Refinement

Refinement on F
$R = 0.035$
$wR = 0.045$
$S = 2.73$
2026 reflections
306 parameters
All H-atom parameters refined

$w = 1/\sigma^2(F_o)$
$(\Delta/\sigma)_{\max} = 0.101$
$\Delta\rho_{\max} = 0.680$ e Å^{-3}
$\Delta\rho_{\min} = -0.600$ e Å^{-3}
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$B_{\rm eq} = (8\pi^2/3)\Sigma_i\Sigma_jU_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
Mo	0.20106 (4)	0.18106 (3)	0.19109 (3)	2.51 (2)
P	0.69192 (16)	−0.00763 (11)	0.23347 (13)	4.33 (7)
N	0.4223 (5)	0.2016 (4)	0.1489 (4)	3.7 (2)
O1	0.2150 (5)	−0.0314 (3)	0.1908 (4)	6.4 (3)
F1	0.7065 (5)	0.1008 (3)	0.2395 (4)	8.5 (3)
F2	0.6767 (5)	−0.1154 (3)	0.2236 (5)	9.3 (3)
F3	0.8005 (7)	−0.0170 (5)	0.3350 (4)	12.1 (4)
F4	0.5751 (8)	0.0032 (4)	0.1382 (6)	16.4 (5)
F5	0.8138 (7)	−0.0122 (4)	0.1730 (6)	13.8 (5)
F6	0.5699 (7)	−0.0044 (5)	0.2983 (7)	16.0 (6)
C1	0.2179 (6)	0.0475 (4)	0.1933 (4)	3.7 (3)
C2	0.1754 (6)	0.2449 (4)	0.0203 (4)	3.9 (3)
C3	0.1053 (8)	0.3040 (4)	0.0825 (5)	4.8 (3)
C4	−0.0054 (7)	0.2545 (5)	0.1153 (5)	4.9 (3)
C5	−0.0063 (7)	0.1655 (5)	0.0756 (5)	4.5 (3)
C6	0.1037 (7)	0.1597 (5)	0.0159 (4)	4.0 (3)
C7	0.3092 (8)	0.2628 (7)	−0.0206 (6)	6.0 (4)
C8	0.4188 (8)	0.1951 (6)	0.0325 (6)	5.5 (4)
C9	0.5030 (9)	0.2844 (6)	0.1922 (8)	5.9 (4)
C11	0.3465 (6)	0.1565 (4)	0.3525 (4)	3.5 (2)
C12	0.2795 (7)	0.2440 (4)	0.3482 (4)	4.0 (3)
C13	0.1309 (7)	0.2395 (4)	0.3354 (4)	4.3 (3)
C14	0.0716 (7)	0.1512 (5)	0.3273 (5)	4.3 (5)
C15	0.1347 (8)	0.0756 (5)	0.4004 (5)	5.0 (3)
C16	0.2969 (7)	0.0805 (5)	0.4178 (5)	4.4 (3)

