# metal-organic compounds

# Poly[di-μ₂-azido-μ₃-pyrazine-2-carboxylato-cadmium(II)]

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The title compound, $[Cd(C_5H_3N_2O_2)(N_3)]_n$, has been prepared by the reaction of pyrazine-2-carboxylic acid, cadmium(II) nitrate and sodium azide. In the structure, the $Cd^{II}$ atom is six-coordinated by two azide anions and three pyrazine-2-carboxylate ligands. Each pyrazine-2-carboxylate ligand bridges three $Cd^{II}$ atoms, whereas the azide ligand bridges two $Cd^{II}$ atoms, resulting in the formation of a two-dimensional metal–organic polymer developing parallel to the (100) plane.

## Related literature

For metal–azide complexes, see: Mondal & Mukherjee (2008); Gu *et al.* (2007); Monfort *et al.* (2000). For the coordination modes of the azide anion, see: Shen *et al.* (2000). For metal–azide complexes with charged ligands, see: Escuer *et al.* (1997). For the synthesis of high-dimensional azide compounds with negatively charged ligands, see: Liu *et al.* (2005).
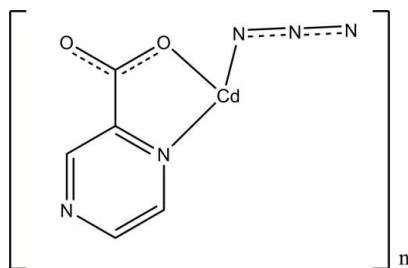


## Experimental

### Crystal data

| | |
|---|---|
| $[Cd(C_5H_3N_2O_2)(N_3)]$ | $V = 760.4$ (3) Å³ |
| $M_r = 277.52$ | $Z = 4$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation |
| $a = 11.857$ (2) Å | $\mu = 2.84$ mm⁻¹ |
| $b = 9.839$ (2) Å | $T = 293$ K |
| $c = 6.6250$ (13) Å | $0.20 \times 0.18 \times 0.15$ mm |
| $\beta = 100.33$ (3)° | |

### Data collection

| | |
|---|---|
| Rigaku SCXmini diffractometer | 7718 measured reflections |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | 1741 independent reflections |
| | 1517 reflections with $I > 2\sigma(I)$ |
| $T_{min} = 0.537$, $T_{max} = 0.643$ | $R_{int} = 0.067$ |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | 118 parameters |
| $wR(F^2) = 0.117$ | H-atom parameters constrained |
| $S = 1.20$ | $\Delta\rho_{max} = 0.74$ e Å⁻³ |
| 1741 reflections | $\Delta\rho_{min} = -1.09$ e Å⁻³ |

Data collection: *SCXmini* (Rigaku, 2006); cell refinement: *PROCESS-AUTO* (Rigaku, 1998); data reduction: *PROCESS-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

## References

Burnett, M. N. & Johnson, C. K. (1996). *ORTEPIII*. Report ORNL-6895. Oak Ridge National Laboratory, Tennessee, USA.

Escuer, A., Vicente, R., Mautner, F. A. & Goher, M. A. S. (1997). *Inorg. Chem.* **36**, 1233–1236.

Gu, Z.-G., Song, Y., Zuo, J.-L. & You, X.-Z. (2007). *Inorg. Chem.* **46**, 9522–9524.

Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.

Liu, F.-C., Zeng, Y.-F., Li, J.-R., Bu, X.-H., Zhang, H.-J. & Ribas, J. (2005). *Inorg. Chem.* **44**, 7298–7300.

Mondal, K.-C. & Mukherjee, P.-S. (2008). *Inorg. Chem.* **47**, 4215–4225.

Monfort, M., Resino, I., Ribas, J. & Stoeckli-Evans, H. (2000). *Angew. Chem. Int. Ed.* **39**, 191–193.

Rigaku (1998). *PROCESS-AUTO*. Rigaku Corporation, Tokyo, Japan.

