Absorption correction: $h = -11 \rightarrow 11$
  none $k = 0 \rightarrow 11$
2075 measured reflections $l = 0 \rightarrow 16$
1993 independent reflections 1 standard reflection
1361 observed reflections   frequency: 30 min
  $[I > 3\sigma(I)]$ intensity variation: $\pm 1.0\%$

Refinement

Refinement on F $(\Delta/\sigma)_{max} = 0.001$
$R = 0.053$ $\Delta\rho_{max} = 0.30$ e Å^{-3}
$wR = 0.059$ $\Delta\rho_{min} = -0.21$ e Å^{-3}
$S = 1.69$ Atomic scattering fac-
1361 reflections   tors from *SHELX*76
164 parameters   (Sheldrick, 1976)
$w = [\sigma^2(|F_o|) + 0.0006|F_o|^2]^{-1}$

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

$$B_{eq} = \tfrac{4}{3}\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
N(1)	0.4467 (3)	0.1739 (3)	0.1267 (2)	3.84 (9)
N(2)	0.2664 (3)	0.2795 (3)	0.3601 (2)	4.3 (1)
O(1)	0.4750 (2)	0.2108 (3)	0.3442 (2)	5.6 (1)
O(2)	0.1529 (2)	0.0485 (3)	0.2619 (2)	4.55 (8)
O(3)	0.2218 (2)	0.2385 (3)	0.1103 (2)	4.99 (9)
C(2)	0.3469 (3)	0.1995 (3)	0.3256 (2)	3.6 (1)
C(3)	0.2711 (3)	0.0805 (3)	0.2619 (2)	3.6 (1)
C(4)	0.3565 (4)	−0.1446 (4)	0.2373 (3)	4.8 (1)
C(5)	0.4402 (5)	−0.2364 (4)	0.2062 (3)	5.8 (1)
C(6)	0.5213 (4)	−0.1908 (5)	0.1486 (3)	5.6 (2)
C(7)	0.5216 (4)	−0.0553 (4)	0.1250 (3)	4.6 (1)
C(8)	0.4395 (3)	0.0386 (4)	0.1564 (2)	3.6 (1)
C(9)	0.3567 (3)	−0.0056 (3)	0.2154 (2)	3.6 (1)
C(10)	0.3394 (3)	0.2652 (4)	0.1023 (2)	3.8 (1)
C(11)	0.3712 (4)	0.3969 (4)	0.0643 (3)	5.0 (1)
C(12)	0.3256 (4)	0.3931 (4)	0.4256 (3)	4.5 (1)
C(13)	0.2808 (9)	0.5206 (6)	0.3764 (5)	14.5 (3)
C(14)	0.293 (1)	0.3835 (8)	0.5173 (5)	15.5 (4)

Table 2. *Geometric parameters* (Å, °)

N(1)—C(8)	1.405 (5)	C(4)—C(5)	1.384 (6)
N(1)—C(10)	1.354 (5)	C(4)—C(9)	1.403 (5)
N(2)—C(2)	1.314 (5)	C(5)—C(6)	1.380 (6)
N(2)—C(12)	1.459 (5)	C(6)—C(7)	1.376 (6)
O(1)—C(2)	1.219 (4)	C(7)—C(8)	1.389 (5)
O(2)—C(3)	1.211 (4)	C(8)—C(9)	1.404 (5)
O(3)—C(10)	1.231 (4)	C(10)—C(11)	1.474 (5)
C(2)—C(3)	1.530 (5)	C(12)—C(13)	1.440 (7)
C(3)—C(9)	1.485 (5)	C(12)—C(14)	1.433 (9)
C(8)—N(1)—C(10)	126.8 (3)	N(1)—C(8)—C(7)	116.6 (3)
C(2)—N(2)—C(12)	121.6 (3)	N(1)—C(8)—C(9)	124.3 (3)
N(2)—C(2)—O(1)	124.9 (3)	C(7)—C(8)—C(9)	119.1 (3)
N(2)—C(2)—C(3)	115.7 (3)	C(3)—C(9)—C(4)	114.8 (3)
O(1)—C(2)—C(3)	119.4 (3)	C(3)—C(9)—C(8)	126.9 (3)
O(2)—C(3)—C(2)	120.1 (3)	C(4)—C(9)—C(8)	118.3 (3)
O(2)—C(3)—C(9)	122.1 (3)	N(1)—C(10)—O(3)	121.6 (3)
C(2)—C(3)—C(9)	117.1 (3)	N(1)—C(10)—C(11)	116.1 (3)
C(5)—C(4)—C(9)	121.7 (4)	O(3)—C(10)—C(11)	122.2 (3)
C(4)—C(5)—C(6)	119.0 (4)	N(2)—C(12)—C(13)	110.8 (4)
C(5)—C(6)—C(7)	120.2 (4)	N(2)—C(12)—C(14)	111.7 (4)
C(6)—C(7)—C(8)	121.6 (4)	C(13)—C(12)—C(14)	112.1 (5)

