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1,6-Anhydro-4-*O*-benzyl-3-deoxy-2-*O*-methyl- β -D-ribo-hexopyranose and 1,6-Anhydro-4-*O*-benzyl-2-*C*-(2-cyanoethyl)-2,3-dideoxy- β -D-ribo-hexopyranose

GRAEME J. GAINSFORD, RICHARD H. FURNEAUX,
JENNIFER M. MASON AND PETER C. TYLER

*New Zealand Institute for Industrial Research
and Development, PO Box 31-310, Lower Hutt,
New Zealand*

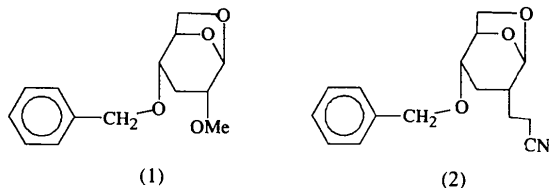
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Abstract

The title compounds, C₁₄H₁₈O₄ and C₁₆H₁₉NO₃, respectively, were obtained during studies of the relationship between structure and herbicidal activity of derivatives of levoglucosenone [Furneaux *et al.* (1989). European Patent Application 0 302 599; Furneaux, Henzell & Tyler (1991). US Patent 5 047 518; Blattner, Furneaux, Mason & Tyler (1991). *Pestic. Sci.* **31**, 419–435; Blattner, Furneaux, Mason & Tyler (1994). *Levoglucosenone and Levoglucosans: Chemistry and Applications*, edited by Z. J. Witczak. ATL Press]. The crystal structures contain independent molecules held together by van der Waals packing forces. The different pendant groups at the C(2) positions have an insignificant effect on the fused dioxolane/pyranose ring conformations. The *O*-benzyl groups adopt different conformations apparently in order to minimize intermolecular non-bonding contacts.

Comment

Crystals of 1,6-anhydro-4-*O*-benzyl-3-deoxy-2-*O*-methyl- β -D-ribo-hexopyranose, (1), and 1,6-anhydro-4-*O*-benzyl-2-*C*-(2-cyanoethyl)-2,3-dideoxy- β -D-ribo-hexopyranose, (2), were prepared during studies of the structure–activity relationships of the potent herbicide (1), derived from levoglucosenone.



The structures consist of the independent molecules shown in Figs. 1 and 2. The bond lengths and angles in the two structures are almost identical, within the ranges found on related sugar structures

(Allen *et al.*, 1987) and display the anomeric effect [mean C(1)—O(5) 1.416, O(5)—C(5) 1.441, C(1)—O(1) 1.430, O(1)—C(6) 1.449 Å (Jeffrey & French, 1978; Noordik & Jeffrey, 1977)]. The molecules have only van der Waals non-bonding contacts, with minimum distances of 2.68 (3) and 2.33 (5) Å for O(1)··H(10) and H(11)··H(14), respectively, in (1), and 2.68 (5) and 2.35 (7) Å for O(1)··H(13) and H(13)··H(14), respectively, in (2).

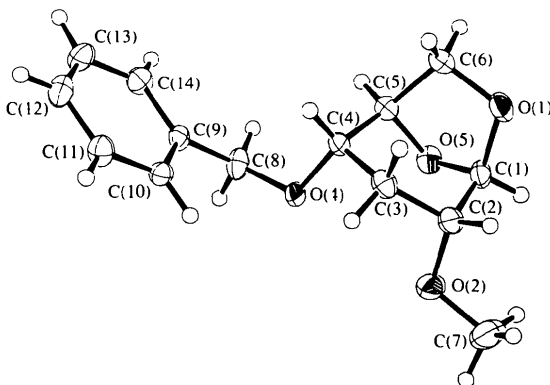


Fig. 1. The structure of (1) showing atom labels, with displacement ellipsoids at the 50% probability level for non-H atoms (Johnson, 1976).

