

Supporting information

for

Bis(imino)-6,7-dihydro-5H-quinoline-cobalt complexes as highly active catalysts for the formation of vinyl-terminated PE waxes; steps towards inhibiting deactivation pathways through targeted ligand design

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Table S1 Crystal data and structure refinement for **Co1** and **Co4**

| | Co1 ·CH ₂ Cl ₂ | Co4 ·2CH ₂ Cl ₂ |
|---|---|--|
| Crystal color | brown | yellow |
| Empirical formula | C ₃₂ H ₃₁ Cl ₂ CoN ₃ ·CH ₂ Cl ₂ | C ₃₄ H ₃₅ Cl ₂ CoN ₃ ·2CH ₂ Cl ₂ |
| Formula weight | 672.35 | 785.33 |
| T (K) | 170(10) | 220(13) |
| Wavelength (Å) | 1.54184 | 1.54184 |
| Crystal system | monoclinic | monoclinic |
| Space group | P21/c | C2/c |
| a /Å | 8.8111(2) | 36.8374(6) |
| b/Å | 14.2113(3) | 12.2282(2) |
| c/Å | 25.8363(4) | 17.1691(2) |
| α/° | 90 | 90 |
| β/° | 95.520(2) | 91.4370(10) |
| γ/° | 90 | 90 |
| Volume/Å ³ | 3220.15(11) | 7731.5(2) |
| Z | 4 | 8 |
| ρ _{calc} /cm ³ | 1.387 | 1.349 |
| μ/mm ⁻¹ | 7.437 | 7.514 |
| F(000) | 1388.0 | 3240.0 |
| Crystal size/mm ³ | 0.15 × 0.1 × 0.08 | 0.15 × 0.08 × 0.03 |
| θ range (°) | 6.874 to 150.922 -10 ≤ h ≤ 10 | 4.8 to 150.932 -46 ≤ h ≤ 46 |
| Limiting indices | -17 ≤ k ≤ 16 -32 ≤ l ≤ 32 | -14 ≤ k ≤ 15 -21 ≤ l ≤ 16 |
| No. of rflns collected | 22545 | 32855 |
| No. unique rflns [R(int)] | 6376(0.0347) | 7691(0.0561) |
| Completeness to θ (%) | 99.98 | 99.75 |
| Goodness of fit on F ² | 0.955 | 1.076 |
| Final R indices [I > 2σ(I)] | R1 = 0.0495 wR2 = 0.1303 | R1 = 0.0657 wR2 = 0.1963 |
| R indices (all data) | R1 = 0.0584 wR2 = 0.1364 | R1 = 0.0849 wR2 = 0.2216 |
| Largest diff peak and hole (e Å ⁻³) | 0.93/-0.65 | 1.18/-0.85 |

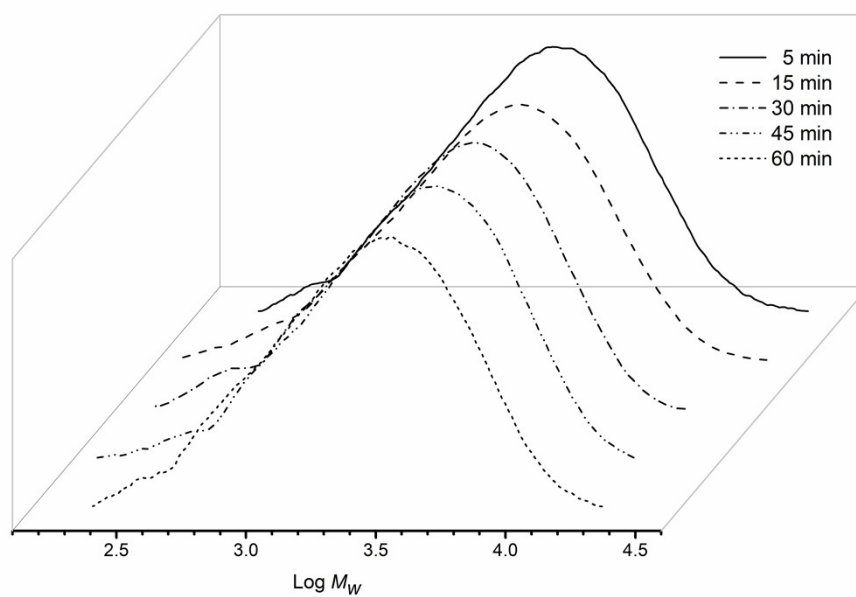


Fig. S1 GPC traces of the polyethylene generated using **Co4/MAO** over different run times (entries 7 and 10 – 13, Table 2)

