

# Poly[[diaquacaesium(I)]bis( $\mu_3$ -3-carboxypyrazine-2-carboxylato)]

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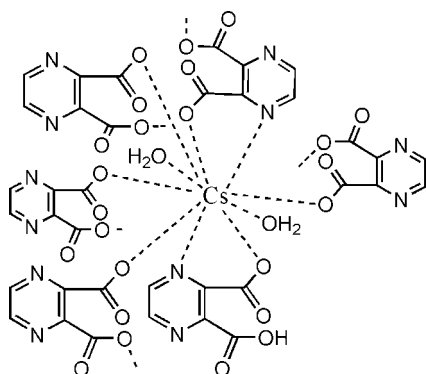
Received 16 May 2007; accepted 25 May 2007

Key indicators: single-crystal X-ray study;  $T = 296$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.019;  $wR$  factor = 0.052; data-to-parameter ratio = 14.4.

The asymmetric unit of the title compound,  $[\text{Cs}(\text{C}_6\text{H}_3\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_2]_n$ , contains one  $\text{Cs}^{\text{I}}$  cation on an inversion centre, one 3-carboxypyrazine-2-carboxylate anion and one water molecule. In the crystal structure, each anion is linked to three cations, while each cation is surrounded by six of the anions. In addition, each cation is coordinated by two water O atoms, raising the coordination number to ten. In the crystal structure, intermolecular  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{O}-\text{H}\cdots\text{N}$  hydrogen bonds contribute to the stabilization of the structure.

## Related literature

For general background, see: Rao *et al.* (2004); Takusagawa & Shimada (1973); Ptasiwicz-Bak & Leciejewicz (1997a); Starosta & Leciejewicz (2005); Ptasiwicz-Bak & Leciejewicz (1997b). For related literature, see: Tombul *et al.* (2006); Harnish *et al.* (1999); Wiesbrock & Schmidbaur (2003); Hu *et al.* (2005).



## Experimental

### Crystal data

$[\text{Cs}(\text{C}_6\text{H}_3\text{N}_2\text{O}_4)_2(\text{H}_2\text{O})_2]$   
 $M_r = 503.15$   
 Triclinic,  $P\bar{1}$   
 $a = 7.4801$  (9) Å  
 $b = 7.6352$  (9) Å  
 $c = 8.6505$  (11) Å  
 $\alpha = 70.031$  (9)°  
 $\beta = 81.126$  (10)°  
 $\gamma = 66.128$  (9)°  
 $V = 424.55$  (10) Å<sup>3</sup>  
 $Z = 1$   
 Mo  $K\alpha$  radiation  
 $\mu = 2.24$  mm<sup>-1</sup>  
 $T = 296$  K  
 $0.52 \times 0.47 \times 0.42$  mm

### Data collection

Stoe IPDSII diffractometer  
 Absorption correction: integration  
 ( $X$ -RED32; Stoe & Cie, 2002)  
 $T_{\text{min}} = 0.382$ ,  $T_{\text{max}} = 0.471$   
 7683 measured reflections  
 1968 independent reflections  
 1949 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.057$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.019$   
 $wR(F^2) = 0.052$   
 $S = 0.98$   
 1968 reflections  
 137 parameters  
 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.45$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.72$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$                              | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{O5}-\text{H3}\cdots\text{O3}^{\text{ii}}$  | 0.83 (1)     | 1.76 (1)           | 2.577 (1)   | 172.70 (3)           |
| $\text{O3}-\text{H4}\cdots\text{N2}^{\text{iii}}$ | 0.79 (1)     | 2.13 (1)           | 2.907 (1)   | 169.64 (3)           |
| $\text{O3}-\text{H5}\cdots\text{O1}^{\text{iv}}$  | 0.64 (1)     | 2.19 (1)           | 2.788 (1)   | 157.14 (3)           |

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

Data collection:  $X$ -AREA (Stoe & Cie, 2002); cell refinement:  $X$ -AREA; data reduction:  $X$ -RED32 (Stoe & Cie, 2002); program(s) used to solve structure:  $SHELXS97$  (Sheldrick, 1997); program(s) used to refine structure:  $SHELXL97$  (Sheldrick, 1997); molecular graphics:  $PLATON$  (Spek, 2003); software used to prepare material for publication:  $enCIFer$  (Allen *et al.*, 2004).

