metal-organic papers

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Potassium 2-methyl-5-nitrobenzenesulfonate

The title compound, $K^+ \cdot C_7H_6NO_5S^-$, consists of a two-dimensional framework of K^+ ions coordinated to 2-methyl-5-nitrobenzenesulfonate anions. The K^+ ion is typically eight-coordinate, surrounded by eight O atoms from six 2-methyl-5-nitrobenzenesulfonate anions.

Comment

The title compound, (I), consists of a two-dimensional framework of K^+ ions coordinated to 2-methyl-5-nitro-benzenesulfonate anions. As shown in Fig. 1, the K^+ ion is coordinated by eight O atoms from six 2-methyl-5-nitro-benzenesulfonate anions, forming a distorted square-anti-prismatic coordination geometry, in which the K—O bond distances range from 2.7751 (14) to 3.0427 (15) Å, with an average bond distance of 2.893 Å. In (I), the K^+ ion is typically eight-coordinate, e.g. $K(OH_2)^+$ in $CaKAsO_4 \cdot 8H_2O$ (Dickens & Brown, 1972). In the 2-methyl-5-nitrobenzenesulfonate anions, the sulfonate groups exhibit a chelating–bridging heptadentate coordination, the O1/O2 atoms and O1/O3 atoms chelate one K^+ ion, and each O atom bridges to another K^+ ion. Only one O atom (O4) of the nitro group coordinates to the K^+ ion, but the N1—O4 and N1—O5 bond distances are almost equivalent [1.219 (2) Å]. The KO_8 polyhedra are each surrounded by five KO_8 polyhedra and condensed to $\{KO_4\}_n$ layers parallel to the (100) plane. The arene rings of the 2-methyl-5-nitrobenzenesulfonate anions are arranged above and below the layers.

(I)
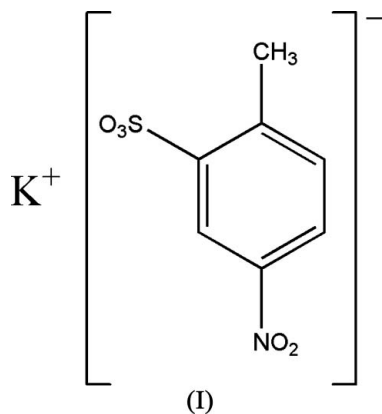
Experimental

Hydrothermal treatment of $KMnO_4$ (1.0 mmol, 0.158 g), 2-methyl-5-nitrobenzenesulfonic acid (1.0 mmol, 0.217 g), water (0.2 ml) and ethanol (1.0 ml) over a period of 2 d at 373 K yielded colorless needle-shaped crystals (yield 32%, based on K).

Crystal data

$K^+ \cdot C_7H_6NO_5S^-$
$M_r = 255.29$
Monoclinic, $P2_1/c$
$a = 14.139\ (4)$ Å
$b = 9.367\ (3)$ Å
$c = 7.124\ (2)$ Å
$\beta = 98.652\ (4)°$
$V = 932.8\ (5)$ Å^3

$Z = 4$
$D_x = 1.818$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.79$ mm^{-1}
$T = 292\ (2)$ K
Needle, colorless
$0.23 \times 0.08 \times 0.06$ mm

Data collection

Bruker SMART APEX-II CCD
  area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan
  (SADABS; Sheldrick, 1996)
  $T_{min} = 0.931$, $T_{max} = 0.947$

5275 measured reflections
2019 independent reflections
1714 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 27.2°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.090$
$S = 1.03$
2019 reflections
138 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0661P)^2]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.009$
$\Delta\rho_{max} = 0.37$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}
Extinction correction: SHELXL97
Extinction coefficient: 0.0011 (3)

Table 1
Selected bond lengths (Å).

K—O1	2.9583 (14)	K—O2^{iii}	2.9113 (13)
K—O1^i	3.0427 (15)	K—O3^{iv}	2.8255 (13)
K—O1^{ii}	2.7751 (14)	K—O3^i	2.8862 (15)
K—O2	2.8228 (16)	K—O4^v	2.9188 (16)

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

H atoms were included at calculated positions and refined as riding, with C—H distances of 0.93–0.96Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHEL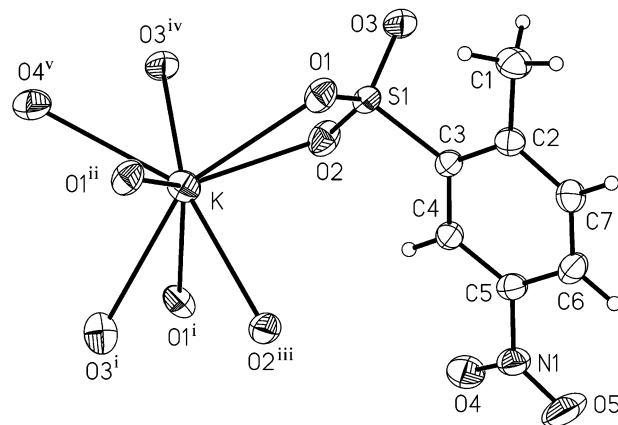XS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 2004); software used to prepare material for publication: SHELXTL.

Figure 1
The coordination environment of the K$^+$ ion, with the atom-numbering scheme, showing displacement ellipsoids drawn at the 50% probability level. [Symmetry codes: (i) $1 - x, y + \frac{1}{2}, \frac{1}{2} - z$; (ii) $1 - x, -y, -z$; (iii) $x, \frac{1}{2} - y, z - \frac{1}{2}$; (iv) $1 - x, -y, 1 - z$; (v) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.]

References

Bruker (2004). SMART (Version 6.0), SAINT (Version 6.0) and SHELXTL (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Dickens, B. & Brown, W. E. (1972). Acta Cryst. B**28**, 3056–3065.
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