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Synthesis, crystal structure and magnetic studies of tetranuclear hydroxo and ligand bridged $[Co_4(\mu_3\text{-}OH)_2(\mu_2\text{-}dea)_2(L\text{-}L)_4]4Cl\cdot 8H_2O$ [H_2dea = diethanolamine, L-L= 2,2′-bipyridine or 1,10-phenanthroline] complexes with mixed valence (Co^{II}_2-Co^{III}_2) defect dicubane core

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Supplementary Information

X-ray crystal structure determination and refinements

Single-crystal X-ray data were collected using graphite- monochromated Mo Kα radiation (λ=0.71073Å). The linear absorption coefficients, scattering factors for the atoms, and the anomalous dispersion corrections were taken from the International Tables for X-ray Crystallography [1]. The data integration and reduction were processed with SAINT Software [2]. An empirical absorption correction was applied to the collected reflections with SADABS [3] using XPREP [4]. The structure was solved by direct methods using SIR-97 [5] and were refined on F^2 by the full-matrix least squares technique using the SHELXL-97 [6] program package. All non-hydrogen atoms were refined with anisotropic displacement parameters.

References:-

[1] International Tables for X-ray Crystallography; Kynoch Press: Birmingham, England, 1974; Vol. IV.

[2] SMART & SAINT Software Reference manuals, Version 6.45; Bruker Analytical X-ray Systems, Inc.: Madison, WI, 2003.

[3] G.M. Sheldrick, SADABS, software for empirical absorption correction, Ver. 2.05; University of Göttingen: Göttingen, Germany, 2002.

[4] XPREP, 5.1 ed.; Siemens Industrial Automation Inc.: Madison, WI, 1995.

[5] G.M. Sheldrick, SHELXL97, Program for Crystal Structure Refinement; University of Göttingen: Göttingen, Germany, 2008.

[6] A. Altomare, M.C. Burla, M. Camalli, G.L. Cascarano, C. Giacovazzo, A. Guagliardi, A.G.G. Moliterni, G. Polidori, R. Spagna, J. Appl. Crystallogr. 32 (1999) 115-119.

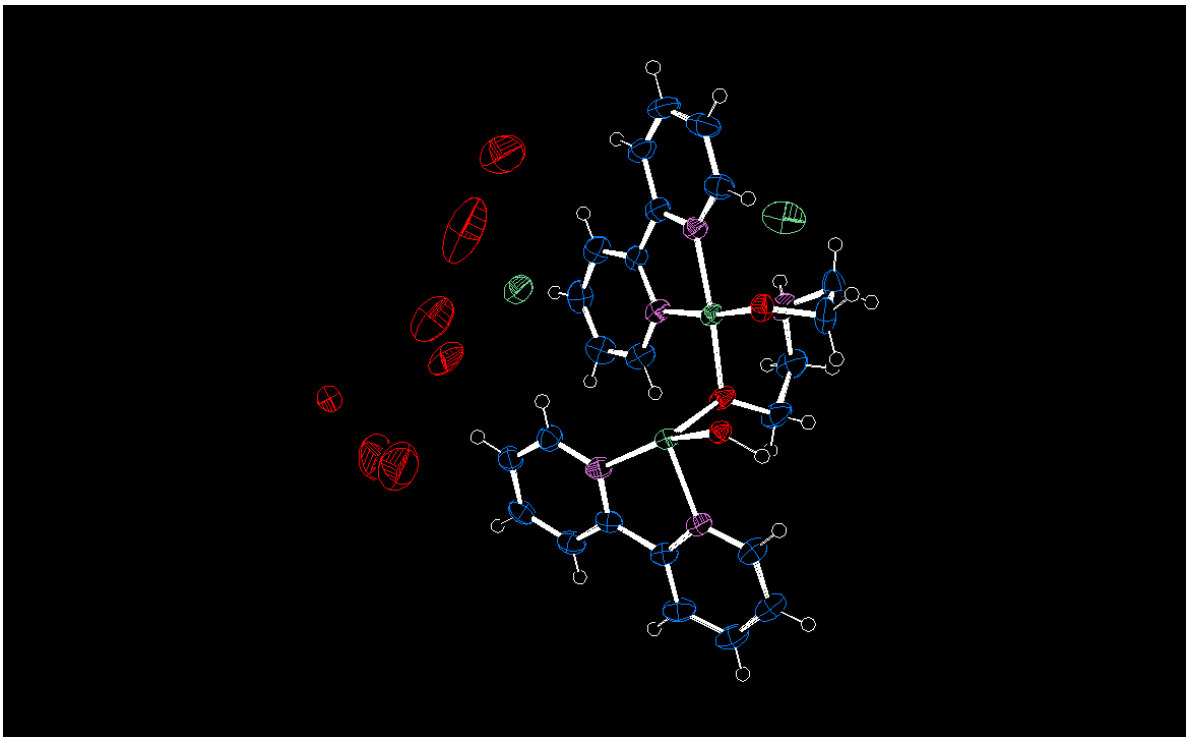

Figure 1S. A perspective view of asymmetric unit of complex **1**.

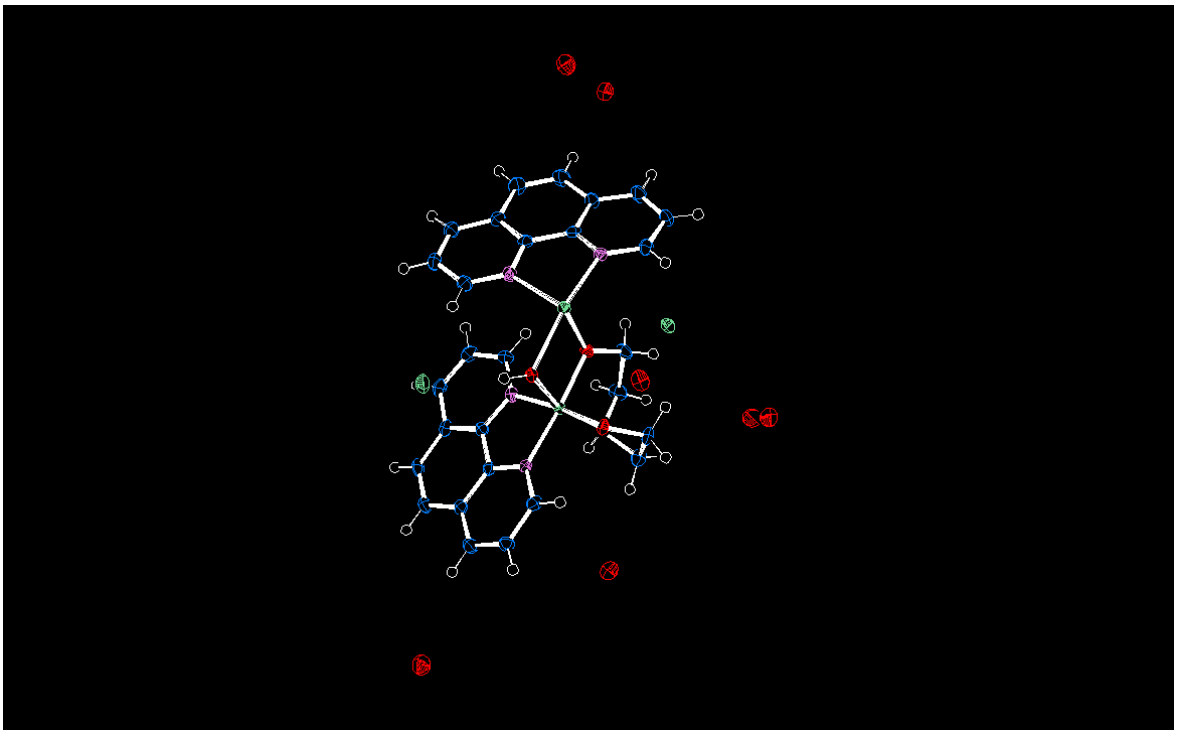

Figure 2S. A perspective view of asymmetric unit of complex **2**.

