

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

## 2-Aminobenzoic acid–4,4'-bipyridine (2/1)

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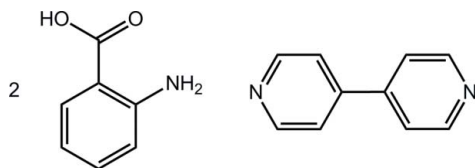
Received 10 August 2013; accepted 13 August 2013

 Key indicators: single-crystal X-ray study;  $T = 98$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.061;  $wR$  factor = 0.159; data-to-parameter ratio = 15.1.

The asymmetric unit of title co-crystal,  $\text{C}_{10}\text{H}_8\text{N}_2 \cdot 2\text{C}_7\text{H}_7\text{NO}_2$ , comprises a centrosymmetric 4,4'-bipyridine molecule, and a 2-aminobenzoic acid molecule in a general position. The latter is effectively planar [ $\text{C}-\text{C}-\text{C}-\text{O}$  torsion angle =  $5.0$  ( $3^\circ$ )] owing to an intramolecular  $\text{N}-\text{H} \cdots \text{O}(\text{carbonyl})$  hydrogen bond. Three-molecule aggregates are formed *via*  $\text{O}-\text{H} \cdots \text{N}(\text{pyridyl})$  hydrogen bonds and these are connected into supramolecular layers in the  $bc$  plane by  $\text{N}-\text{H} \cdots \text{O}(\text{carbonyl})$  hydrogen bonds and  $\pi-\pi$  interactions between pyridyl and benzene rings [inter-centroid distance =  $3.634$  ( $2$ ) Å]. Layers are connected along the  $a$  axis by weak  $\pi-\pi$  interactions between benzene rings [ $3.964$  ( $2$ ) Å].

### Related literature

For co-crystals of 2-aminobenzoic acid with pyridyl derivatives, see: Arman, Kaulgud *et al.* (2012); Arman, Miller & Tiekink (2012).



### Experimental

#### Crystal data

 $\text{C}_{10}\text{H}_8\text{N}_2 \cdot 2\text{C}_7\text{H}_7\text{NO}_2$   
 $M_r = 430.46$   
 Monoclinic,  $P2_1/c$ 
 $a = 10.782$  (5) Å  
 $b = 10.998$  (5) Å  
 $c = 8.951$  (4) Å

 $\beta = 107.215$  ( $7^\circ$ )  
 $V = 1013.9$  (8) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation

 $\mu = 0.10$  mm<sup>-1</sup>  
 $T = 98$  K  
 $0.46 \times 0.11 \times 0.09$  mm

#### Data collection

 Rigaku AFC12/SATURN724 diffractometer  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.723$ ,  $T_{\max} = 1.000$ 

 7849 measured reflections  
 2320 independent reflections  
 1932 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.049$   
 Standard reflections: 0

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.061$   
 $wR(F^2) = 0.159$   
 $S = 1.11$   
 2320 reflections  
 154 parameters  
 4 restraints

 H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\text{max}} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>
**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$\text{N1}-\text{H1n} \cdots \text{O2}$	0.88 (1)	2.02 (2)	2.697 (2)	132 (2)
$\text{O1}-\text{H1o} \cdots \text{N2}^i$	0.85 (1)	1.81 (1)	2.655 (2)	174 (2)
$\text{N1}-\text{H2n} \cdots \text{O2}^{ii}$	0.88 (2)	2.14 (2)	3.002 (3)	170 (2)

 Symmetry codes: (i)  $x, y, z + 1$ ; (ii)  $x, -y + \frac{3}{2}, z - \frac{1}{2}$ .

Data collection: *CrystalClear* (Molecular Structure Corporation & Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

We gratefully thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR-MOHE/SC/03).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZS2276).

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## supporting information

*Acta Cryst.* (2013). E69, o1447 [doi:10.1107/S160053681302271X]

**2-Aminobenzoic acid–4,4'-bipyridine (2/1)**

**Hadi D. Arman and Edward R. T. Tiekink**

**S1. Comment**

The title co-crystal, (I), was formed in continuation of on-going structural studies of co-crystals involving 2-amino-benzoic acid with various pyridyl derivatives (Arman, Kaulgud *et al.*, 2012; Arman, Miller & Tiekink, 2012).

