Supplementary Information

Catalytic Behaviors of Co^{II} and Mn^{II} Compounds Bearing α-Diimine Ligands for Oxidative Polymerization

Gilvan E. S. Lima,[a] Everton V. Nunes,[a] Roberta C. Dantas,[a] Carlos A. de Simone,[b] Mario R. Meneghetti[a] and Simoni M. P. Meneghetti*[a]

[a]Grupo de Catálise e Reatividade Química, Instituto de Química e Biotecnologia, Universidade Federal de Alagoas, 57072-000 Maceió-AL, Brazil

[b]Instituto de Física de São Carlos, Universidade de São Paulo, 13560-970 São Carlos-SP, Brazil

Table S1. Crystal data for complex **1b**

$C_{29}H_{38}CoN_2O_5$	V = 1762.0 (2) $Å^3$
M_r = 553.54	Z = 2
Triclinic, $P\bar{1}$	D_x = 1.043 Mg m^{-3}
a = 10.5870 (7) Å	Mo Kα
b = 10.6420 (9) Å	μ = 0.52 mm^{-1}
c = 17.0440 (12) Å	T = 293 (2) K
α = 99.700 (4)°	Prism, colorless
β = 104.372 (4)°	0.13 × 0.12 × 0.05 mm
γ = 102.850 (5)°	

Table S2. Data collection for complex **1b**

Kappa CCD diffractometer	6008 independent reflections
CCD rotation images, thick slices scans	4807 reflections with I > 2σ (I)
Absorption correction: XABS2	R_{int} = 0.100
T_{min} = 0.599, T_{max} = 0.944	θ_{max} = 25.0°
15289 measured reflections	

*e-mail: simoni.plentz@gmail.com

Table S3. Refinement for complex **1b**

Refinement on F^2	H-atom parameters constrained
R $[F^2 > 2\sigma (F^2)]$ = 0.102	$w = 1 / [\sigma^2(F_o^2) + (0.1811\ P)^2 + 3.3679\ P]$ where $P = (F_o^2 + 2F_c^2)/3$
wR (F^2) = 0.306	$(\Delta / \sigma)_{max}$ = 0.018
S = 1.04	$\Delta\rho_{max}$ = 1.54 e Å^{-3}
6008 reflections	$\Delta\rho_{min}$ = −0.70 e Å^{-3}
334 parameters	Extinction correction: none

Table S4. Selected geometric parameters, bond distance and angle for complex **1b**

Formula	Bond distance / Å (bond angle / degree)	Formula	Bond distance / Å (bond angle / degree)
Co–O3	2.012 (4)	C5–C12	1.496 (7)
Co–O1W	2.065 (4)	C7–C8	1.401 (8)
Co–N1	2.120 (4)	C7–C17	1.517 (9)
Co–N2	2.120 (4)	C1–C2	1.381 (8)
Co–O1	2.153 (5)	C9–C10	1.356 (9)
Co–O2	2.256 (4)	C9–C8	1.381 (9)
O1–C28	1.259 (7)	C2–C3	1.356 (9)
O2–C28	1.261 (7)	C28–C29	1.514 (9)
O3–C20	1.285 (8)	C29–C32	1.483 (13)
O4–C20	1.248 (9)	C29–C30	1.581 (16)
N1–C1	1.336 (7)	C20–C21	1.714 (15)
N1–C5	1.348 (7)	C12–C13	1.498 (8)
N2–C12	1.275 (7)	C12'–C13'	1.511 (9)
N2–C6	1.443 (6)	C12'–C14	1.531 (9)
C11–C10	1.382 (8)	C32–C33	1.469 (16)
C11–C6	1.409 (8)	C30–C31	1.49 (2)
C11–C12'	1.513 (8)	C33–C34	1.261 (17)
C6–C7	1.390 (8)	C34–C35	1.486 (18)
C4–C3	1.382 (8)	C17–C19	1.522 (11)
C4–C5	1.396 (7)	C17–C18	1.528 (10)
O3–Co–O1W	90.89 (17)	N1–C5–C12	115.3 (4)
O3–Co–N1	169.78 (17)	C4–C5–C12	123.2 (5)
O1W–Co–N1	87.52 (17)	C6–C7–C8	117.8 (6)
O3–Co–N2	94.50 (16)	C6–C7–C17	122.4 (5)
O1W–Co–N2	106.25 (16)	C8–C7–C17	119.7 (6)
N1–Co–N2	76.29 (16)	N1–C1–C2	122.0 (5)

