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catena-Poly[dinitratocobalt(II)-μ-2,5-bis-{2-(2-pyridyl)ethynyl}thiophene-*N*:*N'*], $[Co(NO_3)_2(C_{18}H_{10}N_2S)]_3$

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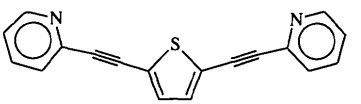
Abstract

The single-crystal X-ray structure of a one-dimensional chain of nitrate-coordinated Co ions connected by rigid rod-like N donor ligands is described.

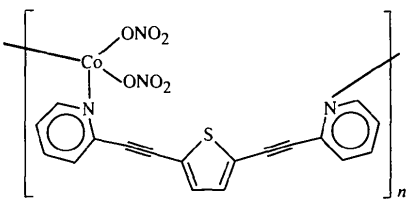
Comment

We have recently begun a program to prepare complexes in which arrays of metal atoms are held together by rigid electron-rich connecting rods (Neenan, Driessen, & Reedijk, 1995). Materials of this type may find application as the building blocks for conducting and photo-conducting solids, or as molecular wires.

Recently, we prepared the ligand 2,5-bis[2-(2-pyridyl)ethynyl]thiophene, (I), and report here the crystal and molecular structure of the infinite polymer, (II), that the ligand forms with cobalt(II) nitrate (see Figs. 1 and 2).



(I)



(II)

In the asymmetric unit $Co_3(L)_3(NO_3)_6$, each Co ion is coordinated to two nitrate ions and to two pyridine N atoms from two different ligands. The Co ions and the ligands form an infinite one-dimensional chain in the [101] direction.

The coordination geometry of the Co ions can be described as highly distorted octahedral, with both pyridine N atoms at distances between 2.06 and 2.09 Å, with two O atoms, one of each nitrate ion, coordinated at distances between 1.98 and 2.06 Å, and another two O atoms, one of each nitrate ion, completing the octahedral coordination at longer distances between 2.36 and 2.52 Å.

In one of the ligands in the asymmetric unit the donor N atoms point in opposite directions, while in the two other ligands the N atoms point in the same direction. The pyridine–thiophene connection is almost linear, as expected for an *sp*–*sp*-coupled system. The pyridine and thiophene rings are planar.

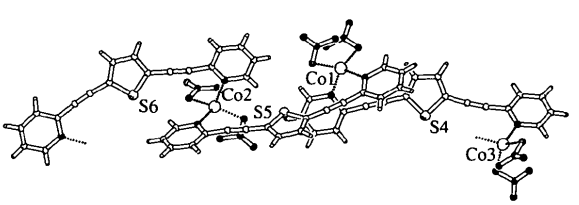
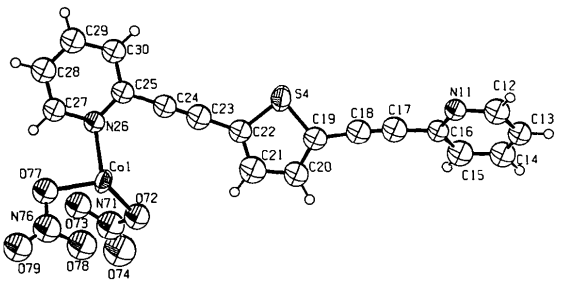
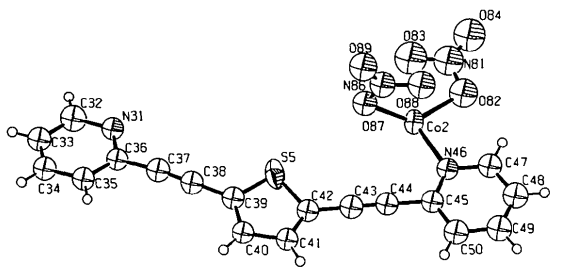