The authors acknowledge the Faculty of Art and Science, Kirikkale University, for financial support and the Faculty of Art and Science, Ondokuz Mayıs University, Turkey, for use of the Stoe IPDS II diffractometer (purchased under grant F.279 of the University Research Fund).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2251).

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**supplementary materials**

*Acta Cryst.* (2007). E63, m1783-m1784 [ doi:10.1107/S1600536807025536 ]

## Poly[[diaquacaesium(I)]bis( $\mu$ -3-3-carboxypyrazine-2-carboxylato)]

M. Tombul, K. Güven and O. Büyükgüngör

### Comment

Metal dicarboxylates are known to form structures with varying dimensionalities, *e.g.* chains or layers, linked by the dicarboxylate anions (Rao *et al.*, 2004). Since the single-crystal X-ray analysis of pyrazine-2,3 dicarboxylic acid was first determined (Takusagawa & Shimada, 1973), a variety of metal-organic compounds of pyrazine-2,3-dicarboxylic acid have been characterized crystallographically, due to growing interest in supramolecular chemistry. These include the calcium (Ptasiewicz-Bak & Leciejewicz, 1997*a*; Starosta & Leciejewicz, 2005) and magnesium (Ptasiewicz-Bak & Leciejewicz, 1997*b*) complexes. The title compound (I), was obtained as a colorless powder during an attempt to synthesize a borate ester product from the reaction of  $\text{Cs}_2\text{CO}_3$  with  $\text{B}(\text{OH})_3$  and pyrazine-2,3-dicarboxylic acid, akin to the result for the sodium complex reported previously by our group (Tombul *et al.*, 2006). We herein report its crystal structure.

The asymmetric unit of the title compound, (I), contains one caesium cation, one pyrazine-2,3-dicarboxylate anion and one water molecule (Fig. 1). The pyrazine-2,3-dicarboxylic acid is deprotonated at one of the carboxylate groups so that the crystal structure consists of  $\text{Cs}^+$  cations and pyrazine-2,3-dicarboxylate anions. Taking a larger domain of the crystal structure, the anion is linked to three cations, while the cation is surrounded by six of the anions, two of which are coordinated by N and O atoms and the remaining four anions are coordinated solely by O atoms. In addition, each caesium atom is coordinated by two water molecules, reaching the coordination number to ten. The inner coordination sphere accommodates eight oxygen atoms ( $\text{O}3$ ,  $\text{O}4$ ,  $\text{O}1^{\text{i}}$ ,  $\text{O}1^{\text{ii}}$ ,  $\text{O}3^{\text{iii}}$ ,  $\text{O}2^{\text{iv}}$ ,  $\text{O}4^{\text{iv}}$  and  $\text{O}3^{\text{v}}$ ), together with two nitrogen atoms ( $\text{N}1$  and  $\text{N}1^{\text{i}}$ ) [Symmetry Codes: (i)  $2 - x, -1 - y, 1 - z$ , (ii)  $1 + x, y, z$ , (iii)  $2 - x, -y, 1 - z$ , (iv)  $1 + x, -1 + y, z$ , (v)  $3 - x, -1 - y, 1 - z$ ]. The Cs—O distances are in the range of 3.099 (1)–3.372 (2) Å, in which they are in accordance with the corresponding values reported for other caesium complexes (Harnish *et al.*, 1999; Wiesbrock & Schmidbaur, 2003; Hu *et al.*, 2005).

In the crystal structure, the intermolecular O—H $\cdots$ O and O—H $\cdots$ N hydrogen bonds (Table 2, Fig. 2) may be effective in the stabilization of the structure.