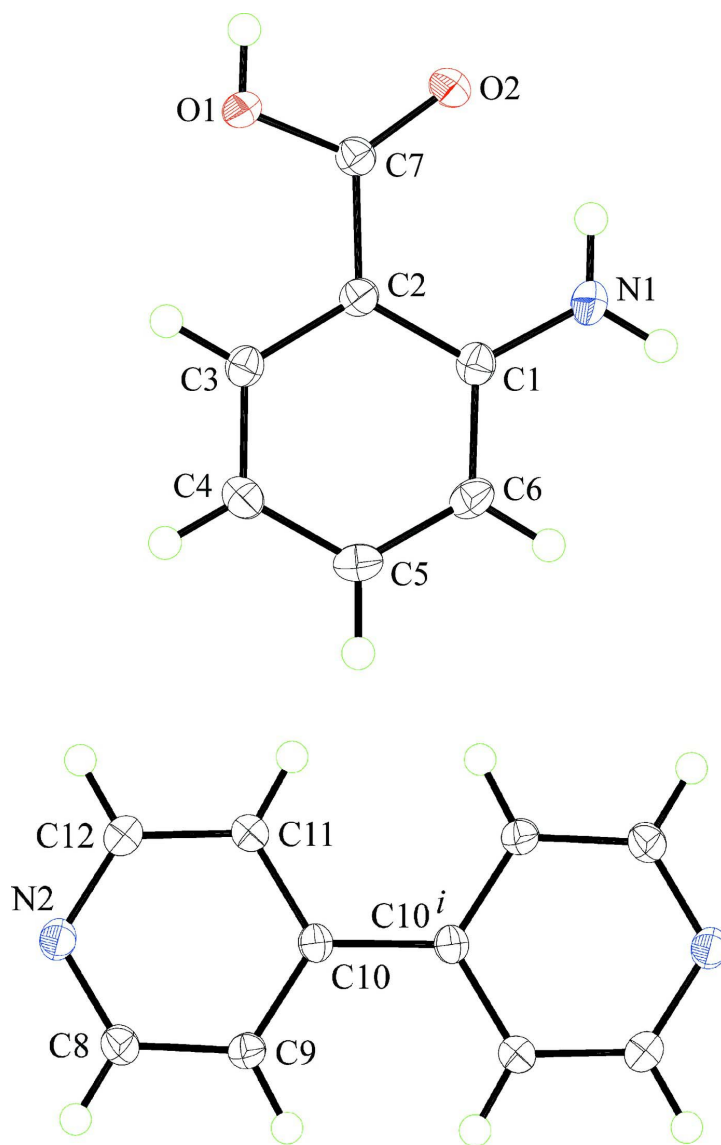
The asymmetric unit contains a molecule of 2-aminobenzoic acid in a general position, and half a molecule of 4,4'-bipyridine disposed about a centre of inversion, Fig. 1. The carboxylic acid is planar owing to the presence of an intramolecular N1—H···O2 hydrogen bond, Table 1, as seen in the C1—C2—C7—O2 torsion angle of 5.0 (3)°. The acid and base associate into a centrosymmetric three-molecule aggregate *via* O1—H···N2 hydrogen bonds, Fig. 2 and Table 1. These assemble into columns along the *c* axis *via*  $\pi$ — $\pi$  interactions between the pyridyl and benzene rings [inter-centroid distance = 3.634 (2) Å], Fig. 2. Supramolecular layers in the *bc* plane are formed by N1—H···O2 hydrogen bonds, Table 1. Connections between layers along the *a* axis are weak  $\pi$ — $\pi$  interactions between benzene rings [inter-centroid distance = 3.964 (2) Å for symmetry operation:  $-x, -y + 1, -z + 1$ ] (Fig. 3.)

