

Inorganic Chemistry

including bioinorganic chemistry

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Table S1. Crystallographic data and structure refinement for **1**.

Empirical formula	C ₃₆ H ₂₄ Cl ₁ Co ₃ N ₆ O ₁₆
Formula weight	1008.85
Temperature	293(2) K
Wavelength	1.54179 Å
Crystal system	cubic
Space group	p 4 ₁ 3 2
Unit cell dimensions	a = 15.287(2) Å
Volume	3572.5(8) Å ³
Z	8
Density (calculated)	1.876 Mg/m ³
Absorption coefficient	12.271 mm ⁻¹
F(000)	2032
Crystal size	0.37 x 0.33 x 0.22 mm
Theta range for data collection	4.09 to 59.18°
Index ranges	0 ≤ h ≤ 17, -16 ≤ k ≤ 16, -11 ≤ l ≤ 12
Reflections collected	2809
Independent reflections	859 [R(int) = 0.1576]
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	819 / 0 / 104
Goodness-of-fit on F ²	0.898
Final R indices [I > 2σ(I)]	R(F ²) = 0.0523, wR(F ²) = 0.0958
R indices (all data)	R(F ²) = 0.1171, wR(F ²) = 0.2023
Absolute structure parameter	0.02(2)
Extinction coefficient	0.00012(7)
Largest diff. peak and hole	0.261 and -0.378 e.Å ⁻³

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Table S2. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Co(1)	23(1)	23(1)	23(1)	-1(1)	1(1)	1(1)
Co(2)	29(1)	29(1)	29(1)	1(1)	1(1)	1(1)
Cl(1)	51(1)	51(1)	51(1)	6(2)	6(2)	-6(2)
O(1)	42(3)	32(3)	38(4)	1(3)	-2(3)	4(3)
O(2)	14(3)	42(3)	48(4)	8(3)	0(3)	-1(2)
N(1)	17(3)	35(4)	23(4)	-3(3)	-3(3)	4(3)
C(1)	20(5)	47(5)	40(5)	-5(4)	1(4)	0(4)
C(2)	20(4)	63(6)	52(6)	0(4)	-2(4)	-7(4)
C(3)	29(5)	72(7)	43(5)	-1(5)	7(4)	-8(5)
C(4)	23(5)	49(5)	37(5)	1(4)	3(4)	-6(4)
C(5)	26(4)	35(5)	18(4)	5(4)	0(4)	-11(3)
C(6)	29(4)	29(4)	28(7)	1(4)	-1(4)	-2(5)
C(7)	34(4)	34(4)	31(7)	6(4)	-6(4)	-7(5)
O(3)	114(16)	154(22)	57(11)	13(12)	50(8)	-13(13)
O(4)	145(15)	145(15)	145(15)	45(12)	-45(12)	45(12)

Table S3. Final Atomic Coordinates^a and Equivalent Isotropic Displacement Parameters^b for Non-Hydrogen Atoms of Compound 1

atom	<i>x/a</i>	<i>y/b</i>	<i>z/c</i>	10 ³ <i>U</i> _{eq} , Å ²
Co(1)	0.3750	0.6250	0.1250	23(1)
Co(2)	0.1048(1)	0.1048(1)	0.1048(1)	29(1)
Cl(1)	0.6250	0.8750	0.1250	51(1)
O(1)	-0.0308(3)	0.1154(3)	0.1107(3)	37(1)
O(2)	0.0944(3)	0.2395(3)	0.1140(4)	35(1)
N(1)	0.2500(3)	0.6175(4)	0.1247(4)	25(2)
C(1)	0.1927(5)	0.6843(6)	0.1287(5)	36(2)
C(2)	0.1025(5)	0.6712(6)	0.1361(6)	45(2)
C(3)	0.0708(6)	0.5872(6)	0.1326(5)	48(2)
C(4)	0.1269(5)	0.5183(5)	0.1306(5)	36(2)
C(5)	0.2181(5)	0.5339(5)	0.1256(5)	26(2)
C(6)	-0.0570(5)	0.1930(5)	0.1250(5)	29(3)
C(7)	0.0166(5)	0.2666(5)	0.1250(5)	33(3)
O(3) ^c	0.6815(12)	0.9178(11)	0.0612(10)	108(7)
O(4) ^d	0.5697(12)	0.9303(12)	0.0697(12)	145(15)

^a Estimated standard deviations in the last significant digits are given in parentheses.

