Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,3-Dimethoxy-10-oxostrychnidinium 2-carboxy-4,5-dichlorobenzoate

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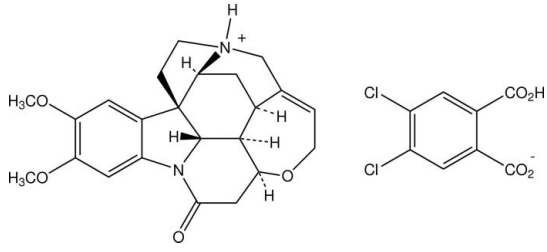
Received 28 September 2007; accepted 30 September 2007

Key indicators: single-crystal X-ray study; T = 130 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.087; data-to-parameter ratio = 12.4.

The structure of the title compound, $C_{23}H_{27}N_2O_4^+\cdot C_8H_3Cl_2O_4^-$, a 1:1 proton-transfer compound of brucine with 4,5-dichlorophthalic acid, has been determined at 130 K. The brucinium cations and the hydrogen phthalate anions associate through single N—H···$O_{carboxylate}$ hydrogen bonds [2.639 (3) Å], giving dimers which are extended *via* weak head-to-tail C—H···$O_{methoxy}$ associations into chains forming down the 2_1 screw axis of the unit cell. The carboxyl proton of the anion gives a short intramolecular O—H···$O_{carboxylate}$ hydrogen bond [2.441 (3) Å].

Related literature

Absolute configuration: (Peerdeman, 1956; Flack, 1983). Similar structures: (Oshikawa *et al.*, 2002; Smith *et al.*, 2005, 2006*a*,*b*; Bialońska & Ciunik, 2004*a*,*b*, 2006; Gould & Walkinshaw, 1984; Mallinson *et al.*, 2003; Bozkurt *et al.*, 2006).



Experimental

Crystal data

$C_{23}H_{27}N_2O_4^+\cdot C_8H_3Cl_2O_4^-$
M_r = 629.47
Monoclinic, $P2_1$
a = 9.5085 (10) Å
b = 12.9946 (13) Å
c = 11.5893 (12) Å
β = 104.110 (2)°
V = 1388.8 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 130 (2) K
0.45 × 0.20 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
T_{min} = 0.86, T_{max} = 0.96
8761 measured reflections
4923 independent reflections
4747 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.087
S = 1.04
4923 reflections
396 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 1604 Friedel pairs
Flack parameter: 0.07 (5)

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

D—H···A	D—H	H···A	D···A	D—H···A
N19—H19···O11*A*	0.90 (3)	1.75 (3)	2.639 (3)	170 (2)
O21*A*—H21*A*···O12*A*	0.84 (5)	1.61 (5)	2.441 (3)	170 (4)
C3*A*—H3*A*···O22*A*	0.93	2.31	2.667 (3)	103
C4—H4···O25	0.93	2.45	2.953 (3)	114
C6*A*—H6*A*···O11*A*	0.93	2.26	2.635 (3)	103
C16—H16···O12*A*	0.98	2.55	3.402 (3)	145
C17—H17*B*···O2^{i}	0.97	2.53	3.441 (3)	156
C18—H18*B*···O3^{i}	0.97	2.48	3.279 (3)	140
C22—H22···O22*A*^{ii}	0.93	2.45	3.316 (3)	155

Symmetry codes: (i) $-x+3, y+\frac{1}{2}, -z+1$; (ii) $x, y+1, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); 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: *PLATON*.

The authors acknowledge financial support from the School of Physical and Chemical Sciences (Queensland University of Technology), the School of Science, Griffith University and the School of Chemistry, the University of Melbourne.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FL2168).

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