Table 2. *Selected geometric parameters* (Å, °)

	(I)	(II)
C(1)—C(2)	1.392 (5)	1.385 (14)
C(2)—C(3)	1.373 (6)	1.396 (14)
C(3)—C(4)	1.373 (6)	1.366 (14)
C(4)—C(5)	1.388 (5)	1.379 (14)
C(5)—C(6)	1.382 (5)	1.407 (14)
C(6)—C(1)	1.387 (5)	1.399 (13)
C(7)—C(6)	1.497 (5)	1.482 (14)
C(7)—N(1)	1.332 (5)	1.315 (13)
C(7)—O(7)	1.232 (4)	1.244 (11)
C(8)—N(1)	1.468 (5)	1.465 (13)
C(8)—C(9)	1.525 (5)	1.501 (14)
C(9)—C(10)	1.496 (5)	1.490 (14)
C(10)—C(11)	-	1.535 (14)
C(11)—C(12)	-	1.537 (14)
C(12)—C(13)	-	1.490 (14)
C(10)—O(101)	1.201 (5)	-
C(10)—O(102)	1.319 (4)	-
C(13)—O(131)	-	1.189 (12)
C(13)—O(132)	-	1.327 (13)
N(2)—C(3)	-	1.473 (13)
N(2)—O(21)	-	1.221 (11)
N(2)—O(22)	-	1.206 (12)
C(8)—N(1)—C(7)	121.7 (3)	122.2 (9)
C(7)—C(6)—C(1)	121.4 (3)	123.3 (10)
C(6)—C(1)—C(2)	119.6 (3)	120.6 (10)
C(5)—C(6)—C(7)	118.9 (3)	117.6 (9)
C(3)—C(2)—C(1)	119.7 (3)	117.7 (9)
C(2)—C(3)—C(4)	120.3 (3)	123.5 (10)
C(3)—C(4)—C(5)	120.1 (3)	118.2 (10)
C(6)—C(5)—C(4)	120.1 (4)	120.9 (9)
C(5)—C(6)—C(1)	120.2 (3)	119.0 (9)
O(7)—C(7)—C(6)	120.2 (3)	120.3 (10)
N(1)—C(7)—C(6)	116.8 (3)	117.7 (9)
N(1)—C(7)—O(7)	123.1 (3)	122.0 (10)
C(9)—C(8)—N(1)	110.1 (3)	110.9 (9)
C(10)—C(9)—C(8)	113.8 (3)	114.0 (9)
C(9)—C(10)—C(11)	-	112.5 (9)
C(10)—C(11)—C(12)	-	113.8 (9)
C(11)—C(12)—C(13)	-	111.4 (8)
O(102)—C(10)—C(9)	113.5 (3)	-
O(101)—C(10)—C(9)	124.3 (3)	-
O(101)—C(10)—O(102)	122.2 (3)	-
O(131)—C(13)—O(132)	-	120.2 (10)
C(12)—C(13)—O(132)	-	115.2 (9)
C(12)—C(13)—O(131)	-	124.5 (10)
C(4)—C(3)—N(2)	-	118.6 (10)
C(2)—C(3)—N(2)	-	117.8 (9)
O(21)—N(2)—C(3)	-	118.2 (9)
O(22)—N(2)—C(3)	-	118.6 (9)
O(22)—N(2)—O(21)	-	123.2 (10)

Standard reflections were recentred every 100 reflections and scanned every hour to check for crystal movement and stability. The structures were solved by direct methods using *SHELXS*86 (Sheldrick, 1985) and refined by full-matrix least-squares analysis using *SHELX*76 (Sheldrick, 1976). For (I), the amino and carboxylic H-atom coordinates were located from a difference Fourier synthesis and refined with isotropic displacement parameters; ring and alkyl H atoms were fixed geometrically and refined with isotropic displacement parameters. For (II), the ring, alkyl and amino H atoms were fixed geometrically and refined with isotropic displacement parameters. The carboxylic H atom could not be located. All non-H atoms were refined with anisotropic displacement parameters. For (II), only very thin needles were obtained. As a result the data set was weak with an associated high *R* factor for the final solution.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71730 (26 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HU1017]