Data were corrected for Lorentz and polarization. The structure was solved by direct methods. H atoms were found in difference synthesis and included as fixed contributors with an overall isotropic temperature factor that refined to $U_{iso} = 0.137$ (5) Å^2. Programs used were: *SHELXS*86 (Sheldrick, 1985), *SHELX*76 (Sheldrick, 1976) and *ORTEP* (Johnson, 1965). The refinement

was by full-matrix least-squares methods. Most of the calculations were performed on a VAX 6420 computer at the Instituto de Fisica e Química de São Carlos.

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Structure of Two 1,3,5-Substituted 2-Pyrazolines, $C_{20}H_{18}N_2O_5$ and $C_{20}H_{20}N_2O_5$

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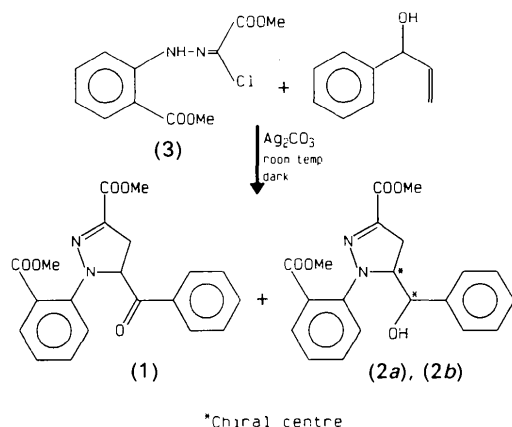
Abstract

The structures of methyl 5-benzoyl-1-(2-methoxycarbonylphenyl)-2-pyrazoline-3-carboxylate (1) and methyl (±)-5-(α-hydroxybenzyl)-1-(2-methoxycarbonylphenyl)-2-pyrazoline-3-carboxylate (2a) are compared. In (1), there is an extensive conjugation involving the N—N=C chain of the pyrazoline ring and the phenyl and carboxy groups bonded at N1 and C3, respectively. In (2a), the presence of a strong hydrogen bond between the hydroxyl group and the methoxycarbonylphenyl group causes the rotation of the latter with respect to the pyrazoline ring by 47°, with a partial loss of conjugation and with the elongation of the N1–phenyl bond.

Comment

Continuing a series of 1,3-dipolar cycloaddition reactions, Garanti (1993) added the chlorhydrazone (3) and Ag_2CO_3 (to generate the corresponding nitrilimmine) to 1-phenyl-2-propen-1-ol, at room temperature in the dark, and obtained three products. The compounds (2a) and (2b) were easily identified as the two expected diastereoisomers, while the recognition of (1) was less obvious; *a posteriori*, the oxidation of (2a) and (2b) to give (1) by means of Ag^+ seems quite reasonable. The present structural study was undertaken to elucidate the structure of (1) and to assign the correct configuration of (2a) and (2b). Because of the smallness of the crystals of (2b), only data for (2a) were collected. Nevertheless, the similarity between the ^{1}H NMR spectra of (2a) and (2b) makes us confident that these compounds are really diastereoisomers.