**S2. Experimental**

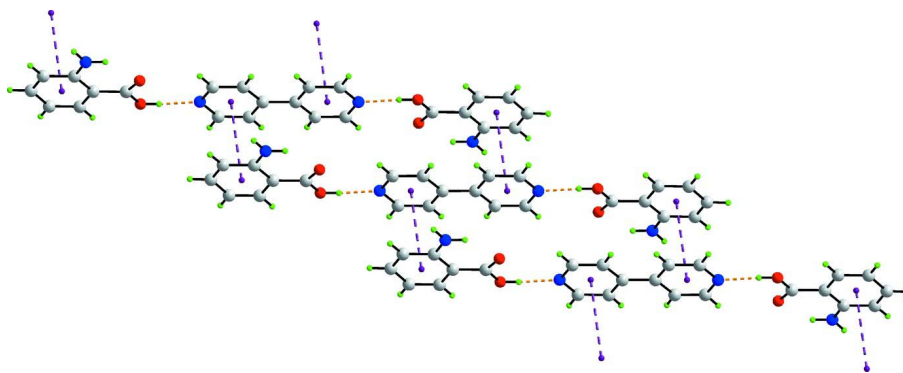
Crystals of (I) were obtained by the co-crystallization of 2-aminobenzoic acid (Sigma-Aldrich, 0.18 mmol) and 4,4'-bipyridine (Sigma-Aldrich, 0.14 mmol) in chloroform solution. Crystals were obtained by slow evaporation.

**S3. Refinement**

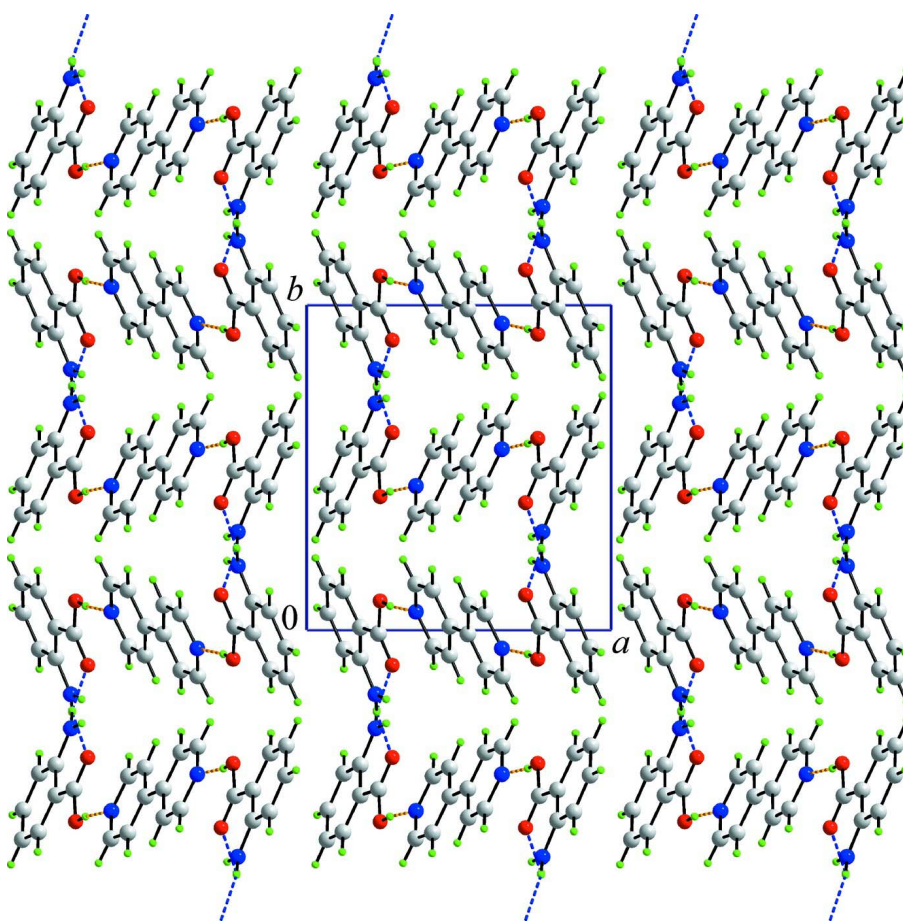
C-bound H-atoms were placed in calculated positions (C—H = 0.95 Å) and were included in the refinement in the riding model approximation with  $U_{\text{iso}}(\text{H})$  set to  $1.2U_{\text{eq}}(\text{C})$ . The O- and N-bound H-atoms were located in a difference Fourier map and were refined with distance restraints of O—H =  $0.84 \pm 0.01$  Å and N—H =  $0.88 \pm 0.01$  Å, and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$  and  $1.5U_{\text{eq}}(\text{O})$ . Owing to being affected by the beam-stop, a reflection, *i.e.* (1 0 0), was omitted from the final cycles of refinement.

