Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

rac-Bis{[1-(9,9-dioxo-10*H*-phenothiazin-10-yl)-2-propyl]dimethylammonium} terephthalate trihydrate

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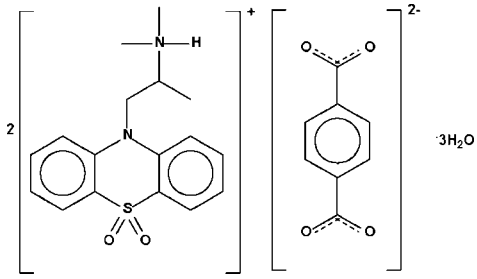
Received 13 November 2007; accepted 14 November 2007

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.161; data-to-parameter ratio = 17.1.

The protonated dioxopromethazinium cation in the title racemic compound, $2C_{17}H_{21}N_2O_2S^+\cdot C_8H_4O_4^{2-}\cdot 3H_2O$, forms an N—H···O hydrogen bond to the terephthalate dianion through the N atom that is not part of a fused ring. The dianion lies on a center of inversion, and the carboxylate O atoms are also acceptors for two water molecules. One of the uncoordinated water molecules lies on a twofold rotation axis. The hydrogen bonds give rise to a sheet structure.

Related literature

For the structure of dioxopromethazinium picrate, see: Harrison *et al.* (2007). This is the only crystal structure study of the dioxopromethazinium cation.



Experimental

Crystal data

$2C_{17}H_{21}N_2O_2S^+\cdot C_8H_4O_4^{2-}\cdot 3H_2O$
M_r = 853.00
Monoclinic, $C2/c$
a = 23.309 (2) Å
b = 7.2258 (6) Å
c = 25.315 (2) Å
β = 91.793 (2)°
V = 4261.7 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.19 mm^{-1}
T = 295 (2) K
0.43 × 0.25 × 0.25 mm

Data collection

Bruker APEX2 area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.865, T_{max} = 0.954
12300 measured reflections
4830 independent reflections
3132 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.161
S = 1.02
4830 reflections
283 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*n*···O3	0.85 (1)	1.82 (1)	2.670 (2)	172 (3)
O1*w*—H1*w*1···O3	0.86 (4)	2.21 (3)	2.953 (4)	145 (5)
O1*w*—H1*w*2···O4^{i}	0.86 (3)	1.99 (2)	2.789 (4)	154 (4)
O2*w*—H2*w*1···O1*w*	0.87 (4)	2.07 (3)	2.836 (4)	146 (5)

Symmetry code: (i) $x, y+1, z$.

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

The authors thank the Science Foundation for Young Teachers of Northeast Normal University (Grant Nos. 20070307 and 20061001) and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2369).

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  doi:10.1107/S1600536807058916

supplementary materials

Acta Cryst. (2007). E**63**, o4830 [**doi:10.1107/S1600536807058916**]

rac-Bis{[1-(9,9-dioxo-10*H*-phenothiazin-10-yl)-2-propyl]dimethylammonium} terephthalate trihydrate

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Comment

There are no crystallographic reports on the antihistamine drug, dioxopromethazine, in the Cambridge Structural Database (Version 5.28, Nov. 2006). The first structural was reported only recently (Harrison *et al.*, 2007); the drug is isolated as its salt with picric acid. The title terephthalate salt exists as a trihydrate (Fig. 1); the cation and anion are linked with the water molecules *via* hydrogen bonding (Table 1) into a layer (Fig. 2).

Experimental

Zinc acetate dihydrate (0.3 mmol, 0.06 g), dioxopromethazine (0.3 mmol, 0.106 g), terephthalic acid (0.2 mmol, 0.033 g), sodium hydroxide (0.4 mmol, 0.016 g) and water (15 ml) were placed in a 25-ml, Teflon-lined, stainless-steel Parr bomb. The bomb was heated from 293 to 443 K in 2 h and a constant temperature was maintained at 443 K for 72 h, after which it was cooled to 298 K. Crystals were isolated from the cool solution.

Refinement

The water and amino hydrogen atoms were located in difference Fourier maps, and were refined with distance restraints of O–H = N–H = 0.85±0.01 Å. Their temperature factors were freely refined. The carbon-bound hydrogen atoms were placed in calculated positions, and were included in the refinement in the riding model approximation.