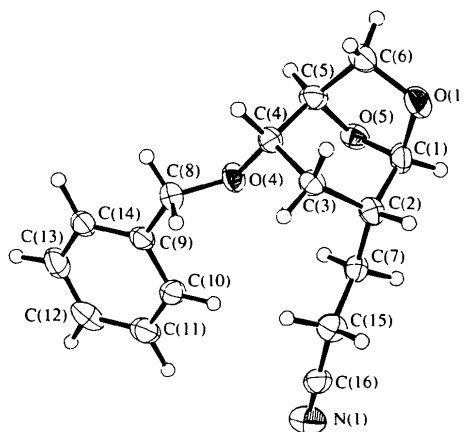


Fig. 2. The structure of (2) showing atom labels, with displacement ellipsoids at the 50% probability level for non-H atoms (Johnson, 1976).

Comparisons of these structures with related compounds 4B {4-*O*-acetyl-2-amino-1,6-anhydro-3-*O*-[(*R*)-1-carboxyethyl]-2-deoxy- β -D-glucopyranose-1',2-lactam, conformer 4B; Keglević, Kojić-Prodić, Banić, Tomić & Puntarec, 1993} and ISO (2,7-anhydro-4,5-*O*-isopropylidene- β -D-*altro*-2-heptulopyranose; Kopf, Abeln & Koll, 1994) suggests how molecular conformations in a crystal can vary when intermolecular hydrogen bonding is present (both reference structures are held together with hydrogen bonds). The 1,6-anhydro moiety five-membered rings adopt envelope conforma-

tions [$Q = 0.411$ and 0.437 \AA , $\varphi = 183.5$ and 185.3° for (1) and (2), respectively (Cremer & Pople, 1975)], very similar to that found in 4B, but different from that in ISO.

The glucopyranose rings in the two structures are almost identical (Table 4), adopting very slightly flattened chair conformations [$Q = 0.620$ and 0.630 \AA , $\theta = 156.7$ and 161.2° , and $\varphi = 174.6$ and 180.3° for (1) and (2), respectively (Cremer & Pople, 1975)]. For the two reference structures, the ring conformation in 4B, affected by adjacent hydrogen bonds (involving the lactam N—H...O atoms) is a distorted boat, while in ISO with an isopropylidene substituent the conformation of the pyranose ring is similar to that found in this work (for ISO, $Q = 0.609 \text{ \AA}$, $\theta = 147.4$, $\varphi = 188.1^\circ$).

Experimental

Crystals of (1) and (2) were synthesized according to known procedures (Furneaux, Henzell & Tyler, 1991; Blattner, Furneaux, Mason & Tyler, 1991; Furneaux, Mason & Tyler, 1994) and obtained from ether/hexane and hexane, respectively.

Compound (1)

Crystal data

$C_{14}H_{18}O_4$
 $M_r = 250.3$
 Tetragonal
 $P4_1$
 $a = 8.535$ (2) \AA
 $c = 17.339$ (6) \AA
 $V = 1263.0$ (7) \AA^3
 $Z = 4$
 $D_x = 1.32 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation
 $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 24 reflections
 $\theta = 4.8$ – 17.0°
 $\mu = 0.103 \text{ mm}^{-1}$
 $T = 138 \text{ K}$
 Needle
 $0.80 \times 0.20 \times 0.20 \text{ mm}$
 Colourless

Data collection

Nicolet R3m four-circle diffractometer
 ω scans
 Absorption correction: none
 2205 measured reflections
 1886 independent reflections
 1604 observed reflections
 $[I > 3\sigma(I)]$

$R_{\text{int}} = 0.016$
 $\theta_{\text{max}} = 30^\circ$
 $h = -7 \rightarrow 8$
 $k = 0 \rightarrow 11$
 $l = 0 \rightarrow 24$
 3 standard reflections monitored every 97 reflections
 intensity decay: 1.5%

Refinement

Refinement on F
 $R = 0.036$
 $wR = 0.043$
 1604 reflections
 234 parameters
 All H-atom parameters refined isotropically
 $w = 1/[\sigma^2(F) + 0.0006F^2]$

$(\Delta/\sigma)_{\text{max}} = 0.015$
 $\Delta\rho_{\text{max}} = 0.16 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
 Extinction correction: none
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (2)

