# Crystal structure of 1-acetylimidazolidine-2,4-dione monohydrate, $C_5H_8N_2O_4$

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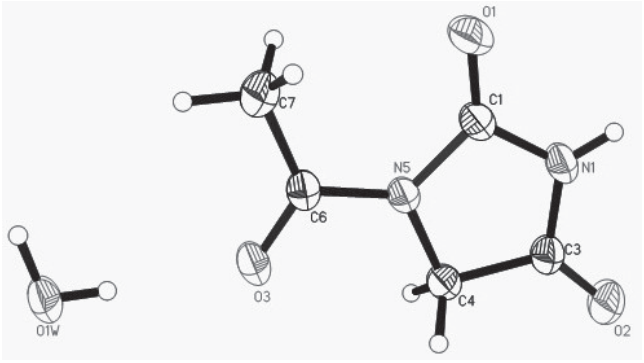


**Abstract**

$C_5H_8N_2O_4$, monoclinic, $P2_1/m$ (no. 11), $a$ = 6.385(2) Å, $b$ = 6.150(2) Å, $c$ = 8.771(2) Å, $\beta$ = 105.698(4)°, $V$ = 331.5 Å$^3$, $Z$ = 2, $R_{gt}(F)$ = 0.0358, $wR_{ref}(F^2)$ = 0.0955, $T$ = 273 K.

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

| | |
|---|---|
| Crystal: | colourless blocks, size 0.29×0.30×0.64 mm |
| Wavelength: | Mo $K_\alpha$ radiation (0.71073 Å) |
| $\mu$: | 1.40 cm$^{-1}$ |
| Diffractometer, scan mode: | Bruker SMART APEX CCD, $\omega$ |
| $2\theta_{max}$: | 51° |
| $N(hkl)_{measured}$, $N(hkl)_{unique}$: | 1922, 680 |
| Criterion for $I_{obs}$, $N(hkl)_{gt}$: | $I_{obs} > 2\ \sigma(I_{obs})$, 589 |
| $N(param)_{refined}$: | 77 |
| Programs: | SHELX [3] |

## Source of material

All reagents and solvents used in this study are commercially available. The synthesis of 1-acetylimidazolidine-2,4-dione was carried out by refluxing hydantoin (2 mol) in $Ac_2O$ ( 2 mL) for 4 h. The reaction mixture was then cooled at RT and poured into ice water. The solid product was filtered off to afford the product. The compound was obtained as colourless crystals (water). **m.p.:** 124 °C. **$^1$H-NMR** (DMSO-$d_6$) δ (ppm): 2.37 (s, 2H, $CH_2$), 4.13 (s, 3H, $CH_3$), 11.50 (s, 1H, NH). **$^{13}$C-NMR** δ: 169.9, 168.5, 154.4, 48.9, 24.2.

## Discussion

Hydantoin (1,3-imidazolidinedione) derivatives display diverse pharmacological properties. Several of these derivatives (mephenythoin, phenytoin, norantoin, ethotoin, methetoin, fosphenytoin) have been used as anticonvulsive drugs [1, 2]. The title structure is composed of a planar imidazolidine-2,4-dione ring (O1-O2/N2-N5/C1/C3-C4) having an acetyl substituant (O3/C6-C7) attached to N5. Additionally one solvent water molecule is present in th title structure. The water molecule apparently plays an important role in the stabilization of this crystal structure *via* O1W–H1W1···O3 hydrogen bonding, that further extended to a two dimensional framework through O1W–H2W1···O3, and N2–H2A···O1W intermolecular hydrogen bondings [3].

**Table 2.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | Occ. | $x$ | $y$ | $z$ | $U_{iso}$ |
|---|---|---|---|---|---|---|
| H(1W1) | 2*e* | | 0.224(4) | ¼ | 0.225(4) | 0.064(8) |
| H(2W1) | 2*e* | | 0.160(5) | ¼ | 0.360(4) | 0.08(1) |
| H(2A) | 2*e* | | –0.444(4) | ¼ | –0.541(3) | 0.053(7) |
| H(4A) | 4*f* | 0.5 | 0.0807 | 0.1215 | –0.2781 | 0.052 |
| H(4B) | 4*f* | 0.5 | 0.0807 | 0.3785 | –0.2781 | 0.052 |
| H(7C) | 2*e* | | –0.2142 | ¼ | 0.1318 | 0.091 |
| H(7B) | 4*f* | 0.5 | –0.3683 | 0.1225 | –0.0094 | 0.091 |
| H(7A) | 4*f* | 0.5 | –0.3683 | 0.3775 | –0.0094 | 0.091 |

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**Table 3.** Atomic coordinates and displacement parameters (in Å$^2$).

| Atom | Site | *x* | *y* | *z* | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| O(1) | 2*e* | –0.5356(2) | ¼ | –0.2890(2) | 0.0343(9) | 0.138(2) | 0.053(1) | 0 | 0.0099(8) | 0 |
| O(1W) | 2*e* | 0.2797(3) | ¼ | 0.3163(2) | 0.046(1) | 0.102(2) | 0.035(1) | 0 | –0.0026(8) | 0 |
| O(2) | 2*e* | –0.0762(3) | ¼ | –0.5779(2) | 0.063(1) | 0.095(1) | 0.0348(9) | 0 | 0.0176(8) | 0 |
| O(3) | 2*e* | 0.0734(2) | ¼ | 0.0040(2) | 0.0451(9) | 0.069(1) | 0.0348(8) | 0 | –0.0022(7) | 0 |
| N(2) | 2*e* | –0.3430(3) | ¼ | –0.4636(2) | 0.040(1) | 0.071(1) | 0.031(1) | 0 | –0.0004(8) | 0 |
| N(5) | 2*e* | –0.1692(3) | ¼ | –0.2182(2) | 0.0328(9) | 0.056(1) | 0.0305(9) | 0 | 0.0053(7) | 0 |
| C(1) | 2*e* | –0.3704(3) | ¼ | –0.3188(3) | 0.035(1) | 0.070(2) | 0.038(1) | 0 | 0.0047(9) | 0 |
| C(3) | 2*e* | –0.1396(3) | ¼ | –0.4650(3) | 0.046(1) | 0.054(1) | 0.034(1) | 0 | 0.0091(9) | 0 |
| C(4) | 2*e* | –0.0104(3) | ¼ | –0.3020(2) | 0.035(1) | 0.058(1) | 0.037(1) | 0 | 0.0081(9) | 0 |
| C(6) | 2*e* | –0.1132(3) | ¼ | –0.0614(2) | 0.044(1) | 0.042(1) | 0.033(1) | 0 | 0.0054(9) | 0 |
| C(7) | 2*e* | –0.2797(4) | ¼ | 0.0195(3) | 0.060(2) | 0.084(2) | 0.041(1) | 0 | 0.018(1) | 0 |

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