Figures

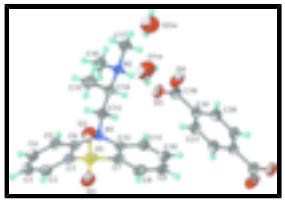

Fig. 1. **Figure 1**. Thermal ellipsoid plot of. Displacement ellipsoids are drawn at the 50% probabability level, and H atoms as spheres of arbitrary radii.

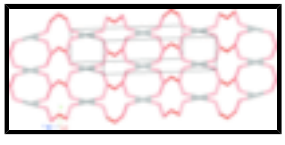

Fig. 2. **Figure 2**. *OLEX* (Dolomanov *et al.*, 2003) representation of the sheet structure.

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Crystal data

$2C_{17}H_{21}N_2O_2S^+\cdot C_8H_4O_4^{2-}\cdot 3H_2O$ $F_{000} = 1808$

M_r = 853.00	D_x = 1.329 Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2051 reflections
a = 23.309 (2) Å	θ = 2.4–22.8º
b = 7.2258 (6) Å	μ = 0.19 mm^{-1}
c = 25.315 (2) Å	T = 295 (2) K
β = 91.793 (2)º	Block, colorless
V = 4261.7 (6) Å^3	0.43 × 0.25 × 0.25 mm
Z = 4	

Data collection

Bruker APEX2 area-detector diffractometer	4830 independent reflections
Radiation source: fine-focus sealed tube	3132 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.034
T = 295(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −30→12
T_{min} = 0.865, T_{max} = 0.954	k = −9→9
12300 measured reflections	l = −29→32

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.161	$w = 1/[\sigma^2(F_o^2) + (0.0868P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.02	$(\Delta/\sigma)_{max}$ = 0.001
4830 reflections	$\Delta\rho_{max}$ = 0.28 e Å^{-3}
283 parameters	$\Delta\rho_{min}$ = −0.30 e Å^{-3}
4 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.21772 (3)	0.48104 (7)	0.59925 (2)	0.0458 (2)
O1	0.18573 (8)	0.3513 (2)	0.56691 (7)	0.0645 (5)
O2	0.24138 (8)	0.4133 (2)	0.64923 (6)	0.0593 (5)
O3	0.43542 (8)	1.1283 (3)	0.62526 (7)	0.0615 (5)
O4	0.48301 (10)	0.8645 (3)	0.63832 (7)	0.0793 (6)

O1w	0.44044 (17)	1.5151 (4)	0.66278 (13)	0.1085 (9)
H1w1	0.429 (2)	1.427 (5)	0.6421 (18)	0.17 (2)*
H1w2	0.4630 (16)	1.603 (4)	0.6535 (18)	0.139 (19)*
O2w	0.5000	1.3494 (7)	0.7500	0.1126 (12)
H2w1	0.482 (2)	1.437 (5)	0.733 (2)	0.17 (2)*
N1	0.26433 (7)	0.8602 (2)	0.61738 (7)	0.0390 (4)
N2	0.38072 (8)	1.0306 (3)	0.71206 (7)	0.0436 (5)
H2n	0.4001 (10)	1.068 (4)	0.6862 (7)	0.067 (8)*
C1	0.17680 (9)	0.6739 (3)	0.61256 (8)	0.0390 (5)
C2	0.11734 (10)	0.6573 (3)	0.61538 (9)	0.0512 (6)
H2	0.0996	0.5459	0.6064	0.061*
C3	0.08490 (11)	0.8041 (4)	0.63130 (10)	0.0570 (7)
H3	0.0452	0.7934	0.6331	0.068*
C4	0.11219 (11)	0.9684 (4)	0.64464 (10)	0.0520 (6)
H4	0.0905	1.0678	0.6561	0.062*
C5	0.17094 (10)	0.9883 (3)	0.64140 (9)	0.0427 (5)
H5	0.1880	1.1007	0.6504	0.051*
C6	0.20495 (9)	0.8414 (3)	0.62471 (8)	0.0359 (5)
C7	0.27294 (10)	0.5792 (3)	0.56471 (8)	0.0426 (5)
C8	0.29983 (12)	0.4765 (3)	0.52557 (10)	0.0542 (6)
H8	0.2853	0.3615	0.5156	0.065*
C9	0.34747 (11)	0.5451 (4)	0.50200 (10)	0.0585 (7)
H9	0.3659	0.4766	0.4765	0.070*
C10	0.36762 (11)	0.7180 (4)	0.51689 (9)	0.0571 (7)
H10	0.3998	0.7651	0.5008	0.069*
C11	0.34165 (10)	0.8222 (3)	0.55458 (9)	0.0488 (6)
H11	0.3565	0.9377	0.5638	0.059*
C12	0.29287 (9)	0.7553 (3)	0.57933 (8)	0.0385 (5)
C13	0.29780 (10)	0.9938 (3)	0.64904 (9)	0.0409 (5)
H13A	0.2720	1.0725	0.6683	0.049*
H13B	0.3198	1.0717	0.6259	0.049*
C14	0.33852 (9)	0.8938 (3)	0.68795 (8)	0.0413 (5)
H14	0.3606	0.8051	0.6675	0.050*
C15	0.30636 (12)	0.7840 (4)	0.72856 (10)	0.0674 (8)
H15A	0.3333	0.7215	0.7518	0.101*
H15B	0.2821	0.6945	0.7109	0.101*
H15C	0.2833	0.8664	0.7487	0.101*
C16	0.35436 (11)	1.1991 (3)	0.73481 (10)	0.0578 (7)
H16A	0.3372	1.2724	0.7069	0.087*
H16B	0.3834	1.2704	0.7532	0.087*
H16C	0.3254	1.1634	0.7590	0.087*
C17	0.42157 (11)	0.9432 (4)	0.75107 (11)	0.0676 (7)
H17A	0.4472	1.0357	0.7654	0.101*
H17B	0.4433	0.8493	0.7338	0.101*
H17C	0.4005	0.8885	0.7791	0.101*
C18	0.46685 (11)	0.9964 (4)	0.61020 (10)	0.0535 (6)
C19	0.48481 (10)	1.0007 (3)	0.55294 (9)	0.0473 (6)
C20	0.51864 (10)	0.8601 (3)	0.53354 (10)	0.0538 (6)
H20	0.5315	0.7657	0.5559	0.065*

