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Supporting information for article:

Conformational polymorphism in a cobalt(II) dithiocarbamate complex

Jetnipat Songkerdthong, Phimphaka Harding and David J. Harding

Computing details

For both structure, data collection: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018) cell refinement: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018); data reduction: *CrysAlis PRO* 1.171.39.46 (Rigaku OD, 2018); program to solve structure: SHELXT (Sheldrick, 2015) program used to refine the data: *SHELXL* 2018/3 (Sheldrick, 2015); molecular graphics: Olex2 1.3 (Dolomanov *et al.*, 2009); software used to prepare material for publication: Olex2 1.3 (Dolomanov *et al.*, 2009). The CCDC numbers for **1a** and **1b** are 2021202 and 2021203, respectively.

Dibutyldithiocarbamate-κ²*S*,*S*′-[hydrotris(3,5-diphenylpyrazol-1-yl-κ*N*²)borato]cobalt(II) Polymorph 1a

Crystal data

[$C_{54}H_{52}BCoN_7S_2$]

M_r = 932.88

Orthorhombic, *Pbca*

T = 150 K

a = 26.26089 (17) Å

b = 12.39989 (8) Å

c = 29.17764 (19) Å

V = 9501.18 (11) Å

Z = 8

Cu $K\alpha$ radiation, λ = 1.54184 Å

Cell measurement from 24286 reflections

θ = 3.0–69.1°

μ = 4.00 mm^{-1}

Block, red

0.27 × 0.19 × 0.14 mm

Data collection

Diffractometer: SuperNova, Single source at offset/far, HyPix3000

Radiation source: micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source

ω scans

Absorption correction: *CrysAlis PRO* 1.171.39.46 (Rigaku Oxford Diffraction, 2018) Analytical numeric absorption correction using a multifaceted crystal model based on expressions derived by R.C. Clark & J.S. Reid. (Clark, R. C. & Reid, J. S. (1995). Acta Cryst. A51, 887-897) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

T_{min} = 0.964, T_{max} = 0.977

41879 measured reflections

8785 independent reflections

7986 reflection with $I > 2\sigma(I)$

R_{int} = 0.039

θ_{max} = 69.3°, θ_{min} = 3.0°

$(\sin \theta/\lambda)_{max}$ = 0.607 Å^{-1}

$h = -31 \rightarrow 31$

$k = -10 \rightarrow 15$

$l = -35 \rightarrow 35$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)]$ = 0.036

$wR(F^2)$ = 0.092

S = 1.03

8785 reflections

662 parameters

69 restraints

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 5.2719P]$ where $P = (F_o^2 + 2F_c^2)/3$

$\Delta\rho_{max} = 0.29$ e Å^{-3}

$\Delta\rho_{min} = -0.44$ e Å^{-3}

Geometric parameters (Å, º)

Co1—S1	2.4449 (5)	C30—H30	0.9500
Co1—S2	2.3531 (5)	C31—C32	1.394 (2)
Co1—N1	2.0901 (14)	C31—C34	1.476 (2)
Co1—N3	2.0733 (15)	C32—H32	0.9500
Co1—N5	2.1774 (14)	C32—C33	1.386 (2)
S1—C46	1.7143 (19)	C33—C40	1.480 (2)
S2—C46	1.7298 (19)	C34—C35	1.391 (2)
N1—N2	1.3692 (18)	C34—C39	1.395 (2)
N1—C1	1.339 (2)	C35—H35	0.9500
N2—C3	1.360 (2)	C35—C36	1.387 (3)
N2—B1	1.549 (2)	C36—H36	0.9500
N3—N4	1.3701 (19)	C36—C37	1.385 (3)
N3—C16	1.350 (2)	C37—H37	0.9500
N4—C18	1.361 (2)	C37—C38	1.387 (3)
N4—B1	1.543 (2)	C38—H38	0.9500
N5—N6	1.3713 (19)	C38—C39	1.386 (3)
N5—C31	1.342 (2)	C39—H39	0.9500
N6—C33	1.360 (2)	C40—C41	1.394 (3)
N6—B1	1.548 (2)	C40—C45	1.392 (3)
N7—C46	1.326 (2)	C41—H41	0.9500
N7—C47	1.497 (4)	C41—C42	1.390 (3)
N7—C51	1.497 (9)	C42—H42	0.9500
N7—C47A	1.535 (11)	C42—C43	1.383 (4)
N7—C51A	1.48 (2)	C43—H43	0.9500
C1—C2	1.398 (2)	C43—C44	1.372 (4)