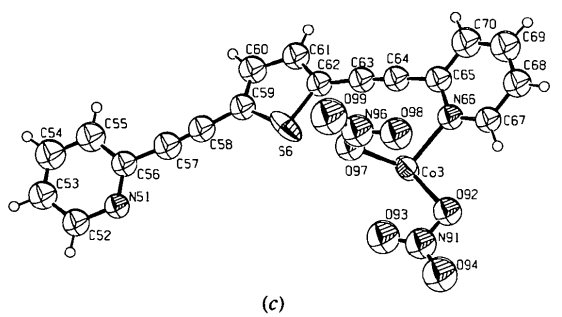
Fig. 1. *PLUTON* (Spek, 1992) projection of the asymmetric unit $Co_3(L)_3(NO_3)_6$.



(*a*)



(*b*)



(*c*)

Fig. 2. Numbering scheme of the non-H atoms of the asymmetric unit. Ellipsoids are shown at the 50% probability level.

Experimental

The synthesis of the ligand is reported elsewhere (Neenan *et al.*, 1995). Addition of a filtered solution of 1 mmol of the ligand in absolute ethanol (5 ml) to $Co(H_2O)_6(NO_3)_2$ in absolute ethanol (5 ml) gave deep-purple oblong blocks upon standing at room temperature for 48 h.

Crystal data

$[Co(NO_3)_2(C_{18}H_{10}N_2S)]_3$
$M_r = 1407.88$
Monoclinic
$P2_1/c$
$a = 15.51\ (1)$ Å
$b = 15.178\ (5)$ Å
$c = 25.66\ (3)$ Å
$\beta = 106.9\ (1)°$
$V = 5780\ (8)$ Å^3
$Z = 4$
$D_x = 1.617$ Mg m^{-3}
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 24 reflections
$\theta = 10$–$12°$
$\mu = 1.034$ mm^{-1}
$T = 293$ K
Oblong block
$0.3 \times 0.2 \times 0.15$ mm
Deep purple

Data collection

Enraf–Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
7028 measured reflections
7028 independent reflections
2925 observed reflections $[I > 2\sigma(I)]$
$\theta_{max} = 21.95°$
$h = -16 \rightarrow 15$
$k = 0 \rightarrow 15$
$l = 0 \rightarrow 26$
3 standard reflections
frequency: 90 min
intensity decay: 12.6% (corrected)

Refinement

Refinement on F
$R = 0.060$
$wR = 0.056$
$S = 2.271$
2921 reflections
391 parameters
H-atom parameters not refined, U fixed
$w = 1/\sigma^2(F)$
$(\Delta/\sigma)_{max} = 0.227$
$\Delta\rho_{max} = 1.1$ e Å^{-3}
$\Delta\rho_{min} = -0.86$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, Tables 2.2B and 2.3.1)

Table 1. *Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)*

U_{iso} for C, N, O; $U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$ for Co and S.

