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Benzyltributylammonium 4-hydroxy-naphthalene-1-sulfonate

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Key indicators

Single-crystal X-ray study

 $T = 296\text{ K}$ Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$

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>.

The title compound, $\text{C}_{19}\text{H}_{34}\text{N}^+\cdot\text{C}_{10}\text{H}_7\text{O}_4\text{S}^-$, is a charge-control agent used in electrophotography. The anions form chains along the b axis through $\text{O}-\text{H}\cdots\text{O}$ 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.

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 $\text{O}-\text{H}\cdots\text{O}$ 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

 $\text{C}_{19}\text{H}_{34}\text{N}^+\cdot\text{C}_{10}\text{H}_7\text{O}_4\text{S}^-$ $M_r = 499.70$ Monoclinic, $P2_1/n$ $a = 14.3810\text{ (11)\AA}$ $b = 9.8124\text{ (7)\AA}$ $c = 19.7757\text{ (15)\AA}$ $\beta = 92.560\text{ (5)^\circ}$ $V = 2787.8\text{ (4)\AA}^3$ $Z = 4$ Cu $K\alpha$ radiation $\mu = 1.29\text{ mm}^{-1}$ $T = 296.1\text{ K}$ $0.20 \times 0.20 \times 0.20\text{ mm}$

Data collection

Rigaku R-Axis RAPID
diffractometerAbsorption correction: multi-scan
(*ABSCOR*; Higashi, 1995) $T_{\min} = 0.745$, $T_{\max} = 0.772$

24226 measured reflections

4902 independent reflections

3490 reflections with $F^2 > 2\sigma(F^2)$ $R_{\text{int}} = 0.036$

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

 $\Delta\rho_{\max} = 0.45\text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.24\text{ e \AA}^{-3}$

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

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O4-H4 \cdots O1^i$	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 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; $U_{iso}(H) = 1.2U_{eq}(\text{parent atom})$.

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.*,

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

2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP III* (Burnett & Johnson, 1996); software used to prepare material for publication: *CrystalStructure*.

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