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6-Oxo-6-(phenylamino)hexanoic Acid [Two Polymorphic Forms, (I) and (II)] and 4-Oxo-4-(*N*-methylphenylamino)-butanoic Acid (III)

N. Feeder and W. Jones*

Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England

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Abstract

Two polymorphs of 6-oxo-6-(phenylamino)hexanoic acid, $C_{12}H_{15}NO_3$, have been observed. In the first, (I), intermolecular hydrogen bonds form ribbons of molecules, while in the second, (II), a more planar molecular conformation allows the hydrogen bonding to extend to form sheets. The structure of (III), $C_{11}H_{13}NO_3$, is also presented and, as a result of the *N*-methyl substitution, hydrogen bonding is restricted to the formation of carboxylic acid dimers.

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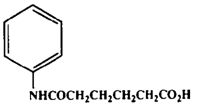
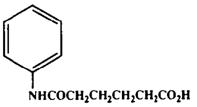
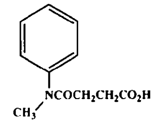
Comment

As part of a general study of the stability of organic peracids and peracid salts (Kariuki & Jones, 1990) and in particular of the role of hydrogen bonding in controlling the crystal structure of peracid and acid amides (Feeder & Jones, 1992), we report here upon two phenylamino carboxylic acids. In the case of 6-oxo-6-(phenylamino)hexanoic acid we have identified two polymorphic forms, (I) and (II), while for 4-oxo-4-(*N*-methylphenylamino)butanoic acid only one, (III), has been observed.


(I)


(II)


(III)

The bond angles and distances found for (I), (II) and (III) are consistent with those observed in *p*-acetanisidide (Haisa, Kashino, Ueno, Shinozaki & Matsuzaki, 1980) and *p*-acetamidobenzoic acid (Kashino, Matsushita, Iwamoto, Yamaguchi & Haisa, 1986). The two C—O bond distances of the carboxyl group in (II) are only just significantly different (5σ), suggesting a partially disordered model. This is uncommon among aliphatic acids (Leiserowitz, 1976). No such disorder is seen in (I) and (III). The bond angles and distances specific to the alkyl chain are similar to those found in 6-(6-aminophenylhexanamido)hexanoic acid monohydrate (Kasai, Yamanaka, Miki, Tanaka, Post & Morawetz, 1981) and 6-aminocaproic acid (Bodor, Bednowitz & Post, 1976).

The molecular geometries of (I) and (II) are such that the benzene rings (*A*) are planar to within 0.004 and 0.014 Å, respectively, and the atoms which represent the amide groups [C(1)N(1)C(7)O(7)C(8)] (*B*) are also planar (to within 0.040 and 0.005 Å, respectively). The dihedral angles are 140.2 for *A*(I)*B*(I) and 21.9° for *A*(II)*B*(II). In (I), the carboxyl group is not planar and the OCOH torsion angle is −13.7°. The OCO group (moiety *C*) makes angles of 119.9 and 21.8° with *A*(I) and *B*(I), respectively, and 32.8 and 11.1° with *A*(II) and *B*(II), respectively. For (III), the molecular geometry is such that the benzene ring *A*(III), the *N*-methyl amide group [C(1)N(1)C(7)O(8)C(8)C(9)] *B*(III), and the carboxyl group *C*(III) are planar to within 0.003, 0.032 and 0.006 Å, respectively. The dihedral angles are 81.5 for *A*(III)*B*(III), 149.6 for *A*(III)*C*(III) and 78.6° for *B*(III)*C*III).