### Experimental

For the preparation of the title compound, (I),  $\text{Cs}_2\text{CO}_3$  (882 mg, 2.7 mmol) was carefully added to an aqueous solution (20 ml) containing pyrazine-2,3-di-carboxylic acid (1680 mg, 10 mmol) and  $\text{B}(\text{OH})_3$  (5 mmol, 0.31 g), until no bubbles escapes. The reaction mixture produced a colorless and clear solution, which was stirred at 333 K for 5 h, until all became solid. The solid product was redissolved in water (10 ml) and allowed to stand for 10 min at room temperature, whereupon transparent and fine crystals were harvested.

## Refinement

The pyrazine H atoms were positioned geometrically with C—H = 0.94 Å and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . H atoms of carboxylate and water molecules were located in difference syntheses and refined isotropically [O—H = 0.64 (4)–0.83 (4) Å and  $U_{\text{iso}}(\text{H}) = 0.057$  (9)–0.066 (9) Å<sup>2</sup>].

## Figures

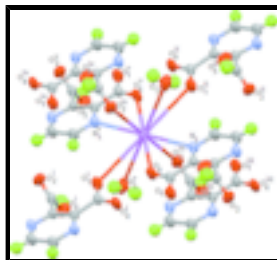


Fig. 1. A segment of the structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level [symmetry codes: (i)  $2 - x, -1 - y, 1 - z$ , (ii)  $1 + x, y, z$ , (iii)  $2 - x, -y, 1 - z$ , (iv)  $1 + x, -1 + y, z$ , (v)  $3 - x, -1 - y, 1 - z$ ].

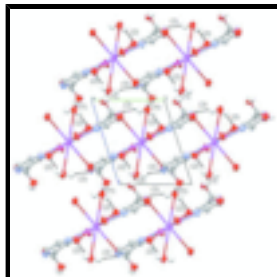


Fig. 2. A packing diagram for (I). The hydrogen bonds are shown as dashed lines [(1) O3—H(4)·N2, (2) O3—H5·O1, (3) O5—H3·O3].

## Poly[[diaquaacsium(II)]bis(μ<sub>3</sub>-3-carboxypyrazine-2-carboxylato)]

### Crystal data

[Cs(C<sub>6</sub>H<sub>3</sub>N<sub>2</sub>O<sub>4</sub>)<sub>2</sub>(H<sub>2</sub>O)<sub>2</sub>]

$M_r = 503.15$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 7.4801$  (9) Å

$b = 7.6352$  (9) Å

$c = 8.6505$  (11) Å

$\alpha = 70.031$  (9)°

$\beta = 81.126$  (10)°

$\gamma = 66.128$  (9)°

$V = 424.55$  (10) Å<sup>3</sup>

$Z = 1$

$F_{000} = 245$

$D_x = 1.968$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 22636 reflections

$\theta = 2.5$ – $28.0$ °

$\mu = 2.24$  mm<sup>-1</sup>

$T = 296$  K

Prism, colorless

$0.52 \times 0.47 \times 0.42$  mm

### Data collection

Stoe IPDS2  
diffractometer

1968 independent reflections

|   |  |
|---|--|
| Monochromator: plane graphite                                     | 1949 reflections with $I > 2\sigma(I)$ |
| Detector resolution: 6.67 pixels $\text{mm}^{-1}$                 | $R_{\text{int}} = 0.057$               |
| $T = 296$ K   | $\theta_{\text{max}} = 27.7^\circ$     |
| rotation method scans   | $\theta_{\text{min}} = 2.5^\circ$      |
| Absorption correction: integration<br>(X-RED32; Stoe & Cie, 2002) | $h = -9 \rightarrow 9$                 |
| $T_{\text{min}} = 0.382$ , $T_{\text{max}} = 0.471$               | $k = -9 \rightarrow 9$                 |
| 7683 measured reflections   | $l = -11 \rightarrow 11$               |