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

Mo—N	2.282 (5)	C2—C3	1.417 (9)
Mo—C1	1.947 (6)	C2—C6	1.410 (9)
Mo—C2	2.368 (5)	C2—C7	1.481 (9)
Mo—C3	2.359 (6)	C3—C4	1.399 (11)
Mo—C4	2.306 (6)	C4—C5	1.390 (11)
Mo—C5	2.279 (6)	C5—C6	1.403 (9)
Mo—C6	2.318 (5)	C7—C8	1.513 (11)
Mo—C11	2.330 (5)	C11—C12	1.419 (8)
Mo—C12	2.237 (5)	C11—C16	1.512 (8)
Mo—C13	2.248 (5)	C12—C13	1.399 (10)
Mo—C14	2.351 (6)	C13—C14	1.399 (10)
N—C8	1.500 (9)	C14—C15	1.505 (9)
N—C9	1.487 (9)	C15—C16	1.525 (10)
O1—C1	1.147 (7)		
N—Mo—C1	93.3 (2)	C6—C2—C7	125.5 (6)
C1—Mo—C11	78.4 (2)	C11—C12—C13	113.7 (6)
C1—Mo—C12	112.3 (2)	C11—C16—C15	110.8 (5)
C1—Mo—C13	113.5 (2)	C12—C11—C16	119.8 (6)
C1—Mo—C14	81.8 (2)	C12—C13—C14	116.1 (6)
C2—C3—C4	108.1 (6)	C13—C14—C15	120.5 (6)
C2—C6—C5	109.1 (6)	C14—C15—C16	110.3 (5)
C2—C7—C8	107.0 (5)	Mo—N—C8	111.3 (4)
C3—C4—C5	109.0 (6)	Mo—N—C9	117.1 (5)
C3—C2—C6	106.5 (5)	Mo—C1—O1	173.8 (5)
C3—C2—C7	127.6 (7)	C8—N—C9	110.6 (6)
C4—C5—C6	107.4 (6)	N—C8—C7	108.2 (6)
C5—Mo—N—C8	−4.9 (4)	C11—C12—C13—C14	−0.1 (4)
C4—Mo—C1—O1	−3.9 (4)	C12—C13—C14—C15	44.5 (5)
C7—C2—C3—C4	−170.6 (10)	C14—C15—C16—C11	−3.2 (4)
C7—C2—C6—C5	170.7 (9)	C16—C11—C12—C13	−45.0 (5)
C2—C3—C4—C5	−0.5 (4)		

All the data processing was carried out on a MicroVAX 3600 computer using the *NRCVAX* program system (Gabe, Le Page, White & Lee, 1987).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: HU1051). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Cadmium(II) Chloride Adduct with an Olefinic Double Betaine: *catena*-Poly[tetraaquadiethanoltris[dichlorocadmium(II)] *cis*-bis(4-dimethylamino-1-pyridinio)butenedioate hydrate]

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Abstract

The structure of a cadmium(II) chloride adduct with an olefinic double betaine {systematic name: *catena*-poly[[(diaquacadmium)-di-μ-chloro-(diethanolcadmium)-di-μ-chloro-(diaquacadmium)-di-μ-chloro] *cis*-bis(4-dimethylamino-1-pyridinio)butenedioate monohydrate]}, $[(CdCl_2)_3(C_2H_6O)_2(H_2O)_4]_n.n(C_{18}H_{20}N_4O_4).nH_2O$, is based on an infinite zigzag chain consisting of a series of corner-sharing $CdCl_2$ quadrilaterals with aqua or ethanol ligands around each Cd^{II} atom, forming a $CdCl_4O_2$ octahedral coordination polyhedron. The olefinic double betaine has no association with the metal atoms, being bound to the aqua and ethanol ligands in the chain and to the lattice water molecule by hydrogen bonding.

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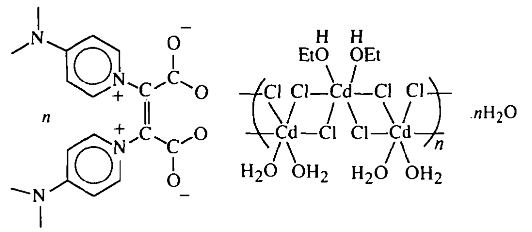
Comment

Betaine ($Me_3N^+CH_2CO_2^-$; trimethylammonioacetate) and its derivatives, considered as neutral structural analogues of the corresponding carboxylate anions, are very good proton acceptors and versatile ligands, and can form water-soluble cadmium complexes in a variety of coordination modes (Chen & Mak, 1991*a*,*b*; Chen, Mak, Huang & Lü, 1992). The present report deals with the preparation and crystal structure of a cadmium chloride adduct with an olefinic double betaine that possesses pairs of *cis* anionic carboxylate groups and positively charged pyridinium substituents, namely *catena*-poly-[[(diaquacadmium)-di-μ-chloro-(diethanolcadmium)-di-μ-chloro-(diaquacadmium)-di-μ-chloro] *cis*-bis(4-dimethylamino-1-pyridinio)butenedioate monohydrate], (I).