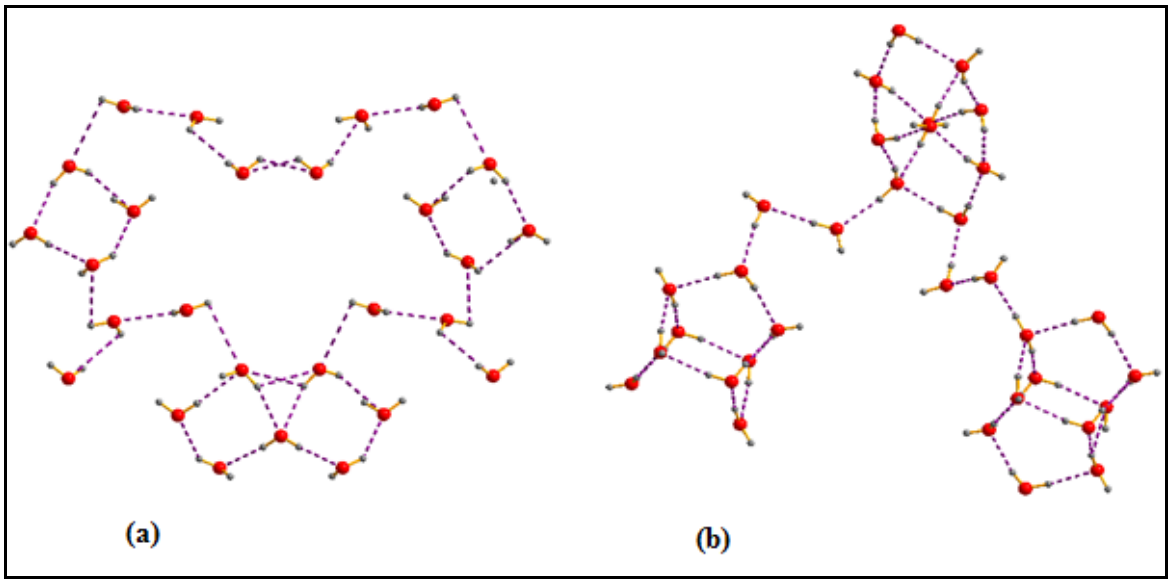

Fig. 3S**.** Water molecules joined through hydrogen bonding (**a**) in compound **1** and (**b**) in compound **2**.

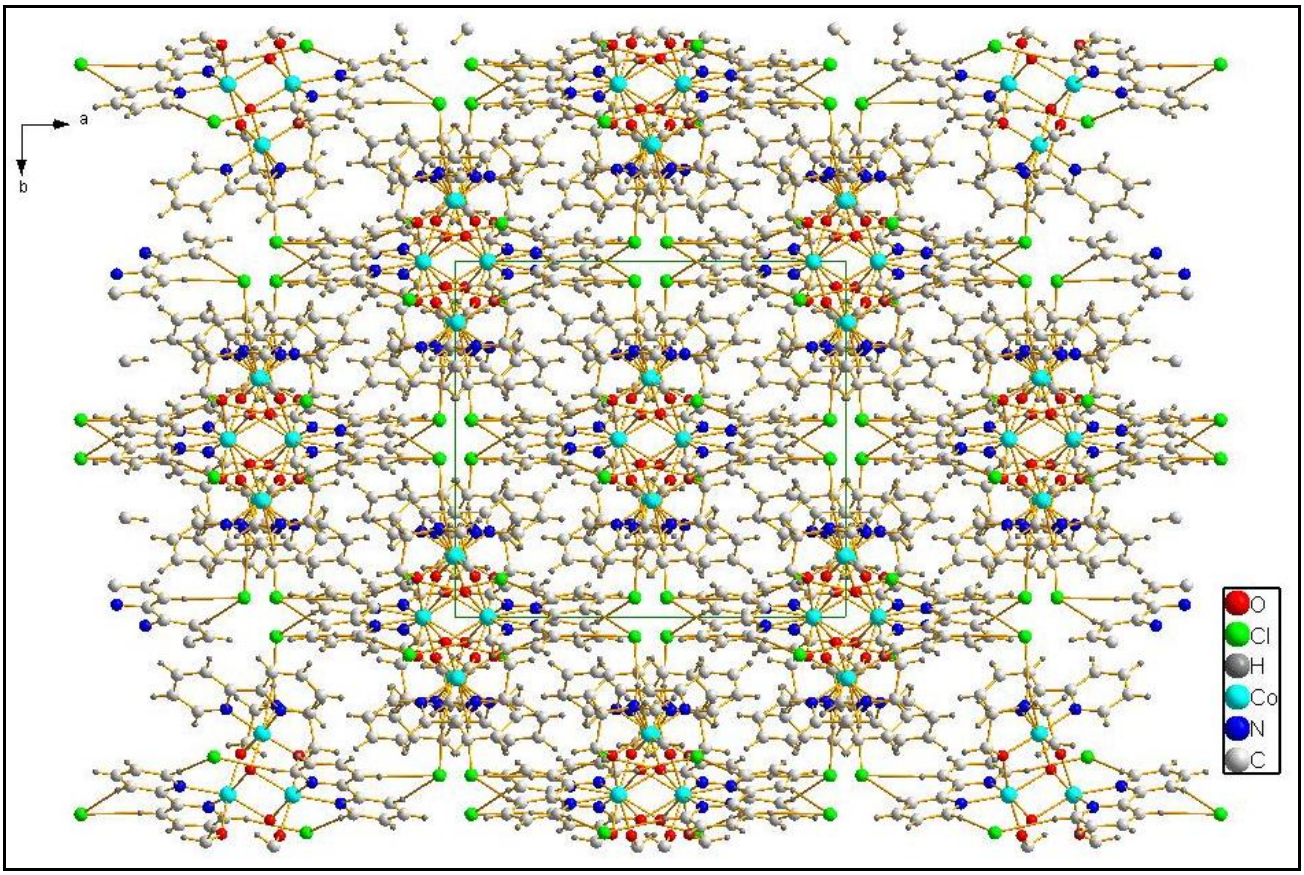

Fig 4S**.** 3D supramolecular network of the complex **1**.