	x	y	z	U_{iso}/U_{eq}
Co1	−0.0684 (1)	0.5517 (1)	0.33260 (6)	0.053 (1)
Co2	−0.2480 (1)	0.5963 (1)	−0.00302 (7)	0.054 (1)
Co3	0.5812 (1)	0.6355 (1)	0.66784 (7)	0.062 (1)
S4	0.2700 (2)	0.7376 (3)	0.5058 (1)	0.069 (2)
S5	−0.0315 (2)	0.4564 (2)	0.1573 (1)	0.071 (2)
S6	−0.4709 (3)	0.5042 (3)	−0.1936 (1)	0.091 (3)
N11	0.5307 (6)	0.7069 (6)	0.7221 (4)	0.049 (3)
C12	0.5881 (8)	0.7131 (8)	0.7737 (5)	0.070 (4)
C13	0.5623 (8)	0.7537 (8)	0.8144 (5)	0.061 (4)
C14	0.4804 (9)	0.7875 (8)	0.8062 (5)	0.070 (4)
C15	0.4196 (8)	0.7832 (8)	0.7537 (6)	0.072 (4)
C16	0.4479 (8)	0.7412 (8)	0.7136 (5)	0.051 (4)
C17	0.3861 (8)	0.7369 (8)	0.6599 (6)	0.070 (4)
C18	0.3280 (8)	0.7330 (8)	0.6179 (5)	0.065 (4)
C19	0.2548 (8)	0.7219 (8)	0.5690 (5)	0.060 (4)
C20	0.1708 (8)	0.6956 (8)	0.5648 (5)	0.066 (4)
C21	0.1181 (9)	0.6852 (8)	0.5099 (6)	0.079 (4)
C22	0.1622 (8)	0.7053 (8)	0.4740 (5)	0.058 (4)
C23	0.1299 (8)	0.6956 (8)	0.4154 (6)	0.068 (4)
C24	0.1018 (8)	0.6872 (8)	0.3681 (5)	0.057 (4)
C25	0.0657 (8)	0.6847 (8)	0.3095 (5)	0.055 (4)
N26	−0.0118 (6)	0.6377 (6)	0.2904 (4)	0.049 (3)
C27	−0.0526 (7)	0.6424 (8)	0.2351 (5)	0.058 (4)
C28	−0.0165 (8)	0.6884 (8)	0.2013 (5)	0.069 (4)
C29	0.0627 (8)	0.7306 (8)	0.2210 (5)	0.069 (4)
C30	0.1064 (8)	0.7312 (8)	0.2767 (5)	0.063 (4)
N31	0.0370 (6)	0.4793 (6)	0.3823 (4)	0.051 (3)
C32	0.0485 (8)	0.4811 (8)	0.4373 (5)	0.072 (4)
C33	0.1165 (8)	0.4337 (8)	0.4738 (5)	0.061 (4)
C34	0.1732 (8)	0.3867 (8)	0.4557 (5)	0.059 (4)
C35	0.1652 (7)	0.3842 (8)	0.4014 (5)	0.055 (4)
C36	0.0956 (8)	0.4290 (7)	0.3648 (5)	0.049 (3)
C37	0.0826 (8)	0.4256 (8)	0.3078 (5)	0.058 (4)
C38	0.0704 (7)	0.4155 (8)	0.2605 (5)	0.056 (4)
C39	0.0517 (7)	0.4012 (8)	0.2029 (5)	0.055 (4)
C40	0.0950 (7)	0.3437 (7)	0.1784 (5)	0.050 (3)
C41	0.0600 (7)	0.3460 (7)	0.1199 (5)	0.052 (4)
C42	−0.0092 (7)	0.4028 (8)	0.1034 (5)	0.051 (3)
C43	−0.0598 (8)	0.4234 (8)	0.0488 (5)	0.058 (4)
C44	−0.1030 (7)	0.4408 (7)	0.0043 (5)	0.054 (4)
C45	−0.1506 (8)	0.4601 (8)	−0.0529 (5)	0.053 (4)
N46	−0.2128 (6)	0.5239 (6)	−0.0618 (4)	0.048 (3)
C47	−0.2560 (8)	0.5444 (8)	−0.1154 (5)	0.059 (4)

