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Pentaaqua(1-vinyl-1*H*-imidazole-κN^3)-cobalt(II) sulfate

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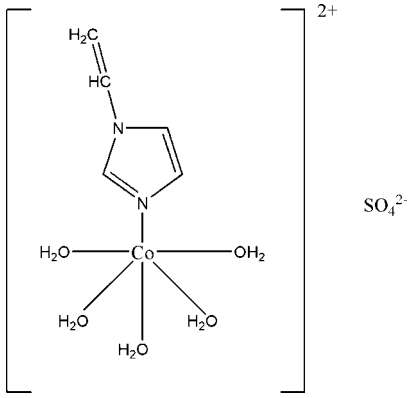
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.041; wR factor = 0.129; data-to-parameter ratio = 12.9.

In the title compound, $[Co(C_5H_6N_2)(H_2O)_5]SO_4$, each Co^{II} ion is coordinated by one N atom from a 1-vinyl-1*H*-imidazole ligand and five water molecules in a distorted octahedral geometry. In the crystal structure, the cations and anions are linked by O—H···O hydrogen bonds into two-dimensional layers parallel to the *ab* plane, with the 1-vinyl-1*H*-imidazole ligands protruding.

Related literature

In the corresponding binuclear cobalt compound $[(pyz)Co_2(H_2O)_{10}](SO_4)_2(H_2O)_2$ (Xie *et al.*, 2004), the two Co^{II} ions have a distorted octahedral environment formed by five water molecules and one N atom from pyz (= pyrazine). In $[Co(viz)_4SiF_6]$ (viz = *N*-vinylimidazole), the Co^{II} ions also have a distorted octahedral environment (Driessen *et al.*, 1982).



Experimental

Crystal data

$[Co(C_5H_6N_2)(H_2O)_5]SO_4$
M_r = 339.19
Triclinic, $P\overline{1}$
a = 6.2070 (12) Å
b = 8.0820 (16) Å
c = 13.409 (3) Å
α = 83.42 (3)°
β = 77.67 (3)°
γ = 82.67 (3)°
V = 649.1 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.52 mm^{-1}
T = 293 (2) K
0.40 × 0.30 × 0.10 mm

Data collection

Bruker SMART 1K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.581, T_{max} = 0.863
2546 measured reflections
2486 independent reflections
2322 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.129
S = 1.06
2486 reflections
193 parameters
15 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected bond lengths (Å).

Co—N1	2.069 (3)	Co—O3	2.103 (3)
Co—O1	2.092 (3)	Co—O4	2.067 (3)
Co—O2	2.141 (3)	Co—O5	2.199 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O5—H5*WA*···O9^{i}	0.85 (3)	1.90 (7)	2.750 (4)	171 (6)
O4—H4*WA*···O6^{ii}	0.85 (3)	1.83 (4)	2.673 (5)	171 (6)
O2—H2*WA*···O7^{iii}	0.85 (3)	1.90 (5)	2.714 (4)	161 (5)
O5—H5*WB*···O8	0.85 (3)	1.99 (4)	2.839 (3)	173 (6)
O2—H2*WB*···O5^{ii}	0.85 (3)	2.10 (5)	2.926 (4)	163 (6)
O4—H4*WB*···O8	0.85 (3)	1.93 (5)	2.752 (4)	162 (7)
O1—H1*WA*···O7^{iv}	0.85 (3)	1.92 (4)	2.765 (4)	169 (6)
O1—H1*WB*···O9^{iii}	0.85 (3)	2.07 (5)	2.818 (4)	146 (6)
O3—H3*WB*···O8^{v}	0.85 (3)	1.88 (5)	2.730 (6)	174 (5)
O3—H3*WA*···O9^{iii}	0.85 (3)	2.10 (5)	2.885 (4)	154 (5)

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x+1, y, z$; (iii) $x+1, y-1, z$; (iv) $x, y-1, z$; (v) $-x+1, -y+2, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and local programs.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2278).

