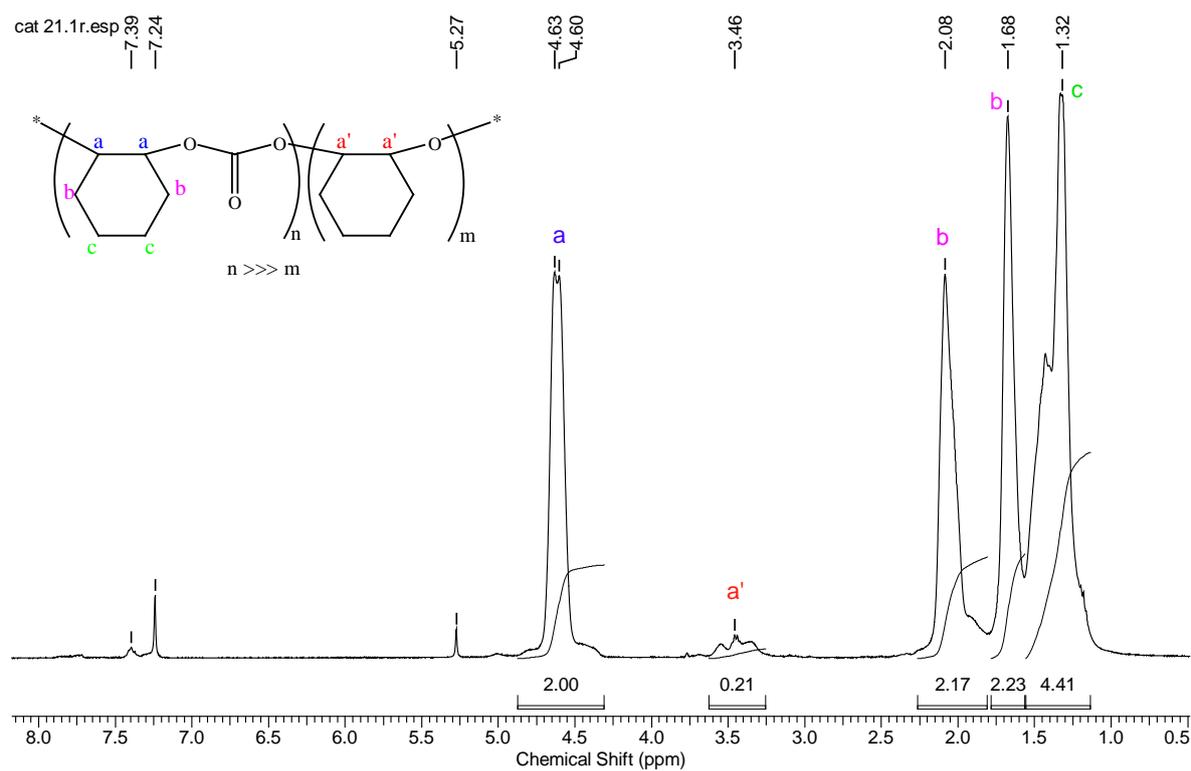


Figure S2. ^1H NMR spectrum of PCHC showing high carbonate content.

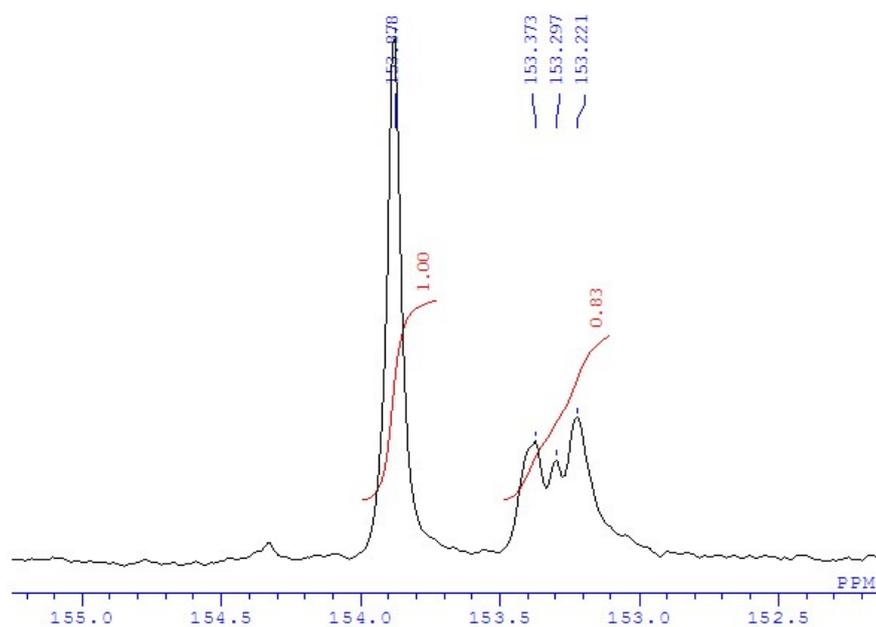


Figure S3. Typical ^{13}C NMR spectrum of PCHC produced using catalysts 1–4 showing the carbonyl region.



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