C48	−0.2383 (8)	0.5001 (9)	−0.1576 (5)	0.071 (4)
C49	−0.1775 (8)	0.4354 (8)	−0.1476 (5)	0.067 (4)
C50	−0.1302 (8)	0.4139 (8)	−0.0935 (5)	0.063 (4)
N51	−0.3007 (6)	0.5044 (6)	0.0392 (4)	0.058 (3)
C52	−0.2599 (8)	0.4992 (8)	0.0945 (5)	0.069 (4)
C53	−0.2880 (9)	0.4352 (9)	0.1245 (5)	0.079 (4)
C54	−0.355 (1)	0.3821 (9)	0.1024 (6)	0.090 (5)
C55	−0.3985 (9)	0.3867 (9)	0.0478 (6)	0.084 (5)
C56	−0.3687 (8)	0.4482 (9)	0.0165 (5)	0.063 (4)
C57	−0.4118 (8)	0.4534 (9)	−0.0413 (6)	0.072 (4)
C58	−0.4529 (8)	0.4548 (8)	−0.0879 (6)	0.067 (4)
C59	−0.5042 (8)	0.4538 (8)	−0.1432 (5)	0.064 (4)
C60	−0.5854 (9)	0.4154 (8)	−0.1636 (5)	0.073 (4)
C61	−0.6213 (8)	0.4269 (8)	−0.2206 (5)	0.069 (4)
C62	−0.5674 (8)	0.4743 (8)	−0.2435 (5)	0.061 (4)
C63	−0.5792 (8)	0.4947 (8)	−0.2976 (6)	0.063 (4)
C64	−0.5831 (8)	0.5125 (8)	−0.3424 (5)	0.062 (4)
C65	−0.5803 (8)	0.5359 (8)	−0.3966 (5)	0.064 (4)
N66	−0.5160 (6)	0.5940 (6)	−0.4007 (4)	0.061 (3)
C67	−0.5101 (8)	0.6182 (8)	−0.4492 (5)	0.063 (4)
C68	−0.5700 (9)	0.5827 (9)	−0.4979 (5)	0.077 (4)
C69	−0.6325 (9)	0.5253 (9)	−0.4939 (6)	0.089 (5)
C70	−0.6416 (9)	0.4996 (9)	−0.4440 (6)	0.085 (5)
N71	−0.1846 (8)	0.6448 (8)	0.3676 (5)	0.086 (4)
O72	−0.1080 (5)	0.6055 (5)	0.3940 (3)	0.070 (3)
O73	−0.1976 (5)	0.6455 (5)	0.3173 (3)	0.074 (3)
O74	−0.2314 (7)	0.6748 (7)	0.3928 (4)	0.114 (4)
N76	−0.1810 (8)	0.4253 (8)	0.2880 (5)	0.086 (4)
O77	−0.1423 (5)	0.4837 (6)	0.2661 (3)	0.072 (3)
O78	−0.1630 (6)	0.4325 (6)	0.3391 (4)	0.095 (3)
O79	−0.2373 (6)	0.3756 (6)	0.2620 (4)	0.089 (3)
N81	−0.3764 (9)	0.7180 (9)	−0.0267 (5)	0.094 (4)
O82	−0.3529 (6)	0.6628 (6)	−0.0562 (4)	0.088 (3)
O83	−0.3306 (6)	0.7123 (7)	0.0216 (4)	0.113 (4)
O84	−0.4342 (7)	0.7708 (7)	−0.0453 (4)	0.109 (4)
N86	−0.1001 (7)	0.6874 (7)	0.0373 (5)	0.070 (3)
O87	−0.1400 (5)	0.6307 (5)	0.0593 (3)	0.065 (2)
O88	−0.1390 (6)	0.6997 (5)	−0.0128 (4)	0.082 (3)
O89	−0.0343 (6)	0.7266 (6)	0.0627 (3)	0.084 (3)
N91	0.7159 (8)	0.7441 (9)	0.6706 (5)	0.092 (4)
O92	0.6414 (6)	0.7231 (5)	0.6316 (3)	0.076 (3)
O93	0.7240 (6)	0.7056 (6)	0.7126 (4)	0.105 (4)
O94	0.7607 (7)	0.8004 (7)	0.6568 (4)	0.115 (4)
N96	0.6764 (8)	0.4859 (9)	0.6834 (5)	0.097 (4)
O97	0.6367 (5)	0.5321 (6)	0.7129 (3)	0.081 (3)
O98	0.6692 (6)	0.5161 (6)	0.6372 (4)	0.097 (3)
O99	0.7171 (7)	0.4209 (8)	0.7006 (4)	0.128 (4)