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supplementary materials

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Pentaaqua(1-vinyl-1*H*-imidazole-κN^3)cobalt(II) sulfate

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Comment

In the title compound, (I) (Fig. 1), the local coordination geometry around the Co centre can be described as a distorted octahedron, formed by one N atom from one *N*-vinylimidazole ligand and five O atoms from five water molecules. The Co—N bond distance is 2.069 (3) Å, compared with a value of 2.097 (2) Å in [Co(*viz*)$_4$SiF$_6$] {*viz* is *N*-vinylimidazole; Driessen *et al.*, 1982}. The Co—O bond distances range from 2.067 (3) to 2.199 (2) Å, compared to the similar Co—O(water) bond distances of 2.087 (3), 2.062 (2) and 2.087 (4) Å in [(pyz)Co$_2$(H$_2$O)$_{10}$](SO$_4$)$_2$(H$_2$O)$_2$ (pyz is pyrazine; Xie *et al.*, 2004).

In the crystal, the cations and anions are linked by O—H···O hydrogen bonds into two-dimensional layers parallell to *ab*-plane with the protruding *N*-vinylimidazole ligands.

Experimental

The title compound was prepared by the reaction of *N*-ethylimidazole (0.48 g, 5 mmol) with CoSO$_4$·7H$_2$O(1.40 g, 5 mmol) by means of hydrothermal synthesis in a stainless-steel reactor with a Teflon liner at 383 K for 24 h. Single crystals suitable for X-ray measurements were obtained by recrystallization from ethanol at room temperature.

Refinement

H atoms bonded to O atoms were located in a difference map and were refined with bonds restraints O—H=0.85 (3) Å, H···H 1.37 (2) Å, and with U_{iso}(H) = 0.1. The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and allowed to ride on their parent atoms with U_{iso}(H) = 1.2 times U_{eq}(C).

Figures

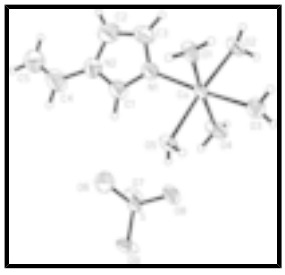
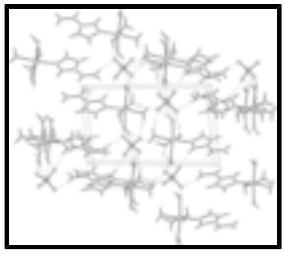


Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.



Pentaaqua(1-vinyl-1*H*-imidazole-κ*N*^{3})cobalt(II) sulfate

Crystal data

$[Co(C_5H_6N_2)(H_2O)_5]SO_4$	$Z = 2$
$M_r = 339.19$	$F_{000} = 350$
Triclinic, $P\overline{1}$	$D_x = 1.735$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.2070$ (12) Å	Cell parameters from 25 reflections
$b = 8.0820$ (16) Å	$\theta = 4$–14º
$c = 13.409$ (3) Å	$\mu = 1.52$ mm^{-1}
$\alpha = 83.42$ (3)º	$T = 293$ (2) K
$\beta = 77.67$ (3)º	Block, pink
$\gamma = 82.67$ (3)º	0.40 × 0.30 × 0.10 mm
$V = 649.1$ (2) Å^3	