C21	0.53353 (10)	0.8595 (3)	0.48071 (10)	0.0525 (6)
H21	0.5560	0.7641	0.4680	0.063*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0613 (4)	0.0344 (3)	0.0419 (3)	−0.0104 (3)	0.0038 (3)	−0.0021 (2)
O1	0.0828 (13)	0.0490 (10)	0.0622 (11)	−0.0274 (9)	0.0092 (10)	−0.0186 (8)
O2	0.0853 (13)	0.0430 (9)	0.0497 (10)	0.0019 (9)	0.0023 (9)	0.0106 (7)
O3	0.0589 (11)	0.0744 (12)	0.0525 (10)	−0.0136 (10)	0.0213 (9)	−0.0146 (9)
O4	0.1029 (16)	0.0857 (15)	0.0502 (11)	−0.0031 (13)	0.0182 (11)	0.0043 (10)
O1w	0.146 (3)	0.0807 (19)	0.100 (2)	0.0050 (19)	0.017 (2)	0.0020 (16)
O2w	0.123 (4)	0.104 (3)	0.110 (3)	0.000	−0.006 (3)	0.000
N1	0.0377 (10)	0.0373 (9)	0.0417 (10)	−0.0083 (8)	−0.0005 (8)	−0.0068 (7)
N2	0.0370 (10)	0.0584 (12)	0.0355 (10)	−0.0061 (9)	0.0041 (8)	−0.0115 (9)
C1	0.0441 (12)	0.0408 (12)	0.0320 (10)	−0.0095 (10)	0.0002 (9)	0.0019 (9)
C2	0.0500 (14)	0.0569 (15)	0.0466 (13)	−0.0216 (12)	0.0008 (11)	−0.0021 (11)
C3	0.0395 (13)	0.0750 (17)	0.0565 (15)	−0.0112 (13)	0.0021 (11)	−0.0017 (13)
C4	0.0481 (14)	0.0596 (15)	0.0486 (14)	0.0003 (12)	0.0033 (11)	−0.0003 (11)
C5	0.0439 (12)	0.0414 (12)	0.0428 (12)	−0.0042 (10)	0.0018 (10)	0.0019 (9)
C6	0.0383 (11)	0.0379 (11)	0.0312 (10)	−0.0070 (9)	−0.0014 (9)	0.0035 (8)
C7	0.0511 (13)	0.0401 (12)	0.0363 (11)	−0.0046 (10)	−0.0019 (10)	−0.0033 (9)
C8	0.0647 (16)	0.0527 (14)	0.0451 (13)	−0.0050 (12)	0.0013 (12)	−0.0143 (11)
C9	0.0564 (15)	0.0792 (18)	0.0399 (13)	0.0016 (14)	0.0009 (12)	−0.0152 (12)
C10	0.0489 (14)	0.0833 (19)	0.0392 (13)	−0.0079 (13)	0.0030 (11)	−0.0059 (12)
C11	0.0443 (13)	0.0582 (14)	0.0438 (12)	−0.0111 (11)	0.0017 (11)	−0.0051 (11)
C12	0.0402 (11)	0.0427 (12)	0.0322 (10)	−0.0021 (10)	−0.0037 (9)	−0.0008 (9)
C13	0.0434 (12)	0.0372 (11)	0.0421 (12)	−0.0080 (9)	−0.0007 (10)	−0.0064 (9)
C14	0.0432 (12)	0.0447 (12)	0.0362 (11)	−0.0055 (10)	0.0030 (9)	−0.0057 (9)
C15	0.0725 (18)	0.084 (2)	0.0454 (14)	−0.0267 (16)	0.0019 (13)	0.0078 (13)
C16	0.0557 (15)	0.0636 (16)	0.0543 (14)	−0.0073 (13)	0.0044 (12)	−0.0241 (12)
C17	0.0533 (15)	0.095 (2)	0.0539 (15)	0.0014 (15)	−0.0074 (13)	−0.0095 (15)
C18	0.0483 (14)	0.0675 (17)	0.0451 (13)	−0.0199 (13)	0.0095 (11)	−0.0105 (12)
C19	0.0370 (12)	0.0612 (15)	0.0441 (12)	−0.0160 (11)	0.0064 (10)	−0.0098 (11)
C20	0.0476 (14)	0.0635 (16)	0.0506 (14)	−0.0053 (12)	0.0054 (11)	−0.0037 (12)
C21	0.0458 (13)	0.0621 (15)	0.0500 (13)	−0.0062 (12)	0.0100 (11)	−0.0114 (12)