C1—C4	1.474 (2)	C44—H44	0.9500
C2—H2	0.9500	C44—C45	1.386 (3)
C2—C3	1.383 (2)	C45—H45	0.9500
C3—C10	1.477 (2)	B1—H1	1.061 (18)
C4—C5	1.393 (3)	C47—H47A	0.9900
C4—C9	1.395 (3)	C47—H47B	0.9900
C5—H5	0.9500	C47—C48	1.505 (5)
C5—C6	1.384 (3)	C48—H48B	0.9900
C6—H6	0.9500	C48—H48A	0.9900
C6—C7	1.379 (3)	C48—C49	1.548 (5)
C7—H7	0.9500	C49—H49B	0.9900
C7—C8	1.384 (3)	C49—H49A	0.9900
C8—H8	0.9500	C49—C50	1.502 (5)
C8—C9	1.382 (3)	C50—H50A	0.9800
C9—H9	0.9500	C50—H50B	0.9800
C10—C11	1.396 (2)	C50—H50C	0.9800
C10—C15	1.396 (2)	C51—H51B	0.9900
C11—H11	0.9500	C51—H51A	0.9900
C11—C12	1.384 (3)	C51—C52	1.502 (6)
C12—H12	0.9500	C52—H52A	0.9900
C12—C13	1.385 (3)	C52—H52B	0.9900
C13—H13	0.9500	C52—C53	1.539 (6)
C13—C14	1.387 (3)	C53—H53A	0.9900
C14—H14	0.9500	C53—H53B	0.9900
C14—C15	1.385 (3)	C53—C54	1.535 (6)
C15—H15	0.9500	C54—H54A	0.9800
C16—C17	1.392 (3)	C54—H54B	0.9800
C16—C19	1.470 (2)	C54—H54C	0.9800
C17—H17	0.9500	C47A—H47C	0.9900
C17—C18	1.383 (2)	C47A—H47D	0.9900
C18—C25	1.473 (2)	C47A—C48A	1.47 (2)

C19—C20	1.393 (3)	C48A—H48C	0.9900
C19—C24	1.396 (3)	C48A—H48D	0.9900
C20—H20	0.9500	C48A—C49A	1.470 (16)
C20—C21	1.388 (3)	C49A—H49C	0.9900
C21—H21	0.9500	C49A—H49D	0.9900
C21—C22	1.385 (3)	C49A—C50A	1.600 (17)
C22—H22	0.9500	C50A—H50D	0.9800
C22—C23	1.381 (3)	C50A—H50E	0.9800
C23—H23	0.9500	C50A—H50F	0.9800
C23—C24	1.388 (3)	C51A—H51D	0.9900
C24—H24	0.9500	C51A—H51C	0.9900
C25—C26	1.401 (3)	C51A—C52A	1.552 (14)
C25—C30	1.395 (3)	C52A—H52D	0.9900
C26—H26	0.9500	C52A—H52C	0.9900
C26—C27	1.383 (3)	C52A—C53A	1.478 (14)
C27—H27	0.9500	C53A—H53C	0.9900
C27—C28	1.384 (3)	C53A—H53D	0.9900
C28—H28	0.9500	C53A—C54A	1.500 (15)
C28—C29	1.386 (3)	C54A—H54D	0.9800
C29—H29	0.9500	C54A—H54E	0.9800
C29—C30	1.386 (3)	C54A—H54F	0.9800
S2—Co1—S1	74.611 (17)	C34—C35—H35	119.8
N1—Co1—S1	103.23 (4)	C36—C35—C34	120.42 (16)
N1—Co1—S2	139.95 (4)	C36—C35—H35	119.8
N1—Co1—N5	80.80 (5)	C35—C36—H36	119.9
N3—Co1—S1	101.53 (4)	C37—C36—C35	120.26 (17)
N3—Co1—S2	123.67 (4)	C37—C36—H36	119.9
N3—Co1—N1	96.20 (5)	C36—C37—H37	120.1
N3—Co1—N5	87.42 (5)	C36—C37—C38	119.82 (17)
N5—Co1—S1	169.60 (4)	C38—C37—H37	120.1
N5—Co1—S2	96.07 (4)	C37—C38—H38	120.0

