

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

1,4-Bis{4-[bis(prop-2-yn-1-yl)amino]-phenoxy}benzene

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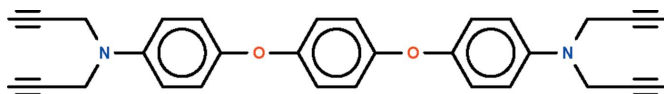
Received 29 January 2011; accepted 30 January 2011

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.063; wR factor = 0.172; data-to-parameter ratio = 15.9.

The asymmetric unit of the title compound, $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_2$, contains two independent molecules, which both lie on centers of inversion. The central phenylene ring is inclined at 61.4 (2)° with respect to the flanking aromatic ring [dihedral angle = 70.7 (3)° in the second molecule].

Related literature

For the only reported crystal structure of a compound possessing a propylamino unit, see: Steiner *et al.* (1999). For the structure of 1,4-bis(4-aminophenoxy)benzene, see: Shems *et al.* (2008).



Experimental

Crystal data

 $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_2$ $M_r = 444.51$

Triclinic, $P\bar{1}$
 $a = 9.8766$ (7) Å
 $b = 11.1635$ (6) Å
 $c = 12.1531$ (9) Å
 $\alpha = 68.687$ (6)°
 $\beta = 69.601$ (7)°
 $\gamma = 88.529$ (5)°

$V = 1162.19$ (13) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 0.08$ mm⁻¹
 $T = 100$ K
 $0.30 \times 0.10 \times 0.05$ mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
 $T_{\min} = 0.712$, $T_{\max} = 1.000$

9192 measured reflections
 5142 independent reflections
 3245 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.063$
 $wR(F^2) = 0.172$
 $S = 1.06$
 5142 reflections
 323 parameters
 4 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.24$ e Å⁻³
 $\Delta\rho_{\min} = -0.33$ e Å⁻³

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank the Higher Education Commission of Pakistan and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: JH2263).

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supplementary materials

Acta Cryst. (2011). E67, o567 [doi:10.1107/S1600536811003862]

1,4-Bis{4-[bis(prop-2-yn-1-yl)amino]phenoxy}benzene

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Comment

1,4-Bis(4-aminophenoxy)benzene is a precursor for the synthesis of polyamides owing the functional amino -NH_2 group that will condense with carboxylic acids (Shemsi *et al.*, 2008). The amino group can be also converted to a dialkylamino group by reaction with an alkyl halide in the presence of potassium carbonate. This strategy is used for the synthesis of the nitrogen-propargyl bond. The unit cell has two independent molecules of $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_2$ (Scheme I) that both lie on a center-of-inversion (Fig. 1). The central phenylene ring is aligned at $61.4(2)^\circ$ with respect to the flanking aromatic ring (the dihedral angle is $70.7(3)^\circ$ for the second molecule). There is only one reported example of the nitrogen-propargyl bond (Steiner *et al.*, 1999).

Experimental

1,4-Bis(4-aminophenoxy)benzene (1 g, 2.2 mmol) was dissolved in ethanol (30 ml) followed by the addition of potassium carbonate (3 g, 21 mmol). The mixture was heated for 1 h. Propargyl bromide (1.5 ml, 15 mmol) was added and the heating was continued for another 8 h. The solvent was evaporated under reduced pressure and the residue was dissolved in a mixture of water (50 ml) and dichloromethane (50 ml). The aqueous layer was extracted three times with dichloromethane and concentrated. The product was recrystallized from ethanol; yield 60%.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C-H 0.95 to 0.99 Å, $U_{\text{iso}}(\text{H})$ $1.2U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding model approximation.

The acetylenic H-atoms were located in a difference Fourier map, and were refined with a distance restraint of C-H 0.95 ± 0.01 Å; their temperature factors were refined.