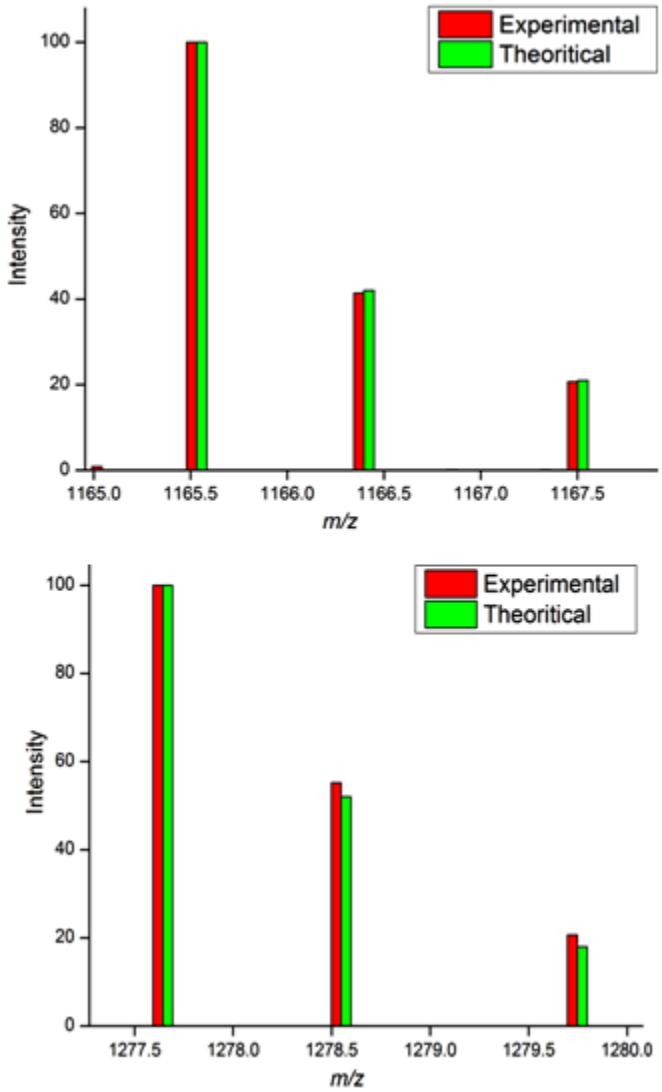

Fig 5S**.** ESI-MS of complexes **1** (top) and **2** (bottom).

Table 1S. Bond Distances (Å) and Bond Angles (^{o}) in **1** and **2**.

Complex 1			
C1—N2	1.347 (7)	C18—H18	0.9300
C1—C2	1.381 (9)	C19—C20	1.379 (8)
C1—H1	0.9300	C19—H19	0.9300
C2—C3	1.358 (10)	C20—N4	1.351 (7)
C2—H2	0.9300	C20—H20	0.9300
C3—C4	1.361 (9)	C21—O2	1.429 (6)
C3—H3	0.9300	C21—C22	1.502 (9)
C4—C5	1.393 (8)	C21—H21A	0.9700
C4—H4	0.9300	C21—H21B	0.9700
C5—N2	1.338 (7)	C22—N5	1.494 (8)
C5—C6	1.465 (8)	C22—H22A	0.9700
C6—N1	1.350 (7)	C22—H22B	0.9700
C6—C7	1.403 (8)	C23—N5	1.473 (9)
C7—C8	1.378 (10)	C23—C24	1.540 (9)
C7—H7	0.9300	C23—H23A	0.9700
C8—C9	1.377 (9)	C23—H23B	0.9700
C8—H8	0.9300	C24—O3	1.415 (7)
C9—C10	1.381 (9)	C24—H24A	0.9700
C9—H9	0.9300	C24—H24B	0.9700
C10—N1	1.338 (8)	N1—Co1	1.949 (5)
C10—H10	0.9300	N2—Co1	1.951 (4)
C11—N3	1.330 (7)	N3—Co2	2.136 (5)
C11—C12	1.389 (8)	N4—Co2	2.110 (5)
C11—H11	0.9300	N5—Co1	1.946 (5)
C12—C13	1.392 (8)	N5—H01	1.00 (7)
C12—H12	0.9300	O1—Co1^{i}	1.928 (3)
C13—C14	1.374 (8)	O1—Co2	2.139 (4)
C13—H13	0.9300	O1—Co2^{i}	2.168 (3)
C14—C15	1.375 (8)	O1—H02	1.04 (10)
C14—H14	0.9300	O2—Co1	1.870 (4)
C15—N3	1.348 (7)	O2—Co2	2.014 (4)
C15—C16	1.498 (8)	O3—Co1	1.870 (4)
C16—N4	1.351 (7)	O3—Co2^{i}	2.051 (4)
C16—C17	1.386 (8)	Co1—O1^{i}	1.928 (3)
C17—C18	1.377 (9)	Co2—O3^{i}	2.051 (4)

C17—H17	0.9300	Co2—O1^{i}	2.168 (3)
C18—C19	1.381 (10)		
N2—C1—C2	121.1 (6)	N5—C23—C24	109.6 (5)
N2—C1—H1	119.5	N5—C23—H23A	109.8
C2—C1—H1	119.5	C24—C23—H23A	109.8
C3—C2—C1	120.1 (6)	N5—C23—H23B	109.8
C3—C2—H2	120.0	C24—C23—H23B	109.8
C1—C2—H2	120.0	H23A—C23—H23B	108.2
C4—C3—C2	119.3 (6)	O3—C24—C23	106.2 (5)
C4—C3—H3	120.4	O3—C24—H24A	110.5
C2—C3—H3	120.4	C23—C24—H24A	110.5
C3—C4—C5	119.2 (6)	O3—C24—H24B	110.5
C3—C4—H4	120.4	C23—C24—H24B	110.5
C5—C4—H4	120.4	H24A—C24—H24B	108.7
N2—C5—C4	121.4 (6)	C10—N1—C6	118.9 (5)
N2—C5—C6	113.7 (5)	C10—N1—Co1	126.2 (4)
C4—C5—C6	124.8 (5)	C6—N1—Co1	114.8 (4)
N1—C6—C7	121.1 (6)	C5—N2—C1	118.9 (5)
N1—C6—C5	114.1 (5)	C5—N2—Co1	115.5 (4)
C7—C6—C5	124.8 (5)	C1—N2—Co1	125.6 (4)
C8—C7—C6	118.9 (6)	C11—N3—C15	118.5 (5)
C8—C7—H7	120.6	C11—N3—Co2	125.4 (4)
C6—C7—H7	120.6	C15—N3—Co2	116.1 (4)
C7—C8—C9	119.7 (6)	C20—N4—C16	117.8 (5)
C7—C8—H8	120.1	C20—N4—Co2	125.2 (4)
C9—C8—H8	120.1	C16—N4—Co2	117.0 (4)
C10—C9—C8	118.6 (6)	C23—N5—C22	115.4 (5)
C10—C9—H9	120.7	C23—N5—Co1	107.7 (4)
C8—C9—H9	120.7	C22—N5—Co1	106.4 (4)
N1—C10—C9	122.7 (6)	C23—N5—H01	113 (4)
N1—C10—H10	118.6	C22—N5—H01	99 (4)
C9—C10—H10	118.6	Co1—N5—H01	115 (4)
N3—C11—C12	122.8 (5)	Co1^{i}—O1—Co2	99.12 (16)
N3—C11—H11	118.6	Co1^{i}—O1—Co2^{i}	98.05 (15)
C12—C11—H11	118.6	Co2—O1—Co2^{i}	93.89 (13)
C11—C12—C13	118.4 (5)	Co1^{i}—O1—H02	109 (5)
C11—C12—H12	120.8	Co2—O1—H02	125 (5)
C13—C12—H12	120.8	Co2^{i}—O1—H02	126 (5)