^b $U_{eq} = 1/3 \sum_i \sum_j a_i a_j \mathbf{a}_i \mathbf{a}_j$. ^c Site occupancy factor 0.167. ^d Site occupancy factor 0.500.

POOR QUALITY ORIGINAL**Table S4.** Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for **1***

Atom	x	y	z
H(1)	2139(5)	7413(6)	1265(5)
H(2)	648(5)	7183(6)	1432(6)
H(3)	107(6)	5775(6)	1316(5)
H(4)	1056(5)	4614(5)	1324(5)

$$U_{\text{iso}} = 54.2 \text{ \AA}^2 \times 10^3$$

Table S5. Non-Essential Bond Lengths (Å) and Angles (deg)^{a,b} for Compound 1

2,2'-Bipyridine Ligand			
N(1)-C(1)	1.347(9)	C(1)-C(2)	1.398(10)
N(1)-C(5)	1.369(9)	C(2)-C(3)	1.373(12)
		C(3)-C(4)	1.359(10)
		C(4)-C(5)	1.416(11)
		C(5)-C(5) ^{iv}	1.423(14)
C(1)-N(1)-C(5)	118.4(6)	C(3)-C(4)-C(5)	119.5(8)
N(1)-C(1)-C(2)	122.4(8)	N(1)-C(5)-C(4)	120.6(6)
C(3)-C(2)-C(1)	118.7(8)	N(1)-C(5)-C(5) ^v	114.1(4)
C(4)-C(3)-C(2)	120.1(8)	C(4)-C(5)-C(5) ^v	125.3(4)
Perchlorate Anion ^b			
Cl(1)-O(3)	1.548(12)	Cl(1)-O(4)	1.470(3)
O(3)-Cl(1)-O(4)	107.6(8)	O(3)-Cl(1)-O(3) ^{iv}	111.2(7)

^aEstimated standard deviations in the last significant digits are given in parentheses.

^bSymmetry code: (iv) $x+1/4$, $y-1/4$, $-z+1/4$; (v) x , y , z .

Table S.6. Least-square planes and dihedral angles.

Weighted least-squares planes through the starred atoms
(Nardelli, Musatti, Domiano & Andreotti Ric.Sci.(1965),15(II-A),807).
Equation of the plane: $m_1X+m_2Y+m_3Z=d$

Plane 1

$m_1 = -.05512(.00298)$
 $m_2 = .01816(.00321)$
 $m_3 = -.99831(.00018)$
 $D = -1.94620(.03058)$

Atom	d	s	d/s	(d/s)**2
N1 *	.0038	.0061	.627	.393
C1 *	.0095	.0073	1.291	1.666
C2 *	-.0307	.0084	-3.648	13.310
C3 *	.0265	.0080	3.338	11.143
C4 *	-.0092	.0081	-1.135	1.289
C5 *	-.0059	.0069	-.854	.729

Sum((d/s)**2) for starred atoms 28.529

Chi-squared at 95% for 3 degrees of freedom: 7.81

The group of atoms deviates significantly from planarity

Plane 2

$m_1 = -.01815(.00356)$
 $m_2 = .05512(.00297)$
 $m_3 = -.99831(.00017)$
 $D = -1.58906(.02828)$

Atom	d	s	d/s	(d/s)**2
N1C *	-.0038	.0061	-.627	.393
C1C *	-.0095	.0073	-1.290	1.663
C2C *	.0307	.0084	3.647	13.299
C3C *	-.0265	.0080	-3.336	11.132
C4C *	.0092	.0081	1.135	1.288
C5C *	.0059	.0069	.853	.727

Sum((d/s)**2) for starred atoms 28.502

Chi-squared at 95% for 3 degrees of freedom: 7.81

The group of atoms deviates significantly from planarity

Plane 3

$m_1 = .00030(.00435)$
 $m_2 = -.00030(.00443)$
 $m_3 = -1.00000(.00000)$
 $D = -1.91200(.04858)$

Atom	d	s	d/s	(d/s)**2
N1 *	.0041	.0061	.663	.440
C5 *	-.0092	.0069	-1.332	1.774
C5C *	.0092	.0069	1.332	1.774
N1C *	-.0041	.0061	-.663	.440
Co1	.0000	.0001	.001	.000