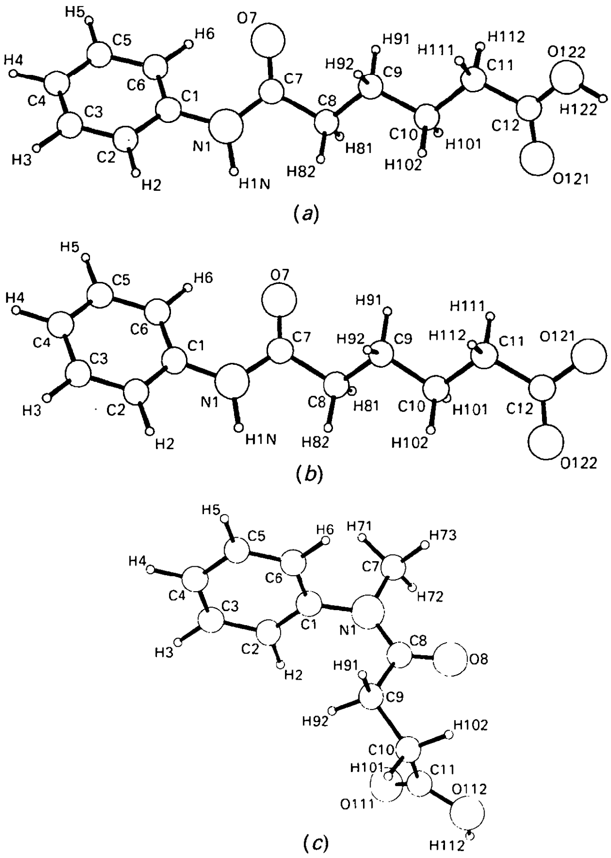


Fig. 1. Atom-numbering scheme for (*a*) (I), (*b*) (II) and (*c*) (III).

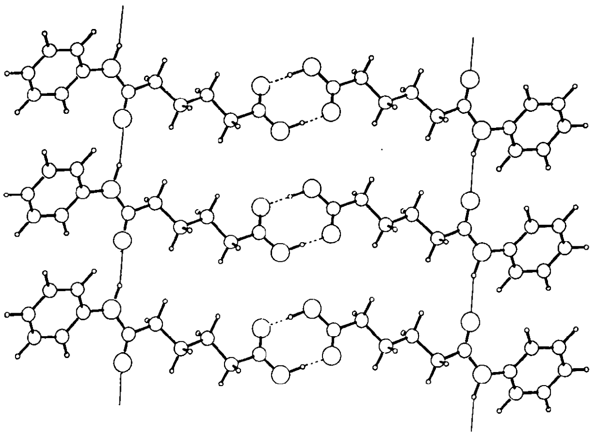


Fig. 2. The ribbon-like structure formed as result of hydrogen bonding in (I), viewed down the *a* axis.

Fig. 2 is a *PLUTO* (Motherwell & Clegg, 1978) plot of (I) illustrating the intermolecular hydrogen bonding. There are two types of hydrogen bond. The first is formed between two carboxyl groups producing a centrosymmetric ring dimer (O—H···O=C 1.583, O···O=C 2.639 Å). This motif is commonly observed for carboxylic acids (Kashino & Haisa, 1980). These dimers are then related by translation along the *b* axis by secondary hydrogen bonding through linear amide–amide contacts (N—H···O=C 1.948, N···O=C 2.988 Å). In this way a ribbon-type structure is produced. This is a very similar arrangement to that seen in one of the polymorphic forms identified for *p*-amidobenzoic acid derivatives (Feeder & Jones, 1993). The dihedral angle for *A*(I)*B*(I) is typical of this mode of hydrogen bonding in aromatic amides (Haisa, Kashino, Ueno, Shinozaki & Matsuzaki, 1980), especially when the amido group is large (Cohen-Addad, 1973). The ribbons interact along the *c* axis, in part through short intermolecular C—H···O contacts, to form 'blocks'. These blocks are then linked along the *a* axis by weak van der Waals interactions through the phenyl groups.

Fig. 3 indicates that the hydrogen bonding in the orthorhombic form (II) results in the formation of sheets rather than ribbons. The carboxylic acid dimers are retained (O···O=C 2.606 Å), as are the linear amide–amide interactions (N—H···O=C 1.838, N···O=C 2.887 Å); however, this time they are between dimers related by a twofold screw operation. These sheets are then stacked along the *a* axis, related by a twofold screw operation.