C14—C13—C12	118.5 (5)	C21—O2—Co1	115.5 (4)
C14—C13—H13	120.8	C21—O2—Co2	134.1 (3)
C12—C13—H13	120.8	Co1—O2—Co2	105.67 (17)
C13—C14—C15	120.1 (5)	C24—O3—Co1	113.7 (4)
C13—C14—H14	120.0	C24—O3—Co2^{i}	134.9 (3)
C15—C14—H14	120.0	Co1—O3—Co2^{i}	104.32 (17)
N3—C15—C14	121.7 (5)	O2—Co1—O3	95.14 (17)
N3—C15—C16	115.1 (5)	O2—Co1—O1^{i}	82.58 (15)
C14—C15—C16	123.2 (5)	O3—Co1—O1^{i}	82.82 (16)
N4—C16—C17	121.9 (5)	O2—Co1—N5	86.10 (19)
N4—C16—C15	114.9 (5)	O3—Co1—N5	87.1 (2)
C17—C16—C15	123.2 (5)	O1^{i}—Co1—N5	164.07 (18)
C18—C17—C16	119.5 (6)	O2—Co1—N1	92.50 (18)
C18—C17—H17	120.2	O3—Co1—N1	171.98 (18)
C16—C17—H17	120.2	O1^{i}—Co1—N1	95.78 (17)
C17—C18—C19	118.9 (6)	N5—Co1—N1	95.9 (2)
C17—C18—H18	120.5	O2—Co1—N2	174.35 (18)
C19—C18—H18	120.5	O3—Co1—N2	90.49 (19)
C20—C19—C18	118.9 (6)	O1^{i}—Co1—N2	97.72 (16)
C20—C19—H19	120.5	N5—Co1—N2	94.6 (2)
C18—C19—H19	120.5	N1—Co1—N2	81.86 (19)
N4—C20—C19	122.8 (6)	O2—Co2—O3^{i}	168.17 (16)
N4—C20—H20	118.6	O2—Co2—N4	89.75 (16)
C19—C20—H20	118.6	O3^{i}—Co2—N4	101.39 (17)
O2—C21—C22	106.0 (5)	O2—Co2—N3	99.45 (17)
O2—C21—H21A	110.5	O3^{i}—Co2—N3	87.07 (16)
C22—C21—H21A	110.5	N4—Co2—N3	76.87 (18)
O2—C21—H21B	110.5	O2—Co2—O1	101.08 (15)
C22—C21—H21B	110.5	O3^{i}—Co2—O1	73.66 (14)
H21A—C21—H21B	108.7	N4—Co2—O1	98.01 (16)
N5—C22—C21	109.5 (5)	N3—Co2—O1	158.81 (16)
N5—C22—H22A	109.8	O2—Co2—O1^{i}	73.53 (14)
C21—C22—H22A	109.8	O3^{i}—Co2—O1^{i}	95.33 (14)
N5—C22—H22B	109.8	N4—Co2—O1^{i}	163.28 (16)
C21—C22—H22B	109.8	N3—Co2—O1^{i}	104.76 (15)
H22A—C22—H22B	108.2	O1—Co2—O1^{i}	86.11 (14)
N2—C1—C2—C3	−1.7 (9)	C24—O3—Co1—N5	−14.7 (4)
C1—C2—C3—C4	−0.2 (9)	Co2^{i}—O3—Co1—N5	−170.0 (2)

C2—C3—C4—C5	1.0 (9)	C24—O3—Co1—N1	−126.6 (12)
C3—C4—C5—N2	0.0 (8)	Co2^{i}—O3—Co1—N1	78.1 (13)
C3—C4—C5—C6	177.9 (5)	C24—O3—Co1—N2	−109.3 (4)
N2—C5—C6—N1	−2.1 (7)	Co2^{i}—O3—Co1—N2	95.37 (19)
C4—C5—C6—N1	179.8 (5)	C23—N5—Co1—O2	−106.1 (4)
N2—C5—C6—C7	177.0 (5)	C22—N5—Co1—O2	18.2 (4)
C4—C5—C6—C7	−1.0 (9)	C23—N5—Co1—O3	−10.8 (4)
N1—C6—C7—C8	1.3 (8)	C22—N5—Co1—O3	113.6 (4)
C5—C6—C7—C8	−177.8 (5)	C23—N5—Co1—O1^{i}	−61.4 (9)
C6—C7—C8—C9	−1.1 (9)	C22—N5—Co1—O1^{i}	62.9 (9)
C7—C8—C9—C10	0.2 (9)	C23—N5—Co1—N1	161.8 (4)
C8—C9—C10—N1	0.5 (9)	C22—N5—Co1—N1	−73.9 (4)
N3—C11—C12—C13	0.2 (9)	C23—N5—Co1—N2	79.5 (4)
C11—C12—C13—C14	0.2 (8)	C22—N5—Co1—N2	−156.2 (4)
C12—C13—C14—C15	0.7 (8)	C10—N1—Co1—O2	2.4 (5)
C13—C14—C15—N3	−1.9 (8)	C6—N1—Co1—O2	178.5 (4)
C13—C14—C15—C16	178.1 (5)	C10—N1—Co1—O3	−159.9 (11)
N3—C15—C16—N4	−3.0 (7)	C6—N1—Co1—O3	16.2 (15)
C14—C15—C16—N4	177.0 (5)	C10—N1—Co1—O1^{i}	−80.4 (5)
N3—C15—C16—C17	176.0 (5)	C6—N1—Co1—O1^{i}	95.8 (4)
C14—C15—C16—C17	−4.0 (8)	C10—N1—Co1—N5	88.8 (5)
N4—C16—C17—C18	−2.7 (9)	C6—N1—Co1—N5	−95.1 (4)
C15—C16—C17—C18	178.4 (5)	C10—N1—Co1—N2	−177.4 (5)
C16—C17—C18—C19	0.4 (9)	C6—N1—Co1—N2	−1.2 (4)
C17—C18—C19—C20	1.4 (9)	C5—N2—Co1—O2	−2.1 (19)
C18—C19—C20—N4	−1.0 (9)	C1—N2—Co1—O2	179 (100)
O2—C21—C22—N5	43.4 (7)	C5—N2—Co1—O3	−177.6 (4)
N5—C23—C24—O3	−43.1 (7)	C1—N2—Co1—O3	3.5 (5)
C9—C10—N1—C6	−0.3 (8)	C5—N2—Co1—O1^{i}	−94.8 (4)
C9—C10—N1—Co1	175.7 (4)	C1—N2—Co1—O1^{i}	86.3 (5)
C7—C6—N1—C10	−0.6 (8)	C5—N2—Co1—N5	95.3 (4)
C5—C6—N1—C10	178.6 (5)	C1—N2—Co1—N5	−83.6 (5)
C7—C6—N1—Co1	−177.0 (4)	C5—N2—Co1—N1	0.0 (4)
C5—C6—N1—Co1	2.2 (6)	C1—N2—Co1—N1	−178.9 (5)
C4—C5—N2—C1	−1.8 (8)	C21—O2—Co2—O3^{i}	136.3 (8)
C6—C5—N2—C1	−179.9 (5)	Co1—O2—Co2—O3^{i}	−16.9 (8)
C4—C5—N2—Co1	179.2 (4)	C21—O2—Co2—N4	−24.2 (6)
C6—C5—N2—Co1	1.1 (6)	Co1—O2—Co2—N4	−177.5 (2)