(I)

The structure of the title adduct comprises an infinite zigzag chain plus the uncoordinated olefinic double betaine and a lattice water molecule (Fig. 1). The coordination geometry about each Cd^{II} atom is octahedral, involving four Cl ligands [Cd—Cl = 2.570 (3)–2.679 (3) Å] and two *cis*-related O atoms [Cd—O = 2.266 (8)–2.380 (7) Å], the most distorted bond angles about the three crystallographically independent cadmium(II) atoms being 86.0 (2), 85.1 (1) and 82.8 (2)°. Such an octahedral environment about Cd^{II} is well documented and indeed preferred for most of the known cadmium(II) carboxylates (Prince, 1987). Unlike atoms Cd(1) and Cd(3), in which the two *cis*-related O atoms are from two aqua ligands, the pair of O atoms around atom Cd(2) belong to two ethanol ligands. Neighbouring Cd^{II} atoms are linked by a pair of bridging Cl ligands [Cd—Cl—Cd = 91.0 (1)–92.4 (1)°] to generate a one-dimensional polymeric chain structure similar to that in the cadmium complex of a betaine derivative $[Cd(Et_3NCH_2CO_2)(\mu\text{-}Cl_2)]_n$ (Chen, Mak, Huang & Lü, 1992); however, in the latter case the *cis*-related positions are occupied by two O atoms of a symmetrical chelating carboxylate group of the betaine ligand, and the coordination geometry about Cd^{II} is much more distorted.

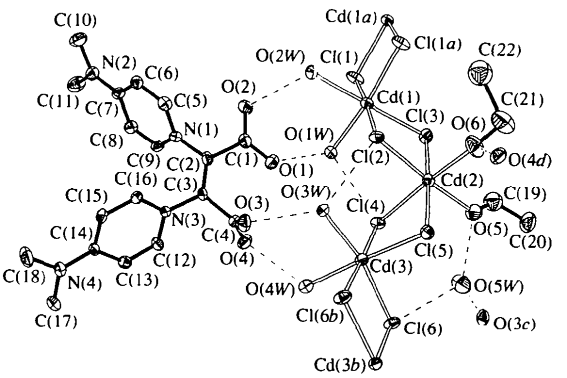


Fig. 1. Perspective view (35% probability displacement ellipsoids) of the structure of the title adduct with the atom-numbering scheme, excluding the H atoms. Each disordered ethanol molecule is shown in one of its two orientations. Hydrogen bonds are indicated by broken lines.

The olefinic double betaine has no direct association with the metal atoms, being bound to the aqua and ethanol ligands in the chain by hydrogen bonds [O···O = 2.689 (10)–2.775 (8) Å]; the lattice water molecule is involved in three hydrogen bonds [O(5*W*)···O(3^i) 2.773 (8), O(5*W*)···Cl(6) 3.228 (9), O(5)···O(5*W*) 2.629 (12) Å; see Table 3]. The configuration of the olefinic double betaine is significantly different from those in its hexahydrated form (Weiss, Roth, Lowack & Bremer, 1990) and its perchloric or nitric acid adducts (Wu & Mak, 1994*a*), in which two carboxylate groups are (i) twisted out of the plane of the central double bond in a conrotatory fashion, and (ii) coplanar with the central double bond, respectively. In the present adduct, one carboxylate group is almost coplanar with the double bond [O(1)—C(1)—C(2)—C(3) = 4.0 (9)°], while the other is orthogonal to it [O(3)—C(4)—C(3)—C(2) = 89.9 (9)°]. Such an arrangement of the two carboxylate groups is known in metal complexes with a coordinated olefinic double-betaine ligand, such as $[Hg_2(C_{18}H_{20}N_4O_4)_2X_4.6HgX_2]_n$ (X = Cl, Br) (Wu & Mak, 1994*b*) and $[Cd_3(C_{18}H_{20}N_4O_4)_3I_2(H_2O)_6]_n$-$[CdI_4]_{2n}.nH_2O$ (Wu & Mak, 1995). Most betaine compounds are versatile ligands and exhibit strong ligation behaviour towards metals. Occurrence of the uncoordinated olefinic double betaine in the present metal complex may be due to its large steric bulk as compared with the coordinated chloro, aqua and ethanol ligands.