The presence of the aforementioned intramolecular hydrogen bond in (2a) gives rise to some differences between the common parts of the two structures. In particular, the phenyl group bonded to N1, the carboxy group bonded to C3 and atoms N1, N2 and C3 in (1) are quite coplanar [the maximum deviation being 0.133 (2) Å for C9]; this favours an extensive conjugation of the whole π system. To the contrary, in (2a) the phenyl group is greatly rotated with respect to the pyrazoline plane, the dihedral angle between the two groups being 47.03 (5)°; as a consequence, the conjugation is partially broken at the N1—C6 bond, which is 0.018 Å longer in (2a) than in (1). As mentioned, the carboxy group and the pyrazoline ring are approximately coplanar but with opposite configurations; in fact, the double bonds N2=C3 and C16=O19
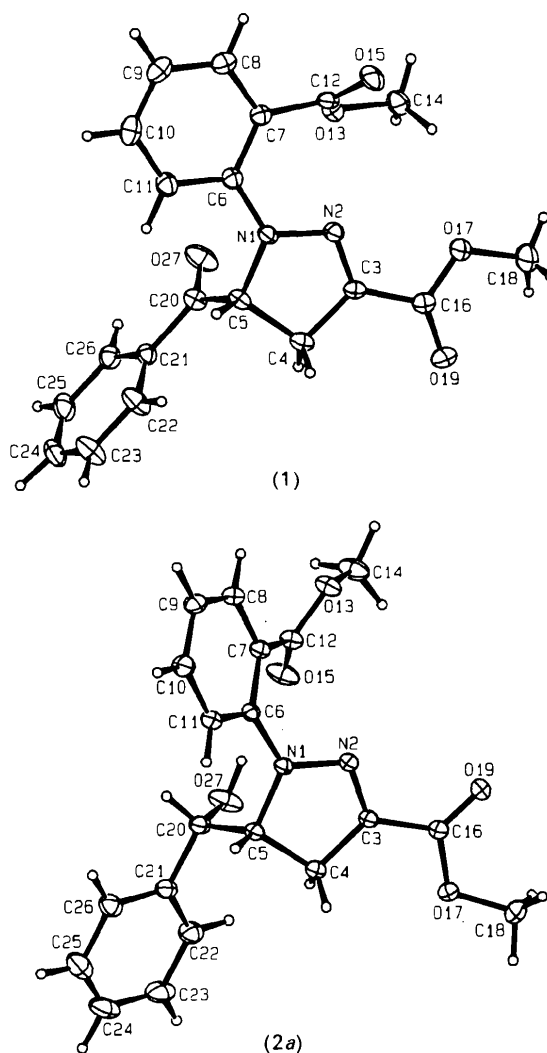

(3)

(1)   (2a), (2b)

*Chiral centre

In spite of the presence of a hydroxyl group, the elution rate for (2a) is higher than for (1) (R_f = 0.15 *versus* 0.06); this can be explained by the fact that the hydroxyl group is engaged in a hydrogen bond [O27···O15 2.834 (1) Å, O27—H27···O15 172 (2)°] that is probably preserved in solution; at the same time, the low elution rate for (2b) (R_f = 0.05) indicates that in this molecule, probably for steric reasons, there is no intramolecular hydrogen bonding and that the hydroxyl group can easily interact with the silica of the chromatographic column.

Bond distances of both structures compare well with literature values (see, for example, Allen, Kennard, Watson, Brammer, Orpen & Taylor, 1987). The conformation of the pyrazoline ring in (2a) is quite planar; in fact, the modulus of the maximum torsion angle, φ_{max}, along the perimeter is 1.5 (2)° and the maximum deviation from the least-squares plane through the ring is only 0.008 (2) Å. The same ring in (1) is much more twisted; φ_{max} is 7.0 (1)°. This value is comparable with that found in the β form of 1,3-diphenyl-5-(p-chlorophenyl)-pyrazoline (φ_{max} = 8.0°; Kimura, Kai, Yasuoka & Kasai, 1977) but less than that found for the α form of the same compound (φ_{max} = 14.6°; Kimura *et al.*, 1977).

Fig. 1. *ORTEPII* plot of the two molecules with the numbering scheme of the non-H atoms. Thermal ellipsoids are drawn at the 20% probability level. H atoms are represented as circles of arbitrary size.

are *anti* in (1) and *syn* in (2a). Also, the conformation of the methoxycarbonyl group bound to phenyl is very different in the two structures, the torsion angle C6—C7—C12—O15 being $-118.6\,(2)$ and $38.8\,(2)°$ in (1) and (2a), respectively.