Crystal data

$C_{16}H_{19}NO_3$
 $M_r = 273.3$
 Orthorhombic
 $P2_12_12_1$
 $a = 6.229$ (2) \AA
 $b = 11.951$ (3) \AA
 $c = 18.865$ (6) \AA
 $V = 1404.4$ (6) \AA^3
 $Z = 4$
 $D_x = 1.29 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 25 reflections
 $\theta = 3.5$ – 15.0°
 $\mu = 0.096 \text{ mm}^{-1}$
 $T = 143 \text{ K}$
 Needle
 $0.60 \times 0.15 \times 0.15 \text{ mm}$
 Colourless

Data collection

Nicolet R3m four-circle diffractometer
 ω scans
 Absorption correction: none
 1862 measured reflections
 1780 independent reflections
 914 observed reflections
 $[I > 3\sigma(I)]$

$R_{\text{int}} = 0.007$
 $\theta_{\text{max}} = 27^\circ$
 $h = 0 \rightarrow 7$
 $k = 0 \rightarrow 15$
 $l = 0 \rightarrow 24$
 3 standard reflections monitored every 97 reflections
 intensity decay: 1.5%

Refinement

Refinement on F
 $R = 0.041$
 $wR = 0.043$
 914 reflections
 241 parameters
 All H-atom parameters refined isotropically, three grouped B factors

$w = 0.3537/[\sigma^2(F) + 0.0005F^2]$
 $(\Delta/\sigma)_{\text{max}} = 0.019$
 $\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$
 Extinction correction: none
 Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2) for (1)

$$U_{\text{eq}} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*a_i\cdot a_j.$$

	x	y	z	U_{eq}
O(1)	1.3948 (2)	-0.0386 (2)	0.3739 (1)	0.0324 (4)
O(2)	1.2912 (2)	0.3760 (2)	0.3997 (1)	0.0370 (5)
O(4)	0.9763 (2)	0.2271 (2)	0.3351 (1)	0.0257 (4)
O(5)	1.1822 (2)	0.0605 (2)	0.4350 (1)	0.0279 (4)
C(1)	1.3381 (2)	0.0953 (3)	0.4145 (2)	0.0273 (6)
C(2)	1.3437 (2)	0.2384 (3)	0.3612 (2)	0.0281 (6)
C(3)	1.2409 (3)	0.2100 (3)	0.2903 (2)	0.0272 (6)
C(4)	1.0906 (2)	0.1192 (2)	0.3064 (2)	0.0232 (5)
C(5)	1.1228 (2)	-0.0097 (3)	0.3652 (2)	0.0263 (5)
C(6)	1.2589 (3)	-0.1154 (3)	0.3412 (2)	0.0326 (6)
C(7)	1.4067 (3)	0.4481 (4)	0.4462 (2)	0.0475 (9)
C(8)	0.8188 (2)	0.1732 (3)	0.3290 (2)	0.0288 (6)
C(9)	0.7553 (2)	0.1730 (2)	0.2476 (1)	0.0215 (5)
C(10)	0.7986 (2)	0.2888 (2)	0.1955 (2)	0.0239 (5)
C(11)	0.7326 (3)	0.2924 (3)	0.1219 (2)	0.0294 (6)
C(12)	0.6247 (3)	0.1792 (3)	0.0993 (2)	0.0330 (6)
C(13)	0.5819 (3)	0.0633 (3)	0.1511 (2)	0.0341 (7)
C(14)	0.6471 (2)	0.0607 (3)	0.2247 (2)	0.0294 (6)

Table 2. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (2)
$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* a_i \cdot a_j$$

