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**Key indicators**

Single-crystal X-ray study
$T = 296$ K
Mean $\sigma$(C–C) = 0.003 Å
$R$ factor = 0.036
$wR$ factor = 0.075
Data-to-parameter ratio = 13.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

# Tetraaquabis(isonicotinamide-κN)cobalt(II) terephthalate dihydrate

In the title compound, $[Co(C_6H_6N_2O)_2(H_2O)_4](C_8H_4O_4)\cdot2H_2O$, the $Co^{II}$ atom (site symmetry $\bar{1}$) exhibits a slightly distorted *trans*-$CoN_2O_4$ octahedral coordination geometry arising from two N-bonded isonicotinamide molecules and four O atoms of water molecules. The uncoordinated centrosymmetric terephthalate anion and uncoordinated water molecules interact with the cation by way of O—H···O and N—H···O hydrogen bonds, generating a three-dimensional network.

## Comment

In an extension of our recent work on supramolecular architectures arising from hydrogen-bonded networks involving transition metal complexes (Li, *et al.*, 2005), we obtained the title compound, (I), using terephthalate, isonicotinamide (inta) and $Co^{II}$ as starting materials.



(I)
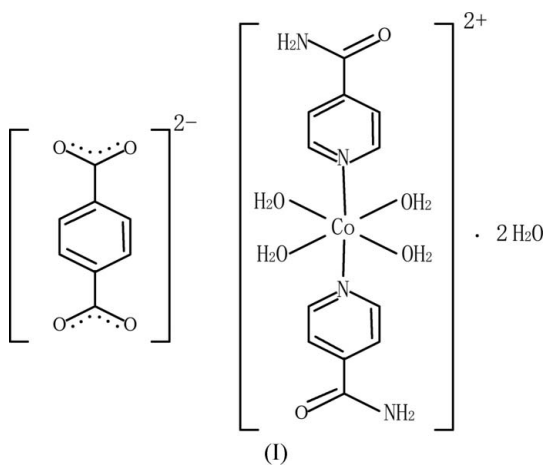
Compound (I) contains $[Co(C_6H_6N_2O)_2(H_2O)_4]^{2+}$ di-cations, $C_8H_4O_4^{2-}$ dianions and water molecules (Fig. 1). The $Co^{II}$ centre (site symmetry $\bar{1}$) shows a slightly distorted *trans*-$CoN_2O_4$ octahedral coordination geometry, being coordinated by two N atoms from two inta molecules and four water O atoms. The Co—O and Co—N distances are normal. An uncoordinated terephthalate dianion and an uncoordinated water molecule complete the structure of (I). The former species is centrosymmetric and its C—O bond lengths suggest delocalization of charge.

Hydrogen-bonding interactions play an important role in generating a three-dimensional network in the crystal structure of (I) (Fig. 2). The component species are linked together by way of O—H···O and N—H···O hydrogen bonds (Table 1). Thus, (I) can be considered to be a three-dimensional supramolecular hydrogen-bonded network.

## Experimental

A mixture of $CoCl_2 \cdot 6H_2O$ (0.5 mmol), terephthalic acid (0.5 mmol) and isonicotinamide (1 mmol) was dissolved in 25 ml $H_2O$ and stirred continuously for about 30 min at 333 K. The pH value was adjusted to about 7 by the addition of 4 M NaOH solution. The mixture was cooled and filtered. After evaporation of the solvent slowly at room temperature for about one month, light-pink crystals of (I) suitable for X-ray crystallographic analysis were obtained.

### Crystal data

| | |
|---|---|
| $[Co(C_6H_6N_2O)_2(H_2O)_4]$- | $\gamma = 106.532\ (2)°$ |
| $(C_8H_4O_4) \cdot 2H_2O$ | $V = 607.06\ (13)\ \text{Å}^3$ |
| $M_r = 575.39$ | $Z = 1$ |
| Triclinic, $P\bar{1}$ | $D_x = 1.574\ \text{Mg m}^{-3}$ |
| $a = 6.4962\ (8)\ \text{Å}$ | Mo $K\alpha$ radiation |
| $b = 9.7585\ (12)\ \text{Å}$ | $\mu = 0.78\ \text{mm}^{-1}$ |
| $c = 11.0145\ (14)\ \text{Å}$ | $T = 296\ (2)$ K |
| $\alpha = 105.270\ (2)°$ | Block, light pink |
| $\beta = 103.908\ (2)°$ | $0.27 \times 0.10 \times 0.09$ mm |