Geometric parameters (Å, °)

S1—O1	1.4377 (17)	C8—H8	0.9300
S1—O2	1.4495 (17)	C9—C10	1.383 (4)
S1—C1	1.728 (2)	C9—H9	0.9300
S1—C7	1.730 (2)	C10—C11	1.371 (3)
O3—C18	1.268 (3)	C10—H10	0.9300
O4—C18	1.241 (3)	C11—C12	1.401 (3)
O1w—H1w1	0.86 (4)	C11—H11	0.9300
O1w—H1w2	0.86 (3)	C13—C14	1.528 (3)
O2w—H2w1	0.87 (4)	C13—H13A	0.9700
N1—C6	1.409 (3)	C13—H13B	0.9700

N1—C12	1.409 (3)	C14—C15	1.515 (3)
N1—C13	1.464 (2)	C14—H14	0.9800
N2—C16	1.488 (3)	C15—H15A	0.9600
N2—C17	1.490 (3)	C15—H15B	0.9600
N2—C14	1.510 (3)	C15—H15C	0.9600
N2—H2n	0.851 (10)	C16—H16A	0.9600
C1—C2	1.395 (3)	C16—H16B	0.9600
C1—C6	1.406 (3)	C16—H16C	0.9600
C2—C3	1.370 (3)	C17—H17A	0.9600
C2—H2	0.9300	C17—H17B	0.9600
C3—C4	1.384 (3)	C17—H17C	0.9600
C3—H3	0.9300	C18—C19	1.522 (3)
C4—C5	1.382 (3)	C19—C21^{i}	1.380 (3)
C4—H4	0.9300	C19—C20	1.386 (3)
C5—C6	1.398 (3)	C20—C21	1.392 (3)
C5—H5	0.9300	C20—H20	0.9300
C7—C12	1.401 (3)	C21—C19^{i}	1.380 (3)
C7—C8	1.401 (3)	C21—H21	0.9300
C8—C9	1.370 (4)		
O1—S1—O2	116.95 (11)	C10—C11—H11	119.9
O1—S1—C1	110.92 (11)	C12—C11—H11	119.9
O2—S1—C1	107.42 (10)	C7—C12—C11	117.5 (2)
O1—S1—C7	111.11 (10)	C7—C12—N1	120.64 (19)
O2—S1—C7	108.12 (11)	C11—C12—N1	121.83 (19)
C1—S1—C7	101.07 (10)	N1—C13—C14	110.54 (16)
H1w1—O1w—H1w2	124 (5)	N1—C13—H13A	109.5
C6—N1—C12	121.67 (16)	C14—C13—H13A	109.5
C6—N1—C13	120.03 (17)	N1—C13—H13B	109.5
C12—N1—C13	118.29 (16)	C14—C13—H13B	109.5
C16—N2—C17	110.67 (19)	H13A—C13—H13B	108.1
C16—N2—C14	114.85 (17)	N2—C14—C15	113.47 (18)
C17—N2—C14	112.7 (2)	N2—C14—C13	109.58 (17)
C16—N2—H2n	105.8 (19)	C15—C14—C13	111.99 (19)
C17—N2—H2n	107.6 (18)	N2—C14—H14	107.2
C14—N2—H2n	104.6 (19)	C15—C14—H14	107.2
C2—C1—C6	121.3 (2)	C13—C14—H14	107.2
C2—C1—S1	119.76 (17)	C14—C15—H15A	109.5
C6—C1—S1	118.69 (16)	C14—C15—H15B	109.5
C3—C2—C1	120.5 (2)	H15A—C15—H15B	109.5
C3—C2—H2	119.8	C14—C15—H15C	109.5
C1—C2—H2	119.8	H15A—C15—H15C	109.5
C2—C3—C4	118.8 (2)	H15B—C15—H15C	109.5
C2—C3—H3	120.6	N2—C16—H16A	109.5
C4—C3—H3	120.6	N2—C16—H16B	109.5
C5—C4—C3	121.6 (2)	H16A—C16—H16B	109.5
C5—C4—H4	119.2	N2—C16—H16C	109.5
C3—C4—H4	119.2	H16A—C16—H16C	109.5
C4—C5—C6	120.7 (2)	H16B—C16—H16C	109.5