	x	y	z	U _{eq}
O(1)	0.5575 (6)	-0.5246 (3)	0.1007 (2)	0.044 (1)
O(4)	0.5852 (5)	-0.1724 (2)	0.0881 (2)	0.035 (1)
O(5)	0.3897 (5)	-0.3729 (3)	0.0539 (2)	0.035 (1)
N(1)	-0.0225 (8)	-0.0889 (4)	0.2846 (2)	0.052 (2)
C(1)	0.3936 (9)	-0.4434 (4)	0.1147 (3)	0.037 (2)
C(2)	0.4462 (8)	-0.3765 (4)	0.1811 (3)	0.030 (2)
C(3)	0.6696 (8)	-0.3236 (4)	0.1723 (3)	0.029 (2)
C(4)	0.7020 (8)	-0.2753 (4)	0.0975 (2)	0.029 (1)
C(5)	0.6158 (9)	-0.3553 (4)	0.0430 (3)	0.035 (2)
C(6)	0.7047 (10)	-0.4729 (4)	0.0510 (3)	0.041 (2)
C(7)	0.2648 (8)	-0.2931 (4)	0.1953 (3)	0.031 (2)
C(8)	0.7053 (10)	-0.0765 (4)	0.1093 (3)	0.036 (2)
C(9)	0.5621 (8)	0.0244 (4)	0.1032 (2)	0.032 (2)
C(10)	0.3691 (9)	0.0297 (4)	0.1400 (3)	0.036 (2)
C(11)	0.2425 (10)	0.1238 (4)	0.1368 (3)	0.043 (2)
C(12)	0.3061 (10)	0.2147 (4)	0.0974 (3)	0.045 (2)
C(13)	0.4970 (11)	0.2101 (4)	0.0596 (3)	0.043 (2)
C(14)	0.6246 (9)	0.1153 (4)	0.0625 (3)	0.035 (2)
C(15)	0.2946 (9)	-0.2292 (4)	0.2649 (3)	0.037 (2)
C(16)	0.1189 (9)	-0.1500 (4)	0.2775 (3)	0.036 (2)

Table 3. Bond lengths (Å) and angles (°)

	(1)	(2)
O(1)—C(1)	1.427 (3)	1.433 (6)
O(1)—C(6)	1.447 (3)	1.450 (6)
O(4)—C(4)	1.431 (2)	1.439 (5)
O(5)—C(1)	1.409 (3)	1.423 (6)
C(1)—C(2)	1.532 (3)	1.522 (7)
C(3)—C(4)	1.524 (3)	1.537 (6)
C(5)—C(6)	1.528 (3)	1.519 (7)
C(9)—C(10)	1.389 (3)	1.389 (7)
C(10)—C(11)	1.394 (3)	1.375 (7)
C(12)—C(13)	1.384 (4)	1.387 (8)
C(2)—C(7)	—	1.530 (7)
C(15)—C(16)	—	1.466 (7)
O(2)—C(2)	1.423 (3)	—
O(2)—C(7)	1.415 (3)	—
O(4)—C(8)	1.425 (2)	1.426 (6)
O(5)—C(5)	1.443 (3)	1.439 (6)
C(2)—C(3)	1.530 (3)	1.537 (7)
C(4)—C(5)	1.525 (3)	1.504 (7)
C(8)—C(9)	1.512 (3)	1.505 (7)
C(9)—C(14)	1.389 (3)	1.387 (6)
C(11)—C(12)	1.391 (3)	1.374 (7)
C(13)—C(14)	1.393 (4)	1.385 (7)
C(7)—C(15)	—	1.530 (7)
C(16)—N(1)	—	1.152 (6)
C(1)—O(1)—C(6)	106.5 (2)	106.3 (4)
C(4)—O(4)—C(8)	114.2 (2)	112.7 (3)
O(1)—C(1)—O(5)	106.0 (2)	105.3 (4)
O(5)—C(1)—C(2)	110.5 (2)	110.9 (3)
O(2)—C(2)—C(3)	109.1 (2)	—
C(2)—C(3)—C(4)	114.6 (2)	111.9 (4)
O(4)—C(4)—C(5)	110.7 (2)	106.1 (4)
O(5)—C(5)—C(4)	108.9 (2)	110.1 (4)
C(4)—C(5)—C(6)	112.4 (2)	113.0 (4)
O(4)—C(8)—C(9)	114.1 (2)	108.2 (4)
C(8)—C(9)—C(14)	120.4 (2)	120.3 (5)
C(9)—C(10)—C(11)	120.2 (2)	120.8 (5)
C(11)—C(12)—C(13)	119.3 (2)	119.5 (5)
C(9)—C(14)—C(13)	121.1 (2)	120.1 (5)
C(7)—C(15)—C(16)	—	111.8 (4)
C(2)—O(2)—C(7)	114.0 (2)	—
C(1)—O(5)—C(5)	102.0 (1)	100.7 (4)
O(1)—C(1)—C(2)	109.3 (2)	110.7 (4)
O(2)—C(2)—C(1)	111.4 (2)	—

