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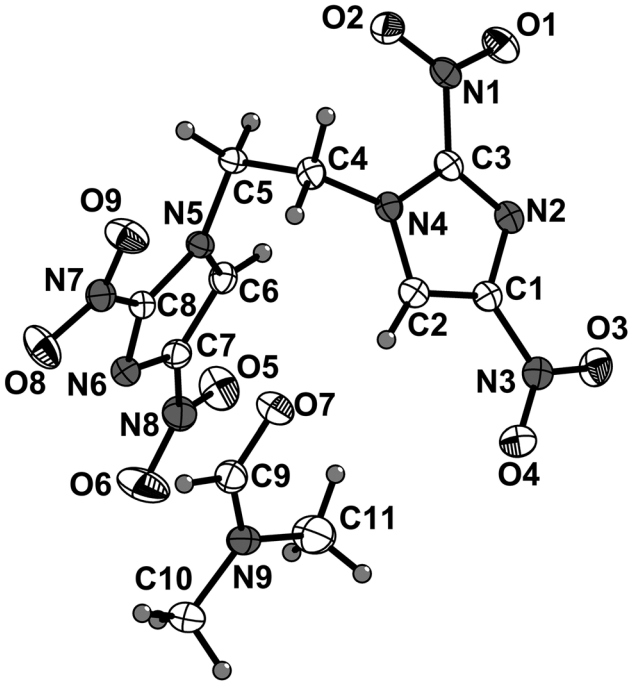
# Crystal structure of 1,2-bis(2,4-dinitro-1*H*-imidazol-1-yl)ethane – dimethylformamide (1/1), $C_{11}H_{13}N_9O_9$

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**Abstract**

$C_{11}H_{13}N_9O_9$, triclinic, $P\bar{1}$ (no. 2), $a$ = 8.6588(3) Å, $b$ = 8.7538(3) Å, $c$ = 11.7312(4) Å, $\alpha$ = 78.230(1)°, $\beta$ = 82.060(1)°, $\gamma$ = 76.031(1)° $V$ = 841.05(5) Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0376, $wR_{ref}(F^2)$ = 0.1006, T = 150.0 K.

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**Table 1:** Data collection and handling.

| | |
|---|---|
| Crystal: | Colourless plate |
| Size: | 0.12 × 0.08 × 0.05 mm |
| Wavelength: | Mo $K\alpha$ radiation (0.71073 Å) |
| $\mu$: | 0.14 mm$^{-1}$ |
| Diffractometer, scan mode: | D8 VENTURE, $\varphi$ and $\omega$ |
| $\theta_{max}$, completeness: | 26.4°, 99% |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$, $R_{int}$: | 9685, 3412, 0.039 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\sigma(I_{obs})$, 2825 |
| $N(param)_{refined}$: | 264 |
| Programs: | Bruker [1], Olex2 [2], SHELX [3, 4] |

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.

## Source of material

All reagents were purchased with analysis grade. In representative experiments, 5 mL $HNO_3$ and 15 mL $H_2SO_4$ were mixed. Then 14 g (50 mmol) 1,2-bis(2-nitro-1*H*-imidazol-1-yl)ethane were added at 293 K. The target compound was obtained by reaction at 348 K for 9 h. The raw product was dissolved in *N*,*N*-dimethylformamide (DMF) and the crystal of the title compound was obtained by slow evaporation at 293 K.

## Experimental details

Using Olex2 [2], the structure was solved and refined with the ShelXL [4] refinement package. All H atoms were positioned geometrically and treated as riding, and $U_{iso}(H) = 1.2U_{eq}(C)$.

## Comment

Bisimidazole moieties bridged by other groups have always been a hot topic [5–8]. These compounds concatenate two imidazole groups and have the features of both

