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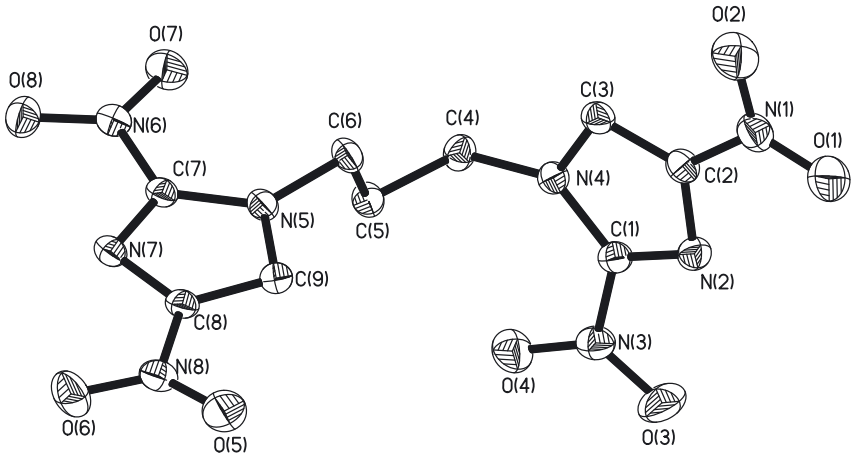
The crystal structure of 1,3-bis(2,4-dinitro-1*H*-imidazol-1-yl)propane



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Abstract

$C_9H_8N_8O_8$, monoclinic, $P2_1/c$ (no. 14), a = 12.0387(3) Å, b = 10.7899(2) Å, c = 11.4310(3) Å, β = 111.536(3)°, V = 1,381.18(6) Å^3, Z = 4, $R_{gt}(F)$ = 0.0499, $wR_{ref}(F^2)$ = 0.1396, T = 293 K.

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Table 1: Data collection and handling.

Crystal:	Yellow block
Size:	0.06 × 0.05 × 0.04 mm
Wavelength:	Cu *K*α radiation (1.54184 Å)
μ:	1.34 mm^{-1}
Diffractometer, scan mode:	XtaLAB Pro II AFC12 (RINC), ω
θ_{max}, completeness:	68.0°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	7,045, 2,476, 0.046
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 2,199
$N(param)_{refined}$:	226
Programs:	Olex2,[1] SHELX,[2,3] Bruker[4]

The molecular structure is shown in the figure (hydrogen atoms are omitted for clarity). Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

Add N,N-dimethylformamide (DMF), 2,4-dinitroimidazole and dibromopropane to the reactor. The temperature of the reactor was raised to 333.15 K and the reaction lasted for 2 h. After the reaction is complete, the temperature of the reactor was lowered to 298.15 K. The reaction solution is filtered and remove the filtrate and retain the yellow solid precipitate. The yellow solid is dissolved in acetone and the solution is volatilized at room temperature to obtain clear yellow crystals.

2 Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

3 Comment

Imidazole compounds are research hotspots in the field of energetic materials in various countries.[5–8] 2,4-Dinitroimidazole is an important imidazole compound that has been widely and deeply studied.[5,9,10] The title compound is obtained by connecting two 2,4-dinitroimidazole molecules using

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
O1	1.18438 (16)	0.79030 (19)	0.64787 (19)	0.0812 (7)
O2	1.02132 (18)	0.89094 (18)	0.59733 (19)	0.0675 (5)
O3	1.13542 (16)	0.41674 (17)	0.35824 (19)	0.0663 (5)
O4	0.95056 (15)	0.40077 (16)	0.23752 (18)	0.0571 (5)
O5	0.59547 (15)	0.26384 (17)	0.63987 (16)	0.0657 (5)
O6	0.42293 (16)	0.20563 (15)	0.52292 (16)	0.0575 (5)
O7	0.42555 (15)	0.57677 (15)	0.11182 (17)	0.0557 (4)
O8	0.28075 (13)	0.46220 (15)	0.11764 (16)	0.0508 (4)
N1	1.08384 (17)	0.80669 (17)	0.58428 (18)	0.0465 (5)
N2	1.08705 (14)	0.62156 (15)	0.46431 (16)	0.0379 (4)
N3	1.03391 (16)	0.45514 (16)	0.31578 (18)	0.0420 (4)
N4	0.90380 (13)	0.63407 (14)	0.31496 (15)	0.0326 (4)
N5	0.57519 (13)	0.48594 (14)	0.34357 (15)	0.0332 (4)
N6	0.38249 (15)	0.50143 (13)	0.16231 (15)	0.0365 (4)
N7	0.42104 (13)	0.36795 (13)	0.34157 (15)	0.0326 (4)
N8	0.51322 (16)	0.26611 (14)	0.54398 (17)	0.0392 (4)
C1	1.00903 (17)	0.57138 (17)	0.36398 (19)	0.0344 (4)
C2	1.02851 (17)	0.72306 (17)	0.48067 (19)	0.0360 (4)
C3	0.91717 (17)	0.73415 (17)	0.3913 (2)	0.0362 (4)
H3	0.861955	0.796813	0.383865	0.043*
C4	0.79625 (17)	0.61045 (19)	0.20181 (19)	0.0377 (5)
H4A	0.820604	0.577546	0.135942	0.045*
H4B	0.755386	0.688346	0.172184	0.045*
C5	0.70969 (17)	0.51995 (18)	0.22555 (19)	0.0370 (4)
H5A	0.647485	0.498188	0.146139	0.044*
H5B	0.751970	0.444701	0.262873	0.044*
C6	0.65347 (17)	0.57563 (17)	0.3124 (2)	0.0374 (5)
H6A	0.716045	0.602714	0.389429	0.045*
H6B	0.606941	0.647797	0.272454	0.045*
C7	0.45936 (16)	0.45113 (15)	0.28139 (18)	0.0305 (4)
C8	0.51756 (16)	0.34862 (16)	0.44696 (18)	0.0328 (4)
C9	0.61365 (17)	0.41861 (17)	0.45144 (19)	0.0356 (4)
H9	0.689054	0.419847	0.514673	0.043*

dibromopropane as a bridge. The title compound is an organic compound with high research value in the preparation of imidazole energetic materials.

The asymmetric unit of the title compound is one 1,3-bis(2,4-dinitro-1H-imidazol-1-yl)propane molecule. The bond lengths and angles are in the expected ranges. The dihedral angle formed by the two imidazole rings in the title compound is 78.740°. In the 2,4-dinitroimidazole molecule connected to C6, the dihedral angles formed by the two nitro groups and imidazole ring are 1.529° and 7.623°. In the 2,4-dinitroimidazole molecule connected to C4, the dihedral angles formed by the two nitro groups and imidazole ring are 5.664° and 12.139°. These dihedral angles have changed slightly compared to 2,4-dinitroimidazole molecule,[11] which may be due to effect of steric hindrance and bridge of C4–C5–C6.

The title compound is a novel imidazole compound formed by the connection of two 2,4-dinitroimidazole molecules with dibromopropane. The title compound is expected to have superior performance than 2,4-dinitroimidazole. There are many similar structures in the field of energetic materials, such as HNS.[12]

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