Fig. 4 shows the packing arrangement for (III) and illustrates the hydrogen-bonding pattern. The carboxyl groups are hydrogen bonded to form centrosymmetric ring dimers (O—H···C=O 1.617, O···C=O 2.616 Å), which are stacked along the *a* axis. Stacks related by a translation along the *b* axis are linked through a van der Waals surface, forming a corrugated sheet.

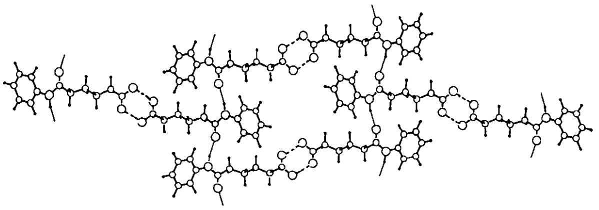


Fig. 3. The sheet-like structure formed as result of hydrogen bonding in (II), viewed down the *a* axis.

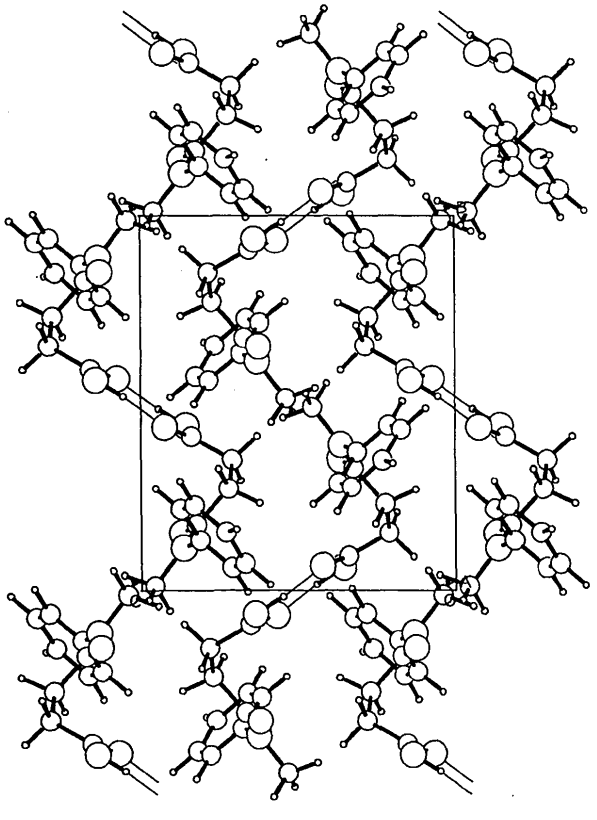


Fig. 4. Packing diagram for (III), viewed down the *a* axis.

Experimental

Crystals of (I) were obtained during the attempted crystallization of the corresponding peracid from ethanol. Crystals of (II) were found in a sample of the corresponding peracid supplied by Solvay Interox PLC. Crystals of (III) were obtained from a sample supplied by Solvay Interox PLC.

Compound (I)

Crystal data

$C_{12}H_{15}NO_3$
$M_r = 221.12$
Monoclinic
$P2_1/c$
$a = 17.198$ (4) Å
$b = 5.140$ (5) Å
$c = 12.976$ (4) Å
$\beta = 96.76$ (2)°
$V = 1139$ Å^3
$Z = 4$
$D_x = 1.29$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71069$ Å
Cell parameters from 25 reflections
$\theta = 8$-$14°$
$\mu = 0.056$ mm^{-1}
$T = 295$ K
Plate-like
0.4 × 0.3 × 0.1 mm
White, transparent

Data collection

Enraf–Nonius CAD-4 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3504 measured reflections
3074 independent reflections
1464 observed reflections [$F > 3\sigma(F)$]

$R_{\rm int} = 0.027$
$\theta_{\rm max} = 25°$
$h = -18 \rightarrow 18$
$k = 0 \rightarrow 7$
$l = 0 \rightarrow 24$
2 standard reflections
frequency: 60 min
intensity variation: none

Refinement

Refinement on F
$R = 0.055$
$wR = 0.055$
$S = 0.821$
1464 reflections
155 parameters
Unit weights applied
$(\Delta/\sigma)_{\rm max} = 0.327$