C2—C1—N2—C5	2.6 (8)	C21—O2—Co2—N3	−100.9 (6)
C2—C1—N2—Co1	−178.5 (4)	Co1—O2—Co2—N3	105.9 (2)
C12—C11—N3—C15	−1.4 (8)	C21—O2—Co2—O1	73.9 (6)
C12—C11—N3—Co2	178.9 (4)	Co1—O2—Co2—O1	−79.37 (19)
C14—C15—N3—C11	2.3 (8)	C21—O2—Co2—O1^{i}	156.4 (6)
C16—C15—N3—C11	−177.8 (5)	Co1—O2—Co2—O1^{i}	3.16 (16)
C14—C15—N3—Co2	−178.0 (4)	C20—N4—Co2—O2	79.5 (5)
C16—C15—N3—Co2	2.0 (6)	C16—N4—Co2—O2	−101.0 (4)
C19—C20—N4—C16	−1.2 (9)	C20—N4—Co2—O3^{i}	−96.5 (5)
C19—C20—N4—Co2	178.3 (4)	C16—N4—Co2—O3^{i}	83.0 (4)
C17—C16—N4—C20	3.1 (8)	C20—N4—Co2—N3	179.3 (5)
C15—C16—N4—C20	−177.9 (5)	C16—N4—Co2—N3	−1.2 (4)
C17—C16—N4—Co2	−176.4 (4)	C20—N4—Co2—O1	−21.6 (5)
C15—C16—N4—Co2	2.6 (6)	C16—N4—Co2—O1	157.9 (4)
C24—C23—N5—C22	−86.9 (6)	C20—N4—Co2—O1^{i}	81.7 (7)
C24—C23—N5—Co1	31.8 (6)	C16—N4—Co2—O1^{i}	−98.8 (6)
C21—C22—N5—C23	80.8 (7)	C11—N3—Co2—O2	−93.3 (5)
C21—C22—N5—Co1	−38.5 (6)	C15—N3—Co2—O2	87.0 (4)
C22—C21—O2—Co1	−28.8 (7)	C11—N3—Co2—O3^{i}	76.8 (5)
C22—C21—O2—Co2	179.9 (4)	C15—N3—Co2—O3^{i}	−102.9 (4)
C23—C24—O3—Co1	34.7 (6)	C11—N3—Co2—N4	179.2 (5)
C23—C24—O3—Co2^{i}	179.8 (4)	C15—N3—Co2—N4	−0.5 (4)
C21—O2—Co1—O3	−80.4 (4)	C11—N3—Co2—O1	101.1 (6)
Co2—O2—Co1—O3	78.61 (19)	C15—N3—Co2—O1	−78.6 (6)
C21—O2—Co1—O1^{i}	−162.5 (4)	C11—N3—Co2—O1^{i}	−18.0 (5)
Co2—O2—Co1—O1^{i}	−3.44 (17)	C15—N3—Co2—O1^{i}	162.3 (4)
C21—O2—Co1—N5	6.3 (4)	Co1^{i}—O1—Co2—O2	171.17 (14)
Co2—O2—Co1—N5	165.3 (2)	Co2^{i}—O1—Co2—O2	72.37 (15)
C21—O2—Co1—N1	102.0 (4)	Co1^{i}—O1—Co2—O3^{i}	2.09 (14)
Co2—O2—Co1—N1	−98.9 (2)	Co2^{i}—O1—Co2—O3^{i}	−96.71 (15)
C21—O2—Co1—N2	104.1 (17)	Co1^{i}—O1—Co2—N4	−97.50 (17)
Co2—O2—Co1—N2	−96.9 (17)	Co2^{i}—O1—Co2—N4	163.70 (16)
C24—O3—Co1—O2	71.1 (4)	Co1^{i}—O1—Co2—N3	−23.3 (5)
Co2^{i}—O3—Co1—O2	−84.19 (18)	Co2^{i}—O1—Co2—N3	−122.1 (4)
C24—O3—Co1—O1^{i}	152.9 (4)	Co1^{i}—O1—Co2—O1^{i}	98.80 (16)
Co2^{i}—O3—Co1—O1^{i}	−2.36 (16)	Co2^{i}—O1—Co2—O1^{i}	0.0

Complex2

Co1—O1	1.870 (2)	C20—C19	1.399 (5)
Co1—O2	1.871 (2)	C20—H20	0.9300
Co1—O01	1.926 (2)	C19—C23	1.418 (5)
Co1—N1	1.936 (3)	C19—C18	1.435 (5)
Co1—N5	1.953 (3)	C28—C27	1.527 (5)
Co1—N4	1.955 (3)	C28—H28A	0.9700
Co2—O2^{i}	2.015 (2)	C28—H28B	0.9700
Co2—O1	2.032 (2)	C17—C18	1.345 (5)
Co2—N2	2.131 (3)	C17—C16	1.437 (5)
Co2—O01	2.140 (2)	C17—H17	0.9300
Co2—O01^{ii}	2.146 (2)	C25—C26	1.516 (5)
Co2—N3	2.148 (3)	C25—H25A	0.9700
O2—C28	1.404 (4)	C25—H25B	0.9700
O2—Co2^{i}	2.015 (2)	C1—C2	1.398 (5)
O1—C25	1.410 (4)	C1—H1	0.9300
O01—Co2^{ii}	2.146 (2)	C7—C11	1.400 (5)
O01—H01	0.81 (4)	C7—C8	1.408 (5)
C12—N5	1.360 (4)	C13—C14	1.401 (5)
C12—C4	1.400 (5)	C13—H13	0.9300
C12—C11	1.423 (5)	C8—C9	1.361 (5)
N1—C27	1.485 (5)	C8—H8	0.9300
N1—C26	1.487 (5)	C18—H18	0.9300
N1—H001	0.78 (4)	C16—C24	1.400 (5)
N4—C10	1.340 (4)	C16—C15	1.409 (5)
N4—C11	1.358 (4)	C24—C23	1.434 (5)
N5—C1	1.336 (4)	C26—H26A	0.9700
C4—C3	1.395 (5)	C26—H26B	0.9700
C4—C5	1.437 (5)	C3—C2	1.366 (5)
N2—C22	1.329 (4)	C3—H3	0.9300
N2—C23	1.362 (4)	C10—C9	1.401 (5)
N3—C13	1.328 (4)	C10—H10	0.9300
N3—C24	1.356 (4)	C27—H27A	0.9700
C6—C5	1.347 (5)	C27—H27B	0.9700
C6—C7	1.442 (5)	C2—H2	0.9300
C6—H6	0.9300	C5—H5	0.9300
C22—C21	1.416 (5)	C9—H9	0.9300
C22—H22	0.9300	C14—C15	1.358 (5)