Rigaku (2006). *SCXmini*. Rigaku Americas Corporation, The Woodlands, Texas, USA.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Shen, Z., Zuo, J.-L., Gao, S., Song, Y., Che, C.-M., Fun, H.-K. & You, X.-Z. (2000). *Angew. Chem. Int. Ed.* **39**, 3633–3635.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

# supporting information

## Poly[di-*μ*₂-azido-*μ*₃-pyrazine-2-carboxylato-cadmium(II)]

### Cai-Yun Li, Pei-Fan Li and Hui-Min Jin

### S1. Comment

Recently, metal azide complexes have attracted great attention.(Mondal & Mukherjee, 2008; Gu *et al.*, 2007). The azide anion have rich coordinated modes. (Shen, *et al.*, 2000). In this sense, lots metal-azide complexes have been reported. (Monfort, *et al.*, 2000). In most of the compounds reported to date, the coligands are neutral organic ligands, while charged ligands are very scarce (Escuer *et al.*, 1997). Synthesizing high-dimensional compounds with azide and negatively charged ligands represents then a challenge for researchers working in this field. (Liu *et al.*, 2005)

In the title compound, the cadmium atom is six coordinated by two azide anions and three pyrazine-2-carboxylate (Fig. 1). Each pyrazine-2-carboxylate bridges three cadmium atoms whereas the azide is bridging two cadmium atoms resulting in the formation of a two dimensional metal organic polymer developping parallel to the (1 0 0) plane.

### S2. Experimental

A mixture of cadmium(II)nitrate and sodium azide (1 mmol), pyrazine-2-carboxylate acid(0.5 mmol), in 10 ml of water was sealed in a Teflon-lined stainless-steel Parr bomb that was heated at 363 K for 48 h. Pink crystals of the title complex were collected after the bomb was allowed to cool to room temperature.Yield 30% based on cadmium(II). Caution:Metal azides may be explosive. Although we have met no problems in this work, only a small amount of them should be prepared and handled with great caution.

### S3. Refinement

Hydrogen atoms were included in calculated positions and treated as riding on their parent C atoms with C—H = 0.93Å and $U_{iso}$(H) = $1.2U_{eq}$(C).
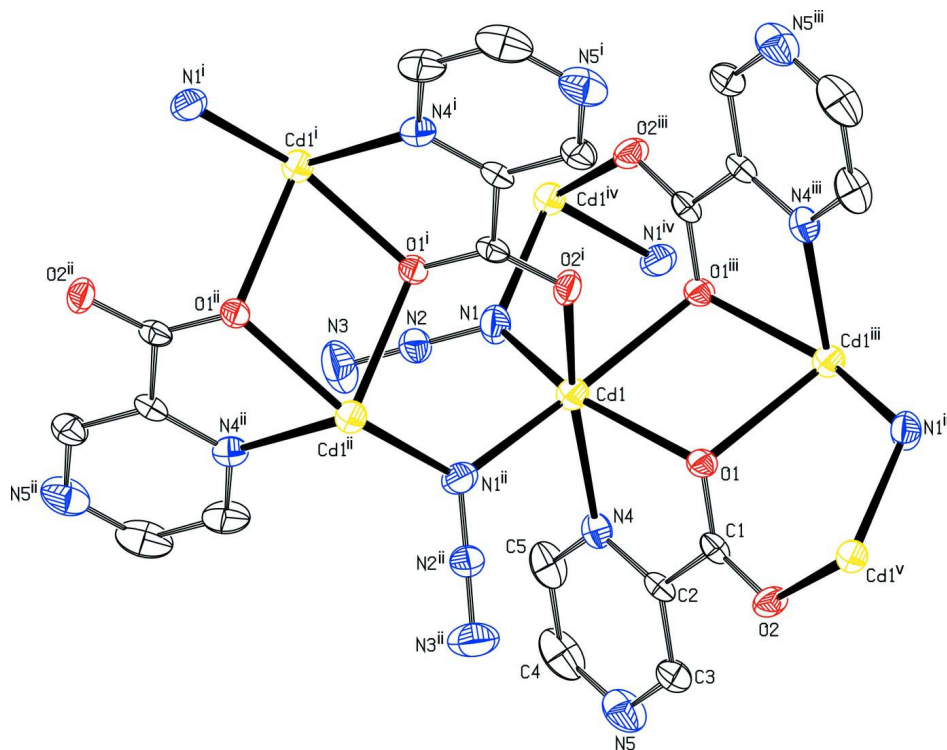
**Figure 1**

A view of the title compound showing the coordination of Cd atom with the atom-labelling scheme. Ellipsoids are drawn at the 50% probability level. H atom have been omitted for clarity. [Symmetry codes: (i) -x+1, y-1/2, -z+1/2; (ii) x, -y+1/2, z-1/2; (iii) -x+1, -y+1, -z+1; (iv) x, -y+1/2, z+1/2; (v) -x+1, y+1/2, -z+1/2]