Figures

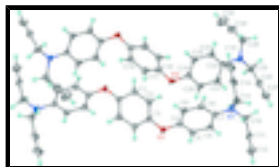


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

1,4-Bis{4-[bis(prop-2-yn-1-yl)amino]phenoxy}benzene

Crystal data

$\text{C}_{30}\text{H}_{24}\text{N}_2\text{O}_2$

$Z = 2$

supplementary materials

$M_r = 444.51$	$F(000) = 468$
Triclinic, $P\bar{1}$	$D_x = 1.270 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 9.8766 (7) \text{ \AA}$	Cell parameters from 2448 reflections
$b = 11.1635 (6) \text{ \AA}$	$\theta = 2.2\text{--}29.2^\circ$
$c = 12.1531 (9) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$\alpha = 68.687 (6)^\circ$	$T = 100 \text{ K}$
$\beta = 69.601 (7)^\circ$	Prism, colorless
$\gamma = 88.529 (5)^\circ$	$0.30 \times 0.10 \times 0.05 \text{ mm}$
$V = 1162.19 (13) \text{ \AA}^3$	

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector	5142 independent reflections
Radiation source: SuperNova (Mo) X-ray Source	3245 reflections with $I > 2\sigma(I)$
Mirror	$R_{\text{int}} = 0.051$
Detector resolution: $10.4041 \text{ pixels mm}^{-1}$	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.2^\circ$
ω scans	$h = -12 \rightarrow 12$
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2010)	$k = -12 \rightarrow 14$
$T_{\text{min}} = 0.712$, $T_{\text{max}} = 1.000$	$l = -13 \rightarrow 15$
9192 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.063$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.172$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.06$	$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2]$
5142 reflections	where $P = (F_o^2 + 2F_c^2)/3$
323 parameters	$(\Delta/\sigma)_{\text{max}} = 0.001$
4 restraints	$\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.33 \text{ e \AA}^{-3}$

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.51131 (17)	0.20860 (14)	0.78479 (13)	0.0252 (4)
O2	1.00539 (17)	0.19216 (14)	0.77617 (13)	0.0247 (4)
N1	0.7243 (2)	0.72196 (18)	0.64767 (16)	0.0242 (5)
N2	1.2235 (2)	0.70018 (18)	0.65456 (17)	0.0240 (5)
C1	0.6093 (2)	-0.0128 (2)	1.0493 (2)	0.0223 (5)
H1	0.6838	-0.0217	1.0835	0.027*