**Figure 1**

Molecular structures of the components of (I), showing atom-labelling scheme and displacement ellipsoids at the 50% probability level: (upper) 2-aminobenzoic acid and (lower) 4,4'-bipyridine. For symmetry code (i):  $-x + 1, -y + 1, -z + 1$ .

**Figure 2**

Detail of the  $\pi$ — $\pi$  interactions between three-molecule aggregates in (I). The O—H $\cdots$ N and  $\pi$ — $\pi$  interactions are shown as orange and purple dashed lines, respectively.

**Figure 3**

Unit-cell contents of (I) viewed in projection down the  $c$  axis. The N—H $\cdots$ O hydrogen bonds are shown blue dashed lines.

## 2-Aminobenzoic acid–4,4'-bipyridine (2/1)

## Crystal data

C<sub>10</sub>H<sub>8</sub>N<sub>2</sub>·2C<sub>7</sub>H<sub>7</sub>NO<sub>2</sub> $M_r = 430.46$ Monoclinic,  $P2_1/c$ 

Hall symbol: -P 2ybc

 $a = 10.782$  (5) Å $b = 10.998$  (5) Å $c = 8.951$  (4) Å $\beta = 107.215$  (7)° $V = 1013.9$  (8) Å<sup>3</sup> $Z = 2$  $F(000) = 452$  $D_x = 1.410$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71069$  Å

Cell parameters from 3691 reflections

 $\theta = 2.0$ – $40.7^\circ$  $\mu = 0.10$  mm<sup>-1</sup> $T = 98$  K

Prism, yellow

 $0.46 \times 0.11 \times 0.09$  mm

## Data collection

Rigaku AFC12K/SATURN724

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega$  scans

Absorption correction: multi-scan

(ABSCOR; Higashi, 1995)

 $T_{\min} = 0.723$ ,  $T_{\max} = 1.000$ 

7849 measured reflections

2320 independent reflections

1932 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.049$  $\theta_{\text{max}} = 27.5^\circ$ ,  $\theta_{\text{min}} = 2.7^\circ$  $h = -13 \rightarrow 13$  $k = -14 \rightarrow 14$  $l = -11 \rightarrow 9$ 

## Refinement

Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.061$  $wR(F^2) = 0.159$  $S = 1.11$ 

2320 reflections

154 parameters

4 restraints

Primary atom site location: structure-invariant

direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0786P)^2 + 0.3371P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} < 0.001$  $\Delta\rho_{\text{max}} = 0.32$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

## Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.24135 (13)	0.41046 (12)	0.79067 (14)	0.0227 (3)
H1O	0.277 (2)	0.426 (2)	0.8863 (13)	0.034*
O2	0.28109 (13)	0.60804 (12)	0.76583 (14)	0.0227 (3)

