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1,2-Di-2-pyridylethylene–phenylsuccinic acid (1/1)

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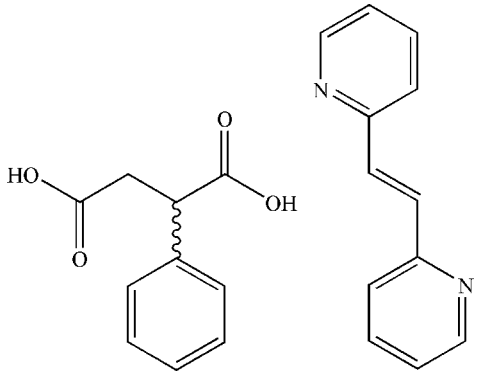
Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.003 Å; R factor = 0.047; wR factor = 0.133; data-to-parameter ratio = 14.2.

In the title 1:1 adduct, $C_{10}H_{10}O_4\cdot C_{12}H_{10}N_2$, the two components are linked by O—H···N hydrogen bonds to form a one-dimensional chain. The dihedral angle between the pyridine rings is 15.68 (8)° These chains are further interconnected by weak intermolecular C—H···O hydrogen bonds and weak C—H···π interactions to generate a three-dimensional network.

Related literature

For (*S*)- and (*R,S*)-phenylsuccinic acids, see: Fischer & Profir (2003*a*,*b*). For weak C—H···O hydrogen bonds, see, for example: Bhogala *et al.* (2005); Wang *et al.* (2008). For C—H···π interactions, see, for example: Fun & Kia (2008).



Experimental

Crystal data

$C_{10}H_{10}O_4\cdot C_{12}H_{10}N_2$ M_r = 376.40
Triclinic, $P\overline{1}$
a = 8.6707 (13) Å
b = 10.9714 (17) Å
c = 11.2013 (17) Å
α = 80.801 (2)°
β = 69.696 (2)°
γ = 77.663 (2)°
V = 972.0 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 291 (2) K
0.34 × 0.33 × 0.29 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.957, T_{max} = 0.975
7261 measured reflections
3605 independent reflections
2369 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.03
3605 reflections
253 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···N1	0.82	1.88	2.699 (2)	176
O1—H1···N2^{i}	0.82	1.88	2.683 (2)	165
C2—H2···O2^{ii}	0.93	2.56	3.472 (3)	164
C11—H11···O3^{iii}	0.93	2.43	3.350 (3)	170
C3—H3···$Cg1^{iv}$	0.93	2.86	3.650 (4)	143

Symmetry codes: (i) $x, y+1, z-1$; (ii) $x-1, y, z+1$; (iii) $x+1, y-1, z$; (iv) $-x, -y+1, -z+1$. $Cg1$ is the centroid of the C15–C20 phenyl ring.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

The authors thank Nanyang Normal University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2134).

References

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supporting information

Acta Cryst. (2009). E**65**, o182 [doi:10.1107/S1600536808040245]

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S1. Comment

The asymmetric unit consists of the two heteromolecular components of the title compound in a (1/1) ratio (Fig.1). These molecules are linked by intermolecular O—H···N hydrogen bonds to form a one-dimensional chain (Table 1, Fig.2). The chains interact with each other *via* weak intermolecular C—H···O hydrogen bonds and C—H···π interactions (Tab 1). *Cg*1 is the centroid of the phenyl ring C15 - C20. These hydrogen bonds, albeit rather weak, link the chains into two-dimensional layers structure (Fig. 3), which are further connected by weak intermolecular C—H···π interactions to generate a three-dimensional supramolecular structure (Fig. 4).

S2. Experimental

1,2-bis(2-pyridyl)ethylene (0.15 mmol), (*R*)-Phenylsuccinic acid (0.15 mmol), and NaOH (0.1 mmol) were added to a H_2O solution (20 ml) in a Teflonlined stainless steel reactor. The mixture was heated at 450 K for 4 d, and then slowly cooled down to room temperature. Colorless crystals of the title compound were obtained.