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

| Atom | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.49627 (18) | 0.25303 (18) | 0.54117 (13) | 0.0191 (3) |
| C2 | 0.46354 (18) | 0.21210 (18) | 0.44190 (13) | 0.0202 (3) |
| H2 | 0.520290 | 0.124787 | 0.405441 | 0.024* |
| C3 | 0.29685 (18) | 0.42433 (18) | 0.48727 (13) | 0.0190 (3) |
| C4 | 0.25624 (18) | 0.32579 (19) | 0.30135 (13) | 0.0205 (3) |
| H4A | 0.138637 | 0.350173 | 0.318980 | 0.025* |
| H4B | 0.288719 | 0.218561 | 0.279143 | 0.025* |
| C5 | 0.30248 (17) | 0.44935 (18) | 0.19916 (13) | 0.0194 (3) |
| H5A | 0.238106 | 0.457319 | 0.133840 | 0.023* |
| H5B | 0.277609 | 0.555197 | 0.223402 | 0.023* |
| C6 | 0.58807 (18) | 0.46915 (19) | 0.19184 (13) | 0.0205 (3) |
| H6 | 0.573842 | 0.540979 | 0.245103 | 0.025* |
| C7 | 0.72678 (18) | 0.40440 (19) | 0.13199 (13) | 0.0211 (3) |
| C8 | 0.55469 (18) | 0.31065 (18) | 0.08136 (12) | 0.0184 (3) |
| C9 | 0.7311 (2) | −0.0545 (2) | 0.20001 (14) | 0.0256 (4) |
| H9 | 0.719104 | −0.102338 | 0.136931 | 0.031* |
| C10 | 1.0173 (2) | −0.1226 (2) | 0.14598 (16) | 0.0362 (4) |
| H10A | 0.982453 | −0.165075 | 0.085140 | 0.054* |
| H10B | 1.088254 | −0.209037 | 0.193688 | 0.054* |
| H10C | 1.074788 | −0.038730 | 0.109362 | 0.054* |
| C11 | 0.9072 (2) | 0.0131 (3) | 0.31526 (18) | 0.0414 (5) |
| H11A | 0.807488 | 0.081588 | 0.342751 | 0.062* |
| H11B | 0.987995 | 0.077065 | 0.287908 | 0.062* |
| H11C | 0.945298 | −0.072706 | 0.379581 | 0.062* |
| N1 | 0.16688 (15) | 0.56357 (16) | 0.48195 (11) | 0.0222 (3) |
| N2 | 0.39335 (15) | 0.38512 (16) | 0.56962 (11) | 0.0207 (3) |
| N3 | 0.62649 (15) | 0.17211 (16) | 0.61035 (11) | 0.0216 (3) |
| N4 | 0.33227 (15) | 0.32359 (15) | 0.40700 (11) | 0.0187 (3) |
| N5 | 0.47384 (14) | 0.40785 (15) | 0.15826 (10) | 0.0180 (3) |
| N6 | 0.70750 (15) | 0.30595 (16) | 0.06250 (11) | 0.0217 (3) |
| N7 | 0.47828 (16) | 0.22097 (16) | 0.02367 (11) | 0.0238 (3) |
| N8 | 0.88256 (16) | 0.43254 (18) | 0.13924 (12) | 0.0279 (3) |
| N9 | 0.87855 (16) | −0.05601 (17) | 0.21981 (12) | 0.0265 (3) |
| O1 | 0.15276 (14) | 0.64737 (14) | 0.55605 (10) | 0.0307 (3) |
| O2 | 0.07898 (13) | 0.59010 (14) | 0.40264 (10) | 0.0270 (3) |
| O3 | 0.65040 (14) | 0.23477 (15) | 0.68883 (10) | 0.0288 (3) |
| O4 | 0.70779 (13) | 0.04601 (14) | 0.58430 (10) | 0.0269 (3) |
| O5 | 0.88761 (15) | 0.53664 (17) | 0.19335 (11) | 0.0369 (3) |
| O6 | 0.99906 (15) | 0.35025 (18) | 0.09252 (13) | 0.0465 (4) |
| O7 | 0.60791 (14) | 0.00429 (15) | 0.25718 (10) | 0.0301 (3) |
| O8 | 0.55945 (16) | 0.15560 (17) | −0.05365 (11) | 0.0372 (3) |
| O9 | 0.33831 (14) | 0.21837 (16) | 0.05561 (11) | 0.0345 (3) |

flexibility and rigidity. The title compound has been reported for the first time in this paper (cf. Figure).

The asymmetric unit of the title structure contains one 1,2-bis(2,4-dinitro-1*H*-imidazol-1-yl)ethane and one dimethylformamide molecule. The nitroimidazole ring are almost flat, and the dihedral angle of the two nitroimidazole rings is 66.50°.

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**Conflict of interest statement:** The authors declare no conflicts of interest regarding this article.

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