C21—C20	1.373 (5)	C14—H14	0.9300
C21—H21	0.9300	C15—H15	0.9300
O1—Co1—O2	95.83 (10)	C20—C19—C23	117.5 (3)
O1—Co1—O01	83.00 (10)	C20—C19—C18	124.0 (3)
O2—Co1—O01	82.88 (10)	C23—C19—C18	118.5 (3)
O1—Co1—N1	85.96 (11)	O2—C28—C27	106.1 (3)
O2—Co1—N1	86.74 (12)	O2—C28—H28A	110.5
O01—Co1—N1	163.98 (12)	C27—C28—H28A	110.5
O1—Co1—N5	173.58 (11)	O2—C28—H28B	110.5
O2—Co1—N5	90.55 (11)	C27—C28—H28B	110.5
O01—Co1—N5	97.16 (11)	H28A—C28—H28B	108.7
N1—Co1—N5	95.10 (12)	C18—C17—C16	120.4 (3)
O1—Co1—N4	90.80 (11)	C18—C17—H17	119.8
O2—Co1—N4	173.29 (11)	C16—C17—H17	119.8
O01—Co1—N4	96.93 (11)	O1—C25—C26	107.1 (3)
N1—Co1—N4	94.80 (12)	O1—C25—H25A	110.3
N5—Co1—N4	82.81 (11)	C26—C25—H25A	110.3
O2^{i}—Co2—O1	169.36 (9)	O1—C25—H25B	110.3
O2^{i}—Co2—N2	102.97 (10)	C26—C25—H25B	110.3
O1—Co2—N2	85.83 (10)	H25A—C25—H25B	108.5
O2^{i}—Co2—O01	97.45 (9)	N5—C1—C2	121.8 (3)
O1—Co2—O01	74.11 (9)	N5—C1—H1	119.1
N2—Co2—O01	159.47 (10)	C2—C1—H1	119.1
O2^{ii}—Co2—O01^{ii}	74.24 (9)	C11—C7—C8	116.5 (3)
O1—Co2—O01^{ii}	98.27 (9)	C11—C7—C6	117.9 (3)
N2—Co2—O01^{ii}	102.11 (10)	C8—C7—C6	125.6 (3)
O01—Co2—O01^{ii}	85.39 (9)	N3—C13—C14	122.5 (3)
O2^{ii}—Co2—N3	89.41 (10)	N3—C13—H13	118.8
O1—Co2—N3	98.40 (10)	C14—C13—H13	118.8
N2—Co2—N3	77.76 (11)	C9—C8—C7	119.0 (3)
O01—Co2—N3	100.53 (10)	C9—C8—H8	120.5
O01^{ii}—Co2—N3	163.27 (10)	C7—C8—H8	120.5
C28—O2—Co1	113.7 (2)	C17—C18—C19	121.9 (3)
C28—O2—Co2^{ii}	132.5 (2)	C17—C18—H18	119.0
Co1—O2—Co2^{ii}	104.77 (10)	C19—C18—H18	119.0
C25—O1—Co1	115.5 (2)	C24—C16—C15	116.9 (3)
C25—O1—Co2	136.5 (2)	C24—C16—C17	119.6 (3)
Co1—O1—Co2	104.35 (10)	C15—C16—C17	123.5 (3)

Co1—O01—Co2	98.51 (10)	N4—C11—C7	124.6 (3)
Co1—O01—Co2^{ii}	98.12 (10)	N4—C11—C12	115.0 (3)
Co2—O01—Co2^{ii}	94.61 (9)	C7—C11—C12	120.4 (3)
Co1—O01—H01	121 (3)	N3—C24—C16	123.2 (3)
Co2—O01—H01	125 (3)	N3—C24—C23	116.8 (3)
Co2^{i}—O01—H01	115 (3)	C16—C24—C23	120.0 (3)
N5—C12—C4	123.5 (3)	N1—C26—C25	108.4 (3)
N5—C12—C11	115.6 (3)	N1—C26—H26A	110.0
C4—C12—C11	120.8 (3)	C25—C26—H26A	110.0
C27—N1—C26	114.8 (3)	N1—C26—H26B	110.0
C27—N1—Co1	107.8 (2)	C25—C26—H26B	110.0
C26—N1—Co1	107.4 (2)	H26A—C26—H26B	108.4
C27—N1—H001	109 (3)	C2—C3—C4	120.1 (3)
C26—N1—H001	109 (3)	C2—C3—H3	119.9
Co1—N1—H001	109 (3)	C4—C3—H3	119.9
C10—N4—C11	117.3 (3)	N2—C23—C19	122.5 (3)
C10—N4—Co1	129.2 (2)	N2—C23—C24	118.0 (3)
C11—N4—Co1	113.5 (2)	C19—C23—C24	119.5 (3)
C1—N5—C12	118.0 (3)	N4—C10—C9	121.4 (3)
C1—N5—Co1	128.9 (2)	N4—C10—H10	119.3
C12—N5—Co1	113.0 (2)	C9—C10—H10	119.3
C3—C4—C12	116.8 (3)	N1—C27—C28	109.3 (3)
C3—C4—C5	125.5 (3)	N1—C27—H27A	109.8
C12—C4—C5	117.7 (3)	C28—C27—H27A	109.8
C22—N2—C23	118.6 (3)	N1—C27—H27B	109.8
C22—N2—Co2	127.2 (2)	C28—C27—H27B	109.8
C23—N2—Co2	113.2 (2)	H27A—C27—H27B	108.3
C13—N3—C24	118.1 (3)	C3—C2—C1	119.8 (3)
C13—N3—Co2	128.2 (2)	C3—C2—H2	120.1
C24—N3—Co2	113.6 (2)	C1—C2—H2	120.1
C5—C6—C7	121.3 (3)	C6—C5—C4	121.7 (3)
C5—C6—H6	119.3	C6—C5—H5	119.2
C7—C6—H6	119.3	C4—C5—H5	119.2
N2—C22—C21	122.2 (3)	C8—C9—C10	121.1 (3)
N2—C22—H22	118.9	C8—C9—H9	119.5
C21—C22—H22	118.9	C10—C9—H9	119.5
C20—C21—C22	119.3 (3)	C15—C14—C13	119.5 (3)
C20—C21—H21	120.4	C15—C14—H14	120.2

C22—C21—H21	120.4	C13—C14—H14	120.2
C21—C20—C19	119.8 (3)	C14—C15—C16	119.8 (3)
C21—C20—H20	120.1	C14—C15—H15	120.1
C19—C20—H20	120.1	C16—C15—H15	120.1

