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Anhydrous 1-methylimidazolidin-2-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.070
wR factor = 0.161
Data-to-parameter ratio = 13.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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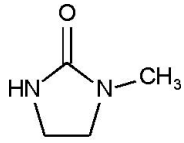
The title compound, $C_4H_8N_2O$, crystallizes from the vapor phase in sheets supported by a one-dimensional hydrogen-bonded network. The molecular unit shows planar ureido $-NCH_3$ groups, but the slight out-of-plane hydrogen-bond geometry may be indicative of some pyramidalization of the ureido $-NH$ groups.

Comment

The imidazolidin-2-one functional group is of primary importance in the transfer of carbon dioxide by biotin-dependent enzymes (Carey *et al.*, 2004; Attwood & Wallace, 2002). It is therefore important that the structural characteristics of this unit be well understood. In the course of our work on biomimetic carbon dioxide fixation, we crystallized anhydrous 1-methylimidazolidin-2-one, (I), and report here its crystal structure.



(I)

The molecular unit in (I) shows the five-membered heterocycle. The ring is only slightly enveloped, with an average internal torsion angle of 4.6° and a mean deviation from planarity of 0.0273 Å. The metrical parameters in the heterocycle are essentially identical to those in unsubstituted imidazolidin-2-one (Kapon & Reisner, 1989), and to those in biotin itself (DeTitta *et al.*, 1976). Methylated atom N2 is planar, indicative of largely sp^2-hybrid character. This is consistent with *N*-silyl-substituted imidazolidin-2-ones (Szalay *et al.*, 2005), as well as with *N*1′-methoxycarbonylbiotin methyl

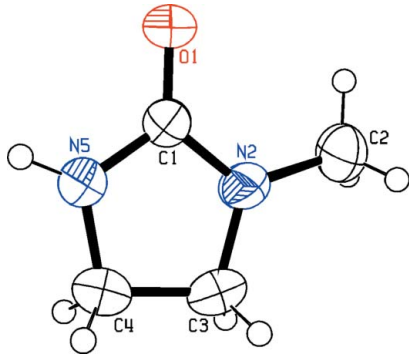


Figure 1
Displacement ellipsoid drawing of (I) (35% probability ellipsoids).

ester (Stallings *et al.*, 1980), which also exhibit essentially planar ureido N atoms. However, the planar N atoms are at variance with some theoretical work which seems to indicate that the N atoms in urea and related molecules have considerable sp^3 character (Meier & Coussens, 1992). Some insight may be gained from the solid state packing in (I), which is supported by a one-dimensional network of hydrogen bonds (O···N = 2.87 Å). Neighboring hydrogen-bonded chains are packed to form a two-dimensional sheet (Fig. 2). The individual hydrogen-bonding interactions are inclined at 19.8° to the heterocycle plane, and may be indicative of some pyramidalization of the —NH group.

Experimental

The title compound was purchased from Aldrich. The microcrystalline powder was placed in a flame-sealed ampoule and the apparatus stored in a 363 K oven for one week. This procedure gave colorless blocks suitable for X-ray diffraction.

Crystal data

$C_4H_8N_2O$
M_r = 100.12
Monoclinic, $P2_1/c$
a = 7.5746 (11) Å
b = 9.3984 (13) Å
c = 7.9482 (11) Å
β = 117.139 (2)°
V = 503.53 (12) Å^3
Z = 4
D_x = 1.321 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1593 reflections
θ = 3.0–31.6°
μ = 0.10 mm^{-1}
T = 298 (2) K
Block, colorless
0.38 × 0.30 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
ω scans
Absorption correction: ψ scan (Blessing, 1995)
T_{min} = 0.94, T_{max} = 0.99
3853 measured reflections
888 independent reflections
712 reflections with $I > 2\sigma(I)$
R_{int} = 0.092
θ_{max} = 25.0°
$h = -9 \rightarrow 9$
$k = -11 \rightarrow 11$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.161
S = 1.16
888 reflections
65 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0535P)^2 + 0.1874P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

H atoms were placed in idealized positions as riding atoms with C—H distances of 0.96 Å for methyl and 0.96 Å for the rest; The N—H distance is 0.86 Å. The isotropic displacement parameters were set at $1.5U_{eq}$ of the parent atom for the methyl H atoms and $1.2U_{eq}$ for the rest.

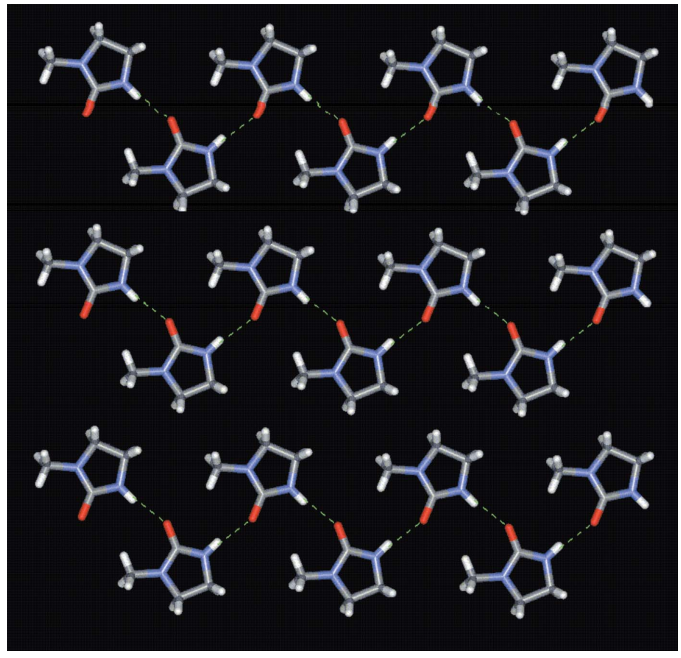


Figure 2
Solid-state packing diagram of (I), viewed down the crystallographic *a* axis.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT-Plus* (Bruker, 1997); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker 1997); software used to prepare material for publication: *SHELXTL*.

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