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Key indicators

Single-crystal X-ray study
 T = 298 K
 Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
 R factor = 0.036
 wR factor = 0.129
 Data-to-parameter ratio = 10.8

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

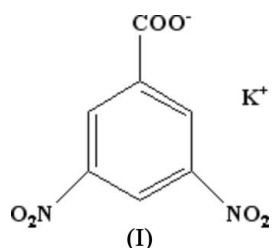
Potassium 3,5-dinitrobenzoate

The title compound, $\text{K}^+\cdot\text{C}_7\text{H}_3\text{N}_2\text{O}_6^-$, crystallized from aqueous solution, is not isostructural with sodium 3,5-dinitrobenzoate. Both the anion and the cation lie on a twofold axis. The K^+ cation is surrounded by eight O atoms and the crystal structure is stabilized by $\pi-\pi$ interactions.

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Comment

During work on crystallization, potassium 3,5-dinitrobenzoate, (I), was obtained as single crystals by evaporation of an aqueous solution at room temperature, and its structure determined. Probably due to the difference in the radii of K^+ and Na^+ cations, compound (I) is not isostructural with the Na salt, sodium 3,5-dinitrobenzoate, whose structure has been reported in the space group $P3_121$ (Jones *et al.*, 2005).



The structure of (I) is shown in Fig. 1. The K^+ cation and 3,5-dinitrobenzoate anion lie on a twofold axis. All atoms of the 3,5-dinitrobenzoate anion are almost coplanar, as observed in the corresponding Na^+ salt. The crystal structure is essentially

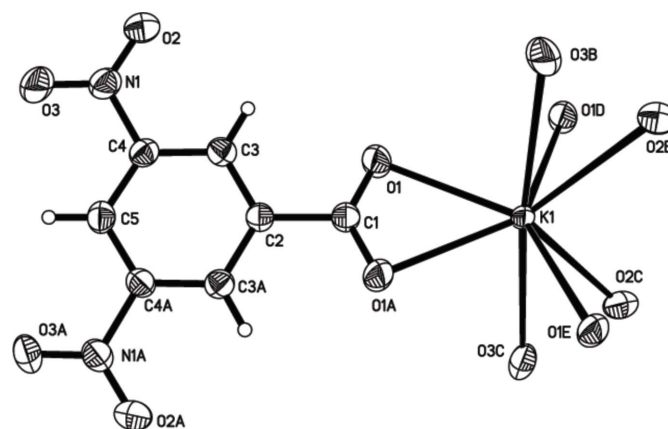


Figure 1
 The ions and complete coordination of the K^+ cation of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Atoms with the suffixes A, B, C, D and E are at the symmetry positions $(1-x, y, \frac{1}{2}-z)$, $(\frac{1}{2}-x, \frac{1}{2}+y, -\frac{1}{2}-z)$, $(\frac{1}{2}+x, \frac{1}{2}+y, z+1)$, $(-x+1, -y+1, -z)$ and $(x, -y+1, \frac{1}{2}+z)$, respectively.

ionic, and each K^+ cation interacts with eight O atoms belonging to nitro and carboxylate groups of four symmetry-related anions (Table 1). The crystal packing is stabilized by intermolecular π - π interactions (4.05 Å) between aromatic rings (Fig. 2), forming a layer structure.

Experimental

3,5-Dinitrobenzoic acid (14.1 mmol) was added to a solution of KOH (14.1 mmol) in water (10 ml). The mixture was stirred for 2 h at 298 K. The solution was then filtered under reduced pressure and set aside for crystallization. After 7 d, pure colourless crystals of (I) were collected from the filtered solution.

Crystal data

$K^+ \cdot C_7H_3N_2O_6^-$	$D_x = 1.791 \text{ Mg m}^{-3}$
$M_r = 250.21$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 1239 reflections
$a = 10.150 (3) \text{ \AA}$	$\theta = 3.0\text{--}27.6^\circ$
$b = 17.715 (4) \text{ \AA}$	$\mu = 0.59 \text{ mm}^{-1}$
$c = 7.066 (2) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 133.075 (3)^\circ$	Block, colourless
$V = 928.1 (4) \text{ \AA}^3$	$0.45 \times 0.32 \times 0.25 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	809 independent reflections
φ and ω scans	667 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 2002)	$R_{\text{int}} = 0.019$
$T_{\text{min}} = 0.777$, $T_{\text{max}} = 0.867$	$\theta_{\text{max}} = 25.0^\circ$
2333 measured reflections	$h = -12 \rightarrow 11$
	$k = -20 \rightarrow 16$
	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0885P)^2 + 0.7104P]$
$R[F^2 > 2\sigma(F^2)] = 0.036$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.129$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.00$	$\Delta\rho_{\text{max}} = 0.21 \text{ e \AA}^{-3}$
809 reflections	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
75 parameters	
H-atom parameters constrained	

Table 1

Selected bond lengths (Å).

K1—O1 ⁱ	2.636 (2)	K1—O3 ⁱⁱ	3.021 (3)
K1—O1	2.801 (2)	K1—O2 ⁱⁱ	3.034 (3)

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

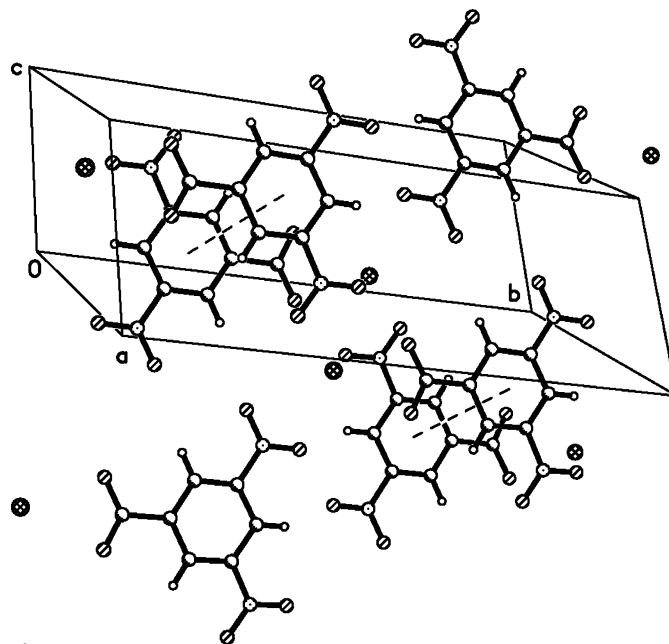


Figure 2

The packing arrangement in the crystal structure of (I). Dashed lines indicate intermolecular π - π interactions.

H atoms were placed in calculated positions and refined as riding, with C—H distances constrained to 0.93 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINTE* (Bruker, 2001); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXTL*.

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References

- Bruker (2001). *SMART* and *SAINTE*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Jones, H. P., Gillon, A. L. & Davey, R. J. (2005). *Acta Cryst.* **E61**, m1131–m1132.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*, University of Göttingen, Germany.
- Sheldrick, G. M. (2001). *SHELXTL*. Version 5. Bruker AXS Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (2002). *SADABS*. University of Göttingen, Germany.