Data collection

Bruker SMART 1K CCD area-detector diffractometer	2486 independent reflections
Radiation source: fine-focus sealed tube	2322 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.032$
$T = 293(2)$ K	$\theta_{max} = 26.0$º
thin–slice ω scans	$\theta_{min} = 1.6$º
Absorption correction: multi-scan (SADABS; Sheldrick, 2004)	$h = -7 \rightarrow 7$
$T_{min} = 0.581$, $T_{max} = 0.863$	$k = -9 \rightarrow 9$
2546 measured reflections	$l = 0 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.129$	$w = 1/[\sigma^2(F_o^2) + (0.0813P)^2 + 0.8585P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
2486 reflections	$\Delta\rho_{max}$ = 0.65 e Å^{-3}
193 parameters	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
15 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Co	0.43720 (6)	0.70331 (5)	0.68120 (3)	0.02540 (18)
S	−0.07835 (12)	1.21755 (9)	0.65627 (6)	0.0268 (2)
O1	0.3863 (4)	0.4501 (3)	0.6951 (2)	0.0382 (6)
O2	0.7417 (4)	0.6427 (3)	0.7345 (2)	0.0389 (6)
O3	0.6202 (4)	0.6508 (3)	0.5351 (2)	0.0405 (6)
O4	0.5035 (5)	0.9498 (3)	0.6461 (3)	0.0453 (7)
O5	0.1416 (4)	0.7796 (3)	0.61441 (19)	0.0317 (5)
O6	−0.2029 (5)	1.0888 (4)	0.7207 (3)	0.0533 (8)
O7	−0.0249 (4)	1.3356 (3)	0.7205 (2)	0.0438 (7)
O8	0.1284 (4)	1.1339 (3)	0.5985 (2)	0.0455 (7)
O9	−0.2087 (5)	1.3086 (3)	0.5828 (2)	0.0454 (7)
N1	0.2553 (5)	0.7268 (4)	0.8283 (2)	0.0366 (7)
N2	−0.0162 (6)	0.7876 (5)	0.9575 (3)	0.0474 (8)
C1	0.0593 (6)	0.8068 (5)	0.8561 (3)	0.0417 (9)
H1A	−0.0193	0.8700	0.8105	0.050*
C2	0.1479 (10)	0.6906 (8)	0.9986 (4)	0.0736 (17)
H2A	0.1466	0.6570	1.0674	0.088*
C3	0.3118 (9)	0.6545 (7)	0.9172 (4)	0.0680 (15)
H3A	0.4448	0.5893	0.9215	0.082*
C4	−0.2297 (9)	0.8587 (8)	1.0087 (4)	0.0685 (15)
H4A	−0.3243	0.9171	0.9685	0.082*
C5	−0.2983 (10)	0.8469 (8)	1.1060 (4)	0.0807 (18)
H5A	−0.2079	0.7893	1.1484	0.097*
H5B	−0.4387	0.8959	1.1342	0.097*
H5WA	0.165 (11)	0.741 (7)	0.556 (5)	0.1*
H4WA	0.597 (8)	1.002 (7)	0.664 (6)	0.1*

H2WA	0.787 (10)	0.540 (5)	0.730 (6)	0.1*
H5WB	0.139 (11)	0.886 (5)	0.604 (5)	0.1*
H2WB	0.839 (8)	0.699 (6)	0.695 (5)	0.1*
H4WB	0.389 (6)	1.018 (6)	0.642 (6)	0.1*
H1WA	0.254 (3)	0.427 (8)	0.700 (6)	0.1*
H1WB	0.471 (8)	0.378 (7)	0.659 (5)	0.1*
H3WA	0.703 (9)	0.559 (4)	0.533 (6)	0.1*
H3WB	0.691 (9)	0.723 (6)	0.494 (5)	0.1*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Co	0.0185 (3)	0.0206 (3)	0.0371 (3)	0.00043 (16)	−0.00718 (18)	−0.00281 (17)
S	0.0177 (4)	0.0223 (4)	0.0407 (5)	0.0007 (3)	−0.0093 (3)	−0.0006 (3)
O1	0.0260 (12)	0.0251 (12)	0.0621 (17)	−0.0017 (10)	−0.0049 (12)	−0.0067 (11)
O2	0.0256 (12)	0.0338 (13)	0.0601 (17)	0.0028 (10)	−0.0165 (12)	−0.0071 (12)
O3	0.0371 (14)	0.0331 (14)	0.0460 (15)	0.0013 (11)	0.0001 (11)	−0.0035 (11)
O4	0.0359 (14)	0.0225 (12)	0.083 (2)	−0.0034 (10)	−0.0257 (14)	−0.0012 (13)
O5	0.0255 (11)	0.0267 (12)	0.0442 (14)	0.0024 (9)	−0.0124 (10)	−0.0045 (10)
O6	0.0424 (16)	0.0540 (18)	0.0659 (19)	−0.0204 (14)	−0.0153 (14)	0.0098 (15)
O7	0.0356 (14)	0.0362 (14)	0.0644 (18)	0.0008 (11)	−0.0208 (13)	−0.0100 (13)
O8	0.0306 (13)	0.0355 (14)	0.0631 (18)	0.0112 (11)	−0.0033 (12)	−0.0019 (12)
O9	0.0458 (16)	0.0413 (15)	0.0507 (16)	0.0193 (12)	−0.0253 (13)	−0.0082 (12)
N1	0.0316 (15)	0.0393 (17)	0.0374 (16)	0.0030 (13)	−0.0070 (13)	−0.0042 (13)
N2	0.0397 (18)	0.055 (2)	0.0436 (18)	−0.0001 (16)	−0.0024 (15)	−0.0039 (16)
C1	0.036 (2)	0.047 (2)	0.042 (2)	0.0025 (17)	−0.0082 (16)	−0.0093 (16)
C2	0.073 (4)	0.092 (4)	0.040 (2)	0.018 (3)	−0.002 (2)	0.009 (2)
C3	0.055 (3)	0.083 (4)	0.053 (3)	0.026 (3)	−0.009 (2)	0.008 (3)
C4	0.050 (3)	0.091 (4)	0.056 (3)	0.017 (3)	−0.005 (2)	−0.010 (3)
C5	0.063 (3)	0.094 (4)	0.065 (3)	0.018 (3)	0.009 (3)	0.004 (3)