Crystal packing of both structures is ruled only by residual forces and weak hydrogen bonds.

Experimental

Compound (1)

Crystal data

$C_{20}H_{18}N_2O_5$
$M_r = 366.37$
Triclinic
$P\bar{1}$
$a = 8.634\,(1)$ Å
$b = 10.310\,(1)$ Å
$c = 10.493\,(1)$ Å
$\alpha = 84.15\,(1)°$
$\beta = 81.32\,(1)°$
$\gamma = 76.41\,(1)°$
$V = 895.4\,(2)$ Å³
$Z = 2$
$D_x = 1.359$ Mg m⁻³

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 12.1\text{-}17.8°$
$\mu = 0.0924$ mm⁻¹
Room temperature
Prism
$0.34 \times 0.34 \times 0.28$ mm
Pale yellow
Crystal source: chemical synthesis (Garanti, 1993)

Data collection

Enraf-Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
3149 measured reflections
3149 independent reflections
2548 observed reflections
$[I_o > 2\sigma(I_o)]$

$\theta_{max} = 25°$
$h = 0 \rightarrow 9$
$k = -11 \rightarrow 12$
$l = -12 \rightarrow 12$
1 standard reflection frequency: 180 min intensity variation: none

Refinement

Refinement on F
$R = 0.035$
$wR = 0.042$
$S = 2.261$
2548 reflections
317 parameters
All H-atom parameters refined
$w = 2F_o\text{Lp}/[\sigma(I_o)^2 + (0.02I_o)^2]^{1/2}$
$(\Delta/\sigma)_{max} = 0.11$

$\Delta\rho_{max} = 0.13$ e Å⁻³
$\Delta\rho_{min} = -0.10$ e Å⁻³
Extinction correction: Stout & Jensen (1968)
Extinction coefficient: $3.9\,(2) \times 10^{-6}$
Atomic scattering factors from *International Tables for X-ray Crystallography* [1974, Vol. IV, Tables 2.2A, 2.3.1 (O, N, C); 2.2C (H)]

Compound (2a)

Crystal data

$C_{20}H_{20}N_2O_5$
$M_r = 368.39$
Monoclinic
$C2/c$

Cell parameters from 25 reflections
$\theta = 10.3\text{-}16.8°$
$\mu = 0.0907$ mm⁻¹

$a = 28.960\,(3)$ Å
$b = 7.984\,(1)$ Å
$c = 18.388\,(2)$ Å
$\beta = 120.55\,(1)°$
$V = 3661.4\,(8)$ Å³
$Z = 8$
$D_x = 1.337$ Mg m⁻³
Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Room temperature
Prism
$0.34 \times 0.28 \times 0.18$ mm
Yellow-orange, strongly dichroic
Crystal source: chemical synthesis (Garanti, 1993)

Data collection

Enraf-Nonius CAD-4 diffractometer
$\theta/2\theta$ scans
Absorption correction: none
3223 measured reflections
3223 independent reflections
2461 observed reflections
$[I_o > 2\sigma(I_o)]$

$\theta_{max} = 25°$
$h = -34 \rightarrow 34$
$k = 0 \rightarrow 9$
$l = 0 \rightarrow 21$
1 standard reflection frequency: 180 min intensity variation: none

Refinement

Refinement on F
$R = 0.035$
$wR = 0.036$
$S = 1.818$
2461 reflections
325 parameters
All H-atom parameters refined
$w = 2F_o\text{Lp}/[\sigma(I_o)^2 + (0.02I_o)^2]^{1/2}$
$(\Delta/\sigma)_{max} = 0.03$

$\Delta\rho_{max} = 0.014$ e Å⁻³
$\Delta\rho_{min} = -0.011$ e Å⁻³
Extinction correction: Stout & Jensen (1968)
Extinction coefficient: $5.6\,(7) \times 10^{-7}$
Atomic scattering factors from *International Tables for X-ray Crystallography* [1974, Vol. IV, Tables 2.2A, 2.3.1 (O, N, C); 2.2C (H)]