### Refinement

|  |   |
|--|---|
| Refinement on $F^2$  | Hydrogen site location: inferred from neighbouring sites  |
| Least-squares matrix: full                                     | H atoms treated by a mixture of independent and constrained refinement                          |
| $R[F^2 > 2\sigma(F^2)] = 0.019$                                | $w = 1/[\sigma^2(F_o^2) + (0.0343P)^2 + 0.0717P]$<br>where $P = (F_o^2 + 2F_c^2)/3$             |
| $wR(F^2) = 0.052$  | $(\Delta/\sigma)_{\text{max}} < 0.001$  |
| $S = 0.98$   | $\Delta\rho_{\text{max}} = 0.45 \text{ e } \text{\AA}^{-3}$                                     |
| 1968 reflections   | $\Delta\rho_{\text{min}} = -0.71 \text{ e } \text{\AA}^{-3}$                                    |
| 137 parameters   | Extinction correction: SHELXL97,<br>$F_c^* = kFc[1 + 0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | Extinction coefficient: 0.187 (6)   |
| Secondary atom site location: difference Fourier map           |   |

### 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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

|     | $x$          | $y$         | $z$        | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|------------|----------------------------------|
| Cs1 | 1.5000       | -0.5000     | 0.5000     | 0.04315 (10)                     |
| O1  | 0.7652 (2)   | -0.1628 (2) | 0.3351 (2) | 0.0447 (3)                       |
| O2  | 0.54073 (19) | 0.3193 (2)  | 0.2006 (2) | 0.0464 (3)                       |
| O3  | 1.6315 (3)   | -0.2774 (3) | 0.1162 (2) | 0.0545 (4)                       |
| H4  | 1.719 (5)    | -0.381 (6)  | 0.118 (4)  | 0.059 (8)*                       |
| H5  | 1.659 (5)    | -0.228 (6)  | 0.147 (4)  | 0.057 (9)*                       |
| O4  | 1.0625 (2)   | -0.3669 (2) | 0.4303 (2) | 0.0500 (4)                       |

## supplementary materials

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|    |            |             |              |            |
|----|------------|-------------|--------------|------------|
| O5 | 0.6999 (2) | 0.1627 (3)  | 0.0154 (2)   | 0.0507 (3) |
| H3 | 0.589 (5)  | 0.202 (6)   | -0.020 (5)   | 0.066 (9)* |
| N1 | 1.1830 (2) | -0.0606 (2) | 0.34310 (19) | 0.0342 (3) |
| N2 | 0.9390 (2) | 0.3245 (2)  | 0.1696 (2)   | 0.0378 (3) |
| C1 | 1.2381 (2) | 0.0943 (3)  | 0.3004 (2)   | 0.0376 (3) |
| H1 | 1.3639     | 0.0727      | 0.3275       | 0.045*     |
| C2 | 1.1156 (3) | 0.2872 (3)  | 0.2169 (3)   | 0.0403 (4) |
| H2 | 1.1579     | 0.3942      | 0.1930       | 0.048*     |
| C3 | 0.8866 (2) | 0.1668 (2)  | 0.20647 (19) | 0.0297 (3) |
| C4 | 1.0056 (2) | -0.0248 (2) | 0.29693 (19) | 0.0286 (3) |
| C5 | 0.6880 (2) | 0.2210 (2)  | 0.1433 (2)   | 0.0331 (3) |
| C6 | 0.9360 (2) | -0.1975 (3) | 0.3563 (2)   | 0.0332 (3) |