C46—S1—Co1	83.38 (6)	C39—C38—C37	119.92 (17)
C46—S2—Co1	85.92 (6)	C39—C38—H38	120.0
N2—N1—Co1	114.87 (10)	C34—C39—H39	119.6
C1—N1—Co1	138.25 (11)	C38—C39—C34	120.72 (17)
C1—N1—N2	106.86 (13)	C38—C39—H39	119.6
N1—N2—B1	120.88 (13)	C41—C40—C33	123.03 (18)
C3—N2—N1	109.74 (13)	C45—C40—C33	117.87 (17)
C3—N2—B1	127.90 (14)	C45—C40—C41	118.99 (18)
N4—N3—Co1	116.75 (10)	C40—C41—H41	120.2
C16—N3—Co1	133.73 (12)	C42—C41—C40	119.6 (2)
C16—N3—N4	106.71 (14)	C42—C41—H41	120.2
N3—N4—B1	118.93 (13)	C41—C42—H42	119.7
C18—N4—N3	109.89 (13)	C43—C42—C41	120.6 (2)
C18—N4—B1	131.04 (14)	C43—C42—H42	119.7
N6—N5—Co1	114.36 (10)	C42—C43—H43	120.0
C31—N5—Co1	136.69 (11)	C44—C43—C42	120.0 (2)
C31—N5—N6	106.66 (13)	C44—C43—H43	120.0
N5—N6—B1	119.25 (13)	C43—C44—H44	120.0
C33—N6—N5	109.66 (13)	C43—C44—C45	120.0 (2)
C33—N6—B1	131.01 (14)	C45—C44—H44	120.0
C46—N7—C47	120.3 (2)	C40—C45—H45	119.6
C46—N7—C51	120.7 (4)	C44—C45—C40	120.7 (2)
C46—N7—C47A	120.8 (6)	C44—C45—H45	119.6
C46—N7—C51A	121.8 (9)	S1—C46—S2	115.25 (10)
C51—N7—C47	117.0 (4)	N7—C46—S1	123.19 (15)
C51A—N7—C47A	107.3 (9)	N7—C46—S2	121.55 (15)
N1—C1—C2	110.03 (15)	N2—B1—H1	108.0 (10)
N1—C1—C4	122.32 (15)	N4—B1—N2	110.60 (13)
C2—C1—C4	127.64 (16)	N4—B1—N6	108.86 (13)
C1—C2—H2	127.1	N4—B1—H1	110.2 (10)
C3—C2—C1	105.72 (15)	N6—B1—N2	107.90 (13)

C3—C2—H2	127.1	N6—B1—H1	111.3 (10)
N2—C3—C2	107.64 (14)	N7—C47—H47A	108.9
N2—C3—C10	123.34 (15)	N7—C47—H47B	108.9
C2—C3—C10	129.00 (15)	N7—C47—C48	113.6 (3)
C5—C4—C1	121.50 (16)	H47A—C47—H47B	107.7
C5—C4—C9	118.60 (16)	C48—C47—H47A	108.9
C9—C4—C1	119.90 (16)	C48—C47—H47B	108.9
C4—C5—H5	119.7	C47—C48—H48B	109.0
C6—C5—C4	120.52 (19)	C47—C48—H48A	109.0
C6—C5—H5	119.7	C47—C48—C49	113.0 (3)
C5—C6—H6	119.9	H48B—C48—H48A	107.8
C7—C6—C5	120.3 (2)	C49—C48—H48B	109.0
C7—C6—H6	119.9	C49—C48—H48A	109.0
C6—C7—H7	120.1	C48—C49—H49B	109.6
C6—C7—C8	119.82 (19)	C48—C49—H49A	109.6
C8—C7—H7	120.1	H49B—C49—H49A	108.1
C7—C8—H8	119.9	C50—C49—C48	110.3 (3)
C9—C8—C7	120.1 (2)	C50—C49—H49B	109.6
C9—C8—H8	119.9	C50—C49—H49A	109.6
C4—C9—H9	119.7	C49—C50—H50A	109.5
C8—C9—C4	120.59 (19)	C49—C50—H50B	109.5
C8—C9—H9	119.7	C49—C50—H50C	109.5
C11—C10—C3	119.71 (15)	H50A—C50—H50B	109.5
C15—C10—C3	121.33 (15)	H50A—C50—H50C	109.5
C15—C10—C11	118.92 (16)	H50B—C50—H50C	109.5
C10—C11—H11	119.7	N7—C51—H51B	108.4
C12—C11—C10	120.64 (17)	N7—C51—H51A	108.4
C12—C11—H11	119.7	N7—C51—C52	115.4 (6)
C11—C12—H12	120.0	H51B—C51—H51A	107.5
C11—C12—C13	120.01 (18)	C52—C51—H51B	108.4
C13—C12—H12	120.0	C52—C51—H51A	108.4