$\Delta\rho_{\rm max} = 0.25$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (II)

Crystal data

$C_{12}H_{15}NO_3$
M_r = 221.12
Orthorhombic
Pcab
a = 24.220 (9) Å
b = 9.675 (6) Å
c = 10.094 (6) Å
V = 2365 Å^3
Z = 8
D_x = 1.24 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 8-13°
μ = 0.054 mm^{-1}
T = 295 K
Rods
0.2 × 0.2 × 0.2 mm
White, transparent

Data collection

Enraf-Nonius CAD-4 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: none
4186 measured reflections
1843 independent reflections
971 observed reflections [$F > 3\sigma(F)$]

$R_{\rm int}$ = 0.045
$\theta_{\rm max}$ = 25°
$h = 0 \rightarrow 28$
$k = 0 \rightarrow 11$
$l = 0 \rightarrow -11$
2 standard reflections
frequency: 60 min
intensity variation: none

Refinement

Refinement on F
R = 0.078
wR = 0.078
S = 0.922
971 reflections
151 parameters
Unit weights applied
$(\Delta/\sigma)_{\rm max}$ = 0.009

$\Delta\rho_{\rm max}$ = 0.26 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.30 e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Compound (III)

Crystal data

$C_{11}H_{13}NO_3$
M_r = 207.2
Monoclinic
$P2_1/c$
a = 9.604 (1) Å
b = 11.457 (2) Å
c = 9.908 (3) Å
β = 96.58 (2)°
V = 1083 Å^3
Z = 4

D_x = 1.258 Mg m^{-3}
Mo $K\alpha$ radiation
λ = 0.71069 Å
Cell parameters from 25 reflections
θ = 11-15°
μ = 0.056 mm^{-1}
T = 295 K
Plate-like
0.4 × 0.3 × 0.2 mm
White

Data collection

Enraf-Nonius CAD-4 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: none
3308 measured reflections
3141 independent reflections
1318 observed reflections [$F > 3\sigma(F)$]

$R_{\rm int}$ = 0.014
$\theta_{\rm max}$ = 30°
$h = -13 \rightarrow 13$
$k = 0 \rightarrow 16$
$l = 0 \rightarrow 13$
2 standard reflections
frequency: 60 min
intensity variation: none

Refinement

Refinement on F
R = 0.060
wR = 0.060
S = 0.798
1318 reflections
144 parameters
Unit weights applied
$(\Delta/\sigma)_{\rm max}$ = 0.059

$\Delta\rho_{\rm max}$ = 0.33 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.22 e Å^{-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* (Å^2)