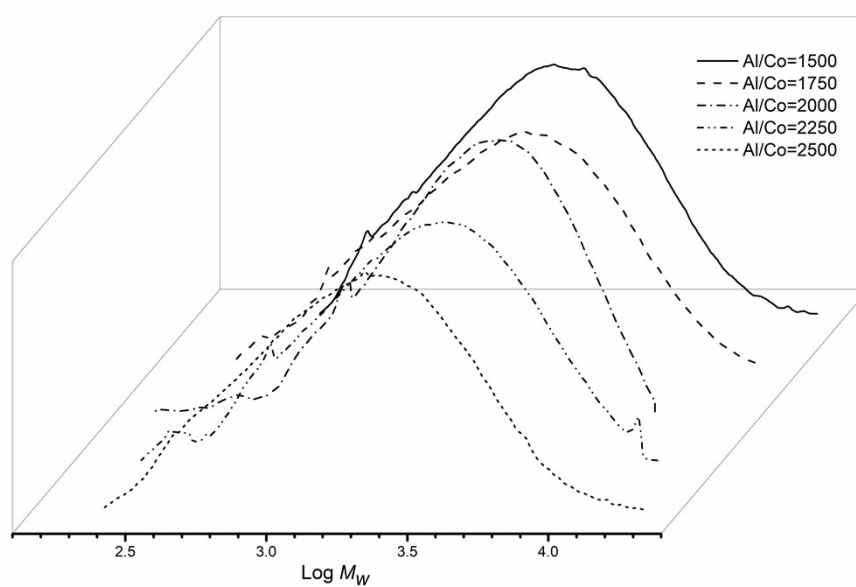


Fig. S2 GPC traces of the polyethylene produced using **Co4/MMAO** at different Al:Co molar ratios (entries 3 and 6 – 9, Table 3).

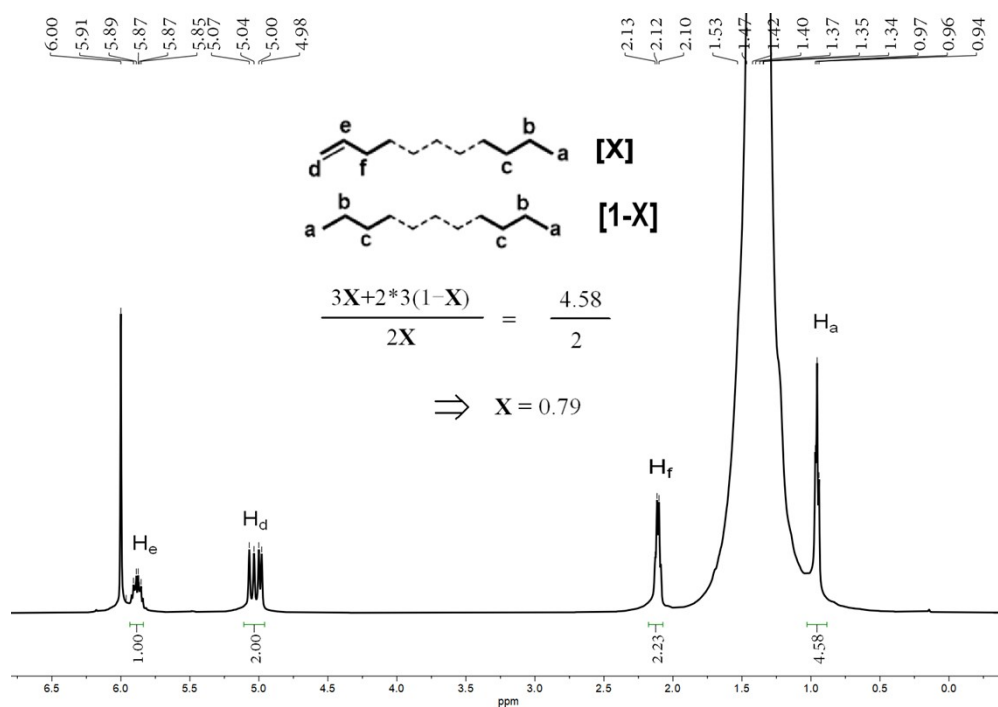


Fig. S3 ¹H NMR spectrum of the polyethylene wax generated using **Co4**/MAO (entry 7, Table 2); recorded in tetrachloroethane-*d*₂ (δH 6.0).



Fig. S4 ¹³C NMR spectrum of the polyethylene sample generated using **Co4**/MAO (entry 7, Table 2); recorded in tetrachloroethane-*d*₂ (δC 74.37).

