Benzyltributylammonium 4-hydroxynaphthalene-1-sulfonate
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The title compound, C_{19}H_{34}N^+\cdotC_{10}H_7O_4S^-\text{-}C_1, 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 (Taniaka, 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.

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^+\cdotC_{10}H_7O_4S^-\text{-} C_1

Mr = 499.70

Monoclinic, $P2_1/n$

$\alpha = 14.3810$ (11) Å

$\beta = 9.8124$ (7) Å

$\gamma = 19.7757$ (15) Å

$\beta = 92.560$ (5)$^\circ$

$V = 2787.8$ (4) Å$^3$

$Z = 4$

Cu Kα radiation

$\mu = 1.29$ 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)

$T_{\text{min}} = 0.745$, $T_{\text{max}} = 0.772$

24226 measured reflections

4902 independent reflections

3490 reflections with $F^2 > 2\sigma(F^2)$

$R_{\text{int}} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$

$wR(F^2) = 0.162$

$\chi^2 = 1.19$

4902 reflections

347 parameters

H-atom parameters constrained

$\Delta\rho_{\text{max}} = 0.45$ e Å$^{-3}$

$\Delta\rho_{\text{min}} = -0.24$ e Å$^{-3}$
Table 1
Hydrogen-bond geometry (Å, °).

| D—H—A | D—H | H—A | D—A | D—H—A |
|--------|------|-----|-----|-------|
| O4—H4 | 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 C4A/C4B are 0.742 (7):0.258 (7), whereas those for C5A/C5B and C6A/C6B 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; $U_{eq}(H) = 1.2U_{eq}$(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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