S3. Refinement

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93 Å (aromatic H) and *U*iso~(H) = 1.2Ueq(C), with C—H = 0.97 Å (CH2) and *U*iso~(H) = 1.2Ueq(C), with C—H = 0.98 Å(CH) and *U*iso~(H) = 1.2Ueq(C) and with O—H = 0.82 Å (OH) and *U*iso~(H) = 1.5Ueq(O).

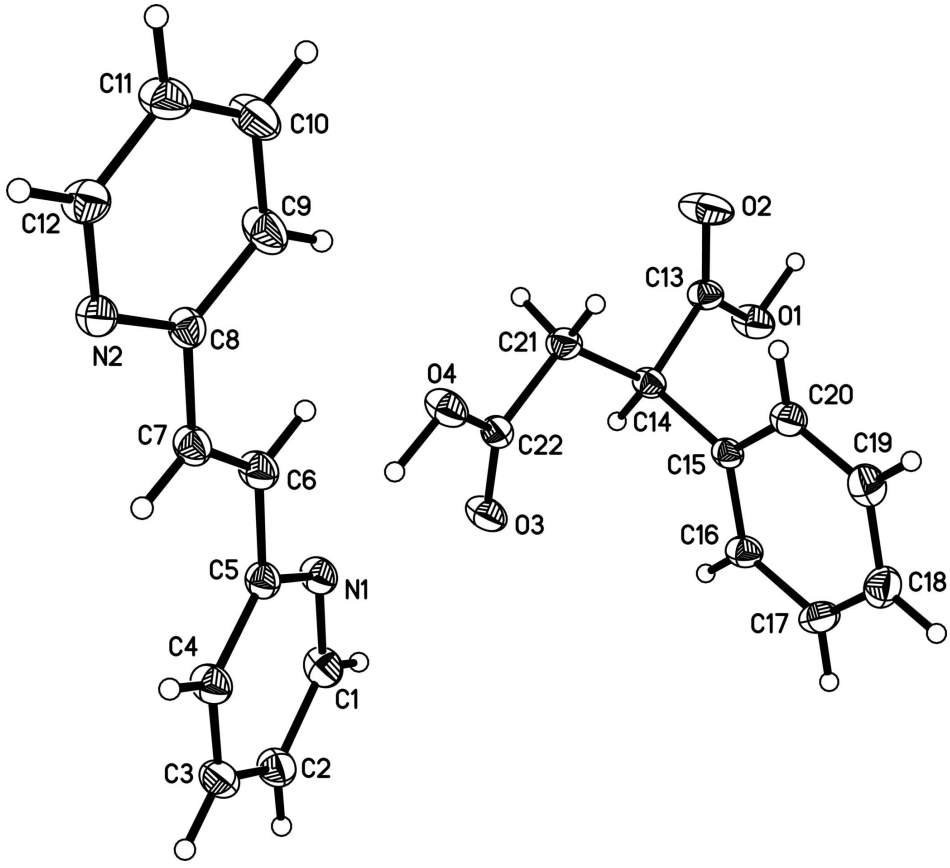

Figure 1

A view of the heteromolecular components of the title compound with the atom labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

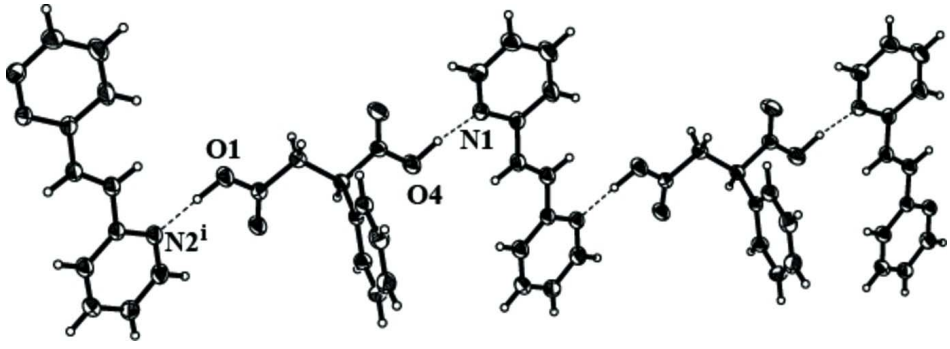

Figure 2

A view of the one-dimensional hydrogen-bonding pattern network.