C4—C5—H5	119.6	N2—C17—H17A	109.5
C6—C5—H5	119.6	N2—C17—H17B	109.5
C5—C6—C1	117.04 (19)	H17A—C17—H17B	109.5
C5—C6—N1	122.36 (18)	N2—C17—H17C	109.5
C1—C6—N1	120.52 (19)	H17A—C17—H17C	109.5
C12—C7—C8	121.0 (2)	H17B—C17—H17C	109.5
C12—C7—S1	118.98 (16)	O4—C18—O3	124.9 (2)
C8—C7—S1	119.79 (18)	O4—C18—C19	118.3 (2)
C9—C8—C7	120.2 (2)	O3—C18—C19	116.7 (2)
C9—C8—H8	119.9	$C21^{i}$—C19—C20	119.1 (2)
C7—C8—H8	119.9	$C21^{i}$—C19—C18	120.9 (2)
C8—C9—C10	118.8 (2)	C20—C19—C18	119.9 (2)
C8—C9—H9	120.6	C19—C20—C21	120.3 (2)
C10—C9—H9	120.6	C19—C20—H20	119.8
C11—C10—C9	122.1 (2)	C21—C20—H20	119.8
C11—C10—H10	118.9	$C19^{i}$—C21—C20	120.6 (2)
C9—C10—H10	118.9	$C19^{i}$—C21—H21	119.7
C10—C11—C12	120.3 (2)	C20—C21—H21	119.7
O1—S1—C1—C2	30.0 (2)	C7—C8—C9—C10	−1.2 (4)
O2—S1—C1—C2	−98.98 (19)	C8—C9—C10—C11	0.3 (4)
C7—S1—C1—C2	147.85 (18)	C9—C10—C11—C12	−0.3 (4)
O1—S1—C1—C6	−155.31 (16)	C8—C7—C12—C11	−2.0 (3)
O2—S1—C1—C6	75.75 (18)	S1—C7—C12—C11	173.08 (17)
C7—S1—C1—C6	−37.42 (18)	C8—C7—C12—N1	177.7 (2)
C6—C1—C2—C3	−1.4 (3)	S1—C7—C12—N1	−7.2 (3)
S1—C1—C2—C3	173.13 (18)	C10—C11—C12—C7	1.1 (3)
C1—C2—C3—C4	−0.2 (4)	C10—C11—C12—N1	−178.6 (2)
C2—C3—C4—C5	1.1 (4)	C6—N1—C12—C7	−29.1 (3)
C3—C4—C5—C6	−0.4 (4)	C13—N1—C12—C7	151.99 (19)
C4—C5—C6—C1	−1.2 (3)	C6—N1—C12—C11	150.5 (2)
C4—C5—C6—N1	175.5 (2)	C13—N1—C12—C11	−28.3 (3)
C2—C1—C6—C5	2.1 (3)	C6—N1—C13—C14	110.7 (2)
S1—C1—C6—C5	−172.56 (15)	C12—N1—C13—C14	−70.4 (2)
C2—C1—C6—N1	−174.62 (19)	C16—N2—C14—C15	−74.7 (3)
S1—C1—C6—N1	10.7 (3)	C17—N2—C14—C15	53.3 (3)
C12—N1—C6—C5	−149.3 (2)	C16—N2—C14—C13	51.3 (2)
C13—N1—C6—C5	29.5 (3)	C17—N2—C14—C13	179.32 (18)
C12—N1—C6—C1	27.2 (3)	N1—C13—C14—N2	168.51 (16)
C13—N1—C6—C1	−153.95 (19)	N1—C13—C14—C15	−64.7 (2)
O1—S1—C7—C12	153.49 (17)	O4—C18—C19—$C21^{i}$	177.7 (2)
O2—S1—C7—C12	−76.9 (2)	O3—C18—C19—$C21^{i}$	−1.2 (3)
C1—S1—C7—C12	35.7 (2)	O4—C18—C19—C20	−0.4 (3)
O1—S1—C7—C8	−31.4 (2)	O3—C18—C19—C20	−179.3 (2)
O2—S1—C7—C8	98.2 (2)	$C21^{i}$—C19—C20—C21	−0.4 (4)
C1—S1—C7—C8	−149.2 (2)	C18—C19—C20—C21	177.7 (2)
C12—C7—C8—C9	2.0 (4)	C19—C20—C21—$C19^{i}$	0.4 (4)
S1—C7—C8—C9	−173.0 (2)		