N1	0.22588 (18)	0.69761 (15)	0.47292 (19)	0.0275 (4)
H1N	0.264 (2)	0.711 (2)	0.5733 (11)	0.041*
H2N	0.233 (2)	0.7512 (18)	0.4034 (19)	0.041*
N2	0.35899 (15)	0.44351 (14)	0.09341 (17)	0.0204 (4)
C1	0.17630 (16)	0.58551 (17)	0.4277 (2)	0.0190 (4)
C2	0.17652 (16)	0.49167 (16)	0.53666 (19)	0.0174 (4)
C3	0.11939 (16)	0.37885 (17)	0.4823 (2)	0.0185 (4)
H3	0.1171	0.3173	0.5558	0.022*
C4	0.06660 (17)	0.35534 (18)	0.3247 (2)	0.0216 (4)
H4	0.0291	0.2784	0.2897	0.026*
C5	0.06951 (17)	0.44668 (19)	0.2180 (2)	0.0225 (4)
H5	0.0343	0.4312	0.1092	0.027*
C6	0.12234 (18)	0.55891 (17)	0.2671 (2)	0.0211 (4)
H6	0.1225	0.6196	0.1916	0.025*
C7	0.23616 (16)	0.51026 (16)	0.7065 (2)	0.0183 (4)
C8	0.35778 (17)	0.35879 (17)	0.2006 (2)	0.0209 (4)
H8	0.3171	0.2831	0.1659	0.025*
C9	0.41319 (17)	0.37652 (16)	0.3599 (2)	0.0190 (4)
H9	0.4122	0.3129	0.4313	0.023*
C10	0.47043 (16)	0.48801 (16)	0.41530 (18)	0.0163 (4)
C11	0.46902 (18)	0.57685 (17)	0.3028 (2)	0.0210 (4)
H11	0.5050	0.6549	0.3341	0.025*
C12	0.41485 (17)	0.55033 (18)	0.1457 (2)	0.0225 (4)
H12	0.4174	0.6110	0.0712	0.027*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0326 (7)	0.0183 (7)	0.0149 (6)	-0.0019 (6)	0.0036 (5)	0.0017 (5)
O2	0.0302 (7)	0.0181 (7)	0.0193 (6)	-0.0021 (6)	0.0065 (5)	-0.0038 (5)
N1	0.0423 (10)	0.0171 (8)	0.0225 (8)	-0.0046 (7)	0.0087 (7)	0.0027 (6)
N2	0.0229 (7)	0.0210 (8)	0.0167 (7)	0.0022 (6)	0.0048 (6)	0.0001 (6)
C1	0.0198 (8)	0.0165 (9)	0.0216 (9)	0.0025 (7)	0.0076 (7)	0.0007 (7)
C2	0.0198 (8)	0.0162 (9)	0.0167 (8)	0.0026 (7)	0.0064 (7)	0.0002 (6)
C3	0.0193 (8)	0.0168 (9)	0.0197 (8)	0.0015 (7)	0.0061 (7)	0.0015 (6)
C4	0.0211 (8)	0.0195 (9)	0.0227 (9)	-0.0018 (7)	0.0043 (7)	-0.0028 (7)
C5	0.0219 (9)	0.0276 (10)	0.0164 (8)	0.0031 (8)	0.0030 (7)	-0.0002 (7)
C6	0.0246 (9)	0.0213 (9)	0.0176 (8)	0.0056 (7)	0.0066 (7)	0.0037 (7)
C7	0.0198 (8)	0.0173 (9)	0.0185 (8)	0.0013 (7)	0.0065 (7)	-0.0016 (6)
C8	0.0239 (9)	0.0186 (9)	0.0197 (8)	0.0004 (7)	0.0059 (7)	-0.0024 (7)
C9	0.0227 (8)	0.0163 (9)	0.0179 (8)	0.0010 (7)	0.0056 (7)	0.0011 (6)
C10	0.0155 (8)	0.0182 (9)	0.0156 (8)	0.0009 (7)	0.0053 (6)	-0.0015 (6)
C11	0.0254 (9)	0.0186 (9)	0.0185 (8)	-0.0040 (7)	0.0054 (7)	-0.0012 (7)
C12	0.0259 (9)	0.0226 (9)	0.0184 (8)	-0.0008 (8)	0.0054 (7)	0.0026 (7)