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

	x	y	z	$U_{\rm eq}$
(I)				
N(1)	0.7077 (2)	−0.2766 (5)	0.8757 (2)	0.046
O(7)	0.7234 (2)	0.1518 (4)	0.9144 (2)	0.059
O(121)	0.9713 (2)	−0.1133 (5)	1.3812 (2)	0.075
O(122)	0.9444 (2)	0.2677 (6)	1.4466 (2)	0.077
C(1)	0.6565 (2)	−0.2561 (6)	0.7817 (2)	0.044
C(2)	0.5987 (2)	−0.4419 (7)	0.7619 (3)	0.056
C(3)	0.5501 (2)	−0.4353 (8)	0.6686 (3)	0.070
C(4)	0.5597 (2)	−0.2455 (8)	0.5963 (3)	0.068
C(5)	0.6172 (2)	−0.0595 (8)	0.6162 (3)	0.062
C(6)	0.6658 (2)	−0.0628 (7)	0.7094 (3)	0.053
C(7)	0.7390 (2)	−0.0759 (6)	0.9339 (2)	0.045
C(8)	0.7978 (2)	−0.1572 (6)	1.0243 (2)	0.049
C(9)	0.8080 (2)	0.0434 (7)	1.1102 (2)	0.050
C(10)	0.8695 (2)	−0.0380 (7)	1.1985 (2)	0.052
C(11)	0.8836 (2)	0.1728 (7)	1.2797 (3)	0.054
C(12)	0.9372 (2)	0.0954 (7)	1.3741 (3)	0.050
(II)				
N(1)	0.6344 (3)	0.0838 (5)	0.3292 (5)	0.043
O(7)	0.6244 (3)	0.2947 (5)	0.2376 (5)	0.069
O(121)	0.5226 (3)	−0.0382 (6)	−0.3533 (5)	0.076
O(122)	0.5301 (3)	0.1611 (6)	−0.4551 (5)	0.073
C(1)	0.6668 (3)	0.1174 (7)	0.4430 (7)	0.041
C(2)	0.6964 (3)	0.0122 (8)	0.4996 (8)	0.056
C(3)	0.7291 (4)	0.0387 (11)	0.6103 (9)	0.071
C(4)	0.7309 (4)	0.1709 (11)	0.6629 (9)	0.074
C(5)	0.7000 (4)	0.2738 (10)	0.6075 (8)	0.073
C(6)	0.6683 (3)	0.2494 (8)	0.4957 (8)	0.059
C(7)	0.6154 (3)	0.1706 (7)	0.2361 (7)	0.046
C(8)	0.5814 (3)	0.1051 (8)	0.1275 (7)	0.048
C(9)	0.6004 (4)	0.1478 (9)	−0.0089 (7)	0.060
C(10)	0.5624 (4)	0.0858 (9)	−0.1131 (7)	0.070
C(11)	0.5746 (4)	0.1415 (9)	−0.2458 (8)	0.071
C(12)	0.5402 (3)	0.0813 (8)	−0.3548 (7)	0.050
(III)				
N(1)	0.2210 (3)	0.8877 (3)	0.1340 (3)	0.049
O(8)	0.4495 (3)	0.8481 (3)	0.1288 (3)	0.068
O(112)	0.6034 (2)	0.5621 (3)	0.1415 (3)	0.061
O(111)	0.3742 (2)	0.5650 (3)	0.0742 (3)	0.050
C(1)	0.0892 (4)	0.8678 (3)	0.1856 (4)	0.050
C(2)	−0.0020 (4)	0.7850 (4)	0.1247 (5)	0.074
C(3)	−0.1346 (5)	0.7746 (4)	0.1677 (7)	0.095
C(4)	−0.1740 (5)	0.8462 (5)	0.2674 (6)	0.092
C(5)	−0.0825 (5)	0.9288 (5)	0.3270 (5)	0.081
C(6)	0.0496 (4)	0.9396 (4)	0.2862 (4)	0.063
C(7)	0.2250 (4)	0.9880 (4)	0.0418 (4)	0.064
C(8)	0.3390 (4)	0.8258 (3)	0.1740 (4)	0.048
C(9)	0.3278 (4)	0.7298 (3)	0.2759 (4)	0.052
C(10)	0.4588 (4)	0.6528 (4)	0.2871 (4)	0.054
C(11)	0.4756 (4)	0.5905 (3)	0.1587 (4)	0.047

Table 2. *Selected geometric parameters* (Å, °)