Experimental

The olefinic double betaine in its hexahydrated form was synthesized by a literature method (Weiss *et al.*, 1990). The title adduct was prepared by dissolving $CdCl_2$ (81.3 mg, 0.40 mmol) and the double betaine (92.8 mg, 0.20 mmol) in hot water (10 ml). The resulting colourless solution was cooled and covered with ethanol (5 ml). Slow diffusion at room temperature for several days yielded colourless plate-like crystals.

Crystal data

$[Cd_3Cl_6(C_2H_6O)_2(H_2O)_4]$.- $C_{18}H_{20}N_4O_4.H_2O$	Mo $K\alpha$ radiation λ = 0.71073 Å

$M_r = 1088.5$
Triclinic
$P\bar{1}$
$a = 10.082\ (1)$ Å
$b = 10.746\ (2)$ Å
$c = 19.155\ (9)$ Å
$\alpha = 95.81\ (2)°$
$\beta = 98.05\ (2)°$
$\gamma = 112.63\ (1)°$
$V = 1869.0\ (12)$ Å^3
$Z = 2$
$D_x = 1.934$ Mg m^{-3}

Cell parameters from 25 reflections
$\theta = 6.0$–$12.5°$
$\mu = 2.175$ mm^{-1}
$T = 293$ K
Plate
$0.40 \times 0.30 \times 0.10$ mm
Colourless

Data collection

Siemens $R3m/V$ diffractometer
ω scans
Absorption correction:
ψ scan (Kopfmann & Huber, 1968)
$T_{\min} = 0.522$, $T_{\max} = 0.741$
6924 measured reflections
6519 independent reflections

5435 observed reflections $[F > 4\sigma(F)]$
$R_{\rm int} = 0.022$
$\theta_{\max} = 25.0°$
$h = 0 \rightarrow 11$
$k = -12 \rightarrow 11$
$l = -22 \rightarrow 22$
3 standard reflections monitored every 97 reflections
intensity decay: 1.1%

Refinement

Refinement on F
$R = 0.051$
$wR = 0.072$
$S = 1.93$
5435 reflections
416 parameters
H-atom parameters not refined
$w = 1/[\sigma^2(F) + 0.0005F^2]$
$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 1.58$ e Å^{-3}
$\Delta\rho_{\min} = -0.75$ e Å^{-3}
Extinction correction: $F^* = F[1 + (0.02\chi \times F^2/\sin 2\theta)]^{-1/4}$
Extinction coefficient: $\chi = 0.00031\ (6)$
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