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å²) *for compound* (2a)

$$U_{eq} = \tfrac{1}{3}\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
O13	0.1838 (1)	0.29896 (9)	0.03049 (9)	0.0483 (3)
O15	0.2934 (1)	0.1370 (1)	−0.1039 (1)	0.0610 (4)
O17	−0.1214 (1)	0.3946 (1)	−0.2178 (1)	0.0648 (4)
O19	−0.3898 (1)	0.4335 (1)	−0.1784 (1)	0.0680 (4)
O27	−0.2124 (1)	0.3204 (1)	0.3031 (1)	0.0788 (4)
N1	−0.1150 (1)	0.1545 (1)	0.1082 (1)	0.0435 (3)
N2	−0.0973 (1)	0.2253 (1)	−0.0070 (1)	0.0401 (3)
C3	−0.2372 (2)	0.2873 (1)	−0.0344 (1)	0.0414 (4)
C4	−0.3735 (2)	0.2616 (1)	0.0637 (1)	0.0499 (5)
C5	−0.2824 (2)	0.1763 (1)	0.1699 (1)	0.0433 (5)
C6	0.0169 (2)	0.0786 (1)	0.1629 (1)	0.0413 (4)
C7	0.1755 (2)	0.0801 (1)	0.1085 (1)	0.0409 (4)
C8	0.3013 (2)	−0.0073 (2)	0.1621 (1)	0.0528 (5)
C9	0.2748 (2)	−0.0904 (2)	0.2704 (2)	0.0634 (6)
C10	0.1190 (2)	−0.0873 (2)	0.3264 (2)	0.0643 (6)
C11	−0.0087 (2)	−0.0052 (1)	0.2732 (1)	0.0540 (5)
C12	0.2210 (1)	0.1726 (1)	−0.0016 (1)	0.0423 (4)
C14	0.2098 (2)	0.3977 (2)	−0.0738 (2)	0.0585 (5)
C16	−0.2590 (2)	0.3778 (1)	−0.1505 (1)	0.0483 (5)
C18	−0.1339 (2)	0.4932 (1)	−0.3267 (2)	0.1017 (8)
C20	−0.3062 (2)	0.2539 (1)	0.2907 (1)	0.0480 (4)
C21	−0.4503 (2)	0.2496 (1)	0.3875 (1)	0.0423 (4)
C22	−0.5569 (2)	0.1714 (2)	0.3792 (2)	0.0691 (6)
C23	−0.6887 (2)	0.1721 (2)	0.4722 (2)	0.0799 (7)
C24	−0.7150 (2)	0.2497 (2)	0.5738 (2)	0.0655 (6)
C25	−0.6113 (2)	0.3282 (2)	0.5833 (1)	0.0638 (6)
C26	−0.4790 (2)	0.3283 (2)	0.4915 (1)	0.0528 (5)

Table 2. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *for compound* (2a)

$$U_{\text{eq}} = \tfrac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j.$$