Geometric parameters (Å, °)

Co—N1	2.069 (3)	O4—H4WB	0.85 (3)
Co—O1	2.092 (3)	O5—H5WA	0.85 (3)
Co—O2	2.141 (3)	O5—H5WB	0.85 (3)
Co—O3	2.103 (3)	N1—C1	1.303 (5)
Co—O4	2.067 (3)	N1—C3	1.361 (6)
Co—O5	2.199 (2)	N2—C1	1.338 (5)
S—O6	1.463 (3)	N2—C2	1.376 (6)
S—O7	1.467 (3)	N2—C4	1.437 (6)
S—O8	1.476 (3)	C1—H1A	0.9300
S—O9	1.479 (3)	C2—C3	1.354 (7)
O1—H1WA	0.85 (3)	C2—H2A	0.9300
O1—H1WB	0.85 (3)	C3—H3A	0.9300
O2—H2WA	0.85 (3)	C4—C5	1.279 (7)
O2—H2WB	0.86 (3)	C4—H4A	0.9300
O3—H3WA	0.85 (3)	C5—H5A	0.9300
O3—H3WB	0.85 (3)	C5—H5B	0.9300

O4—H4WA	0.85 (3)		
O4—Co—N1	97.60 (13)	H3WA—O3—H3WB	107 (6)
O4—Co—O1	172.04 (12)	Co—O4—H4WA	130 (5)
N1—Co—O1	90.19 (12)	Co—O4—H4WB	114 (4)
O4—Co—O3	88.68 (13)	H4WA—O4—H4WB	108 (5)
N1—Co—O3	173.68 (11)	Co—O5—H5WA	108 (5)
O1—Co—O3	83.56 (11)	Co—O5—H5WB	104 (5)
O4—Co—O2	90.23 (11)	H5WA—O5—H5WB	107 (6)
N1—Co—O2	92.21 (12)	C1—N1—C3	105.0 (4)
O1—Co—O2	91.12 (11)	C1—N1—Co	128.0 (3)
O3—Co—O2	86.96 (11)	C3—N1—Co	126.9 (3)
O4—Co—O5	85.84 (10)	C1—N2—C2	106.7 (4)
N1—Co—O5	91.87 (11)	C1—N2—C4	124.2 (4)
O1—Co—O5	92.29 (10)	C2—N2—C4	129.1 (4)
O3—Co—O5	89.36 (11)	N1—C1—N2	112.4 (4)
O2—Co—O5	174.67 (10)	N1—C1—H1A	123.8
O6—S—O7	109.97 (19)	N2—C1—H1A	123.8
O6—S—O8	108.12 (19)	C3—C2—N2	105.1 (4)
O7—S—O8	109.66 (17)	C3—C2—H2A	127.4
O6—S—O9	110.33 (18)	N2—C2—H2A	127.4
O7—S—O9	109.81 (16)	C2—C3—N1	110.7 (4)
O8—S—O9	108.92 (17)	C2—C3—H3A	124.6
Co—O1—H1WA	117 (5)	N1—C3—H3A	124.6
Co—O1—H1WB	123 (5)	C5—C4—N2	124.4 (5)
H1WA—O1—H1WB	107 (6)	C5—C4—H4A	117.8
Co—O2—H2WA	110 (5)	N2—C4—H4A	117.8
Co—O2—H2WB	108 (5)	C4—C5—H5A	120.0
H2WA—O2—H2WB	107 (6)	C4—C5—H5B	120.0
Co—O3—H3WA	115 (5)	H5A—C5—H5B	120.0
Co—O3—H3WB	123 (5)		
O4—Co—N1—C1	68.8 (4)	C2—N2—C1—N1	1.7 (6)
O1—Co—N1—C1	−109.5 (4)	C4—N2—C1—N1	−178.5 (4)
O2—Co—N1—C1	159.3 (3)	C1—N2—C2—C3	−1.3 (7)
O5—Co—N1—C1	−17.2 (3)	C4—N2—C2—C3	178.9 (5)
O4—Co—N1—C3	−114.5 (4)	N2—C2—C3—N1	0.6 (7)
O1—Co—N1—C3	67.1 (4)	C1—N1—C3—C2	0.4 (7)
O2—Co—N1—C3	−24.0 (4)	Co—N1—C3—C2	−176.8 (4)
O5—Co—N1—C3	159.4 (4)	C1—N2—C4—C5	−176.7 (6)
C3—N1—C1—N2	−1.3 (5)	C2—N2—C4—C5	3.1 (10)
Co—N1—C1—N2	175.9 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H5WA···O9^{i}	0.85 (3)	1.90 (7)	2.750 (4)	171 (6)
O4—H4WA···O6^{ii}	0.85 (3)	1.83 (4)	2.673 (5)	171 (6)
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O3—H3WB···O8^{v}	0.85 (3)	1.88 (5)	2.730 (6)	174 (5)
O3—H3WA···O9^{iii}	0.85 (3)	2.10 (5)	2.885 (4)	154 (5)