C2	0.6174 (2)	0.0957 (2)	0.9431 (2)	0.0243 (5)
H2	0.6977	0.1611	0.9038	0.029*
C3	0.5073 (2)	0.1073 (2)	0.89530 (19)	0.0211 (5)
C4	0.5691 (2)	0.3332 (2)	0.7564 (2)	0.0212 (5)
C5	0.6303 (2)	0.4110 (2)	0.6295 (2)	0.0220 (5)
H5	0.6387	0.3760	0.5671	0.026*
C6	0.6796 (2)	0.5397 (2)	0.5924 (2)	0.0216 (5)
H6	0.7206	0.5927	0.5047	0.026*
C7	0.6698 (2)	0.5927 (2)	0.68269 (19)	0.0205 (5)
C8	0.6062 (2)	0.5121 (2)	0.8109 (2)	0.0225 (5)
H8	0.5976	0.5460	0.8739	0.027*
C9	0.5554 (2)	0.3838 (2)	0.8474 (2)	0.0232 (5)
H9	0.5114	0.3308	0.9348	0.028*
C10	0.7819 (3)	0.8070 (2)	0.5142 (2)	0.0249 (5)
H10A	0.8515	0.7620	0.4663	0.030*
H10B	0.8367	0.8851	0.5052	0.030*
C11	0.6713 (3)	0.8483 (2)	0.4560 (2)	0.0257 (5)
C12	0.5809 (3)	0.8773 (3)	0.4114 (2)	0.0346 (6)
C13	0.6654 (3)	0.7857 (2)	0.7376 (2)	0.0264 (6)
H13A	0.5603	0.7558	0.7841	0.032*
H13B	0.6760	0.8803	0.6901	0.032*
C14	0.7383 (3)	0.7593 (2)	0.8296 (2)	0.0280 (6)
C15	0.7930 (3)	0.7348 (3)	0.9058 (3)	0.0416 (7)
C16	1.0318 (2)	-0.1219 (2)	1.0003 (2)	0.0219 (5)
H16	1.0540	-0.2052	1.0006	0.026*
C17	1.0369 (2)	-0.0226 (2)	0.8889 (2)	0.0231 (5)
H17	1.0618	-0.0381	0.8128	0.028*
C18	1.0058 (2)	0.0986 (2)	0.88900 (19)	0.0212 (5)
C19	1.0600 (2)	0.3185 (2)	0.74796 (19)	0.0212 (5)
C20	0.9869 (2)	0.4191 (2)	0.69923 (19)	0.0236 (5)
H20	0.9004	0.4016	0.6876	0.028*
C21	1.0402 (2)	0.5458 (2)	0.6673 (2)	0.0244 (5)
H21	0.9900	0.6148	0.6333	0.029*
C22	1.1676 (2)	0.5732 (2)	0.68473 (19)	0.0204 (5)
C23	1.2417 (2)	0.4694 (2)	0.73047 (19)	0.0220 (5)
H23	1.3296	0.4859	0.7406	0.026*
C24	1.1894 (2)	0.3433 (2)	0.76112 (19)	0.0222 (5)
H24	1.2416	0.2740	0.7910	0.027*
C25	1.1369 (3)	0.8061 (2)	0.6209 (2)	0.0268 (6)
H25A	1.1674	0.8791	0.6381	0.032*
H25B	1.0332	0.7765	0.6748	0.032*
C26	1.1529 (2)	0.8513 (2)	0.4870 (2)	0.0239 (5)
C27	1.1667 (3)	0.8879 (2)	0.3791 (2)	0.0323 (6)
C28	1.3208 (3)	0.7176 (2)	0.7156 (2)	0.0273 (6)
H28A	1.3485	0.8115	0.6881	0.033*
H28B	1.4106	0.6782	0.6865	0.033*
C29	1.2574 (3)	0.6603 (2)	0.8560 (2)	0.0308 (6)
C30	1.2069 (4)	0.6076 (3)	0.9671 (3)	0.0454 (8)
H12	0.506 (2)	0.895 (3)	0.377 (2)	0.055 (9)*