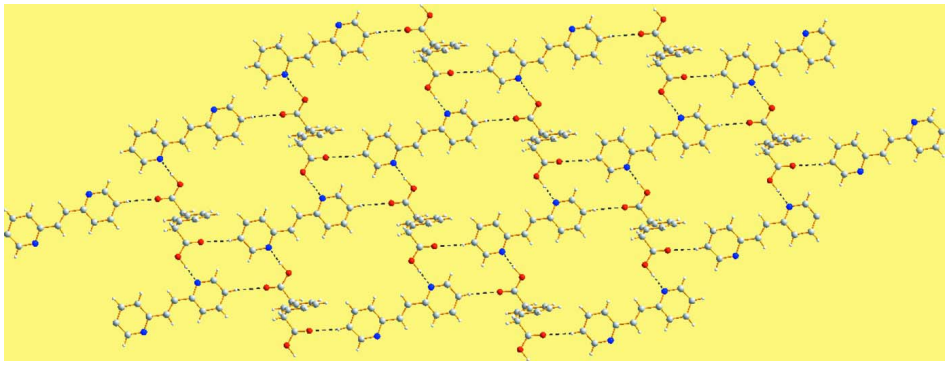

Figure 3

The crystal packing of (I), showing the two-dimensional structure.

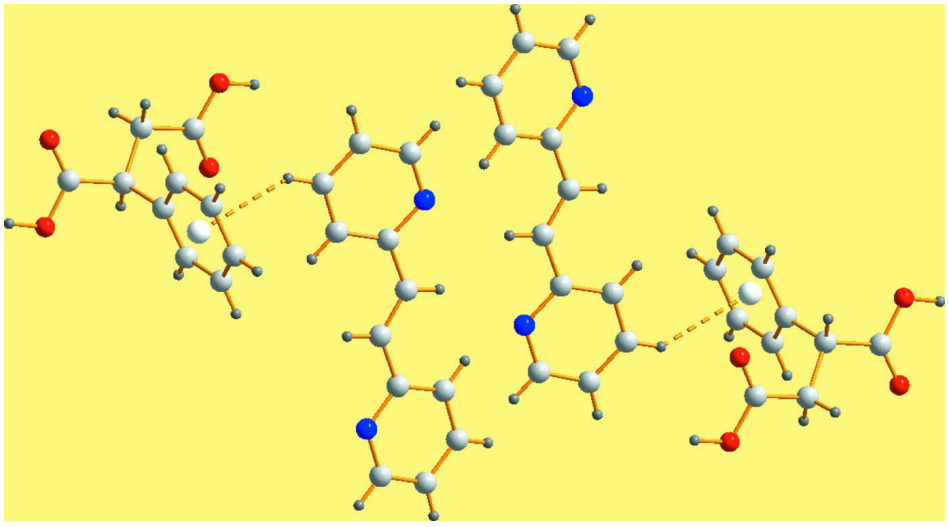

Figure 4

A view of the C—H···π interactions in the crystal structure of the title compound.