C12—C13—H13	120.1	C51—C52—H52A	109.3
C12—C13—C14	119.88 (18)	C51—C52—H52B	109.3
C14—C13—H13	120.1	C51—C52—C53	111.6 (5)
C13—C14—H14	119.8	H52A—C52—H52B	108.0
C15—C14—C13	120.31 (18)	C53—C52—H52A	109.3
C15—C14—H14	119.8	C53—C52—H52B	109.3
C10—C15—H15	119.9	C52—C53—H53A	109.5
C14—C15—C10	120.24 (17)	C52—C53—H53B	109.5
C14—C15—H15	119.9	H53A—C53—H53B	108.1
N3—C16—C17	109.61 (15)	C54—C53—C52	110.8 (4)
N3—C16—C19	122.34 (16)	C54—C53—H53A	109.5
C17—C16—C19	127.94 (16)	C54—C53—H53B	109.5
C16—C17—H17	126.8	C53—C54—H54A	109.5
C18—C17—C16	106.40 (15)	C53—C54—H54B	109.5
C18—C17—H17	126.8	C53—C54—H54C	109.5
N4—C18—C17	107.37 (15)	H54A—C54—H54B	109.5
N4—C18—C25	124.88 (15)	H54A—C54—H54C	109.5
C17—C18—C25	127.74 (16)	H54B—C54—H54C	109.5
C20—C19—C16	120.84 (17)	N7—C47A—H47C	110.0
C20—C19—C24	119.20 (18)	N7—C47A—H47D	110.0
C24—C19—C16	119.93 (18)	H47C—C47A—H47D	108.4
C19—C20—H20	119.7	C48A—C47A—N7	108.5 (12)
C21—C20—C19	120.67 (19)	C48A—C47A—H47C	110.0
C21—C20—H20	119.7	C48A—C47A—H47D	110.0
C20—C21—H21	120.1	C47A—C48A—H48C	108.8
C22—C21—C20	119.7 (2)	C47A—C48A—H48D	108.8
C22—C21—H21	120.1	C47A—C48A—C49A	113.9 (13)
C21—C22—H22	120.0	H48C—C48A—H48D	107.7
C23—C22—C21	120.01 (19)	C49A—C48A—H48C	108.8
C23—C22—H22	120.0	C49A—C48A—H48D	108.8
C22—C23—H23	119.7	C48A—C49A—H49C	110.5

C22—C23—C24	120.7 (2)	C48A—C49A—H49D	110.5
C24—C23—H23	119.7	C48A—C49A—C50A	106.2 (15)
C19—C24—H24	120.1	H49C—C49A—H49D	108.7
C23—C24—C19	119.7 (2)	C50A—C49A—H49C	110.5
C23—C24—H24	120.1	C50A—C49A—H49D	110.5
C26—C25—C18	118.51 (16)	C49A—C50A—H50D	109.5
C30—C25—C18	122.93 (16)	C49A—C50A—H50E	109.5
C30—C25—C26	118.55 (17)	C49A—C50A—H50F	109.5
C25—C26—H26	119.7	H50D—C50A—H50E	109.5
C27—C26—C25	120.65 (19)	H50D—C50A—H50F	109.5
C27—C26—H26	119.7	H50E—C50A—H50F	109.5
C26—C27—H27	119.9	N7—C51A—H51D	109.4
C26—C27—C28	120.26 (19)	N7—C51A—H51C	109.4
C28—C27—H27	119.9	N7—C51A—C52A	111.0 (17)
C27—C28—H28	120.2	H51D—C51A—H51C	108.0
C27—C28—C29	119.64 (19)	C52A—C51A—H51D	109.4
C29—C28—H28	120.2	C52A—C51A—H51C	109.4
C28—C29—H29	119.8	C51A—C52A—H52D	110.8
C28—C29—C30	120.5 (2)	C51A—C52A—H52C	110.8
C30—C29—H29	119.8	H52D—C52A—H52C	108.9
C25—C30—H30	119.8	C53A—C52A—C51A	104.6 (13)
C29—C30—C25	120.40 (18)	C53A—C52A—H52D	110.8
C29—C30—H30	119.8	C53A—C52A—H52C	110.8
N5—C31—C32	110.28 (15)	C52A—C53A—H53C	110.4
N5—C31—C34	121.76 (14)	C52A—C53A—H53D	110.4
C32—C31—C34	127.79 (15)	C52A—C53A—C54A	106.7 (13)
C31—C32—H32	127.2	H53C—C53A—H53D	108.6
C33—C32—C31	105.56 (15)	C54A—C53A—H53C	110.4
C33—C32—H32	127.2	C54A—C53A—H53D	110.4
N6—C33—C32	107.81 (14)	C53A—C54A—H54D	109.5
N6—C33—C40	125.34 (15)	C53A—C54A—H54E	109.5

C32—C33—C40	126.85 (16)	C53A—C54A—H54F	109.5
C35—C34—C31	120.44 (15)	H54D—C54A—H54E	109.5
C35—C34—C39	118.84 (16)	H54D—C54A—H54F	109.5
C39—C34—C31	120.70 (15)	H54E—C54A—H54F	109.5

Dibutyldithiocarbamate-κ²*S*,*S*′-[hydrotris(3,5-diphenylpyrazol-1-yl-κ*N*²)borato]cobalt(II) Polymorph 1b