C(1)—C(2)—C(3)	109.9 (2)	108.7 (4)
O(4)—C(4)—C(3)	108.1 (2)	111.6 (4)
C(3)—C(4)—C(5)	109.7 (2)	110.0 (4)
O(5)—C(5)—C(6)	101.9 (2)	101.9 (4)
O(1)—C(6)—C(5)	103.6 (2)	103.2 (4)
C(8)—C(9)—C(10)	120.7 (2)	120.8 (4)
C(10)—C(9)—C(14)	118.8 (2)	118.9 (5)
C(10)—C(11)—C(12)	120.6 (2)	120.4 (6)
C(12)—C(13)—C(14)	120.0 (2)	120.3 (5)
C(15)—C(7)—C(2)	—	112.7 (4)
C(15)—C(16)—N(1)	—	177.0 (5)

Table 4. Torsion angles (°)

	(1)*	(2)†
C(6)—O(1)—C(1)—O(5)	25.5	25.3
C(1)—O(1)—C(6)—C(5)	1.7	3.5
C(7)—O(2)—C(2)—C(3)	-156.9	—
C(8)—O(4)—C(4)—C(5)	-79.3	-152.1
C(5)—O(5)—C(1)—O(1)	-43.2	-44.7
C(1)—O(5)—C(5)—C(4)	-76.4	-74.6
C(2)—C(3)—C(4)—O(4)	82.0	74.5
O(4)—C(4)—C(5)—O(5)	-60.5	-60.3
C(3)—C(4)—C(5)—O(5)	58.7	60.6
O(5)—C(5)—C(6)—O(1)	-27.2	-30.4
O(4)—C(8)—C(9)—C(10)	-35.3	57.7
C(8)—C(9)—C(10)—C(11)	-176.4	177.3
O(1)—C(1)—C(2)—O(2)	-178.8	—
O(1)—C(1)—C(2)—C(7)	—	-178.5
O(2)—C(2)—C(3)—C(4)	-85.5	—
C(7)—C(2)—C(3)—C(4)	—	-80.1
C(3)—C(2)—C(7)—C(15)	—	-62.8
C(6)—O(1)—C(1)—C(2)	-93.6	-94.7
C(8)—O(4)—C(4)—C(3)	160.5	88.1
C(4)—O(4)—C(8)—C(9)	-72.6	-175.1
C(5)—O(5)—C(1)—C(2)	75.0	75.1
C(1)—O(5)—C(5)—C(6)	42.6	45.6
O(1)—C(1)—C(2)—C(3)	60.1	55.6
O(5)—C(1)—C(2)—C(3)	-56.1	-60.9
C(1)—C(2)—C(3)—C(4)	36.9	42.4
C(2)—C(3)—C(4)—C(5)	-38.8	-43.0
O(4)—C(4)—C(5)—C(6)	-172.7	-173.5
C(3)—C(4)—C(5)—C(6)	-53.5	-52.6
C(4)—C(5)—C(6)—O(1)	89.3	87.7
O(4)—C(8)—C(9)—C(14)	147.6	-124.5
O(5)—C(1)—C(2)—O(2)	64.9	—
O(5)—C(1)—C(2)—C(7)	—	64.9
C(7)—O(2)—C(2)—C(1)	81.6	—
C(1)—C(2)—C(7)—C(15)	—	174.9
C(2)—C(7)—C(15)—C(16)	—	-179.8
C(7)—C(15)—C(16)—N(1)	—	-5.8

* E.s.d. range: 0.1–0.3°.

† E.s.d. range: 0.3–0.6°.