Sum((d/s)**2) for starred atoms 4.429

Chi-squared at 95% for 1 degrees of freedom: 3.84

The group of atoms deviates significantly from planarity

Plane 4

$m_1 = -.00053(.00426)$
 $m_2 = 1.00000(.00000)$
 $m_3 = .00053(.00433)$

D = 9.55233 (.03948)

Atom	d	s	d/s	(d/s)**2
N1B *	-.0036	.0060	-.608	.370
C5B *	.0094	.0072	1.309	1.712
C5D *	-.0094	.0072	-1.309	1.712
N1D *	.0036	.0060	.608	.370
Co1	.0000	.0001	.000	.000

=====

Sum((d/s)**2) for starred atoms 4.164

Chi-squared at 95% for 1 degrees of freedom: 3.84

The group of atoms deviates significantly from planarity

Plane 5

m1 = -1.00000 (.00000)

m2 = .00105 (.00391)

m3 = .00105 (.00394)

D = -5.72052 (.04127)

Atom	d	s	d/s	(d/s)**2
N1A *	-.0027	.0049	-.550	.303
C5A *	.0099	.0070	1.412	1.993
N1E *	.0027	.0049	.550	.303
C5E *	-.0099	.0070	-1.412	1.993
Co1	.0000	.0001	-.002	.000

=====

Sum((d/s)**2) for starred atoms 4.591

Chi-squared at 95% for 1 degrees of freedom: 3.84

The group of atoms deviates significantly from planarity

Plane 6

m1 = -.11849 (.00241)

m2 = .12227 (.00267)

m3 = -.98540 (.00060)

D = -1.41689 (.01091)

Atom	d	s	d/s	(d/s)**2
O1 *	.0201	.0050	3.987	15.899
C6 *	-.0021	.0013	-1.671	2.791
C7 *	.0022	.0013	1.703	2.900
O2 *	-.0237	.0055	-4.325	18.704
Co2	-.1559	.0012	-127.389	16227.930

=====

Sum((d/s)**2) for starred atoms 40.294

Chi-squared at 95% for 1 degrees of freedom: 3.84

The group of atoms deviates significantly from planarity

Plane 7

m1 = .98550 (.00091)

m2 = .10787 (.00420)

m3 = -.13098 (.00409)

D = 1.38998 (.01324)

Atom	d	s	d/s	(d/s)**2
O1A *	-.0034	.0049	-.697	.486
C6A *	.0127	.0073	1.752	3.070
C7A *	-.0133	.0074	-1.786	3.189
O2A *	.0036	.0051	.717	.514
Co2	.1520	.0012	123.931	15358.960

=====

Sum((d/s)**2) for starred atoms 7.259

Chi-squared at 95% for 1 degrees of freedom: 3.84

The group of atoms deviates significantly from planarity

Plane 8
 m1 = .13064(.00407)
 m2 = -.98556(.00086)
 m3 = -.10770(.00383)
 D = -1.39137(.01332)

Atom	d	s	d/s	(d/s)**2
O1B *	.0040	.0053	.750	.562
C6B *	-.0126	.0073	-1.734	3.006
C7B *	.0132	.0074	1.767	3.123
O2B *	-.0034	.0049	-.687	.472
Co2	-.1510	.0012	-122.693	15053.480

Sum((d/s)**2) for starred atoms 7.162

Chi-squared at 95% for 1 degrees of freedom: 3.84

The group of atoms deviates significantly from planarity

Dihedral angles formed by LSQ-planes

Plane	- plane	angle (e.s.d.)
1	2	3.00(.25)
1	3	3.35(.29)
1	4	88.99(.30)
1	5	86.90(.29)
1	6	7.03(.22)
1	7	85.50(.29)
1	8	85.27(.28)
2	3	3.35(.30)
2	4	86.87(.30)
2	5	89.02(.30)
2	6	6.96(.23)
2	7	83.18(.32)
2	8	87.09(.28)
3	4	90.05(.35)
3	5	90.08(.34)
3	6	9.83(.27)
3	7	82.46(.32)
3	8	83.80(.34)
4	5	89.91(.32)
4	6	83.00(.29)
4	7	83.84(.35)
4	8	170.30(.31)
5	6	83.25(.27)
5	7	170.24(.32)
5	8	97.57(.34)
6	7	88.54(.27)
6	8	91.71(.27)
7	8	87.91(.36)