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Crystal data

$C_{10}H_{10}O_4 \cdot C_{12}H_{10}N_2$
$M_r = 376.40$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.6707\ (13)$ Å
$b = 10.9714\ (17)$ Å
$c = 11.2013\ (17)$ Å
$\alpha = 80.801\ (2)°$
$\beta = 69.696\ (2)°$
$\gamma = 77.663\ (2)°$
$V = 972.0\ (3)$ Å^3
$Z = 2$
$F(000) = 396$
$D_x = 1.286$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1614 reflections
$\theta = 2.5–26.0°$
$\mu = 0.09$ mm^{-1}
$T = 291$ K
Block, colorless
0.34 × 0.33 × 0.29 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.957, T_{max} = 0.975
7261 measured reflections
3605 independent reflections
2369 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 25.5°, θ_{min} = 2.5°
h = −10→10
k = −13→13
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.133
S = 1.03
3605 reflections
253 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0553P)^2 + 0.1924P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.47679 (18)	0.96437 (13)	−0.17709 (14)	0.0637 (5)
H1	0.5453	0.9815	−0.2464	0.096*
O2	0.6712 (2)	0.79683 (17)	−0.17226 (16)	0.0896 (7)
O3	0.27415 (18)	0.75636 (14)	0.27577 (13)	0.0620 (4)
O4	0.45071 (18)	0.57475 (13)	0.26650 (13)	0.0618 (4)
H4	0.3867	0.5601	0.3387	0.093*
N1	0.2501 (2)	0.51408 (15)	0.50443 (15)	0.0485 (4)
N2	0.66326 (19)	0.01005 (14)	0.57849 (15)	0.0454 (4)
C1	0.1106 (3)	0.5966 (2)	0.5536 (2)	0.0546 (6)
H1A	0.0995	0.6764	0.5110	0.065*
C2	−0.0168 (3)	0.5695 (2)	0.6635 (2)	0.0567 (6)
H2	−0.1108	0.6295	0.6947	0.068*
C3	−0.0007 (3)	0.4507 (2)	0.7260 (2)	0.0561 (6)
H3	−0.0845	0.4289	0.7999	0.067*
C4	0.1410 (3)	0.3649 (2)	0.6774 (2)	0.0531 (5)
H4A	0.1531	0.2846	0.7187	0.064*
C5	0.2663 (2)	0.39814 (18)	0.56644 (18)	0.0434 (5)
C6	0.4216 (3)	0.31193 (19)	0.5089 (2)	0.0503 (5)
H6	0.4894	0.3386	0.4284	0.060*
C7	0.4745 (2)	0.20028 (18)	0.56004 (19)	0.0470 (5)
H7	0.4071	0.1742	0.6409	0.056*
C8	0.6279 (2)	0.11358 (18)	0.50279 (18)	0.0440 (5)
C9	0.7339 (3)	0.1334 (2)	0.3775 (2)	0.0657 (7)
H9	0.7090	0.2046	0.3256	0.079*
C10	0.8761 (3)	0.0464 (2)	0.3313 (2)	0.0720 (7)