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

$$U_{\rm eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$U_{\rm eq}$
Cd(1)	0.4852 (1)	0.0236 (1)	0.0948 (1)	0.030 (1)
Cd(2)	0.6344 (1)	−0.0964 (1)	0.2529 (1)	0.034 (1)
Cd(3)	0.4728 (1)	0.0074 (1)	0.4029 (1)	0.030 (1)
Cl(1)	0.3052 (2)	−0.0958 (2)	−0.0249 (1)	0.045 (1)
Cl(2)	0.6497 (2)	0.1379 (2)	0.2201 (1)	0.033 (1)
Cl(3)	0.5190 (2)	−0.2022 (2)	0.1184 (1)	0.042 (1)
Cl(4)	0.3664 (2)	−0.1583 (2)	0.2823 (1)	0.035 (1)
Cl(5)	0.7280 (2)	0.0033 (2)	0.3895 (1)	0.037 (1)
Cl(6)	0.4095 (2)	−0.1854 (2)	0.4790 (1)	0.039 (1)
O(1*W*)	0.2911 (6)	−0.0209 (6)	0.1518 (3)	0.039 (2)
O(2*W*)	0.4579 (6)	0.2266 (5)	0.0716 (3)	0.042 (2)
O(3*W*)	0.5063 (6)	0.1971 (5)	0.3509 (3)	0.037 (2)
O(4*W*)	0.2417 (6)	0.0029 (6)	0.4198 (3)	0.045 (3)
O(5*W*)	0.4920 (9)	−0.3936 (7)	0.3784 (4)	0.077 (4)
O(5)	0.6239 (9)	−0.3038 (7)	0.2733 (4)	0.071 (4)
C(19)†	0.595 (2)	−0.4213 (16)	0.2224 (8)	0.071 (6)
C(19′)†	0.695 (6)	−0.379 (3)	0.240 (3)	0.06 (2)
C(20)	0.6475 (14)	−0.5185 (12)	0.2541 (6)	0.074 (6)
O(6)	0.8738 (7)	−0.0322 (8)	0.2417 (4)	0.070 (3)
C(21)	0.9298 (16)	−0.0885 (15)	0.1911 (7)	0.098 (8)
C(22)†	0.942 (3)	0.009 (3)	0.1277 (15)	0.113 (12)
C(22′)†	0.992 (2)	−0.176 (2)	0.2320 (11)	0.057 (7)
O(1)	0.2867 (8)	0.2082 (7)	0.2203 (3)	0.054 (3)
O(2)	0.2647 (8)	0.3086 (7)	0.1266 (3)	0.055 (3)
O(3)	0.3275 (7)	0.3300 (6)	0.3733 (3)	0.043 (2)
O(4)	0.1178 (6)	0.1461 (6)	0.3417 (3)	0.043 (2)
N(1)	0.0910 (6)	0.4217 (6)	0.1802 (3)	0.027 (2)
N(2)	−0.1149 (8)	0.6032 (7)	0.0507 (3)	0.040 (3)
N(3)	0.0671 (6)	0.4108 (6)	0.3259 (3)	0.025 (2)
N(4)	−0.1335 (7)	0.6063 (7)	0.4443 (3)	0.037 (3)
C(1)	0.2439 (9)	0.2826 (8)	0.1864 (4)	0.038 (3)
C(2)	0.1612 (8)	0.3520 (7)	0.2231 (4)	0.031 (3)
C(3)	0.1421 (7)	0.3416 (7)	0.2899 (4)	0.024 (3)
C(4)	0.2022 (9)	0.2629 (8)	0.3365 (4)	0.032 (3)
C(5)	0.1709 (8)	0.5342 (8)	0.1537 (4)	0.032 (3)
C(6)	0.1067 (8)	0.5952 (8)	0.1120 (4)	0.032 (3)
C(7)	−0.0487 (9)	0.5445 (8)	0.0921 (4)	0.033 (3)
C(8)	−0.1279 (9)	0.4260 (8)	0.1214 (4)	0.035 (3)
C(9)	−0.0575 (8)	0.3707 (7)	0.1625 (4)	0.031 (3)
C(10)	−0.0362 (11)	0.7254 (9)	0.0229 (5)	0.055 (4)
C(11)	−0.2748 (10)	0.5476 (11)	0.0283 (5)	0.060 (5)
C(12)	−0.0468 (8)	0.3378 (7)	0.3575 (4)	0.028 (3)
C(13)	−0.1117 (8)	0.4005 (7)	0.3956 (4)	0.030 (3)
C(14)	−0.0683 (8)	0.5446 (7)	0.4053 (4)	0.028 (3)
C(15)	0.0500 (8)	0.6170 (7)	0.3732 (4)	0.030 (3)
C(16)	0.1122 (8)	0.5500 (7)	0.3348 (4)	0.031 (3)
C(17)	−0.2527 (9)	0.5296 (9)	0.4775 (5)	0.044 (4)
C(18)	−0.0908 (11)	0.7524 (9)	0.4555 (5)	0.055 (4)

† Site occupancy factors for C(19) and C(19′) are 0.79 (4) and 0.21 (4), respectively, and for C(22) and C(22′) are 0.53 (2) and 0.47 (2), respectively.