supplementary materials

H15	0.838 (3)	0.720 (3)	0.966 (2)	0.055 (9)*
H27	1.177 (3)	0.911 (3)	0.2929 (12)	0.059 (9)*
H30	1.167 (3)	0.570 (3)	1.0577 (10)	0.075 (11)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0315 (9)	0.0200 (8)	0.0219 (9)	0.0000 (7)	-0.0140 (7)	-0.0015 (6)
O2	0.0334 (9)	0.0205 (9)	0.0209 (9)	0.0019 (7)	-0.0148 (7)	-0.0039 (6)
N1	0.0316 (11)	0.0219 (10)	0.0180 (10)	0.0034 (9)	-0.0101 (8)	-0.0054 (8)
N2	0.0283 (11)	0.0203 (10)	0.0230 (10)	0.0053 (9)	-0.0135 (9)	-0.0039 (8)
C1	0.0214 (12)	0.0224 (12)	0.0256 (12)	0.0055 (10)	-0.0126 (10)	-0.0082 (9)
C2	0.0210 (12)	0.0222 (12)	0.0249 (13)	-0.0025 (10)	-0.0069 (10)	-0.0049 (9)
C3	0.0226 (12)	0.0210 (12)	0.0184 (12)	0.0029 (10)	-0.0088 (10)	-0.0046 (9)
C4	0.0198 (11)	0.0215 (12)	0.0211 (12)	0.0029 (10)	-0.0100 (9)	-0.0043 (9)
C5	0.0223 (12)	0.0249 (13)	0.0209 (12)	0.0063 (10)	-0.0095 (10)	-0.0099 (9)
C6	0.0223 (12)	0.0245 (12)	0.0153 (11)	0.0063 (10)	-0.0068 (9)	-0.0049 (9)
C7	0.0195 (11)	0.0203 (12)	0.0197 (12)	0.0059 (10)	-0.0094 (9)	-0.0035 (9)
C8	0.0222 (12)	0.0275 (13)	0.0201 (12)	0.0089 (10)	-0.0105 (10)	-0.0094 (9)
C9	0.0209 (12)	0.0263 (13)	0.0169 (12)	0.0039 (10)	-0.0061 (9)	-0.0029 (9)
C10	0.0272 (13)	0.0220 (12)	0.0232 (12)	0.0003 (10)	-0.0094 (10)	-0.0057 (9)
C11	0.0305 (14)	0.0217 (12)	0.0215 (12)	0.0025 (11)	-0.0099 (10)	-0.0038 (9)
C12	0.0382 (16)	0.0354 (15)	0.0340 (15)	0.0100 (13)	-0.0195 (13)	-0.0115 (12)
C13	0.0298 (13)	0.0209 (12)	0.0283 (13)	0.0044 (11)	-0.0116 (11)	-0.0081 (10)
C14	0.0234 (13)	0.0341 (14)	0.0246 (13)	-0.0012 (11)	-0.0039 (10)	-0.0135 (11)
C15	0.0351 (16)	0.061 (2)	0.0308 (15)	-0.0072 (14)	-0.0113 (13)	-0.0200 (14)
C16	0.0236 (12)	0.0189 (12)	0.0252 (12)	0.0062 (10)	-0.0110 (10)	-0.0090 (9)
C17	0.0234 (12)	0.0268 (13)	0.0193 (12)	0.0038 (10)	-0.0070 (10)	-0.0099 (10)
C18	0.0179 (11)	0.0254 (13)	0.0193 (12)	0.0019 (10)	-0.0088 (9)	-0.0051 (9)
C19	0.0246 (12)	0.0211 (12)	0.0148 (11)	-0.0003 (10)	-0.0057 (9)	-0.0045 (9)
C20	0.0198 (12)	0.0291 (13)	0.0184 (12)	0.0035 (10)	-0.0086 (9)	-0.0036 (9)
C21	0.0241 (12)	0.0255 (13)	0.0194 (12)	0.0085 (10)	-0.0092 (10)	-0.0032 (9)
C22	0.0213 (12)	0.0215 (12)	0.0135 (11)	0.0029 (10)	-0.0054 (9)	-0.0021 (9)
C23	0.0193 (12)	0.0278 (13)	0.0195 (12)	0.0056 (10)	-0.0096 (9)	-0.0073 (9)
C24	0.0232 (12)	0.0254 (13)	0.0180 (12)	0.0072 (10)	-0.0099 (9)	-0.0061 (9)
C25	0.0311 (14)	0.0238 (13)	0.0223 (12)	0.0069 (11)	-0.0085 (10)	-0.0065 (10)
C26	0.0216 (12)	0.0218 (12)	0.0269 (13)	0.0054 (10)	-0.0092 (10)	-0.0074 (10)
C27	0.0332 (15)	0.0343 (15)	0.0312 (16)	0.0047 (12)	-0.0151 (12)	-0.0114 (12)
C28	0.0250 (13)	0.0241 (13)	0.0332 (14)	0.0040 (10)	-0.0126 (11)	-0.0093 (10)
C29	0.0367 (14)	0.0318 (14)	0.0358 (16)	0.0162 (12)	-0.0211 (12)	-0.0193 (12)
C30	0.067 (2)	0.0478 (18)	0.0350 (18)	0.0323 (16)	-0.0280 (16)	-0.0231 (14)

