Crystal structure of 4-formyl-3-methylsydnone, $C_4H_4N_2O_3$

A. Hergold-Brundic

The University of Zagreb, Faculty of Science, Laboratory of General and Inorganic Chemistry, Ulica kralja Zvonimira 8, P.O.Box 153, 10000 Zagreb, Croatia

A. Nagl

The University of Zagreb, Faculty of Textile-technology, Pierottijeva 6, 10000 Zagreb, Croatia

L. Špoljaric-Lukacic

PLIVA, Research Institute, Prilaz baruna Filipovica 29, 10000 Zagreb, Croatia

and M. Šindler-Kulyk

The University of Zagreb, Faculty of Chemical Engineering and Technology, Department of Organic Chemistry, Marulicev trg 20, 10000 Zagreb, Croatia

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Source of material: The 4-formyl-3-methylsydnone was prepared by Vilsmeier reaction (see ref. 1).

$C_4H_4N_2O_3$, monoclinic, $P12_1/n1$ (No. 14), $a = 5.471(1)$ Å, $b = 8.484(2)$ Å, $c = 11.694(2)$ Å, $\beta = 91.23(4)^\circ$, $V = 542.7$ Å³, $Z = 4$, $R(F) = 0.060$, $R_w(F) = 0.060$.

Table 1. Parameters used for the X-ray data collection

Crystal:	yellowish, prismatic, size 0.51 x 0.18 x 0.76 mm
Wavelength:	Cu $K\alpha$ radiation (1.54183 Å)
μ :	11.43 cm ⁻¹
Diffractometer:	Philips PW1100 updated by Stoe
Scan mode:	$\omega/2\theta$
$T_{\text{measurement}}$:	293 K
$2\theta_{\text{max}}$:	60°
$N(hkl)_{\text{unique}}$:	889
Criterion for F_o :	$F_o > 2 \sigma(F_o)$
$N(\text{param})_{\text{refined}}$:	90
Program:	SHELX-76

Table 2. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{iso}
H(41)	4e	0.1431(7)	0.1902(5)	0.9087(3)	0.10(1)
H(42)	4e	0.3275(7)	0.3601(5)	0.8995(3)	0.10(1)
H(43)	4e	0.35(1)	0.236(7)	1.000(5)	0.10(1)
H(3)	4e	0.323(8)	0.160(5)	0.566(4)	0.07(1)

Table 3. Final atomic coordinates and displacement parameters (in Å²)

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> ₁₁	<i>U</i> ₂₂	<i>U</i> ₃₃	<i>U</i> ₁₂	<i>U</i> ₁₃	<i>U</i> ₂₃
O(1)	4e	0.1284(5)	0.2831(4)	0.6853(2)	0.060(2)	0.057(2)	0.059(2)	0.018(2)	-0.011(1)	-0.001(2)
O(2)	4e	0.7533(6)	-0.0203(4)	0.6187(3)	0.074(2)	0.060(2)	0.068(2)	0.014(2)	0.013(2)	-0.007(2)
O(3)	4e	0.8013(5)	0.0115(3)	0.8113(2)	0.043(2)	0.050(2)	0.065(2)	0.006(1)	-0.006(1)	0.006(2)
N(1)	4e	0.4918(5)	0.1518(3)	0.8489(2)	0.035(2)	0.030(2)	0.043(2)	-0.004(1)	-0.008(1)	0.001(1)
N(2)	4e	0.6773(6)	0.0834(4)	0.8989(3)	0.048(2)	0.044(2)	0.056(2)	-0.001(2)	-0.010(2)	0.005(2)
C(1)	4e	0.6771(7)	0.0372(5)	0.7059(3)	0.052(2)	0.038(2)	0.049(2)	-0.001(2)	0.002(2)	0.002(2)
C(2)	4e	0.4776(6)	0.1329(4)	0.7346(3)	0.042(2)	0.029(2)	0.037(2)	-0.000(2)	-0.002(2)	-0.001(2)
C(3)	4e	0.2982(8)	0.1989(5)	0.6580(4)	0.056(3)	0.039(2)	0.045(2)	0.002(2)	-0.007(2)	0.001(2)
C(4)	4e	0.3243(7)	0.2373(5)	0.9239(3)	0.052(2)	0.056(3)	0.038(2)	0.001(2)	-0.003(2)	-0.007(2)

References

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