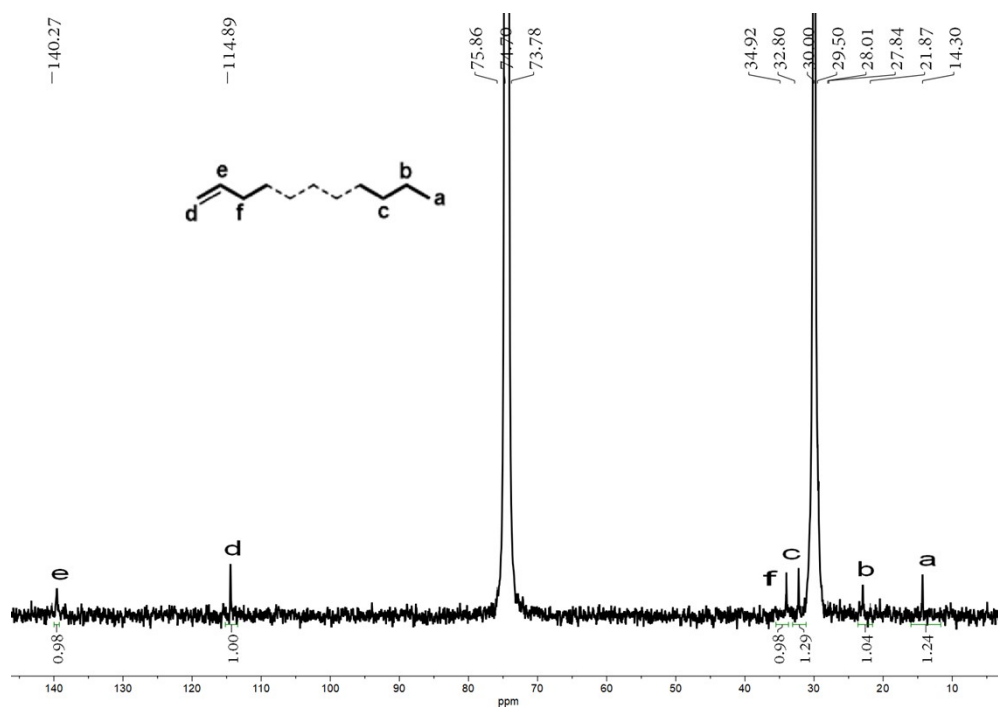


Fig. S5 Inverse-gated decoupled ^{13}C NMR spectrum of the polyethylene wax generated using **Co4**/MAO (entry 7, Table 2); recorded in tetrachloroethane- d_2 (δC 74.70).

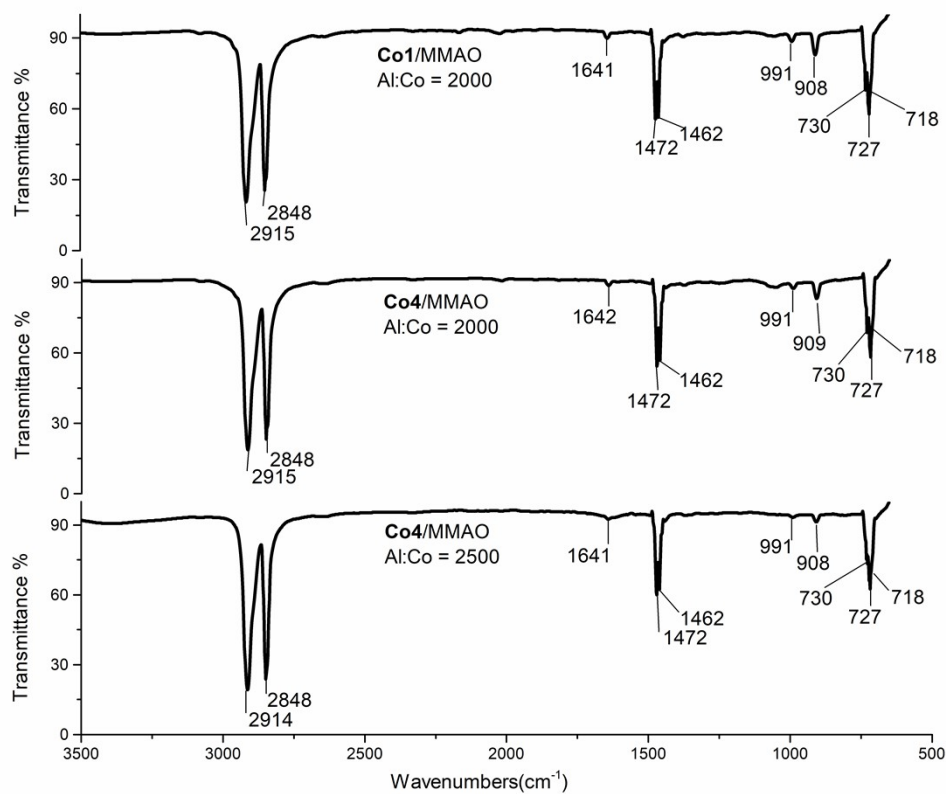


Fig. S6 FT-IR spectra of the polyethylene generated using **Co1**/MMAO (top, entry 15, Table 3) and **Co4**/MMAO (middle, entry 3, Table 3 and bottom, entry 9, Table 3)