O1—Co1—O2—C28	−69.0 (2)	N3—Co2—N2—C22	−175.1 (3)
O01—Co1—O2—C28	−151.1 (2)	O2^{i}—Co2—N2—C23	−93.5 (2)
N1—Co1—O2—C28	16.6 (2)	O1—Co2—N2—C23	92.5 (2)
N5—Co1—O2—C28	111.7 (2)	O01—Co2—N2—C23	80.3 (4)
N4—Co1—O2—C28	120.1 (9)	O01^{ii}—Co2—N2—C23	−169.9 (2)
O1—Co1—O2—Co2^{ii}	82.41 (11)	N3—Co2—N2—C23	−7.0 (2)
O01—Co1—O2—Co2^{ii}	0.24 (10)	O2^{ii}—Co2—N3—C13	−75.0 (3)
N1—Co1—O2—Co2^{ii}	168.02 (13)	O1—Co2—N3—C13	97.7 (3)
N5—Co1—O2—Co2^{ii}	−96.91 (12)	N2—Co2—N3—C13	−178.4 (3)
N4—Co1—O2—Co2^{ii}	−88.5 (9)	O01—Co2—N3—C13	22.5 (3)
O2—Co1—O1—C25	81.2 (2)	O01^{ii}—Co2—N3—C13	−87.1 (4)
O01—Co1—O1—C25	163.3 (2)	O2^{ii}—Co2—N3—C24	109.2 (2)
N1—Co1—O1—C25	−5.1 (2)	O1—Co2—N3—C24	−78.0 (2)
N5—Co1—O1—C25	−104.9 (10)	N2—Co2—N3—C24	5.8 (2)
N4—Co1—O1—C25	−99.9 (2)	O01—Co2—N3—C24	−153.3 (2)
O2—Co1—O1—Co2	−80.90 (11)	O01^{ii}—Co2—N3—C24	97.2 (4)
O01—Co1—O1—Co2	1.17 (10)	C23—N2—C22—C21	0.0 (5)
N1—Co1—O1—Co2	−167.19 (13)	Co2—N2—C22—C21	167.5 (3)
N5—Co1—O1—Co2	93.0 (10)	N2—C22—C21—C20	2.4 (5)
N4—Co1—O1—Co2	98.05 (12)	C22—C21—C20—C19	−1.8 (6)
O2^{ii}—Co2—O1—C25	−119.0 (5)	C21—C20—C19—C23	−1.0 (5)
N2—Co2—O1—C25	27.1 (3)	C21—C20—C19—C18	179.6 (4)
O01—Co2—O1—C25	−157.3 (3)	Co1—O2—C28—C27	−36.8 (3)
O01^{ii}—Co2—O1—C25	−74.5 (3)	Co2^{ii}—O2—C28—C27	−177.9 (2)
N3—Co2—O1—C25	104.1 (3)	Co1—O1—C25—C26	27.2 (4)
O2^{ii}—Co2—O1—Co1	37.2 (5)	Co2—O1—C25—C26	−178.5 (2)
N2—Co2—O1—Co1	−176.66 (12)	C12—N5—C1—C2	−1.0 (5)
O01—Co2—O1—Co1	−1.08 (10)	Co1—N5—C1—C2	−178.0 (2)
O01^{ii}—Co2—O1—Co1	81.69 (11)	C5—C6—C7—C11	1.3 (5)
N3—Co2—O1—Co1	−99.71 (12)	C5—C6—C7—C8	−177.4 (4)
O1—Co1—O01—Co2	−1.08 (10)	C24—N3—C13—C14	0.3 (5)
O2—Co1—O01—Co2	95.72 (10)	Co2—N3—C13—C14	−175.3 (3)
N1—Co1—O01—Co2	45.7 (4)	C11—C7—C8—C9	2.7 (5)
N5—Co1—O01—Co2	−174.62 (10)	C6—C7—C8—C9	−178.5 (3)

N4—Co1—O01—Co2	−91.04 (11)	C16—C17—C18—C19	−0.7 (6)
O1—Co1—O01—Co2^{ii}	−97.02 (10)	C20—C19—C18—C17	177.4 (4)
O2—Co1—O01—Co2^{ii}	−0.22 (9)	C23—C19—C18—C17	−2.0 (6)
N1—Co1—O01—Co2^{ii}	−50.2 (4)	C18—C17—C16—C24	2.2 (6)
N5—Co1—O01—Co2^{ii}	89.44 (11)	C18—C17—C16—C15	−178.3 (4)
N4—Co1—O01—Co2^{ii}	173.02 (10)	C10—N4—C11—C7	0.9 (5)
O2^{ii}—Co2—O01—Co1	−172.35 (9)	Co1—N4—C11—C7	−179.7 (3)
O1—Co2—O01—Co1	1.03 (9)	C10—N4—C11—C12	−178.8 (3)
N2—Co2—O01—Co1	13.7 (3)	Co1—N4—C11—C12	0.6 (4)
O01^{ii}—Co2—O01—Co1	−98.94 (11)	C8—C7—C11—N4	−3.1 (5)
N3—Co2—O01—Co1	96.86 (11)	C6—C7—C11—N4	178.0 (3)
O2^{ii}—Co2—O01—Co2^{ii}	−73.42 (9)	C8—C7—C11—C12	176.6 (3)
O1—Co2—O01—Co2^{ii}	99.97 (10)	C6—C7—C11—C12	−2.3 (5)
N2—Co2—O01—Co2^{ii}	112.6 (3)	N5—C12—C11—N4	1.6 (4)
O01^{ii}—Co2—O01—Co2^{ii}	0.0	C4—C12—C11—N4	−178.8 (3)
N3—Co2—O01—Co2^{ii}	−164.21 (10)	N5—C12—C11—C7	−178.1 (3)
O1—Co1—N1—C27	105.3 (2)	C4—C12—C11—C7	1.4 (5)
O2—Co1—N1—C27	9.2 (2)	C13—N3—C24—C16	−1.0 (5)
O01—Co1—N1—C27	58.8 (5)	Co2—N3—C24—C16	175.2 (3)
N5—Co1—N1—C27	−81.0 (2)	C13—N3—C24—C23	180.0 (3)
N4—Co1—N1—C27	−164.2 (2)	Co2—N3—C24—C23	−3.8 (4)
O1—Co1—N1—C26	−19.0 (2)	C15—C16—C24—N3	0.6 (5)
O2—Co1—N1—C26	−115.1 (2)	C17—C16—C24—N3	−179.8 (3)
O01—Co1—N1—C26	−65.5 (5)	C15—C16—C24—C23	179.5 (3)
N5—Co1—N1—C26	154.7 (2)	C17—C16—C24—C23	−0.9 (5)
N4—Co1—N1—C26	71.5 (2)	C27—N1—C26—C25	−82.2 (4)
O1—Co1—N4—C10	−1.9 (3)	Co1—N1—C26—C25	37.8 (3)
O2—Co1—N4—C10	169.1 (8)	O1—C25—C26—N1	−41.8 (4)
O01—Co1—N4—C10	81.2 (3)	C12—C4—C3—C2	0.3 (5)
N1—Co1—N4—C10	−87.9 (3)	C5—C4—C3—C2	−179.4 (3)
N5—Co1—N4—C10	177.6 (3)	C22—N2—C23—C19	−3.0 (5)
O1—Co1—N4—C11	178.8 (2)	Co2—N2—C23—C19	−172.2 (3)
O2—Co1—N4—C11	−10.2 (10)	C22—N2—C23—C24	176.7 (3)
O01—Co1—N4—C11	−98.1 (2)	Co2—N2—C23—C24	7.5 (4)
N1—Co1—N4—C11	92.8 (2)	C20—C19—C23—N2	3.5 (5)
N5—Co1—N4—C11	−1.7 (2)	C18—C19—C23—N2	−177.1 (3)
C4—C12—N5—C1	0.0 (5)	C20—C19—C23—C24	−176.2 (3)
C11—C12—N5—C1	179.5 (3)	C18—C19—C23—C24	3.2 (5)