## Geometric parameters (Å, °)

O1—C7	1.323 (2)	C4—C5	1.393 (3)
O1—H1O	0.845 (10)	C4—H4	0.9500
O2—C7	1.233 (2)	C5—C6	1.376 (3)
N1—C1	1.357 (2)	C5—H5	0.9500
N1—H1N	0.882 (9)	C6—H6	0.9500
N1—H2N	0.876 (9)	C8—C9	1.387 (2)
N2—C12	1.340 (3)	C8—H8	0.9500
N2—C8	1.341 (2)	C9—C10	1.396 (3)
C1—C6	1.412 (2)	C9—H9	0.9500
C1—C2	1.420 (2)	C10—C11	1.400 (2)
C2—C3	1.407 (3)	C10—C10 <sup>i</sup>	1.484 (3)
C2—C7	1.479 (2)	C11—C12	1.385 (2)
C3—C4	1.380 (2)	C11—H11	0.9500
C3—H3	0.9500	C12—H12	0.9500
C7—O1—H1O	109.8 (17)	C5—C6—H6	119.4
C1—N1—H1N	118.5 (15)	C1—C6—H6	119.4
C1—N1—H2N	120.5 (15)	O2—C7—O1	122.21 (16)
H1N—N1—H2N	120.1 (16)	O2—C7—C2	123.99 (16)
C12—N2—C8	117.25 (15)	O1—C7—C2	113.76 (15)
N1—C1—C6	119.95 (16)	N2—C8—C9	123.08 (17)
N1—C1—C2	122.33 (16)	N2—C8—H8	118.5
C6—C1—C2	117.72 (17)	C9—C8—H8	118.5
C3—C2—C1	119.46 (15)	C8—C9—C10	119.95 (16)
C3—C2—C7	119.36 (15)	C8—C9—H9	120.0
C1—C2—C7	121.18 (16)	C10—C9—H9	120.0
C4—C3—C2	121.65 (16)	C9—C10—C11	116.62 (16)
C4—C3—H3	119.2	C9—C10—C10 <sup>i</sup>	122.0 (2)
C2—C3—H3	119.2	C11—C10—C10 <sup>i</sup>	121.4 (2)
C3—C4—C5	118.65 (18)	C12—C11—C10	119.66 (17)
C3—C4—H4	120.7	C12—C11—H11	120.2
C5—C4—H4	120.7	C10—C11—H11	120.2
C6—C5—C4	121.28 (17)	N2—C12—C11	123.39 (17)
C6—C5—H5	119.4	N2—C12—H12	118.3
C4—C5—H5	119.4	C11—C12—H12	118.3
C5—C6—C1	121.18 (16)		
N1—C1—C2—C3	177.74 (16)	C1—C2—C7—O2	5.0 (3)
C6—C1—C2—C3	-2.4 (2)	C3—C2—C7—O1	6.9 (2)
N1—C1—C2—C7	-2.5 (3)	C1—C2—C7—O1	-172.86 (16)
C6—C1—C2—C7	177.36 (15)	C12—N2—C8—C9	-1.2 (3)
C1—C2—C3—C4	2.2 (3)	N2—C8—C9—C10	1.9 (3)
C7—C2—C3—C4	-177.63 (16)	C8—C9—C10—C11	-0.5 (3)
C2—C3—C4—C5	-0.6 (3)	C8—C9—C10—C10 <sup>i</sup>	179.24 (19)
C3—C4—C5—C6	-0.7 (3)	C9—C10—C11—C12	-1.3 (3)
C4—C5—C6—C1	0.3 (3)	C10 <sup>i</sup> —C10—C11—C12	178.92 (19)

N1—C1—C6—C5	-178.94 (17)	C8—N2—C12—C11	-0.7 (3)
C2—C1—C6—C5	1.2 (3)	C10—C11—C12—N2	2.0 (3)
C3—C2—C7—O2	-175.22 (16)		

Symmetry code: (i)  $-x+1, -y+1, -z+1$ .

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1n $\cdots$ O2	0.88 (1)	2.02 (2)	2.697 (2)	132 (2)
O1—H1o $\cdots$ N2 <sup>ii</sup>	0.85 (1)	1.81 (1)	2.655 (2)	174 (2)
N1—H2n $\cdots$ O2 <sup>iii</sup>	0.88 (2)	2.14 (2)	3.002 (3)	170 (2)

Symmetry codes: (ii)  $x, y, z+1$ ; (iii)  $x, -y+3/2, z-1/2$ .