### Atomic displacement parameters ( $\text{\AA}^2$ )

|     | $U^{11}$     | $U^{22}$     | $U^{33}$     | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| Cs1 | 0.03439 (11) | 0.03736 (11) | 0.04492 (12) | -0.00218 (7) | -0.00804 (6) | -0.00818 (7) |
| O1  | 0.0369 (6)   | 0.0391 (7)   | 0.0612 (8)   | -0.0182 (6)  | -0.0151 (6)  | -0.0086 (6)  |
| O2  | 0.0287 (6)   | 0.0499 (8)   | 0.0663 (9)   | -0.0114 (6)  | -0.0034 (6)  | -0.0280 (7)  |
| O3  | 0.0501 (8)   | 0.0445 (8)   | 0.0754 (11)  | -0.0075 (7)  | -0.0265 (8)  | -0.0279 (8)  |
| O4  | 0.0350 (6)   | 0.0290 (6)   | 0.0762 (10)  | -0.0138 (5)  | -0.0103 (7)  | 0.0014 (6)   |
| O5  | 0.0401 (7)   | 0.0623 (9)   | 0.0481 (7)   | -0.0066 (7)  | -0.0147 (6)  | -0.0247 (7)  |
| N1  | 0.0282 (6)   | 0.0320 (6)   | 0.0403 (7)   | -0.0109 (5)  | -0.0050 (5)  | -0.0073 (6)  |
| N2  | 0.0341 (7)   | 0.0291 (6)   | 0.0481 (8)   | -0.0135 (6)  | -0.0073 (6)  | -0.0049 (6)  |
| C1  | 0.0286 (7)   | 0.0393 (9)   | 0.0472 (9)   | -0.0163 (7)  | -0.0045 (7)  | -0.0101 (7)  |
| C2  | 0.0349 (8)   | 0.0347 (8)   | 0.0539 (10)  | -0.0185 (7)  | -0.0047 (7)  | -0.0084 (7)  |
| C3  | 0.0275 (7)   | 0.0299 (7)   | 0.0315 (6)   | -0.0110 (6)  | -0.0027 (6)  | -0.0083 (6)  |
| C4  | 0.0277 (6)   | 0.0282 (7)   | 0.0310 (6)   | -0.0116 (6)  | -0.0018 (6)  | -0.0088 (5)  |
| C5  | 0.0305 (7)   | 0.0286 (7)   | 0.0394 (8)   | -0.0109 (6)  | -0.0069 (6)  | -0.0073 (6)  |
| C6  | 0.0338 (7)   | 0.0299 (7)   | 0.0378 (7)   | -0.0145 (6)  | -0.0042 (6)  | -0.0084 (6)  |

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

|                                     |           |       |           |
|-------------------------------------|-----------|-------|-----------|
| Cs1 <sup>i</sup> —O1 <sup>ii</sup>  | 3.188 (2) | O4—C6 | 1.268 (2) |
| Cs1 <sup>i</sup> —O1 <sup>iii</sup> | 3.188 (2) | O5—C5 | 1.305 (2) |
| Cs1 <sup>i</sup> —O2 <sup>iv</sup>  | 3.249 (1) | O5—H3 | 0.83 (4)  |
| Cs1 <sup>i</sup> —O2 <sup>v</sup>   | 3.249 (2) | N1—C1 | 1.325 (2) |
| Cs1—O3                              | 3.372 (2) | N1—C4 | 1.338 (2) |
| Cs1 <sup>i</sup> —O3 <sup>ii</sup>  | 3.372 (2) | N2—C2 | 1.333 (2) |
| Cs1—O4                              | 3.099 (1) | N2—C3 | 1.336 (2) |
| Cs1 <sup>i</sup> —O4 <sup>ii</sup>  | 3.099 (1) | C1—C2 | 1.384 (3) |
| Cs1—N1                              | 3.188 (2) | C1—H1 | 0.9400    |
| Cs1 <sup>i</sup> —N1 <sup>ii</sup>  | 3.188 (2) | C2—H2 | 0.9400    |
| O1—C6                               | 1.226 (2) | C4—C3 | 1.387 (2) |
| O2—C5                               | 1.200 (2) | C5—C3 | 1.509 (2) |
| O3—H4                               | 0.79 (4)  | C6—C4 | 1.511 (2) |
| O3—H5                               | 0.64 (4)  |       |           |