Table 2. *Selected geometric parameters (Å, °)*

Co1—N26	2.05 (1)	Co2—O83	2.37 (1)
Co1—N31	2.072 (8)	Co2—O87	2.020 (7)
Co1—O72	2.024 (9)	Co2—O88	2.373 (9)
Co1—O73	2.396 (8)	Co3—N11	2.09 (1)
Co1—O77	2.039 (8)	Co3—N66^{i}	2.055 (9)
Co1—O78	2.37 (1)	Co3—O92	2.002 (9)
Co2—N46	2.06 (1)	Co3—O93	2.425 (9)
Co2—N51	2.07 (1)	Co3—O97	1.991 (8)
Co2—O82	2.059 (8)	Co3—O98	2.53 (1)
N26—Co1—N31	106.3 (4)	N51—Co2—O88	154.3 (3)
N26—Co1—O72	115.4 (4)	O82—Co2—O83	55.1 (4)
N26—Co1—O73	90.1 (3)	O82—Co2—O87	135.4 (3)
N26—Co1—O77	95.9 (4)	O82—Co2—O88	93.2 (3)
N26—Co1—O78	153.4 (3)	O83—Co2—O87	89.2 (3)
N31—Co1—O72	95.7 (4)	O83—Co2—O88	89.7 (3)
N31—Co1—O73	152.7 (4)	O87—Co2—O88	57.3 (3)
N31—Co1—O77	113.5 (3)	N11—Co3—N66^{i}	113.9 (4)
N31—Co1—O78	86.9 (3)	N11—Co3—O92	106.3 (4)
O72—Co1—O73	57.2 (3)	N11—Co3—O93	85.7 (4)
O72—Co1—O77	129.2 (3)	N11—Co3—O97	101.8 (4)
O72—Co1—O78	85.3 (4)	N11—Co3—O98	157.0 (3)
O73—Co1—O77	85.6 (3)	N66^{i}—Co3—O92	97.6 (4)
O73—Co1—O78	87.7 (3)	N66^{i}—Co3—O93	151.9 (4)
O77—Co1—O78	57.5 (4)	N66^{i}—Co3—O97	110.0 (4)
N46—Co2—N51	104.6 (4)	N66^{i}—Co3—O98	80.9 (4)
N46—Co2—O82	95.9 (4)	O92—Co3—O93	56.2 (3)
N46—Co2—O83	150.3 (3)	O92—Co3—O97	127.8 (4)
N46—Co2—O87	112.4 (4)	O92—Co3—O98	88.0 (4)
N46—Co2—O88	85.8 (4)	O93—Co3—O97	83.7 (3)
N51—Co2—O82	108.7 (4)	O93—Co3—O98	87.7 (3)
N51—Co2—O83	92.0 (4)	O97—Co3—O98	55.6 (4)
N51—Co2—O87	97.0 (4)		

Symmetry code: (i) $1+x, y, 1+z$.

Only Co and S atoms were refined anisotropically; all the other non-H atoms were refined isotropically.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *Xtal ADDREF SORTRF* (Hall, Flack & Stewart, 1992). Program(s) used to solve structure: *Xtal SIMPEL*. Program(s) used to refine structure: *Xtal CRYLSQ*. Molecular graphics: *PLUTON* (Spek, 1992). Software used to prepare material for publication: *Xtal BONDLA CIFIO*.

The authors are indebted to Mr S. Gorter for his assistance in the collection and processing of the diffraction data.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: NA1163). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Neodymium Hexacyanocobaltate(III) Tetrahydrate

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Abstract

Neodymium hexacyanocobaltate(III) tetrahydrate, $NdCo(CN)_6.4H_2O$, crystallizes in the orthorhombic space group *Cmcm*. The structure consists of octahedrally coordinated Co atoms and eight-coordinate Nd atoms linked by non-linear cyanide bridges, which produce an undulation throughout the polymeric array. Two water molecules are coordinated to the Nd atoms and