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

Cd(1)—Cl(1)	2.577 (2)	Cd(1)—Cl(2)	2.596 (2)
Cd(1)—Cl(3)	2.650 (3)	Cd(1)—Cl(1$^{\rm i}$)	2.570 (3)
Cd(1)—O(1*W*)	2.288 (6)	Cd(1)—O(2*W*)	2.378 (7)
Cd(2)—Cl(2)	2.608 (2)	Cd(2)—Cl(3)	2.614 (2)
Cd(2)—Cl(4)	2.679 (3)	Cd(2)—Cl(5)	2.617 (2)
Cd(2)—O(5)	2.266 (8)	Cd(2)—O(6)	2.290 (7)
Cd(3)—Cl(4)	2.582 (2)	Cd(3)—Cl(5)	2.638 (3)
Cd(3)—Cl(6)	2.583 (2)	Cd(3)—Cl(6$^{\rm ii}$)	2.609 (2)
Cd(3)—O(3*W*)	2.289 (6)	Cd(3)—O(4*W*)	2.380 (7)
O(5)—C(19)	1.420 (18)	O(5)—C(19′)	1.44 (6)
C(19)—C(20)	1.48 (2)	C(19′)—C(20)	1.45 (4)
O(6)—C(21)	1.386 (19)	C(21)—C(22)	1.66 (4)
C(21)—C(22′)	1.53 (3)	O(1)—C(1)	1.241 (12)
O(2)—C(1)	1.233 (11)	O(3)—C(4)	1.249 (9)
O(4)—C(4)	1.240 (9)	N(1)—C(2)	1.451 (11)
N(1)—C(5)	1.363 (9)	N(1)—C(9)	1.359 (9)
N(2)—C(7)	1.322 (12)	N(2)—C(10)	1.448 (12)
N(2)—C(11)	1.467 (12)	N(3)—C(3)	1.440 (11)
N(3)—C(12)	1.377 (9)	N(3)—C(16)	1.370 (9)
N(4)—C(14)	1.342 (12)	N(4)—C(17)	1.445 (11)
N(4)—C(18)	1.443 (11)	C(1)—C(2)	1.510 (14)
C(2)—C(3)	1.329 (11)	C(3)—C(4)	1.509 (12)
C(5)—C(6)	1.331 (12)	C(6)—C(7)	1.425 (11)
C(7)—C(8)	1.436 (11)	C(8)—C(9)	1.318 (13)
C(12)—C(13)	1.338 (12)	C(13)—C(14)	1.422 (11)
C(14)—C(15)	1.412 (10)	C(15)—C(16)	1.351 (13)
Cl(1)—Cd(1)—Cl(2)	175.7 (1)	Cl(1)—Cd(1)—O(2*W*)	86.7 (1)
Cl(1)—Cd(1)—O(1*W*)	89.6 (1)	Cl(2)—Cd(1)—Cl(3)	86.9 (1)
Cl(1)—Cd(1)—Cl(1$^{\rm i}$)	88.5 (1)	Cl(2)—Cd(1)—O(2*W*)	93.5 (1)
Cl(2)—Cd(1)—O(1*W*)	86.1 (1)	Cl(3)—Cd(1)—O(1*W*)	93.9 (2)
Cl(2)—Cd(1)—Cl(1$^{\rm i}$)	95.8 (1)	Cl(3)—Cd(1)—Cl(1$^{\rm i}$)	92.8 (1)
Cl(3)—Cd(1)—O(2*W*)	178.8 (2)	O(1*W*)—Cd(1)—Cl(1$^{\rm i}$)	173.1 (2)
O(1*W*)—Cd(1)—O(2*W*)	87.3 (2)	Cl(2)—Cd(2)—Cl(3)	87.4 (1)
O(2*W*)—Cd(1)—Cl(1$^{\rm i}$)	86.0 (2)	Cl(2)—Cd(2)—Cl(5)	93.0 (1)
Cl(2)—Cd(2)—Cl(4)	91.8 (1)	Cl(2)—Cd(2)—O(6)	88.3 (2)
Cl(2)—Cd(2)—O(5)	175.8 (2)	Cl(3)—Cd(2)—Cl(5)	175.3 (1)
Cl(3)—Cd(2)—Cl(4)	90.2 (1)	Cl(3)—Cd(2)—O(6)	96.6 (2)
Cl(3)—Cd(2)—O(5)	89.1 (2)	Cl(4)—Cd(2)—O(5)	90.4 (2)
Cl(4)—Cd(2)—Cl(5)	85.1 (1)	Cl(5)—Cd(2)—O(5)	90.7 (2)
Cl(4)—Cd(2)—O(6)	173.3 (2)	O(5)—Cd(2)—O(6)	89.9 (3)
Cl(5)—Cd(2)—O(6)	88.1 (2)	Cl(4)—Cd(3)—Cl(6)	94.3 (1)
Cl(4)—Cd(3)—Cl(5)	86.7 (1)	Cl(4)—Cd(3)—O(4*W*)	94.1 (1)
Cl(4)—Cd(3)—O(3*W*)	93.4 (1)	Cl(5)—Cd(3)—Cl(6)	94.0 (1)
Cl(4)—Cd(3)—Cl(6$^{\rm ii}$)	176.6 (1)	Cl(5)—Cd(3)—O(4*W*)	176.8 (2)