Crystal data

$C_{54}H_{52}BCoN_7S_2$
M_r = 932.88
Triclinic, $P\overline{1}$
T = 150 K
a = 11.69503 (10) Å
b = 15.27162 (13) Å
c = 15.43643 (16) Å
α = 117.4408 (9)°
β = 100.7910 (8)°
γ = 94.2199 (7)°
V = 2362.76 (4) Å^3
Z = 2
F(000) = 978
D_x = 1.311 Mg m^{-3}
Cu Kα radiation, λ = 1.54184 Å
Cell parameters from 22677 reflections
θ = 3.3–68.4°
μ = 4.02 mm^{-1}
Block red
0.26 × 0.22 × 0.18 mm

Data collection

Rigaku SuperNova Single source at offset/far, HyPix3000
Radiation source: micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: Multi-scan *CrysAlis PRO* 1.171.40.81a (Rigaku Oxford Diffraction, 2020) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.
T_{min} = 0.631, T_{max} = 1.000
31970 measured reflections
8636 independent reflections
8250 reflections with $I > 2σ(I)$
R_{int} = 0.048
$θ_{max}$ = 68.5°, $θ_{min}$ = 3.3°
$(\sin θ/λ)_{max}$ = 0.603 Å^{-1}
h = −14→12
k = −18→18
l = −18→18

Refinement

Refinement on F^2
$R[F^2 > 2σ(F^2)]$ = 0.035
$wR(F^2)$ = 0.093
S = 1.05
8636 reflections
630 parameters

37 restraints

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.7689P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$, = 0.46 e Å^{-3}

$\Delta\rho_{min}$ = −0.31 e Å^{-3}

Geometric parameters (Å, º)

Co1—S1	2.4030 (5)	C27—C28	1.388 (3)
Co1—S2	2.3892 (5)	C28—H28	0.9300
Co1—N1	2.1371 (14)	C28—C29	1.377 (3)
Co1—N3	2.0804 (13)	C29—H29	0.9300
Co1—N5	2.1480 (13)	C29—C30	1.387 (3)
S1—C46	1.7169 (18)	C30—H30	0.9300
S2—C46	1.7199 (18)	C31—C32	1.399 (2)
N1—N2	1.3737 (18)	C31—C34	1.476 (2)
N1—C1	1.344 (2)	C32—H32	0.9300
N2—C3	1.358 (2)	C32—C33	1.382 (2)
N2—B1	1.556 (2)	C33—C40	1.476 (2)
N3—N4	1.3735 (18)	C34—C35	1.386 (2)
N3—C16	1.339 (2)	C34—C39	1.391 (3)
N4—C18	1.362 (2)	C35—H35	0.9300
N4—B1	1.541 (2)	C35—C36	1.391 (3)
N5—N6	1.3691 (18)	C36—H36	0.9300
N5—C31	1.341 (2)	C36—C37	1.373 (3)
N6—C33	1.357 (2)	C37—H37	0.9300
N6—B1	1.542 (2)	C37—C38	1.383 (3)
N7—C46	1.331 (2)	C38—H38	0.9300
N7—C47	1.470 (2)	C38—C39	1.387 (3)
N7—C51	1.481 (3)	C39—H39	0.9300
N7—C51A	1.588 (8)	C40—C41	1.397 (2)
C1—C2	1.398 (2)	C40—C45	1.392 (2)

C1—C4	1.470 (2)	C41—H41	0.9300
C2—H2	0.9300	C41—C42	1.385 (3)
C2—C3	1.382 (2)	C42—H42	0.9300
C3—C10	1.480 (2)	C42—C43	1.382 (3)
C4—C5	1.395 (2)	C43—H43	0.9300
C4—C9	1.396 (2)	C43—C44	1.385 (3)
C5—H5	0.9300	C44—H44	0.9300
C5—C6	1.385 (2)	C44—C45	1.388 (2)
C6—H6	0.9300	C45—H45	0.9300
C6—C7	1.387 (3)	C47—H47A	0.9700
C7—H7	0.9300	C47—H47B	0.9700
C7—C8	1.384 (3)	C47—C48	1.517 (3)
C8—H8	0.9300	C48—H48A	0.9700
C8—C9	1.387 (3)	C48—H48B	0.9700
C9—H9	0.9300	C48—C49	1.516 (3)
C10—C11	1.394 (2)	C49—H49A	0.9700
C10—C15	1.393 (3)	C49—H49B	0.9700
C11—H11	0.9300	C49—C50	1.506 (3)
C11—C12	1.389 (3)	C50—H50A	0.9600
C12—H12	0.9300	C50—H50B	0.9600
C12—C13	1.379 (3)	C50—H50C	0.9600
C13—H13	0.9300	B1—H1	1.060 (18)
C13—C14	1.386 (3)	C51—H51A	0.9700
C14—H14	0.9300	C51—H51B	0.9700
C14—C15	1.389 (3)	C51—C52	1.512 (4)
C15—H15	0.9300	C52—H52A	0.9700
C16—C17	1.394 (2)	C52—H52B	0.9700
C16—C19	1.481 (2)	C52—C53	1.527 (5)
C17—H17	0.9300	C53—H53A	0.9700
C17—C18	1.381 (2)	C53—H53B	0.9700