Symmetry codes: (i) −*x*, −*y*+2, −*z*+1; (ii) *x*+1, *y*, *z*; (iii) *x*+1, *y*−1, *z*; (iv) *x*, *y*−1, *z*; (v) −*x*+1, −*y*+2, −*z*+1.

Fig. 1

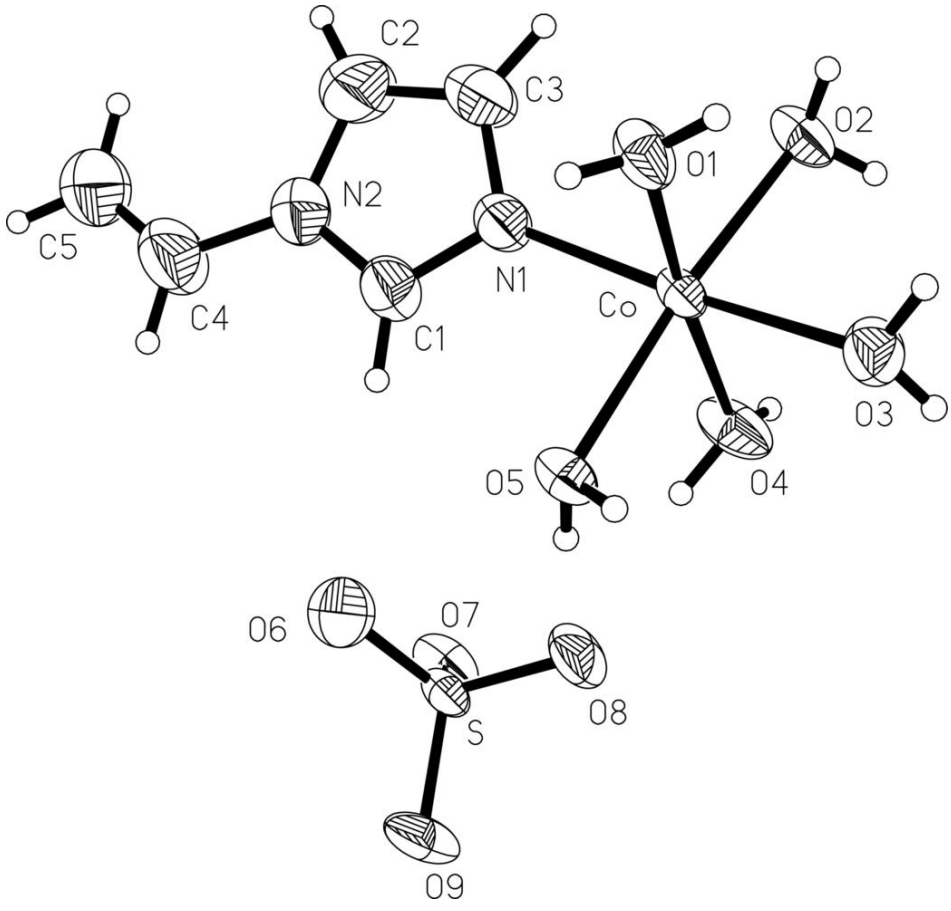

Fig. 2