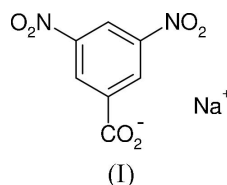
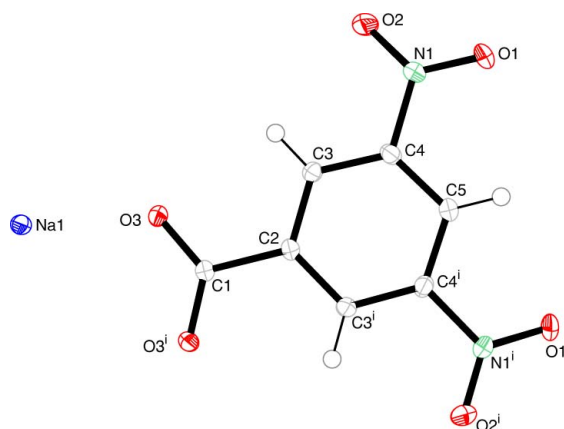


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h.jones-2@postgrad.manchester.ac.uk**Key indicators**Single-crystal X-ray study
 $T = 150$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.025
 wR factor = 0.066
Data-to-parameter ratio = 7.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**Sodium 3,5-dinitrobenzoate**Sodium 3,5-dinitrobenzoate, $\text{Na}^+\cdot\text{C}_7\text{H}_3\text{N}_2\text{O}_6^-$, was obtained
by evaporation at room temperature of an aqueous solution of
ethylenediammonium 3,5-dinitrobenzoate in sodium hydroxide.
The structure is trigonal and the benzoate ion has twofold
crystallographic symmetry.

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CommentDuring work on crystallization of the salt ethylenedi-
ammonium 3,5-dinitrobenzoate, an aqueous solution of the
salt at pH 12 was prepared and allowed to evaporate at room
temperature, giving red prisms of sodium 3,5-dinitrobenzoate
(NaDNB), (I). The crystal structure was not found in the
Cambridge Structural Database (CSD, Version 5.25; Allen,
2002) and hence its structure was determined by single-crystal
X-ray diffraction at 150 K.The benzoate ion is on a twofold axis of symmetry, passing
through the carboxylate group (Fig. 1).**Experimental**3,5-Dinitrobenzoic acid (Aldrich, 99%) was dissolved in sodium
hydroxide solution and a solution of ethylenediamine (Aldrich, 99%)
was added. The solution was filtered and the pH recorded as 12.14.
The solution pH was measured using an Accumet Basic AB15 pH**Figure 1**View of NaDNB, showing the whole benzoate anion. Displacement
ellipsoids are drawn at the 50% probability level. [Symmetry code: (i)
 $x - y, -y, -z + \frac{2}{3}$]

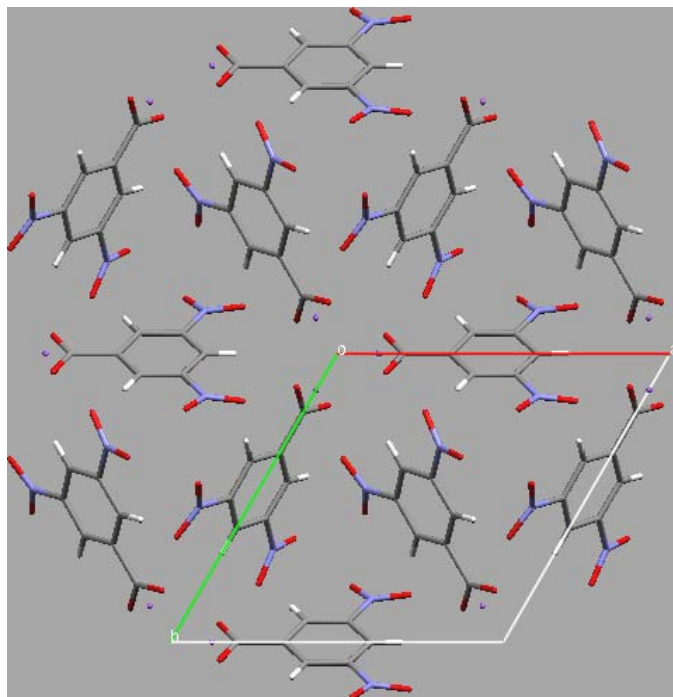


Figure 2
The packing of sodium 3,5-dinitrobenzoate, viewed along the *c* axis, showing the threefold symmetry.

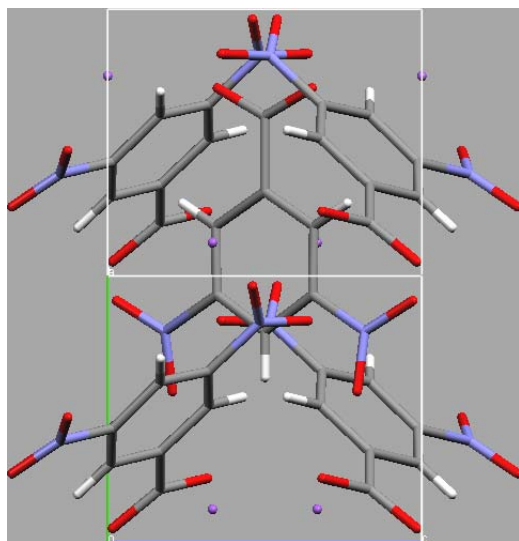


Figure 3
The twofold axis of symmetry perpendicular to the *c* axis.

meter with an Accumet glass calomel pH electrode. The solution was allowed to evaporate to dryness in air at room temperature. Crystals of ethylenediammonium 3,5-dinitrobenzoate, sodium hydroxide and red prisms of sodium 3,5-dinitrobenzoate formed.

Crystal data

$\text{Na}^+ \cdot \text{C}_7\text{H}_3\text{N}_2\text{O}_6^-$
 $M_r = 234.1$
 Trigonal, $P3_121$
 $a = 10.7701 (5) \text{ \AA}$
 $c = 6.3526 (2) \text{ \AA}$
 $V = 638.15 (5) \text{ \AA}^3$
 $Z = 3$
 $D_x = 1.828 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 Cell parameters from 2522 reflections
 $\theta = 1.0\text{--}27.5^\circ$
 $\mu = 0.20 \text{ mm}^{-1}$
 $T = 150 \text{ K}$
 Prism, red
 $0.25 \times 0.25 \times 0.25 \text{ mm}$

Data collection

Nonius KappaCCD diffractometer
 Thick-slice ϕ and ω scans
 Absorption correction: multi-scan (Blessing, 1995)
 $T_{\text{min}} = 0.796, T_{\text{max}} = 0.951$
 3498 measured reflections
 554 independent reflections

537 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -12 \rightarrow 13$
 $k = -8 \rightarrow 13$
 $l = -8 \rightarrow 8$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.026$
 $wR(F^2) = 0.066$
 $S = 1.09$
 554 reflections
 76 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0336P)^2 + 0.1582P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
 Extinction correction: *SHELXL97*
 Extinction coefficient: 0.14 (2)

In the absence of significant anomalous dispersion effects, Friedel pairs were merged. The choice of space group $P3_121$ rather than $P3_221$ is arbitrary. All H atoms were positioned geometrically and refined as riding, with $\text{C-H} = 0.93\text{--}0.98 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SORTAV* (Blessing, 1987,1989, *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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