H10	0.9480	0.0595	0.2485	0.086*
C11	0.9108 (3)	−0.0587 (2)	0.4075 (2)	0.0624 (6)
H11	1.0050	−0.1187	0.3775	0.075*
C12	0.8017 (3)	−0.07322 (19)	0.5304 (2)	0.0549 (6)
H12	0.8252	−0.1445	0.5827	0.066*
C13	0.5369 (2)	0.85814 (19)	−0.12306 (19)	0.0462 (5)
C14	0.4165 (2)	0.81888 (18)	0.00741 (18)	0.0427 (5)
H14	0.3682	0.8931	0.0550	0.051*
C15	0.2750 (2)	0.77139 (17)	−0.01329 (17)	0.0399 (5)
C16	0.1120 (2)	0.83595 (19)	0.02700 (19)	0.0488 (5)
H16	0.0881	0.9074	0.0694	0.059*
C17	−0.0154 (3)	0.7948 (2)	0.0046 (2)	0.0588 (6)
H17	−0.1236	0.8394	0.0316	0.071*
C18	0.0169 (3)	0.6883 (2)	−0.0573 (2)	0.0635 (6)
H18	−0.0688	0.6612	−0.0723	0.076*
C19	0.1789 (3)	0.6220 (2)	−0.0970 (2)	0.0603 (6)
H19	0.2018	0.5498	−0.1381	0.072*
C20	0.3064 (3)	0.66335 (19)	−0.07542 (19)	0.0497 (5)
H20	0.4145	0.6186	−0.1026	0.060*
C21	0.5086 (2)	0.7212 (2)	0.08432 (18)	0.0501 (5)
H21A	0.5541	0.6462	0.0396	0.060*
H21B	0.6013	0.7538	0.0899	0.060*
C22	0.3968 (2)	0.68718 (19)	0.21791 (18)	0.0438 (5)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0595 (9)	0.0537 (9)	0.0538 (9)	−0.0004 (7)	−0.0032 (7)	0.0158 (7)
O2	0.0579 (10)	0.0906 (13)	0.0669 (11)	0.0189 (9)	0.0120 (9)	0.0282 (9)
O3	0.0591 (9)	0.0598 (10)	0.0442 (8)	0.0097 (8)	−0.0023 (7)	0.0005 (7)
O4	0.0653 (10)	0.0513 (9)	0.0446 (8)	0.0079 (7)	−0.0029 (7)	0.0062 (7)
N1	0.0520 (10)	0.0422 (10)	0.0428 (9)	−0.0012 (8)	−0.0126 (8)	0.0046 (8)
N2	0.0471 (9)	0.0384 (9)	0.0450 (9)	−0.0050 (7)	−0.0134 (8)	0.0056 (7)
C1	0.0621 (14)	0.0425 (12)	0.0498 (13)	0.0039 (10)	−0.0165 (11)	0.0013 (10)
C2	0.0534 (13)	0.0584 (14)	0.0490 (13)	0.0073 (11)	−0.0135 (10)	−0.0080 (11)
C3	0.0525 (13)	0.0640 (15)	0.0420 (12)	−0.0079 (11)	−0.0068 (10)	0.0006 (11)
C4	0.0551 (13)	0.0464 (12)	0.0479 (12)	−0.0053 (10)	−0.0107 (10)	0.0051 (10)
C5	0.0458 (11)	0.0419 (11)	0.0398 (11)	−0.0055 (9)	−0.0141 (9)	0.0012 (9)
C6	0.0508 (12)	0.0475 (12)	0.0425 (11)	−0.0031 (10)	−0.0098 (9)	0.0052 (9)
C7	0.0514 (12)	0.0457 (12)	0.0387 (11)	−0.0053 (9)	−0.0122 (9)	0.0011 (9)
C8	0.0495 (11)	0.0413 (11)	0.0397 (11)	−0.0062 (9)	−0.0150 (9)	−0.0005 (9)
C9	0.0788 (16)	0.0581 (15)	0.0403 (12)	0.0049 (12)	−0.0092 (11)	0.0063 (11)
C10	0.0762 (17)	0.0708 (17)	0.0427 (13)	0.0047 (13)	0.0013 (12)	−0.0010 (12)
C11	0.0553 (13)	0.0549 (14)	0.0608 (14)	0.0042 (11)	−0.0055 (11)	−0.0083 (12)
C12	0.0521 (12)	0.0431 (12)	0.0600 (14)	−0.0005 (10)	−0.0148 (11)	0.0038 (10)
C13	0.0405 (11)	0.0446 (12)	0.0451 (11)	−0.0064 (9)	−0.0083 (9)	0.0060 (9)
C14	0.0421 (10)	0.0409 (11)	0.0375 (10)	−0.0041 (8)	−0.0072 (8)	0.0005 (8)
C15	0.0393 (10)	0.0417 (11)	0.0325 (10)	−0.0047 (8)	−0.0081 (8)	0.0034 (8)