|             |              |             |             |
|-------------|--------------|-------------|-------------|
| H4—O3—H5    | 109 (4)      | N2—C3—C5    | 113.30 (14) |
| C5—O5—H3    | 109 (2)      | C4—C3—C5    | 124.88 (13) |
| C1—N1—C4    | 117.24 (15)  | N1—C4—C3    | 120.82 (14) |
| C2—N2—C3    | 116.75 (15)  | N1—C4—C6    | 117.40 (15) |
| N1—C1—C2    | 121.84 (15)  | C3—C4—C6    | 121.66 (14) |
| N1—C1—H1    | 119.1        | O2—C5—O5    | 125.96 (17) |
| C2—C1—H1    | 119.1        | O2—C5—C3    | 121.64 (15) |
| N2—C2—C1    | 121.40 (15)  | O5—C5—C3    | 112.19 (14) |
| N2—C2—H2    | 119.3        | O1—C6—O4    | 126.00 (15) |
| C1—C2—H2    | 119.3        | O1—C6—C4    | 118.73 (16) |
| N2—C3—C4    | 121.81 (14)  | O4—C6—C4    | 115.22 (14) |
| C4—N1—C1—C2 | 2.4 (3)      | C6—C4—C3—C5 | -6.3 (2)    |
| C1—N1—C4—C3 | 0.7 (2)      | O2—C5—C3—N2 | -69.7 (2)   |
| C1—N1—C4—C6 | -175.48 (15) | O5—C5—C3—N2 | 105.33 (18) |
| C3—N2—C2—C1 | -0.1 (3)     | O2—C5—C3—C4 | 109.1 (2)   |
| C2—N2—C3—C4 | 3.2 (2)      | O5—C5—C3—C4 | -75.9 (2)   |
| C2—N2—C3—C5 | -177.92 (16) | O1—C6—C4—N1 | 170.21 (16) |
| N1—C1—C2—N2 | -2.8 (3)     | O4—C6—C4—N1 | -7.3 (2)    |
| N1—C4—C3—N2 | -3.7 (2)     | O1—C6—C4—C3 | -6.0 (2)    |
| C6—C4—C3—N2 | 172.36 (15)  | O4—C6—C4—C3 | 176.54 (16) |
| N1—C4—C3—C5 | 177.61 (15)  |             |             |

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

*Hydrogen-bond geometry* ( $\text{\AA}, ^\circ$ )

| $D-H\cdots A$              | $D-H$    | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------|----------|-------------|-------------|---------------|
| $O5^i-H3^i\cdots O3^{vi}$  | 0.83 (1) | 1.76 (1)    | 2.577 (1)   | 172.70 (3)    |
| $O3^i-H4^i\cdots N2^{iv}$  | 0.79 (1) | 2.13 (1)    | 2.907 (1)   | 169.64 (3)    |
| $O3^i-H5^i\cdots O1^{iii}$ | 0.64 (1) | 2.19 (1)    | 2.788 (1)   | 157.14 (3)    |