Cl(5)—Cd(3)—O(3*W*)	95.3 (2)	Cl(5)—Cd(3)—Cl(6$^{\rm ii}$)	91.7 (1)
Cl(6)—Cd(3)—O(3*W*)	168.2 (2)	Cl(6)—Cd(3)—Cl(6$^{\rm ii}$)	88.8 (1)
Cl(6)—Cd(3)—O(4*W*)	82.8 (2)	O(3*W*)—Cd(3)—Cl(6$^{\rm ii}$)	83.8 (1)
O(3*W*)—Cd(3)—O(4*W*)	87.8 (2)	Cd(1)—Cl(1)—Cd(1$^{\rm i}$)	91.5 (1)
O(4*W*)—Cd(3)—Cl(6$^{\rm ii}$)	87.8 (1)	Cd(1)—Cl(3)—Cd(2)	91.0 (1)
Cd(1)—Cl(2)—Cd(2)	92.4 (1)	Cd(2)—Cl(5)—Cd(3)	91.7 (1)
Cd(2)—Cl(4)—Cd(3)	91.5 (1)	Cd(2)—O(5)—C(19)	128.3 (8)
Cd(3)—Cl(6)—Cd(3$^{\rm ii}$)	91.2 (1)	O(5)—C(19)—C(20)	111.9 (11)
Cd(2)—O(5)—C(19′)	126 (2)	Cd(2)—O(6)—C(21)	128.2 (6)
O(5)—C(19′)—C(20)	113 (4)	O(6)—C(21)—C(22′)	103.5 (13)
O(6)—C(21)—C(22)	103.7 (16)	C(2)—N(1)—C(9)	119.9 (6)
C(2)—N(1)—C(5)	121.4 (6)	C(7)—N(2)—C(10)	123.0 (7)
C(5)—N(1)—C(9)	118.5 (7)	C(10)—N(2)—C(11)	114.7 (8)
C(7)—N(2)—C(11)	122.3 (7)	C(3)—N(3)—C(16)	122.0 (6)
C(3)—N(3)—C(12)	119.9 (6)	C(14)—N(4)—C(17)	121.7 (7)
C(14)—N(4)—C(18)	122.7 (7)	C(17)—N(4)—C(18)	115.5 (8)
O(1)—C(1)—O(2)	126.9 (10)	O(1)—C(1)—C(2)	116.6 (8)
O(2)—C(1)—C(2)	116.4 (9)	N(1)—C(2)—C(1)	117.1 (7)
N(1)—C(2)—C(3)	120.3 (8)	C(1)—C(2)—C(3)	122.4 (8)
N(3)—C(3)—C(2)	122.7 (8)	N(3)—C(3)—C(4)	113.3 (6)
C(2)—C(3)—C(4)	123.9 (8)	O(3)—C(4)—O(4)	126.2 (8)
O(3)—C(4)—C(3)	115.3 (7)	O(4)—C(4)—C(3)	117.7 (7)
N(1)—C(5)—C(6)	121.5 (7)	C(5)—C(6)—C(7)	121.6 (7)
N(2)—C(7)—C(6)	122.6 (7)	N(2)—C(7)—C(8)	122.6 (8)
C(6)—C(7)—C(8)	114.7 (8)	C(7)—C(8)—C(9)	120.6 (7)
N(1)—C(9)—C(8)	123.0 (7)	N(3)—C(12)—C(13)	121.3 (7)
C(12)—C(13)—C(14)	122.2 (7)	N(4)—C(14)—C(13)	121.6 (7)
N(4)—C(14)—C(15)	123.0 (7)	C(13)—C(14)—C(15)	115.4 (8)
C(14)—C(15)—C(16)	120.7 (7)	N(3)—C(16)—C(15)	122.6 (7)
Cl(1)—Cd(1)—Cl(3)	92.9 (1)		
O(1)—C(1)—C(2)—C(3)	4.0 (9)	O(3)—C(4)—C(3)—C(2)	89.9 (9)
C(5)—N(1)—C(2)—C(3)	119.6 (8)	C(12)—N(3)—C(3)—C(2)	127.4 (8)