C16	0.0436 (11)	0.0463 (12)	0.0477 (12)	−0.0027 (9)	−0.0091 (9)	0.0012 (9)
C17	0.0378 (11)	0.0715 (16)	0.0586 (14)	−0.0083 (11)	−0.0134 (10)	0.0115 (12)
C18	0.0639 (15)	0.0765 (17)	0.0579 (14)	−0.0299 (13)	−0.0258 (12)	0.0094 (13)
C19	0.0706 (16)	0.0599 (14)	0.0529 (13)	−0.0190 (12)	−0.0183 (12)	−0.0052 (11)
C20	0.0473 (12)	0.0501 (13)	0.0457 (12)	−0.0033 (10)	−0.0113 (9)	−0.0025 (10)
C21	0.0409 (11)	0.0568 (13)	0.0450 (12)	−0.0067 (9)	−0.0094 (9)	0.0039 (10)
C22	0.0433 (11)	0.0477 (12)	0.0370 (10)	−0.0047 (9)	−0.0117 (9)	−0.0018 (9)

Geometric parameters (Å, º)

O1—C13	1.315 (2)	C9—H9	0.9300
O1—H1	0.8200	C10—C11	1.365 (3)
O2—C13	1.204 (2)	C10—H10	0.9300
O3—C22	1.209 (2)	C11—C12	1.380 (3)
O4—C22	1.324 (2)	C11—H11	0.9300
O4—H4	0.8200	C12—H12	0.9300
N1—C1	1.347 (2)	C13—C14	1.531 (3)
N1—C5	1.352 (2)	C14—C15	1.529 (3)
N2—C12	1.344 (2)	C14—C21	1.532 (3)
N2—C8	1.352 (2)	C14—H14	0.9800
C1—C2	1.380 (3)	C15—C16	1.391 (3)
C1—H1A	0.9300	C15—C20	1.399 (3)
C2—C3	1.381 (3)	C16—C17	1.389 (3)
C2—H2	0.9300	C16—H16	0.9300
C3—C4	1.378 (3)	C17—C18	1.383 (3)
C3—H3	0.9300	C17—H17	0.9300
C4—C5	1.395 (3)	C18—C19	1.390 (3)
C4—H4A	0.9300	C18—H18	0.9300
C5—C6	1.474 (3)	C19—C20	1.387 (3)
C6—C7	1.326 (3)	C19—H19	0.9300
C6—H6	0.9300	C20—H20	0.9300
C7—C8	1.465 (3)	C21—C22	1.513 (3)
C7—H7	0.9300	C21—H21A	0.9700
C8—C9	1.398 (3)	C21—H21B	0.9700
C9—C10	1.382 (3)		

C13—O1—H1	109.5	N2—C12—H12	118.2
C22—O4—H4	109.5	C11—C12—H12	118.2
C1—N1—C5	118.17 (17)	O2—C13—O1	123.53 (18)
C12—N2—C8	118.53 (17)	O2—C13—C14	123.50 (18)
N1—C1—C2	123.70 (19)	O1—C13—C14	112.95 (16)
N1—C1—H1A	118.1	C15—C14—C13	108.73 (16)
C2—C1—H1A	118.1	C15—C14—C21	112.41 (16)
C1—C2—C3	118.01 (19)	C13—C14—C21	110.86 (15)
C1—C2—H2	121.0	C15—C14—H14	108.2
C3—C2—H2	121.0	C13—C14—H14	108.2
C4—C3—C2	119.24 (19)	C21—C14—H14	108.2
C4—C3—H3	120.4	C16—C15—C20	118.20 (19)