	(I)	(II)	(III)
C(1)—C(2)	1.380 (4)	1.368 (10)	1.382 (5)
C(2)—C(3)	1.388 (5)	1.393 (11)	1.394 (7)
C(3)—C(4)	1.376 (5)	1.386 (12)	1.370 (8)
C(4)—C(5)	1.378 (5)	1.365 (12)	1.378 (7)
C(5)—C(6)	1.387 (4)	1.385 (10)	1.381 (5)
C(6)—C(1)	1.389 (4)	1.384 (10)	1.379 (5)
C(1)—N(1)	1.422 (4)	1.429 (8)	1.437 (4)
C(7)—N(1)	1.352 (4)	1.342 (9)	1.471 (5)
C(7)—O(7)	1.221 (4)	1.220 (8)	-
C(8)—O(8)	-	-	1.226 (4)
C(8)—N(1)	-	-	1.358 (4)
C(7)—C(8)	1.515 (4)	1.511 (9)	-
C(8)—C(9)	1.513 (4)	1.509 (9)	1.505 (5)
C(9)—C(10)	1.524 (4)	1.521 (10)	1.531 (5)
C(10)—C(11)	1.511 (4)	1.474 (11)	1.484 (5)
C(11)—C(12)	1.498 (4)	1.498 (10)	-
C(11)—O(111)	-	-	1.244 (4)
C(11)—O(112)	-	-	1.299 (4)
C(12)—O(121)	1.220 (4)	1.232 (9)	-
C(12)—O(122)	1.287 (4)	1.316 (9)	-
C(1)—N(1)—C(7)	126.0 (3)	127.6 (7)	115.6 (4)
C(8)—N(1)—C(1)	-	-	123.5 (4)
C(7)—N(1)—C(8)	-	-	120.7 (4)
C(2)—C(1)—N(1)	117.9 (3)	117.0 (8)	119.6 (5)
C(6)—C(1)—N(1)	121.6 (3)	122.1 (6)	119.3 (4)
C(6)—C(1)—C(2)	120.5 (3)	120.9 (7)	120.8 (5)
C(3)—C(2)—C(1)	119.4 (4)	119.7 (8)	118.8 (6)
C(4)—C(3)—C(2)	120.3 (4)	119.6 (9)	120.4 (6)
C(3)—C(4)—C(5)	120.3 (3)	119.9 (8)	120.4 (6)
C(6)—C(5)—C(4)	120.0 (4)	120.9 (9)	119.9 (6)
C(5)—C(6)—C(1)	119.5 (3)	118.9 (8)	119.8 (5)
O(7)—C(7)—N(1)	123.5 (3)	123.0 (7)	-
C(8)—C(7)—N(1)	114.0 (3)	115.7 (6)	-
C(8)—C(7)—O(7)	122.4 (3)	121.3 (7)	-
C(7)—C(8)—C(9)	113.1 (3)	112.3 (6)	-
N(1)—C(8)—O(8)	-	-	120.8 (5)
C(9)—C(8)—O(8)	-	-	122.0 (4)
C(9)—C(8)—N(1)	-	-	117.2 (4)
C(8)—C(9)—C(10)	112.1 (3)	109.7 (6)	110.4 (4)
C(11)—C(10)—C(9)	111.6 (3)	111.3 (7)	112.6 (4)
C(12)—C(11)—C(10)	114.4 (3)	114.4 (7)	-
O(112)—C(11)—O(111)	-	-	122.1 (5)
C(10)—C(11)—O(111)	-	-	122.4 (4)
C(10)—C(11)—O(112)	-	-	115.4 (4)
O(122)—C(12)—O(121)	123.1 (3)	120.3 (7)	-
C(11)—C(12)—O(121)	122.6 (3)	123.2 (8)	-
C(11)—C(12)—O(122)	114.3 (3)	116.5 (7)	-

As far as possible similar conditions were used for the data collection and refinement of all three structures. Standard reflections were recentred every 100 reflections and scanned every hour to check for crystal movement and stability. The structures were solved by direct methods using *SHELXS*86 (Sheldrick, 1985) and refined by full-matrix least-squares analysis using *SHELX*76 (Sheldrick, 1976). The ring, alkyl and amino H atoms were fixed geometrically and refined with isotropic displacement parameters. The carboxylic H-atom coordinates for (I) and (III) were located from the difference Fourier syntheses. For (II), the carboxylic H-atom coordinates could not be located. All non-H atoms were refined with anisotropic displacement parameters. The high R factor found for (II) is associated with poor crystal quality and the fact that the crystal was present in the peracid and could not otherwise be obtained by recrystallization.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71729 (39 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: HU1018]

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2-Phthalimidoethanoic Acid Monohydrate (I) and 6-Phthalimidohexanoic Acid Monohydrate (II)

N. Feeder and W. Jones*

Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, England

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Abstract

The hydrogen-bond networks of two ω-phthalimidoaliphatic carboxylic acid monohydrates, $C_{10}H_7NO_4.H_2O$ (I) and $C_{14}H_{15}NO_4.H_2O$ (II), have been investigated.

Comment

As part of a general study of the stability of organic peracids and peracid salts (Kariuki & Jones, 1990),

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