**Poly[di-$\mu_2$-azido-$\mu_3$-pyrazine-2-carboxylato-cadmium(II)]**

*Crystal data*

| | |
|---|---|
| [Cd(C$_5$H$_3$N$_2$O$_2$)(N$_3$)] | $F(000) = 528$ |
| $M_r = 277.52$ | $D_x = 2.424$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 7230 reflections |
| $a = 11.857$ (2) Å | $\theta = 3.1$–27.5° |
| $b = 9.839$ (2) Å | $\mu = 2.84$ mm$^{-1}$ |
| $c = 6.6250$ (13) Å | $T = 293$ K |
| $\beta = 100.33$ (3)° | Block, yellow |
| $V = 760.4$ (3) Å$^3$ | $0.2 \times 0.18 \times 0.15$ mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Rigaku SCXmini diffractometer | 7718 measured reflections |
| Radiation source: fine-focus sealed tube | 1741 independent reflections |
| Graphite monochromator | 1517 reflections with $I > 2\sigma(I)$ |
| $\omega$ scans | $R_{int} = 0.067$ |
| Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995) | $\theta_{max} = 27.5°$, $\theta_{min} = 3.5°$ |
| | $h = -15 \rightarrow 15$ |
| | $k = -12 \rightarrow 12$ |
| $T_{min} = 0.537$, $T_{max} = 0.643$ | $l = -8 \rightarrow 8$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.046$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.117$ | |
| $S = 1.20$ | H-atom parameters constrained |
| 1741 reflections | $w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 2.6851P]$ |
| 118 parameters | where $P = (F_o^2 + 2F_c^2)/3$ |
| 0 restraints | $(\Delta/\sigma)_{max} < 0.001$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{max} = 0.74$ e Å$^{-3}$ |
| | $\Delta\rho_{min} = -1.09$ e Å$^{-3}$ |

*Special details*

**Geometry**. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cd1 | 0.42263 (4) | 0.36045 (4) | 0.34194 (7) | 0.02481 (18) |
| N1 | 0.3555 (5) | 0.1927 (5) | 0.5059 (8) | 0.0287 (12) |
| N2 | 0.2937 (5) | 0.1135 (5) | 0.4006 (8) | 0.0248 (12) |
| N3 | 0.2327 (6) | 0.0399 (7) | 0.3035 (10) | 0.0466 (17) |
| N4 | 0.2558 (4) | 0.4910 (5) | 0.3100 (7) | 0.0231 (11) |
| N5 | 0.0689 (5) | 0.6646 (7) | 0.1984 (10) | 0.0390 (15) |
| O1 | 0.4718 (3) | 0.5816 (4) | 0.3145 (6) | 0.0197 (8) |
| O2 | 0.4043 (4) | 0.7823 (4) | 0.1835 (6) | 0.0250 (9) |
| C1 | 0.3913 (5) | 0.6650 (6) | 0.2480 (8) | 0.0198 (12) |
| C2 | 0.2694 (5) | 0.6193 (6) | 0.2517 (8) | 0.0194 (12) |
| C3 | 0.1769 (5) | 0.7052 (7) | 0.1982 (9) | 0.0277 (14) |
| H3A | 0.1898 | 0.7942 | 0.1609 | 0.033* |
| C4 | 0.0571 (6) | 0.5372 (9) | 0.2550 (11) | 0.0422 (19) |
| H4A | −0.0162 | 0.5044 | 0.2575 | 0.051* |
| C5 | 0.1493 (6) | 0.4509 (8) | 0.3106 (10) | 0.0327 (16) |
| H5B | 0.1362 | 0.3623 | 0.3494 | 0.039* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cd1 | 0.0233 (3) | 0.0213 (3) | 0.0287 (3) | −0.00024 (18) | 0.00174 (19) | 0.00118 (18) |
| N1 | 0.038 (3) | 0.023 (3) | 0.024 (3) | −0.008 (2) | 0.002 (2) | −0.001 (2) |
| N2 | 0.022 (3) | 0.025 (3) | 0.027 (3) | −0.003 (2) | 0.003 (2) | 0.000 (2) |
| N3 | 0.051 (4) | 0.047 (4) | 0.040 (3) | −0.023 (3) | 0.001 (3) | −0.004 (3) |
| N4 | 0.022 (3) | 0.025 (3) | 0.023 (2) | −0.004 (2) | 0.005 (2) | −0.003 (2) |