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2n···O3	0.85 (1)	1.82 (1)	2.670 (2)	172 (3)
O1w—H1w1···O3	0.86 (4)	2.21 (3)	2.953 (4)	145 (5)
O1w—H1w2···O4^{ii}	0.86 (3)	1.99 (2)	2.789 (4)	154 (4)
O2w—H2w1···O1w	0.87 (4)	2.07 (3)	2.836 (4)	146 (5)

Symmetry codes: (ii) *x*, *y*+1, *z*.

Fig. 1

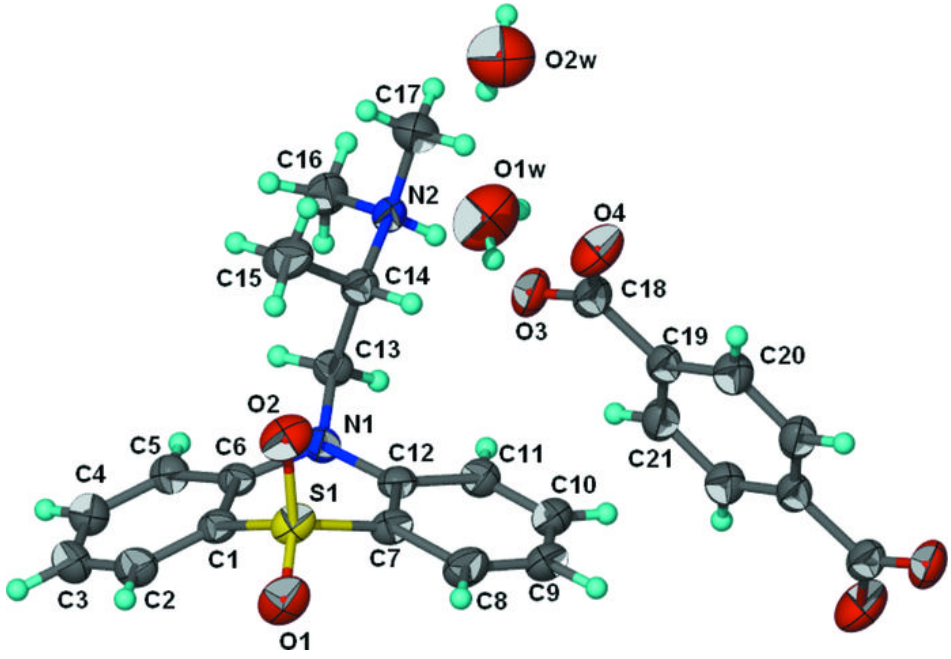
O2w
C17
C16
O1w
N2
O4
C15
C14
C18
O3
C19
C20
C13
O2
N1
C5
C6
C12
C11
C21
C4
S1
C10
C1
C7
C3
C2
C8
C9
O1

Fig. 2