Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Bis(dicyclohexylammonium) adipate monohydrate

Yang-Yi Yang,[a] Xiao-Ming Chen[a] and Seik Weng Ng[b]*

[a]School of Chemistry and Chemical Engineering, Zhongshan University, Guangzhou 510275, People's Republic of China, and [b]Institute of Postgraduate Studies and Research, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: h1nswen@umcsd.um.edu.my

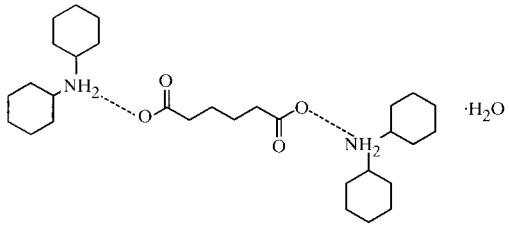
Received 31 January 2000
Accepted 9 February 2000

Data validation number: IUC0000043

In the asymmetric unit of the title compound, $2C_{12}H_{24}N^+\cdot C_6H_8O_4^{2-}\cdot H_2O$, the carboxylate ion lies about an inversion center, the water molecule is on a twofold axis and the *sec*-ammonium cation is in a general position. Cations link the oxygen ends of two adjacent carboxylate anions to form an eight-membered ring [N···O 2.683 (3) and 2.711 (3) Å]. The ion pair propagates as a linear chain and adjacent chains are linked through the water molecules [O···O 2.966 (3) Å] into layers.

Comment

Dicyclohexylammonium monoalkanoates, $[(\text{cyclo-}C_6H_{11})_2NH_2][RCH_2CO_2]$ (*R* is an electron-withdrawing group), typically exist as dimeric ion pairs, in which the two NH_2 units link two CO_2 units to form an eight-membered N···O═C═O···N···O═C═O··· ring, or as linear hydrogen-bonded chains (Ng *et al.*, 1999). The ring architecture probably requires sterically bulky *R* groups; the *R* = $(CH_3)_2NCS_2$ derivative adopts the ring architecture, but the compound has water molecules that link adjacent dimers [$O_{water}\cdots O_{carboxyl}$ 2.784 (6) and 3.029 (7) Å; Ng, 1992]. In the title compound, (I), both carboxyl ends of the centrosymmetric adipate dianion are engaged in a similar type of ring formation to give rise to a chain and adjacent chains are linked through the lattice water molecule [$O_{water}\cdots O$ 2.966 (3) Å] to form layers. The water molecule lies on a twofold axis.



(I)

A layer structure is also adopted by *m*-xylylammonium adipate, which crystallizes as a monohydrate, but its $N\cdots O_{carboxyl}$ hydrogen bonds in the chains are somewhat longer. The chains are links into layers through the lattice water molecules (Moritani & Kashino, 1991). A chain structure is also adopted by anhydrous piperazinium adipate, which displays hydrogen bonds (Vanier & Brisse, 1983) that are somewhat longer than those in the dicyclohexylammonium salt. Slightly longer hydrogen bonds are also noted in hexamethylediammonium adipate (Brown, 1966).

Experimental

Dicyclohexylamine, adipic acid and bis(tributyltin) oxide in a 2:2:1 molar stoichiometry were heated in a small volume of ethanol in an attempt to synthesize dicyclohexylammonium succinatotributylstannate. The procedure had been used to prepare the tributylstannate derivatives of oxalic (Ng *et al.*, 1990), malonic (Ng *et al.*, 1992) and succinic (Ng & Holecek, 1998) acids, but the reaction with adipic acid gave the organic salt as a hydrate. The Cu radiation powder diffractogram of the bulk compound is identical to the diffractogram that is calculated from the atomic coordinates by *POWDIS* (McArdle & Cunningham, 1998).

Crystal data

$2C_{12}H_{24}N^+\cdot C_6H_8O_4^{2-}\cdot H_2O$	D_x = 1.132 Mg m^{-3}
M_r = 526.78	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 25 reflections
a = 10.155 (3) Å	θ = 7.0–14.0°
b = 15.638 (5) Å	μ = 0.075 mm^{-1}
c = 20.102 (6) Å	T = 298 (2) K
β = 104.56 (1)°	Parallelepiped, colorless
V = 3089.8 (16) Å^3	0.50 × 0.50 × 0.40 mm
Z = 4	

Data collection

Siemens *R*3*m* diffractometer	R_{int} = 0.089
ω scans	θ_{max} = 25°
Absorption correction: empirical ψ scan (North *et al.*, 1968)	$h = 0 \rightarrow 12$
T_{min} = 0.912, T_{max} = 1.000	$k = 0 \rightarrow 18$
2879 measured reflections	$l = -23 \rightarrow 23$
2715 independent reflections	2 standard reflections every 118 reflections
1461 reflections with $I > 2\sigma(I)$	intensity decay: none

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0754P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.059	$(\Delta/\sigma)_{max}$ = 0.001
$wR(F^2)$ = 0.159	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
S = 0.977	$\Delta\rho_{min}$ = −0.18 e Å^{-3}
2715 reflections	Extinction correction: *SHELXL*97
181 parameters	Extinction coefficient: 0.017 (1)
H atoms treated by a mixture of independent and constrained refinement	

The N- and O-bonded H atoms were located and refined.

Data collection: *XSCANS* (Siemens, 1990); cell refinement: *XSCANS*; data reduction: *SHELXTL-Plus* (Sheldrick, 1990); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

We thank the National Science Foundation of China (grant No. 29625102) and the University of Malaya for supporting this work.

References

Brown, C. J. (1966). *Acta Cryst.* **21**, 185–190.
McArdle, P. & Cunningham, D. (1998). *J. Appl. Cryst.* **31**, 826.
Moritani, Y. & Kashino, S. (1991). *Acta Cryst.* C**47**, 990–992.
Ng, S. W. (1992). *J. Crystallogr. Spectrosc. Res.* **22**, 615–618.
Ng, S. W. & Holecek, J. (1998). *Acta Cryst.* C**54**, 750–752.
Ng, S. W., Kumar Das, V. G., Hossain, M. B., Goerlitz, F. & van der Helm, D. (1990). *J. Organomet. Chem.* **390**, 19–38.
Ng, S. W., Kumar Das, V. G., Skelton, B. W. & White, A. H. (1992). *J. Organomet. Chem.* **430**, 139–148.
Ng, S. W., Shanmuga Sundara Raj, S. & Fun, H.-K. (1999). *Acta Cryst.* C**55**, 2145–2147.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Sheldrick, G. M. (1990). *SHELXTL-Plus.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1990). *XSCANS User's Manual.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Vanier, M. & Brisse, F. (1983). *Acta Cryst.* C**39**, 914–915.