| | | | | | |
|------|------------|------------|------------|--------------|--------------|--------------|
| N5 | 0.018 (3) | 0.054 (4) | 0.044 (3) | 0.002 (3) | 0.004 (3) | −0.008 (3) |
| O1 | 0.014 (2) | 0.020 (2) | 0.025 (2) | −0.0004 (16) | 0.0012 (16) | 0.0018 (17) |
| O2 | 0.023 (2) | 0.018 (2) | 0.033 (2) | −0.0007 (17) | 0.0035 (18) | 0.0075 (18) |
| C1 | 0.018 (3) | 0.026 (3) | 0.013 (3) | −0.004 (2) | 0.000 (2) | −0.001 (2) |
| C2 | 0.015 (3) | 0.028 (3) | 0.014 (2) | −0.001 (2) | −0.001 (2) | −0.002 (2) |
| C3 | 0.019 (3) | 0.031 (4) | 0.031 (3) | 0.000 (3) | −0.001 (3) | −0.001 (3) |
| C4 | 0.018 (4) | 0.071 (6) | 0.040 (4) | −0.012 (3) | 0.011 (3) | −0.010 (4) |
| C5 | 0.022 (3) | 0.043 (4) | 0.034 (4) | −0.016 (3) | 0.010 (3) | −0.003 (3) |

*Geometric parameters (Å, º)*

| | | | |
|-------------------------|--------------|--------------------|--------------|
| Cd1—N1 | 2.202 (5) | N5—C4 | 1.324 (10) |
| Cd1—O2$^i$ | 2.226 (4) | N5—C3 | 1.342 (8) |
| Cd1—O1 | 2.268 (4) | O1—C1 | 1.275 (7) |
| Cd1—N4 | 2.336 (5) | O2—C1 | 1.250 (7) |
| Cd1—O1$^{ii}$ | 2.460 (4) | C1—C2 | 1.517 (8) |
| N1—N2 | 1.203 (7) | C2—C3 | 1.380 (8) |
| N1—Cd1$^{iii}$ | 2.286 (5) | C3—H3A | 0.9300 |
| N2—N3 | 1.138 (8) | C4—C5 | 1.381 (11) |
| N4—C5 | 1.324 (8) | C4—H4A | 0.9300 |
| N4—C2 | 1.339 (8) | C5—H5B | 0.9300 |
| | | | |
| N1—Cd1—O2$^i$ | 101.42 (19) | C2—N4—Cd1 | 113.6 (4) |
| N1—Cd1—O1 | 151.56 (18) | C4—N5—C3 | 115.6 (6) |
| O2$^i$—Cd1—O1 | 94.12 (15) | C1—O1—Cd1 | 117.2 (4) |
| N1—Cd1—N1$^{iv}$ | 102.45 (15) | C1—O1—Cd1$^{ii}$ | 113.3 (3) |
| O2$^i$—Cd1—N1$^{iv}$ | 90.68 (18) | Cd1—O1—Cd1$^{ii}$ | 104.11 (15) |
| O1—Cd1—N1$^{iv}$ | 101.01 (17) | C1—O2—Cd1$^v$ | 121.1 (4) |
| N1—Cd1—N4 | 94.7 (2) | O2—C1—O1 | 125.6 (5) |
| O2$^i$—Cd1—N4 | 163.79 (17) | O2—C1—C2 | 117.0 (5) |
| O1—Cd1—N4 | 71.99 (16) | O1—C1—C2 | 117.4 (5) |
| N1$^{iv}$—Cd1—N4 | 84.05 (18) | N4—C2—C3 | 121.3 (6) |
| N1—Cd1—O1$^{ii}$ | 83.47 (16) | N4—C2—C1 | 116.7 (5) |
| O2$^i$—Cd1—O1$^{ii}$ | 80.03 (14) | C3—C2—C1 | 122.0 (5) |
| O1—Cd1—O1$^{ii}$ | 75.89 (15) | N5—C3—C2 | 122.2 (6) |
| N1$^{iv}$—Cd1—O1$^{ii}$ | 169.88 (17) | N5—C3—H3A | 118.9 |
| N4—Cd1—O1$^{ii}$ | 103.82 (15) | C2—C3—H3A | 118.9 |
| N2—N1—Cd1 | 115.8 (4) | N5—C4—C5 | 122.6 (6) |
| N2—N1—Cd1$^{iii}$ | 119.1 (4) | N5—C4—H4A | 118.7 |
| Cd1—N1—Cd1$^{iii}$ | 124.0 (2) | C5—C4—H4A | 118.7 |
| N3—N2—N1 | 178.0 (7) | N4—C5—C4 | 121.7 (7) |
| C5—N4—C2 | 116.6 (6) | N4—C5—H5B | 119.1 |
| C5—N4—Cd1 | 128.9 (5) | C4—C5—H5B | 119.1 |

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