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



Fig. 1

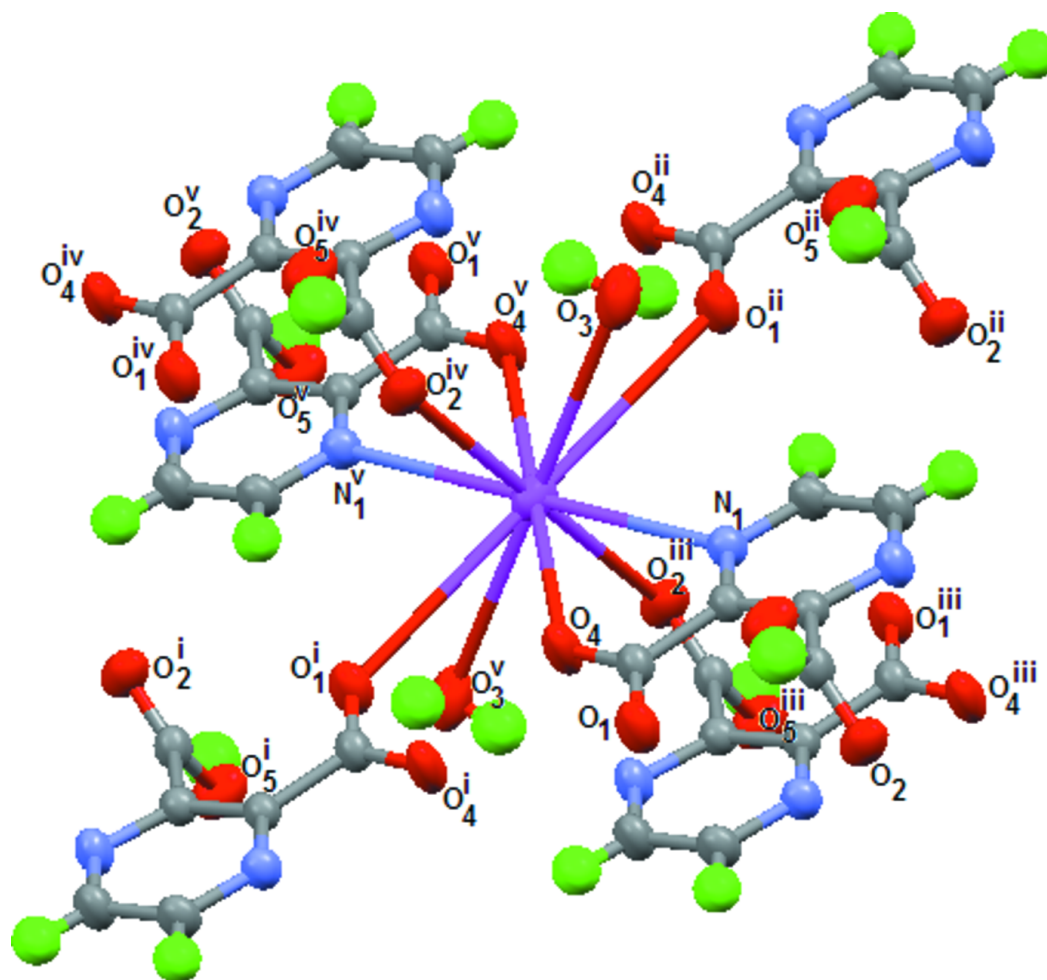
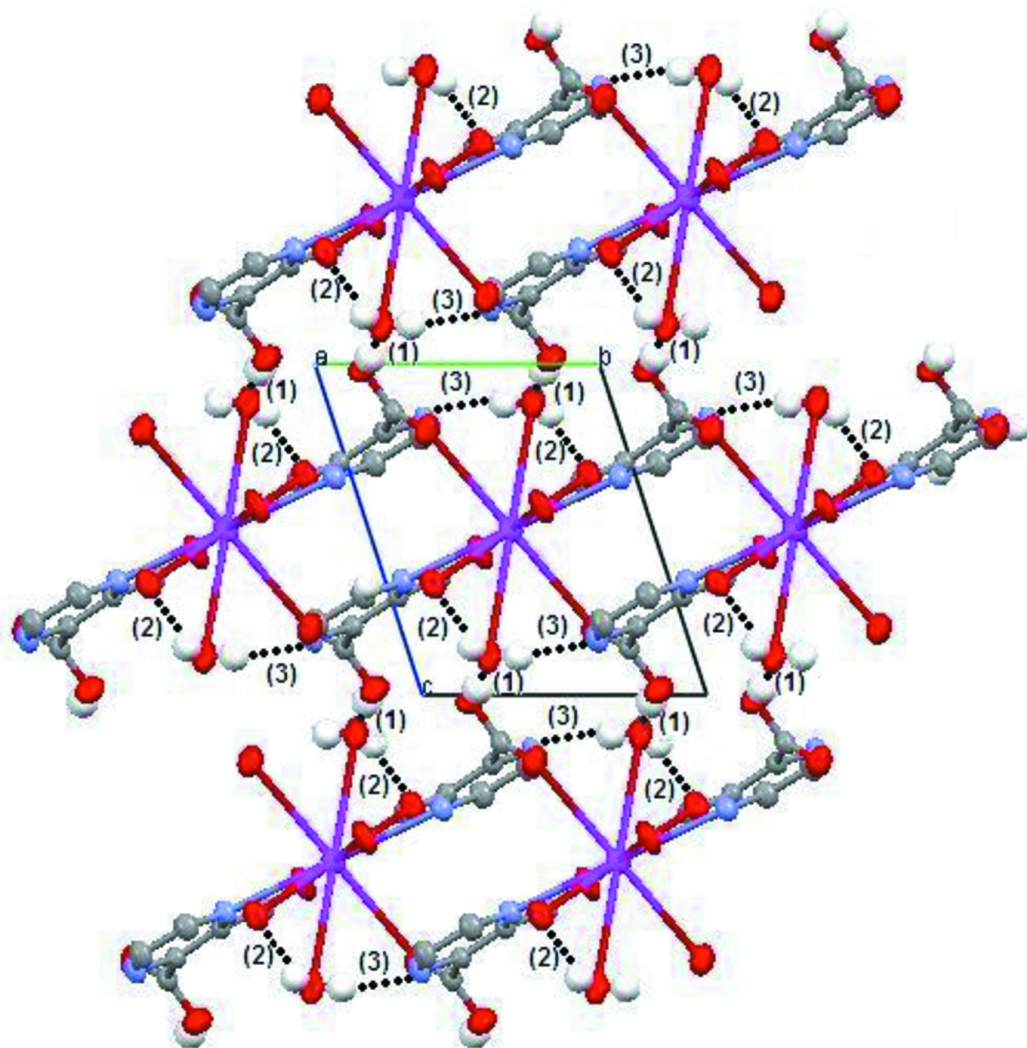


