Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Benzyltributylammonium 4-hydroxynaphthalene-1-sulfonate

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
Some non-H atoms missing
Disorder in main residue
R factor = 0.049
wR factor = 0.162
Data-to-parameter ratio = 14.1

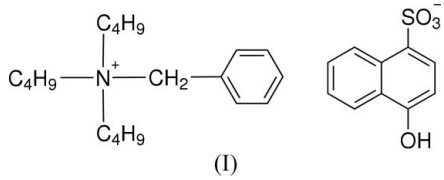
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 30 December 2006
Accepted 9 April 2007

The title compound, $C_{19}H_{34}N^+\cdot C_{10}H_7O_4S^-$, is a charge-control agent used in electrophotography. The anions form chains along the b axis through O—H···O hydrogen bonding.

Comment

The title compound, (I), is an ammonium salt used widely as a charge-control agent (CCA) of the positive type for toners in electrophotography (Tanaka, 1995). CCAs are usually added to toners to create a desired charge level and polarity (Nash *et al.*, 2001). However, the charge-control mechanism of CCA is not fully understood at the moment. We have, therefore, determined the title crystal structure as a step to elucidating the mechanism.



(I)

Fig. 1 shows the asymmetric unit of (I). The ions have no crystallographically imposed symmetry. Fig. 2 shows a hydrogen-bonded chain along the b axis, formed by O—H···O hydrogen bonding (Table 1).

Experimental

Compound (I) was obtained from Orient Chemical Industries Ltd, and was recrystallized from a methanol solution. After 48 h, a number of colorless crystals were obtained in the form of blocks.

Crystal data

$C_{19}H_{34}N^+\cdot C_{10}H_7O_4S^-$
M_r = 499.70
Monoclinic, $P2_1/n$
a = 14.3810 (11) Å
b = 9.8124 (7) Å
c = 19.7757 (15) Å
β = 92.560 (5)°
V = 2787.8 (4) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 1.29 mm^{-1}
T = 296.1 K
0.20 × 0.20 × 0.20 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.745, T_{max} = 0.772
24226 measured reflections
4902 independent reflections
3490 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.036

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.162
S = 1.19
4902 reflections
347 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

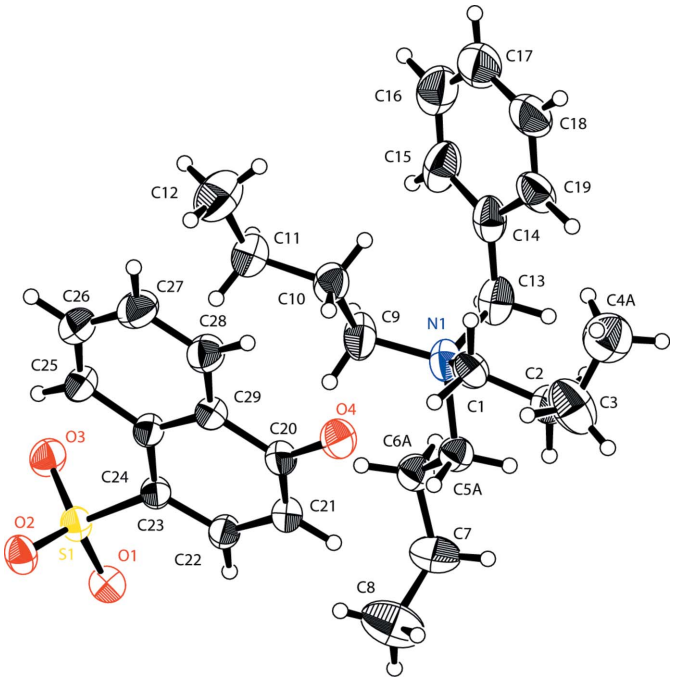


Figure 1
The asymmetric unit of (I), showing 30% probability displacement ellipsoids and only the major disorder components.

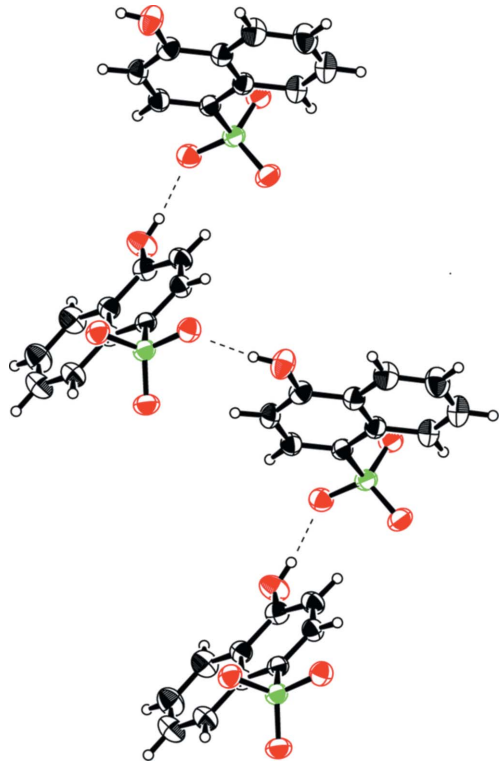


Figure 2
The formation of a hydrogen-bonded (dashed lines) chain.

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O1^{i}	0.82	1.85	2.657 (2)	169

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

C4, C5 and C6 were found to be disordered over two sites each. The site occupancies for C4*A*/C4*B* are 0.742 (7):0.258 (7), whereas those for for C5*A*/C5*B* and C6*A*/C6*B* are 0.460 (6):0.540 (6). These atoms were isotropically refined. All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.93 Å (aromatic), 0.96 Å (methyl) or 0.97 Å (methylene), and O—H = 0.82 Å; U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

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