C18—C25	1.478 (2)	C53—C54	1.499 (7)
C19—C20	1.383 (3)	C54—H54C	0.9600
C19—C24	1.393 (3)	C54—H54A	0.9600
C20—H20	0.9300	C54—H54B	0.9600
C20—C21	1.398 (3)	C51A—H51C	0.9700
C21—H21	0.9300	C51A—H51D	0.9700
C21—C22	1.367 (3)	C51A—C52A	1.535 (14)
C22—H22	0.9300	C52A—H52C	0.9700
C22—C23	1.378 (3)	C52A—H52D	0.9700
C23—H23	0.9300	C52A—C53A	1.548 (13)
C23—C24	1.383 (3)	C53A—H53C	0.9700
C24—H24	0.9300	C53A—H53D	0.9700
C25—C26	1.392 (2)	C53A—C54A	1.465 (14)
C25—C30	1.397 (2)	C54A—H54F	0.9600
C26—H26	0.9300	C54A—H54D	0.9600
C26—C27	1.387 (3)	C54A—H54E	0.9600
C27—H27	0.9300		

S2—Co1—S1	74.746 (16)	N5—C31—C34	123.94 (15)
N1—Co1—S1	101.13 (4)	C32—C31—C34	125.97 (15)
N1—Co1—S2	161.55 (4)	C31—C32—H32	127.1
N1—Co1—N5	82.10 (5)	C33—C32—C31	105.87 (14)
N3—Co1—S1	109.37 (4)	C33—C32—H32	127.1
N3—Co1—S2	108.76 (4)	N6—C33—C32	107.52 (14)
N3—Co1—N1	89.62 (5)	N6—C33—C40	123.86 (14)
N3—Co1—N5	92.96 (5)	C32—C33—C40	128.57 (15)
N5—Co1—S1	157.38 (4)	C35—C34—C31	119.74 (16)
N5—Co1—S2	95.05 (4)	C35—C34—C39	118.66 (17)
C46—S1—Co1	84.51 (6)	C39—C34—C31	121.43 (16)
C46—S2—Co1	84.88 (6)	C34—C35—H35	119.7
N2—N1—Co1	113.93 (9)	C34—C35—C36	120.59 (19)

C1—N1—Co1	136.42 (11)	C36—C35—H35	119.7
C1—N1—N2	106.47 (13)	C35—C36—H36	119.8
N1—N2—B1	120.91 (12)	C37—C36—C35	120.3 (2)
C3—N2—N1	109.72 (12)	C37—C36—H36	119.8
C3—N2—B1	129.02 (13)	C36—C37—H37	120.1
N4—N3—Co1	117.84 (10)	C36—C37—C38	119.74 (18)
C16—N3—Co1	134.87 (11)	C38—C37—H37	120.1
C16—N3—N4	106.88 (13)	C37—C38—H38	119.9
N3—N4—B1	118.44 (12)	C37—C38—C39	120.2 (2)
C18—N4—N3	109.68 (13)	C39—C38—H38	119.9
C18—N4—B1	131.87 (13)	C34—C39—H39	119.7
N6—N5—Co1	114.09 (10)	C38—C39—C34	120.52 (19)
C31—N5—Co1	138.64 (11)	C38—C39—H39	119.7
C31—N5—N6	106.64 (12)	C41—C40—C33	121.71 (15)
N5—N6—B1	120.78 (12)	C45—C40—C33	119.27 (15)
C33—N6—N5	110.09 (13)	C45—C40—C41	119.01 (16)
C33—N6—B1	128.94 (13)	C40—C41—H41	120.0
C46—N7—C47	122.22 (16)	C42—C41—C40	120.03 (17)
C46—N7—C51	121.38 (17)	C42—C41—H41	120.0
C46—N7—C51A	115.0 (3)	C41—C42—H42	119.7
C47—N7—C51	115.75 (17)	C43—C42—C41	120.54 (17)
C47—N7—C51A	113.8 (3)	C43—C42—H42	119.7
N1—C1—C2	110.20 (14)	C42—C43—H43	120.0
N1—C1—C4	122.40 (14)	C42—C43—C44	119.95 (17)
C2—C1—C4	127.33 (15)	C44—C43—H43	120.0
C1—C2—H2	127.2	C43—C44—H44	120.1
C3—C2—C1	105.55 (14)	C43—C44—C45	119.82 (18)
C3—C2—H2	127.2	C45—C44—H44	120.1
N2—C3—C2	108.02 (14)	C40—C45—H45	119.7
N2—C3—C10	123.39 (14)	C44—C45—C40	120.64 (16)