O3–Co–O1	95.12 (18)	C10–C9–C8	120.8 (5)
O1W–Co–O1	154.96 (16)	C9–C8–C7	120.3 (6)
N1–Co–O1	90.54 (17)	C3–C2–C1	120.1 (5)
N2–Co–O1	97.50 (17)	C2–C3–C4	118.9 (5)
O3–Co–O2	93.88 (17)	C9–C10–C11	121.6 (6)
O1W–Co–O2	95.97 (15)	O1–C28–O2	120.4 (5)
N1–Co–O2	96.33 (16)	O1–C28–C29	121.3 (6)
N2–Co–O2	156.08 (18)	O2–C28–C29	118.2 (6)
O1–Co–O2	59.43 (16)	C32–C29–C28	111.7 (7)
C28–O1–Co	92.0 (4)	C32–C29–C30	123.1 (12)
C28–O2–Co	87.3 (3)	C28–C29–C30	107.7 (7)
C20–O3–Co	129.5 (4)	O4–C20–O3	124.7 (6)
C1–N1–C5	118.6 (5)	O4–C20–C21	127.6 (8)
C1–N1–Co	126.4 (4)	O3–C20–C21	107.7 (8)
C5–N1–Co	115.0 (3)	N2–C12–C5	115.4 (5)
C12–N2–C6	121.1 (4)	N2–C12–C13	125.7 (5)
C12–N2–Co	117.8 (3)	C5–C12–C13	118.9 (5)
C6–N2–Co	121.1 (3)	C13'–C12'–C11	110.2 (5)
C10–C11–C6	117.5 (5)	C13'–C12'–C14	110.2 (6)
C10–C11–C12'	121.2 (5)	C11–C12'–C14	113.2 (5)
C6–C11–C12'	121.2 (5)	C33–C32–C29	114.9 (11)
C7–C6–C11	121.9 (5)	C31–C30–C29	114.4 (13)
C7–C6–N2	119.1 (5)	C34–C33–C32	128.0 (12)
C11–C6–N2	119.0 (5)	C33–C34–C35	129.6 (15)
C3–C4–C5	118.9 (5)	C7–C17–C19	110.3 (6)
C3–C4–H4	120.5	C7–C17–C18	112.3 (6)
C5–C4–H4	120.5	C19–C17–C18	110.7 (6)
N1–C5–C4	121.5 (5)		
C10–C11–C6–C7	−0.1 (8)	Co–O2–C28–O1	8.9 (6)
C12'–C11–C6–C7	179.3 (5)	Co–O2–C28–C29	−167.7 (6)
C10–C11–C6–N2	176.6 (5)	O1–C28–C29–C32	59.7 (11)
C12'–C11–C6–N2	−4.0 (8)	O2–C28–C29–C32	−123.7 (9)
C12–N2–C6–C7	−82.7 (7)	O1–C28–C29–C30	−78.3 (13)
Co–N2–C6–C7	96.4 (5)	O2–C28–C29–C30	98.2 (13)
C12–N2–C6–C11	100.5 (6)	Co–O3–C20–O4	1.5 (12)
Co–N2–C6–C11	−80.4 (6)	Co–O3–C20–C21	−179.2 (9)
C1–N1–C5–C4	0.5 (8)	C6–N2–C12–C5	174.0 (5)
Co–N1–C5–C4	−179.3 (4)	Co–N2–C12–C5	−5.2 (7)

C1–N1–C5–C12	−177.1 (5)	C6–N2–C12–C13	−3.4 (9)
Co–N1–C5–C12	3.1 (6)	Co–N2–C12–C13	177.4 (5)
C3–C4–C5–N1	0.0 (9)	N1–C5–C12–N2	1.3 (8)
C3–C4–C5–C12	177.4 (6)	C4–C5–C12–N2	−176.2 (5)
C11–C6–C7–C8	0.0 (9)	N1–C5–C12–C13	178.9 (5)
N2–C6–C7–C8	−176.7 (5)	C4–C5–C12–C13	1.4 (9)
C11–C6–C7–C17	179.7 (6)	C10–C11–C12'–C13'	71.6 (7)
N2–C6–C7–C17	3.0 (9)	C6–C11–C12'–C13'	−107.8 (6)
C5–N1–C1–C2	−0.9 (9)	C10–C11–C12'–C14	−52.3 (8)
Co–N1–C1–C2	178.9 (5)	C6–C11–C12'–C14	128.3 (6)
C10–C9–C8–C7	1.1 (11)	C28–C29–C32–C33	73.5 (12)
C6–C7–C8–C9	−0.5 (10)	C30–C29–C32–C33	−155.9 (11)
C17–C7–C8–C9	179.8 (6)	C32–C29–C30–C31	46 (2)
N1–C1–C2–C3	0.8 (10)	C28–C29–C30–C31	177.7 (17)
C1–C2–C3–C4	−0.2 (10)	C29–C32–C33–C34	109 (2)
C5–C4–C3–C2	−0.2 (10)	C32–C33–C34–C35	170.7 (19)
C8–C9–C10–C11	−1.2 (11)	C6–C7–C17–C19	−115.0 (7)
C6–C11–C10–C9	0.7 (9)	C8–C7–C17–C19	64.7 (8)
C12'|–C11–C10–C9	−178.7 (6)	C6–C7–C17–C18	121.0 (7)
Co–O1–C28–O2	−9.3 (6)	C8–C7–C17–C18	−59.3 (9)
Co–O1–C28–C29	167.2 (6)		