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The crystal structure of dipentaerthritol hexanitrate, $C_{10}H_{16}N_6O_{19}$

Table 1: Data collection and handling.

Crystal:	Colourless plate
Size:	0.19 × 0.08 × 0.03 mm
Wavelength:	Mo K α radiation (0.71073 Å)
μ :	0.17 mm ⁻¹
Diffractometer, scan mode:	Bruker D8 Venture, φ and ω
$\theta_{\max}$, completeness:	26.6°, 99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	10747, 4240, 0.082
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 2391
$N(\text{param})_{\text{refined}}$:	316
Programs:	Bruker [1], SHELX [2, 3], Diamond [4]

Source of material

Pentaerythritol, 10.0 g, was added slowly, with stirring, to 60.0 g of 98% nitric acid which has been cooled to 10 °C. While the pentaerythritol was being introduced the temperature was maintained between 15 and 20 °C. The reaction was then stirred for 15 min at 15–20 °C. The crude product was separated from solution by drowning over five volumes of crushed ice with stirring. Then collected by filtration. The production was washed repeatedly with water until neutral and dried at 50 °C for 2 h.

Experimental details

Hydrogen atoms were added using riding models.

Comment

Dipentaerythritol hexanitrate is one of the primary by-products at the production progress of pentaerythritol tetranitrate [5, 6]. The performance of dipentaerythritol hexanitrate, such as thermal stability and detonation property, is worse than that of pentaerythritol tetranitrate [7, 8]. The mechanical sensitivity is higher than pentaerythritol tetranitrate [5]. The dipentaerythritol hexanitrate is not commercially available because of its properties [9]. The title compound was obtained from

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Abstract

$C_{10}H_{16}N_6O_{19}$, monoclinic, $C2/c$ (no. 15), $a = 29.980(5)$ Å, $b = 8.4695(17)$ Å, $c = 20.719(4)$ Å, $\beta = 128.124(7)^\circ$, $V = 4138.7(16)$ Å³, $Z = 8$, $R_{\text{gt}}(F) = 0.0587$, $wR_{\text{ref}}(F^2) = 0.1683$, $T = 170$ K.

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The molecular structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\text{\AA}^2$).

Atom	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.71855 (13)	0.3535 (3)	0.8293 (2)	0.0358 (8)
H1A	0.746882	0.423515	0.834015	0.043*
H1B	0.707369	0.399982	0.861289	0.043*
C2	0.66656 (13)	0.3332 (3)	0.7391 (2)	0.0321 (8)
C3	0.63526 (13)	0.4913 (3)	0.7078 (2)	0.0358 (8)
H3A	0.601963	0.482635	0.649183	0.043*
H3B	0.621880	0.522216	0.739338	0.043*
C4	0.62441 (14)	0.2145 (4)	0.7296 (2)	0.0361 (8)
H4A	0.588124	0.217529	0.673183	0.043*
H4B	0.639931	0.106030	0.741406	0.043*
C5	0.68452 (13)	0.2772 (4)	0.6891 (2)	0.0344 (8)
H5A	0.708292	0.358810	0.689445	0.041*
H5B	0.707372	0.179691	0.713695	0.041*
C6	0.65204 (14)	0.2026 (4)	0.5581 (2)	0.0351 (8)
H6A	0.675452	0.105640	0.580594	0.042*
H6B	0.674995	0.287657	0.558827	0.042*
C7	0.59925 (13)	0.1729 (3)	0.4702 (2)	0.0336 (8)
C8	0.61710 (14)	0.1192 (4)	0.4190 (2)	0.0384 (8)
H8A	0.636913	0.016330	0.438898	0.046*
H8B	0.583585	0.108090	0.360632	0.046*
C9	0.56092 (14)	0.0469 (3)	0.4662 (2)	0.0392 (9)
H9A	0.547721	0.081073	0.497551	0.047*
H9B	0.527430	0.027259	0.408613	0.047*
C10	0.56507 (13)	0.3269 (4)	0.4367 (2)	0.0368 (8)
H10A	0.553765	0.361376	0.470369	0.044*
H10B	0.587527	0.411980	0.436210	0.044*
N1	0.78068 (13)	0.1871 (4)	0.9444 (2)	0.0491 (8)
N2	0.65123 (12)	0.7602 (3)	0.69566 (18)	0.0402 (7)
N3	0.57333 (12)	0.1801 (3)	0.7828 (2)	0.0414 (7)
N4	0.56583 (14)	−0.2252 (3)	0.49890 (19)	0.0453 (8)
N5	0.67803 (13)	0.2064 (4)	0.3893 (2)	0.0475 (8)
N6	0.48145 (12)	0.4179 (3)	0.3094 (2)	0.0414 (7)
O1	0.79217 (11)	0.3066 (3)	0.98354 (16)	0.0589 (8)
O2	0.79822 (12)	0.0553 (3)	0.96848 (18)	0.0701 (9)
O3	0.74174 (10)	0.1963 (2)	0.85912 (15)	0.0432 (6)
O4	0.61607 (9)	0.2632 (2)	0.78896 (14)	0.0382 (6)
O5	0.56675 (11)	0.2231 (3)	0.83125 (18)	0.0518 (7)
O6	0.54948 (10)	0.0753 (3)	0.73238 (17)	0.0497 (7)
O7	0.67466 (9)	0.6085 (2)	0.71824 (14)	0.0389 (6)
O8	0.68293 (10)	0.8575 (3)	0.70196 (17)	0.0520 (7)
O9	0.60366 (10)	0.7781 (3)	0.67285 (17)	0.0484 (7)
O10	0.63592 (8)	0.2468 (2)	0.60715 (13)	0.0355 (5)
O11	0.65470 (10)	0.2402 (2)	0.42830 (15)	0.0423 (6)
O12	0.66665 (12)	0.0814 (3)	0.35489 (19)	0.0663 (9)
O13	0.70832 (13)	0.3082 (3)	0.3958 (2)	0.0660 (9)
O14	0.49297 (10)	0.5422 (3)	0.34460 (16)	0.0518 (7)
O15	0.51560 (9)	0.2889 (2)	0.35382 (14)	0.0401 (6)
O16	0.44332 (10)	0.3871 (3)	0.23875 (16)	0.0484 (7)
O17	0.59547 (10)	−0.0943 (2)	0.50216 (15)	0.0422 (6)
O18	0.59524 (12)	−0.3414 (3)	0.52829 (17)	0.0568 (8)
O19	0.51673 (12)	−0.2088 (3)	0.46983 (18)	0.0574 (8)

purification progress of pentaerythritol tetranitrate. The understanding of crystal structure of dipentaerythritol hexanitrate may affect the application of pentaerythritol tetranitrate. The crystal structure of the title compound was analyzed and refined using the SHELXL program [2, 3].

As shown in the figure, the symmetric unit of the title compound is the dimer of pentaerythritol tetranitrate. The molecule structure of title compound is similar to the pentaerythritol tetranitrat [10]. C5-O10 and C6-O10 bond lengths are 1.418(6) to 1.421(4) $\text{\AA}$, respectively. The other C-O bond lengths range from 1.445(4) to 1.458(4) $\text{\AA}$. The C-C bond length range from 1.507(5) to 1.536(4) $\text{\AA}$. All bond lengths and angles are in the expected ranges.

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