	x	y	z	U_{eq}
O13	0.26412 (3)	0.0909 (1)	0.10907 (6)	0.0527 (3)
O15	0.35304 (4)	0.0766 (2)	0.18216 (6)	0.0665 (4)
O17	0.43736 (4)	0.7242 (1)	0.18797 (6)	0.0536 (3)
O19	0.35191 (4)	0.6521 (2)	0.09910 (7)	0.0693 (4)
O27	0.46132 (4)	0.1365 (2)	0.30774 (7)	0.0709 (5)
N1	0.38070 (4)	0.3531 (2)	0.30264 (6)	0.0388 (4)
N2	0.36267 (4)	0.4391 (2)	0.22953 (6)	0.0375 (4)
C3	0.40191 (5)	0.5237 (2)	0.23404 (8)	0.0373 (5)
C4	0.45400 (5)	0.5009 (2)	0.31541 (8)	0.0459 (6)
C5	0.43856 (5)	0.3773 (2)	0.36341 (8)	0.0370 (6)
C6	0.34428 (4)	0.2616 (2)	0.31621 (7)	0.0337 (5)
C7	0.30666 (5)	0.1552 (2)	0.25318 (8)	0.0370 (5)
C8	0.26743 (5)	0.0809 (2)	0.26480 (9)	0.0465 (5)
C9	0.26693 (5)	0.1032 (2)	0.33853 (9)	0.0525 (6)
C10	0.30591 (5)	0.2007 (2)	0.40194 (8)	0.0504 (6)
C11	0.34394 (5)	0.2812 (2)	0.39050 (8)	0.0416 (5)
C12	0.31148 (5)	0.1072 (2)	0.17946 (8)	0.0440 (5)
C14	0.26550 (6)	0.0243 (3)	0.03675 (9)	0.0675 (6)
C16	0.39280 (5)	0.6370 (2)	0.16533 (8)	0.0435 (5)
C18	0.43452 (6)	0.8489 (2)	0.1294 (1)	0.0627 (6)
C20	0.46699 (5)	0.2073 (2)	0.38216 (8)	0.0437 (5)
C21	0.52604 (5)	0.2218 (2)	0.44692 (9)	0.0464 (6)
C22	0.56362 (6)	0.2597 (2)	0.4238 (1)	0.0607 (6)
C23	0.61709 (6)	0.2762 (3)	0.4840 (1)	0.0798 (9)
C24	0.63428 (7)	0.2512 (2)	0.5677 (1)	0.0835 (10)
C25	0.59808 (7)	0.2118 (3)	0.5919 (1)	0.0771 (9)
C26	0.54353 (6)	0.1976 (2)	0.5311 (1)	0.0580 (7)

Table 3. *Comparison of selected bond distances* (Å) *and angles* (°) *in compounds* (1) *and* (2a)

	(1)	(2a)
O13—C12	1.332 (1)	1.330 (1)
O13—C14	1.446 (2)	1.452 (2)
O15—C12	1.203 (1)	1.204 (2)
O17—C16	1.326 (1)	1.333 (1)
O17—C18	1.449 (2)	1.438 (2)
O19—C16	1.205 (1)	1.197 (1)
O27—C20	1.206 (2)	1.411 (2)
N1—N2	1.354 (1)	1.356 (1)
N1—C5	1.467 (1)	1.480 (1)
N1—C6	1.388 (1)	1.406 (2)
N2—C3	1.286 (1)	1.288 (2)
C3—C4	1.497 (2)	1.501 (1)
C3—C16	1.465 (1)	1.465 (2)
C4—C5	1.541 (1)	1.534 (2)
C5—C20	1.530 (1)	1.533 (2)
C7—C12	1.488 (1)	1.482 (2)
C20—C21	1.489 (2)	1.512 (1)
C12—O13—C14	115.6 (1)	115.6 (1)
C16—O17—C18	116.2 (1)	116.7 (1)
C5—N1—C6	125.3 (1)	126.7 (1)
N2—N1—C6	121.4 (1)	119.6 (1)
N2—N1—C5	113.1 (1)	113.6 (1)
N1—N2—C3	108.7 (1)	108.6 (1)
N2—C3—C16	122.2 (1)	120.2 (1)
N2—C3—C4	114.3 (1)	114.0 (1)
C4—C3—C16	123.4 (1)	125.7 (1)
C3—C4—C5	101.3 (1)	102.3 (1)
N1—C5—C4	102.0 (1)	101.5 (1)
C4—C5—C20	110.6 (1)	114.7 (1)
N1—C5—C20	110.9 (1)	109.1 (1)
O15—C12—C7	124.3 (1)	124.9 (1)
O13—C12—C7	111.6 (1)	112.7 (1)
O13—C12—O15	123.8 (1)	122.3 (1)
O19—C16—C3	122.5 (2)	126.2 (2)
O17—C16—C3	113.2 (1)	109.4 (1)
O17—C16—O19	124.3 (1)	124.4 (2)
O27—C20—C5	119.8 (1)	110.6 (1)
C5—C20—C21	118.4 (1)	111.9 (1)
O27—C20—C21	121.8 (1)	108.8 (1)

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71465 (44 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: NA1050]

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N-Methylnitrilotriacetamide, C7H14N4O3

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Abstract

The title compound is one of the possible chelating ligands used in our study of metal complexes with the various derivatives of amidated nitrilotriacetic acid. The molecules form a three-dimensional hydrogen-bonding