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

Table 3. *Hydrogen-bond parameters (Å, °)*

The donor atom is given first in each hydrogen bond.

O(1*W*)···O(1)	2.689 (10)	O(1*W*)···Cl(4)	3.175 (6)
O(2*W*)···O(2)	2.718 (11)	O(3*W*)···O(3)	2.748 (10)
O(3*W*)···Cl(2)	3.189 (7)	O(4*W*)···O(4)	2.754 (10)
O(5*W*)···O(3$^{\rm i}$)	2.773 (8)	O(5*W*)···Cl(6)	3.228 (9)
O(5)···O(5*W*)	2.629 (12)	O(6)···(O4$^{\rm ii}$)	2.775 (8)
O(1)···O(1*W*)···Cl(4)	101.4 (2)	O(3)···O(3*W*)···Cl(2)	134.7 (2)
O(5)···O(5*W*)···O(3$^{\rm i}$)	121.3 (3)	O(5)···O(5*W*)···Cl(6)	118.0 (3)
O(3$^{\rm i}$)···O(5*W*)···Cl(6)	116.1 (3)	O(3*W*)···O(3)···O(5*W*$^{\rm iii}$)	107.1 (3)

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

The structure was solved by direct methods and all non-H atoms were refined anisotropically except the disordered C atoms of the ethanol molecules [C(19), C(19′), C(22) and C(22′)]. The H atoms of the double-betaine molecule were generated geometrically (C—H = 0.96 Å), and the H atoms of the water and ethanol molecules were located in difference Fourier maps. All H atoms were assigned displacement parameters and included in the structure-factor calculations. All computations were performed on a PC 486 computer.

Data collection: *P3/PC Diffractometer Control Program* (Siemens, 1989). Cell refinement: *P3/PC Diffractometer Control Program*. Data reduction: *SHELXTL-Plus XDISK* (Sheldrick, 1987). Program(s) used to solve structure: *SHELXTL/PC XS* (Sheldrick, 1990). Program(s) used to refine structure: *SHELXTL/PC XLS*. Molecular graphics: *SHELXTL/PC XP*. Software used to prepare material for publication: *SHELXTL/PC XPUBL*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KH1054). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Polymeric Cadmium(II) Nitrate Adduct of a Flexible Double Betaine: $[\mathrm{Cd_2}(L)_2(\mathrm{NO_3})_2(\mathrm{H_2O})_3]_n(\mathrm{NO_3})_{2n}$ [*L* = *meso*-2,5-Bis(trimethylammonio)adipate]

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Abstract

The title complex, *catena*-poly[(diaquacadmium)-μ-[*meso*-2,5-bis(trimethylammonio)adipato-*O*,*O*′:*O*″,*O*‴]-(aquadinitratocadmium)-μ-[*meso*-2,5-bis(trimethylammonio)adipato-*O*,*O*′:*O*″,*O*‴] dinitrate], $[\mathrm{Cd_2}(L)_2(\mathrm{NO_3})_2(\mathrm{H_2O})_3]_n(\mathrm{NO_3})_{2n}$ [L = $^-\mathrm{O_2CCH(Me_3N^+)CH_2CH_2CH(Me_3N^+)CO_2^-}$], consists of an infinite zigzag chain in which the two independent $\mathrm{Cd^{II}}$ atoms, lying on separate crystallographic C_2 axes, have approximately pentagonal bipyramidal and very dis-

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