Fig. 2



## Poly[[diaquacaesium(II)]bis( $\mu_3$ -3-carboxypyrazine-2-carboxylato)]. Corrigendum

Mustafa Tombul,<sup>a\*</sup> Kutalmış Güven<sup>b</sup> and Orhan Büyükgüngör<sup>c</sup>

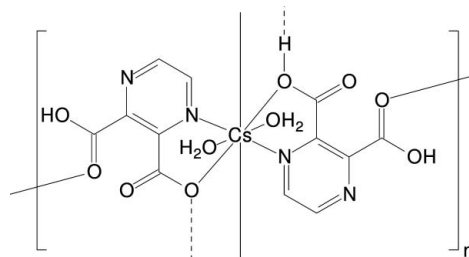
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Received 19 February 2008; accepted 19 February 2008

Corrections are made to the formulation and scheme in Tombul, Güven & Büyükgüngör [*Acta Cryst.* (2007) E63, m1783–m1784].

The structure reported by Tombul, Güven & Büyükgüngör [*Acta Cryst.* (2007) E63, m1783–m1784] was incorrectly

formulated. The compound is actually poly[diaqua( $\mu_2$ -3-carboxypyrazine-2-carboxylato)( $\mu_2$ -pyrazine-2,3-dicarboxylic acid)caesium(I)],  $[\text{Cs}(\text{C}_6\text{H}_3\text{N}_2\text{O}_4)(\text{C}_6\text{H}_4\text{N}_2\text{O}_4)(\text{H}_2\text{O})_2]_n$ . A disordered H atom was omitted in the structural analysis, which leads to protonation of half the organic ligands and corrects the charge imbalance of the original structure. The compound is isostructural with the corresponding potassium complex, which is fully described by Tombul, Güven & Svoboda [*Acta Cryst.* (2008), E64, m246–m247]. Inclusion of the missing atom makes no significant difference to the refinement results and affects only the interpretation of the structure. A corrected scheme is shown below.



### References

- Tombul, M., Güven, K. & Büyükgüngör, O. (2007). *Acta Cryst.* E63, m1783–m1784.  
Tombul, M., Güven, K. & Svoboda, I. (2008). *Acta Cryst.* E64, m246–m247.