C2—C3—C10	128.52 (15)	C44—C45—H45	119.7
C5—C4—C1	121.37 (15)	S1—C46—S2	115.64 (10)
C5—C4—C9	118.67 (15)	N7—C46—S1	122.51 (14)
C9—C4—C1	119.93 (15)	N7—C46—S2	121.81 (14)
C4—C5—H5	119.6	N7—C47—H47A	108.6
C6—C5—C4	120.82 (16)	N7—C47—H47B	108.6
C6—C5—H5	119.6	N7—C47—C48	114.60 (16)
C5—C6—H6	120.0	H47A—C47—H47B	107.6
C5—C6—C7	120.06 (17)	C48—C47—H47A	108.6
C7—C6—H6	120.0	C48—C47—H47B	108.6
C6—C7—H7	120.2	C47—C48—H48A	108.9
C8—C7—C6	119.58 (16)	C47—C48—H48B	108.9
C8—C7—H7	120.2	H48A—C48—H48B	107.7
C7—C8—H8	119.7	C49—C48—C47	113.36 (16)
C7—C8—C9	120.54 (17)	C49—C48—H48A	108.9
C9—C8—H8	119.7	C49—C48—H48B	108.9
C4—C9—H9	119.8	C48—C49—H49A	108.9
C8—C9—C4	120.33 (17)	C48—C49—H49B	108.9
C8—C9—H9	119.8	H49A—C49—H49B	107.7
C11—C10—C3	118.69 (15)	C50—C49—C48	113.24 (18)
C15—C10—C3	122.17 (16)	C50—C49—H49A	108.9
C15—C10—C11	119.13 (16)	C50—C49—H49B	108.9
C10—C11—H11	120.0	C49—C50—H50A	109.5
C12—C11—C10	119.97 (17)	C49—C50—H50B	109.5
C12—C11—H11	120.0	C49—C50—H50C	109.5
C11—C12—H12	119.8	H50A—C50—H50B	109.5
C13—C12—C11	120.39 (18)	H50A—C50—H50C	109.5
C13—C12—H12	119.8	H50B—C50—H50C	109.5
C12—C13—H13	119.9	N2—B1—H1	110.8 (10)
C12—C13—C14	120.22 (17)	N4—B1—N2	108.59 (13)

C14—C13—H13	119.9	N4—B1—N6	109.61 (13)
C13—C14—H14	120.2	N4—B1—H1	110.5 (10)
C13—C14—C15	119.62 (18)	N6—B1—N2	109.24 (13)
C15—C14—H14	120.2	N6—B1—H1	108.1 (10)
C10—C15—H15	119.7	N7—C51—H51A	109.6
C14—C15—C10	120.63 (17)	N7—C51—H51B	109.6
C14—C15—H15	119.7	N7—C51—C52	110.4 (2)
N3—C16—C17	109.77 (14)	H51A—C51—H51B	108.1
N3—C16—C19	124.93 (14)	C52—C51—H51A	109.6
C17—C16—C19	125.25 (15)	C52—C51—H51B	109.6
C16—C17—H17	126.8	C51—C52—H52A	109.2
C18—C17—C16	106.32 (14)	C51—C52—H52B	109.2
C18—C17—H17	126.8	C51—C52—C53	112.0 (3)
N4—C18—C17	107.34 (14)	H52A—C52—H52B	107.9
N4—C18—C25	125.59 (15)	C53—C52—H52A	109.2
C17—C18—C25	127.05 (15)	C53—C52—H52B	109.2
C20—C19—C16	121.62 (16)	C52—C53—H53A	108.6
C20—C19—C24	119.10 (17)	C52—C53—H53B	108.6
C24—C19—C16	118.87 (16)	H53A—C53—H53B	107.5
C19—C20—H20	120.1	C54—C53—C52	114.8 (4)
C19—C20—C21	119.75 (19)	C54—C53—H53A	108.6
C21—C20—H20	120.1	C54—C53—H53B	108.6
C20—C21—H21	119.8	C53—C54—H54C	109.5
C22—C21—C20	120.48 (19)	C53—C54—H54A	109.5
C22—C21—H21	119.8	C53—C54—H54B	109.5
C21—C22—H22	119.9	H54C—C54—H54A	109.5
C21—C22—C23	120.20 (18)	H54C—C54—H54B	109.5
C23—C22—H22	119.9	H54A—C54—H54B	109.5
C22—C23—H23	120.1	N7—C51A—H51C	111.0
C22—C23—C24	119.86 (19)	N7—C51A—H51D	111.0