C2—C3—H3	120.4	C16—C15—C14	120.81 (18)
C3—C4—C5	120.13 (19)	C20—C15—C14	120.98 (17)
C3—C4—H4A	119.9	C17—C16—C15	120.7 (2)
C5—C4—H4A	119.9	C17—C16—H16	119.6
N1—C5—C4	120.74 (17)	C15—C16—H16	119.6
N1—C5—C6	115.87 (17)	C18—C17—C16	120.7 (2)
C4—C5—C6	123.39 (18)	C18—C17—H17	119.7
C7—C6—C5	126.66 (19)	C16—C17—H17	119.7
C7—C6—H6	116.7	C17—C18—C19	119.3 (2)
C5—C6—H6	116.7	C17—C18—H18	120.4
C6—C7—C8	126.93 (19)	C19—C18—H18	120.4
C6—C7—H7	116.5	C20—C19—C18	120.1 (2)
C8—C7—H7	116.5	C20—C19—H19	120.0
N2—C8—C9	120.45 (18)	C18—C19—H19	120.0
N2—C8—C7	116.06 (17)	C19—C20—C15	121.01 (19)
C9—C8—C7	123.49 (18)	C19—C20—H20	119.5
C10—C9—C8	119.6 (2)	C15—C20—H20	119.5
C10—C9—H9	120.2	C22—C21—C14	112.58 (16)
C8—C9—H9	120.2	C22—C21—H21A	109.1
C11—C10—C9	119.9 (2)	C14—C21—H21A	109.1
C11—C10—H10	120.0	C22—C21—H21B	109.1
C9—C10—H10	120.0	C14—C21—H21B	109.1
C10—C11—C12	118.0 (2)	H21A—C21—H21B	107.8
C10—C11—H11	121.0	O3—C22—O4	123.46 (18)
C12—C11—H11	121.0	O3—C22—C21	123.82 (18)
N2—C12—C11	123.6 (2)	O4—C22—C21	112.68 (16)

C5—N1—C1—C2	−0.1 (3)	O2—C13—C14—C15	−104.5 (2)
N1—C1—C2—C3	−0.5 (3)	O1—C13—C14—C15	74.0 (2)
C1—C2—C3—C4	0.6 (3)	O2—C13—C14—C21	19.5 (3)
C2—C3—C4—C5	0.0 (3)	O1—C13—C14—C21	−161.95 (18)
C1—N1—C5—C4	0.7 (3)	C13—C14—C15—C16	−114.07 (19)
C1—N1—C5—C6	−179.70 (18)	C21—C14—C15—C16	122.80 (19)
C3—C4—C5—N1	−0.6 (3)	C13—C14—C15—C20	64.7 (2)
C3—C4—C5—C6	179.8 (2)	C21—C14—C15—C20	−58.5 (2)
N1—C5—C6—C7	171.0 (2)	C20—C15—C16—C17	−0.8 (3)
C4—C5—C6—C7	−9.4 (3)	C14—C15—C16—C17	178.00 (17)
C5—C6—C7—C8	179.33 (19)	C15—C16—C17—C18	0.5 (3)
C12—N2—C8—C9	−0.3 (3)	C16—C17—C18—C19	0.2 (3)
C12—N2—C8—C7	179.38 (18)	C17—C18—C19—C20	−0.5 (3)
C6—C7—C8—N2	173.9 (2)	C18—C19—C20—C15	0.3 (3)
C6—C7—C8—C9	−6.4 (4)	C16—C15—C20—C19	0.4 (3)
N2—C8—C9—C10	−0.2 (3)	C14—C15—C20—C19	−178.39 (18)
C7—C8—C9—C10	−179.9 (2)	C15—C14—C21—C22	−62.5 (2)
C8—C9—C10—C11	0.9 (4)	C13—C14—C21—C22	175.58 (17)
C9—C10—C11—C12	−0.9 (4)	C14—C21—C22—O3	−26.4 (3)
C8—N2—C12—C11	0.3 (3)	C14—C21—C22—O4	155.70 (18)
C10—C11—C12—N2	0.4 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···N1	0.82	1.88	2.699 (2)	176
O1—H1···N2^{i}	0.82	1.88	2.683 (2)	165
C2—H2···O2^{ii}	0.93	2.56	3.472 (3)	164
C11—H11···O3^{iii}	0.93	2.43	3.350 (3)	170
C3—H3···*Cg*1^{iv}	0.93	2.86	3.650 (4)	143

Symmetry codes: (i) *x*, *y*+1, *z*−1; (ii) *x*−1, *y*, *z*+1; (iii) *x*+1, *y*−1, *z*; (iv) −*x*, −*y*+1, −*z*+1.