### Data collection

| | |
|---|---|
| Bruker APEX CCD area-detector diffractometer | 3427 measured reflections |
| | 2329 independent reflections |
| $\omega$ and $\varphi$ scans | 2091 reflections with $I > 2\sigma(I)$ |
| Absorption correction: multi-scan (SADABS; Bruker, 2002) | $R_{int} = 0.031$ |
| | $\theta_{max} = 26.0°$ |
| $T_{min} = 0.910$, $T_{max} = 0.940$ | |

### Refinement

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0537P)^2$ |
| $R[F^2 > 2\sigma(F^2)] = 0.036$ | $+ 0.1097P]$ |
| $wR(F^2) = 0.075$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.02$ | $(\Delta/\sigma)_{max} < 0.001$ |
| 2329 reflections | $\Delta\rho_{max} = 0.30$ e Å$^{-3}$ |
| 168 parameters | $\Delta\rho_{min} = -0.37$ e Å$^{-3}$ |
| H-atom parameters constrained | |

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|---|---|---|---|---|
| $N2-H1N \cdots O3W^i$ | 0.93 | 2.00 | 2.856 (2) | 152 |
| $O1W-H1W \cdots O1^{ii}$ | 0.85 | 1.93 | 2.676 (2) | 146 |
| $O1W-H2W \cdots O2^{iii}$ | 0.85 | 1.91 | 2.664 (2) | 147 |
| $O2W-H3W \cdots O3^{iii}$ | 0.87 | 1.88 | 2.746 (2) | 172 |
| $O2W-H4W \cdots O2^{iv}$ | 0.91 | 1.87 | 2.757 (2) | 165 |
| $O3W-H5W \cdots O2^{iii}$ | 0.93 | 2.13 | 3.041 (3) | 166 |
| $O3W-H6W \cdots O3^v$ | 0.87 | 1.92 | 2.780 (2) | 167 |

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

The C-bound H atoms were positioned geometrically (C—H = 0.93 Å) and refined using a riding model with $U_{iso}(H) = 1.2U_{eq}(C)$. The O- and N-bound H atoms were located in difference maps and refined as riding in their as-found relative positions (O—H = 0.85– 0.93 Å and N—H = 0.90–0.93 Å), with $U_{iso}(H) = 1.2U_{eq}(O,N)$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve
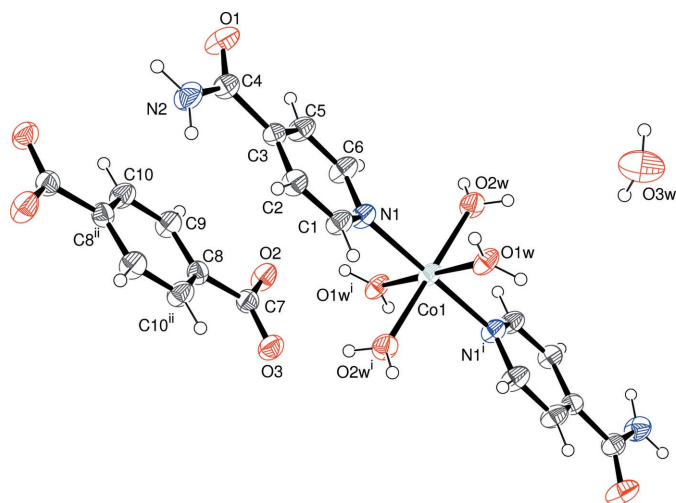


**Figure 1**
The structure of the components of (I), showing 40% probability displacement ellipsoids (arbitrary spheres for the H atoms). [Symmetry codes: (i) $1 - x$, $1 - y$, $1 - z$; (ii) $1 - x$, $2 - y$, $2 - z$.]
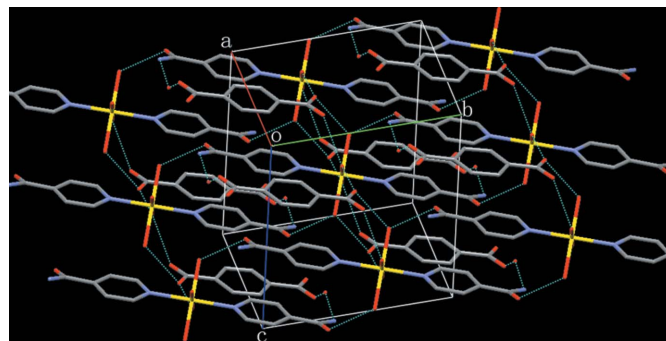


**Figure 2**
The three-dimensional hydrogen-bonding network (dashed lines) in (I). H atoms have been omitted.

structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg, 1999); software used to prepare material for publication: SHELXL97.

### References

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