Data were collected using graphite-monochromated radiation, stationary background. No crystal decomposition was noted. The structures were determined by direct methods. Full-matrix refinement (*SHELX76*; Sheldrick, 1976). Data processing was via Nicolet/*R3m* software (Siemens, 1983), *SHELXTL* (Sheldrick, 1984) and a local version of *ORTEPII* (Johnson, 1976). H and non-H atoms were refined with isotropic and anisotropic displacement parameters, respectively.

Lists of structure factors, anisotropic displacement parameters, least-squares-planes data, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: KH1035). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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4,6-Dimethoxy-3-methyl-1,3,5-triazin-2(3H)-one and 6-Methoxy-3,5-dimethyl-1,3,5-triazine-2,4(3H,5H)-dione

EIDIT HANDELSMAN-BENORY, MARK BOTOSHANSKY AND MENAHEM KAFTORY

Department of Chemistry, Technion-Israel Institute of Technology, Haifa 32000, Israel

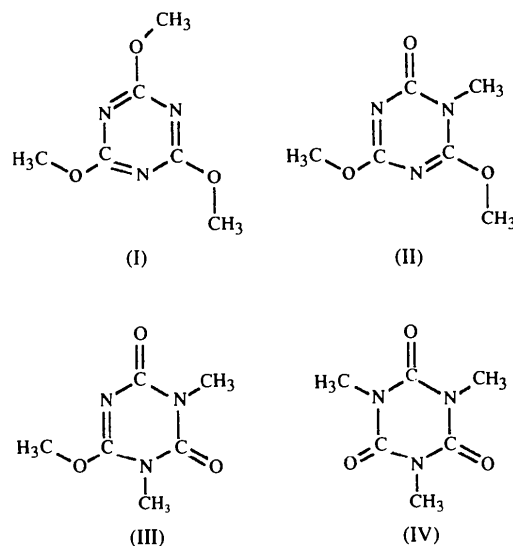
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Abstract

2,4,6-Trimethoxy-1,3,5-triazine, (I), undergoes methyl transfer in a few stages to 1,3,5-trimethyl-2,4,6-trioxohexahydro-*s*-triazine, (IV). The crystal structures of the two intermediates, 4,6-dimethoxy-3-methyl-1,3,5-triazin-2(3H)-one, (II) (C₆H₉N₃O₃), and 6-methoxy-3,5-dimethyl-1,3,5-triazine-2,4(3H,5H)-dione, (III) (C₆H₉N₃O₃), are described. Molecules of (II) form a layer structure made up of infinite ribbons. Molecules of (III) related by an inversion centre are arranged in pairs.

Comment

More than 120 years ago Hoffman & Olshausen (1870), and later Klason (1885), gathered evidence that alkyl derivatives of cyanuric acid and its thio analogues undergo alkyl migration. By the end of the 1960's the rearrangement of methyl groups in these systems had been investigated by Tosato and co-workers (Paolini, Tosato & Cignitti, 1968; Tosato, 1979, 1982, 1984). The lack of topochemical studies prompted us to study the crystal structures and the thermal behaviour of the four different compounds (I)–(IV) involved in the methyl rearrangement (Kaftory & Handelsman-Benory, 1994). The crystal structures of (I) (Glowka & Iwanicka, 1989) and (IV) (Belaj & Nachbaur, 1987) have been published; we describe here the crystal structures of (II) and (III).



In many aspects the crystal structure of (II) resembles the crystal structure of (I). However, the asymmetric unit of (II) consists of two independent molecules and there are pseudosymmetry elements such as an inversion centre and rotation/screw axis in the crystal structure. The possibility of a higher symmetric space group was eliminated after a careful check of the intensities. The relatively high *R* value (0.078) obtained for (III) is due to the instability of the crystal, for which the intensities decayed by 9.4% during the intensity measurements.

Both molecules (II) and (III) are planar and display bond lengths and angles comparable with those described for (I) and (IV). The most interesting structural feature of both compounds is their packing arrangement. The packing is strongly dependent on special intermolecular H₃CO...N(lone-pair electrons) interactions. This type of interaction effects the packing in the same way as hydrogen bonds. Compound (II) forms a planar ribbon structure consisting of molecules arranged in infinite trimers made up by interactions between lone-pair electrons of one molecule and