C4—C12—N5—Co1	177.5 (3)	N3—C24—C23—N2	−2.5 (5)
C11—C12—N5—Co1	−3.0 (4)	C16—C24—C23—N2	178.5 (3)
O1—Co1—N5—C1	−175.2 (8)	N3—C24—C23—C19	177.2 (3)
O2—Co1—N5—C1	−1.3 (3)	C16—C24—C23—C19	−1.8 (5)
O01—Co1—N5—C1	−84.2 (3)	C11—N4—C10—C9	1.7 (5)
N1—Co1—N5—C1	85.5 (3)	Co1—N4—C10—C9	−177.6 (2)
N4—Co1—N5—C1	179.7 (3)	C26—N1—C27—C28	88.7 (4)
O1—Co1—N5—C12	7.7 (11)	Co1—N1—C27—C28	−31.0 (3)
O2—Co1—N5—C12	−178.4 (2)	O2—C28—C27—N1	43.7 (4)
O01—Co1—N5—C12	98.7 (2)	C4—C3—C2—C1	−1.2 (5)
N1—Co1—N5—C12	−91.6 (2)	N5—C1—C2—C3	1.6 (5)
N4—Co1—N5—C12	2.6 (2)	C7—C6—C5—C4	0.6 (5)
N5—C12—C4—C3	0.4 (5)	C3—C4—C5—C6	178.1 (4)
C11—C12—C4—C3	−179.2 (3)	C12—C4—C5—C6	−1.5 (5)
N5—C12—C4—C5	−180.0 (3)	C7—C8—C9—C10	−0.4 (5)
C11—C12—C4—C5	0.5 (5)	N4—C10—C9—C8	−2.0 (6)
O2^{ii}—Co2—N2—C22	98.4 (3)	N3—C13—C14—C15	1.0 (6)
O1—Co2—N2—C22	−75.6 (3)	C13—C14—C15—C16	−1.4 (6)
O01—Co2—N2—C22	−87.8 (4)	C24—C16—C15—C14	0.7 (5)
O01^{i}—Co2—N2—C22	22.0 (3)	C17—C16—C15—C14	−178.9 (4)

Symmetry code: (i) −*x*, −*y*, −*z*+1, (ii) −*x*, −*y*, −*z*+2.

Table 2S: Hydrogen bonding parameter of complexes **1** and **2**.

Complex 1

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7*W*—H7*A*···Cl1	0.85	2.89	3.167 (19)	101
O7*W*—H7*B*···O5*W*^{i}	0.85	2.10	2.945	175
O5*W*—H5*A*···O3*W*^{ii}	0.85	2.21	2.98 (3)	151
O5*W*—H5*B*···O7*W*^{iii}	0.85	2.43	2.945 (6)	120
O4*W*—H4*A*···O7*W*^{iv}	0.85	2.24	2.94 (2)	139
O4*W*—H4*B*···O2*W*^{v}	0.85	2.55	3.07 (3)	120
O1*W*—H1*C*···O1*W*^{vi}	0.85	2.15	2.69 (5)	122

O1*W*—H1*B*···O2*W*	0.85	2.11	2.82 (4)	140
O3*W*—H3*A*···O4*W*^{ii}	0.85	2.03	2.87 (6)	174
O2*W*—H2*A*···O1*W*	0.85	2.27	2.82 (4)	123
O6*W*—H6*B*···O5*W*^{vii}	0.85	2.92	3.09 (4)	94
O6*W*—H6*A*···O2*W*^{viii}	0.85	2.26	2.71 (5)	114
N1—H1*A*···Cl2	1.0 (3)	2.1 (3)	3.07 (2)	166 (25)
O01—H01···Cl1	0.82 (8)	2.35 (10)	3.159 (14)	169 (28)
	Complex 2			
N1—H001···Cl1^{ix}	0.78 (3)	2.43 (3)	3.200 (3)	168 (3)
O3*W*—H03′···O6*W*^{x}	0.856 (18)	2.03 (2)	2.858 (4)	163 (3)
O5*W*—H05···Cl1^{xi}	0.873 (18)	2.34 (2)	3.197 (3)	167 (3)
O6*W*—H06′···O4*W*^{xii}	0.882 (19)	2.03 (2)	2.880 (4)	161 (4)
O1*W*—H01′···O6*W*^{xiv}	0.867 (18)	2.04 (2)	2.902 (4)	171 (4)
O1*W*—H01···O7*W*	0.882 (19)	1.95 (2)	2.820 (4)	171 (4)
O7*W*—H07···O5*W*^{xiii}	0.867 (19)	1.96 (2)	2.820 (4)	169 (4)
O4*W*—H04′···O7*W*^{xv}	0.870 (19)	2.00 (2)	2.823 (3)	157 (4)
O7*W*—H07′···O3*W*^{xvi}	0.86 (2)	1.92 (3)	2.762 (4)	165 (6)
O2*W*—H02′···Cl1	0.873 (19)	2.47 (2)	3.336 (3)	171 (4)
O3*W*—H03···O4*W*	0.863 (19)	2.03 (2)	2.870 (4)	163 (5)
O4*W*—H04···Cl2^{xiii}	0.872 (19)	2.31 (2)	3.174 (3)	173 (4)
O6*W*—H06···Cl1^{xvii}	0.82 (6)	2.37 (6)	3.166 (3)	165 (6)
O5*W*—H05′···O2*W*^{ix}	0.89 (2)	2.09 (2)	2.969 (4)	169 (7)
O2*W*—H02···O1*W*^{xviii}	0.89 (2)	1.91 (3)	2.785 (4)	165 (10)

Symmetry codes: (i) $x-1/2, y-1/2, z$; (ii) $-x+1/2, -y+1/2, -z+1$; (iii) $x+1/2, y+1/2, z$; (iv) $-x-1/2, y+1/2, -z+1/2$; (v) $-x, -y+1, -z+1$; (vi) $-x, y, -z+3/2$; (vii) $-x, y, -z+1/2$; (viii) $x-1/2, -y+1/2, z-1/2$. (ix) $-x, y-1, -z+1$; (x) $-x, y, -z+1$; (xi) $x, y-1, z$; (xii) $x-1, -y-1, z-1$; (xiii) $-x, -y, -z+2$; (xiv) $x, y+1, z+1$; (xv) $-x, y-1, -z+2$; (xvi) $x-1, -y, z$; (xvii) $x-1, -y, z-1$; (xviii) $-x, -y+1, -z+2$.