C24—C23—H23	120.1	H51C—C51A—H51D	109.0
C19—C24—H24	119.7	C52A—C51A—N7	103.6 (6)
C23—C24—C19	120.58 (18)	C52A—C51A—H51C	111.0
C23—C24—H24	119.7	C52A—C51A—H51D	111.0
C26—C25—C18	123.76 (15)	C51A—C52A—H52C	108.9
C26—C25—C30	118.79 (16)	C51A—C52A—H52D	108.9
C30—C25—C18	117.41 (16)	C51A—C52A—C53A	113.5 (9)
C25—C26—H26	119.8	H52C—C52A—H52D	107.7
C27—C26—C25	120.35 (17)	C53A—C52A—H52C	108.9
C27—C26—H26	119.8	C53A—C52A—H52D	108.9
C26—C27—H27	119.9	C52A—C53A—H53C	110.0
C26—C27—C28	120.19 (19)	C52A—C53A—H53D	110.0
C28—C27—H27	119.9	H53C—C53A—H53D	108.4
C27—C28—H28	120.0	C54A—C53A—C52A	108.4 (10)
C29—C28—C27	119.96 (17)	C54A—C53A—H53C	110.0
C29—C28—H28	120.0	C54A—C53A—H53D	110.0
C28—C29—H29	119.9	C53A—C54A—H54F	109.5
C28—C29—C30	120.11 (18)	C53A—C54A—H54D	109.5
C30—C29—H29	119.9	C53A—C54A—H54E	109.5
C25—C30—H30	119.7	H54F—C54A—H54D	109.5
C29—C30—C25	120.56 (18)	H54F—C54A—H54E	109.5
C29—C30—H30	119.7	H54D—C54A—H54E	109.5
N5—C31—C32	109.88 (14)		

Powder X-ray Diffraction and UV-Vis Spectroscopic Data

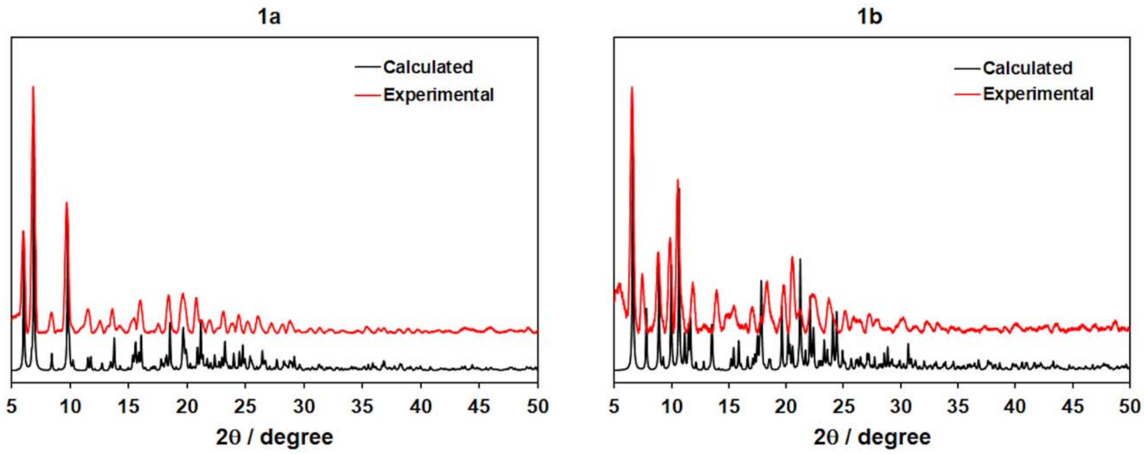

Figure S1 Powder X-ray Diffraction data comparing the calculated and experimental diffractograms of polymorphs **1a** and **1b**.

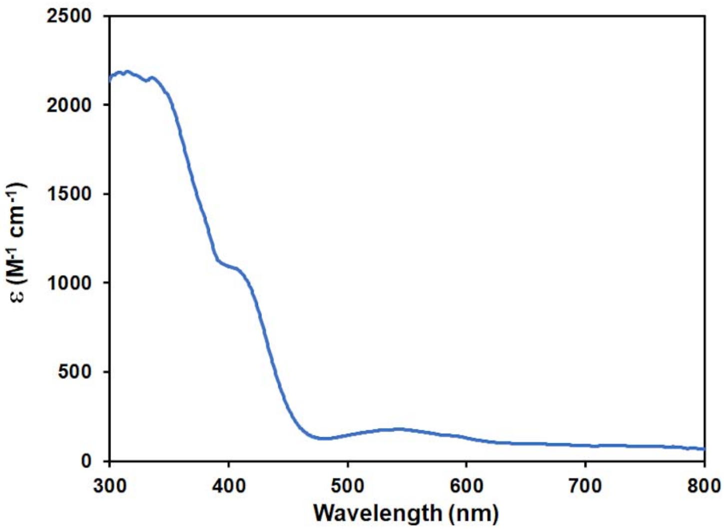

Figure S2 UV-Vis spectrum of [$Tp^{Ph2}Co(S_2CNBu_2)$] in CH_2Cl_2 at room temperature.