Geometric parameters (\AA , $^\circ$)

O1—C4	1.391 (3)	C13—C14	1.472 (3)
O1—C3	1.395 (2)	C13—H13A	0.9900
O2—C18	1.391 (2)	C13—H13B	0.9900
O2—C19	1.399 (3)	C14—C15	1.175 (3)
N1—C7	1.410 (3)	C15—H15	0.95 (1)

N1—C10	1.457 (3)	C16—C18 ⁱⁱ	1.384 (3)
N1—C13	1.463 (3)	C16—C17	1.389 (3)
N2—C22	1.404 (3)	C16—H16	0.9500
N2—C28	1.458 (3)	C17—C18	1.380 (3)
N2—C25	1.461 (3)	C17—H17	0.9500
C1—C3 ⁱ	1.378 (3)	C18—C16 ⁱⁱ	1.384 (3)
C1—C2	1.391 (3)	C19—C20	1.380 (3)
C1—H1	0.9500	C19—C24	1.388 (3)
C2—C3	1.384 (3)	C20—C21	1.388 (3)
C2—H2	0.9500	C20—H20	0.9500
C3—C1 ⁱ	1.378 (3)	C21—C22	1.405 (3)
C4—C5	1.379 (3)	C21—H21	0.9500
C4—C9	1.381 (3)	C22—C23	1.399 (3)
C5—C6	1.385 (3)	C23—C24	1.382 (3)
C5—H5	0.9500	C23—H23	0.9500
C6—C7	1.399 (3)	C24—H24	0.9500
C6—H6	0.9500	C25—C26	1.467 (3)
C7—C8	1.400 (3)	C25—H25A	0.9900
C8—C9	1.385 (3)	C25—H25B	0.9900
C8—H8	0.9500	C26—C27	1.181 (3)
C9—H9	0.9500	C27—H27	0.950 (10)
C10—C11	1.477 (3)	C28—C29	1.481 (3)
C10—H10A	0.9900	C28—H28A	0.9900
C10—H10B	0.9900	C28—H28B	0.9900
C11—C12	1.180 (3)	C29—C30	1.178 (4)
C12—H12	0.96 (1)	C30—H30	0.956 (10)
C4—O1—C3	120.48 (16)	C14—C13—H13B	109.1
C18—O2—C19	116.42 (16)	H13A—C13—H13B	107.8
C7—N1—C10	119.60 (18)	C15—C14—C13	177.7 (3)
C7—N1—C13	118.73 (18)	C14—C15—H15	177.1 (18)
C10—N1—C13	115.86 (18)	C18 ⁱⁱ —C16—C17	119.6 (2)
C22—N2—C28	117.61 (17)	C18 ⁱⁱ —C16—H16	120.2
C22—N2—C25	119.25 (19)	C17—C16—H16	120.2
C28—N2—C25	116.15 (19)	C18—C17—C16	119.9 (2)
C3 ⁱ —C1—C2	119.6 (2)	C18—C17—H17	120.0
C3 ⁱ —C1—H1	120.2	C16—C17—H17	120.0
C2—C1—H1	120.2	C17—C18—C16 ⁱⁱ	120.50 (19)
C3—C2—C1	119.4 (2)	C17—C18—O2	117.25 (19)
C3—C2—H2	120.3	C16 ⁱⁱ —C18—O2	122.1 (2)
C1—C2—H2	120.3	C20—C19—C24	120.5 (2)
C1 ⁱ —C3—C2	121.0 (2)	C20—C19—O2	118.4 (2)
C1 ⁱ —C3—O1	115.80 (19)	C24—C19—O2	121.0 (2)
C2—C3—O1	123.04 (19)	C19—C20—C21	119.8 (2)
C5—C4—C9	120.1 (2)	C19—C20—H20	120.1
C5—C4—O1	116.31 (19)	C21—C20—H20	120.1
C9—C4—O1	123.34 (19)	C20—C21—C22	120.8 (2)

supplementary materials

C4—C5—C6	120.4 (2)	C20—C21—H21	119.6
C4—C5—H5	119.8	C22—C21—H21	119.6
C6—C5—H5	119.8	C23—C22—N2	119.9 (2)
C5—C6—C7	120.7 (2)	C23—C22—C21	118.0 (2)
C5—C6—H6	119.7	N2—C22—C21	122.11 (19)
C7—C6—H6	119.7	C24—C23—C22	121.2 (2)
C6—C7—C8	117.8 (2)	C24—C23—H23	119.4
C6—C7—N1	121.92 (19)	C22—C23—H23	119.4
C8—C7—N1	120.2 (2)	C23—C24—C19	119.6 (2)
C9—C8—C7	121.2 (2)	C23—C24—H24	120.2
C9—C8—H8	119.4	C19—C24—H24	120.2
C7—C8—H8	119.4	N2—C25—C26	112.17 (19)
C4—C9—C8	119.8 (2)	N2—C25—H25A	109.2
C4—C9—H9	120.1	C26—C25—H25A	109.2
C8—C9—H9	120.1	N2—C25—H25B	109.2
N1—C10—C11	114.87 (19)	C26—C25—H25B	109.2
N1—C10—H10A	108.5	H25A—C25—H25B	107.9
C11—C10—H10A	108.5	C27—C26—C25	179.6 (3)
N1—C10—H10B	108.5	C26—C27—H27	175.8 (18)
C11—C10—H10B	108.5	N2—C28—C29	113.99 (19)
H10A—C10—H10B	107.5	N2—C28—H28A	108.8
C12—C11—C10	177.9 (3)	C29—C28—H28A	108.8
C11—C12—H12	176.0 (17)	N2—C28—H28B	108.8
N1—C13—C14	112.7 (2)	C29—C28—H28B	108.8
N1—C13—H13A	109.1	H28A—C28—H28B	107.6
C14—C13—H13A	109.1	C30—C29—C28	176.1 (3)
N1—C13—H13B	109.1	C29—C30—H30	177 (2)
C3 ⁱ —C1—C2—C3	0.5 (4)	C18 ⁱⁱ —C16—C17—C18	0.6 (4)
C1—C2—C3—C1 ⁱ	-0.5 (4)	C16—C17—C18—C16 ⁱⁱ	-0.6 (4)
C1—C2—C3—O1	-175.8 (2)	C16—C17—C18—O2	-176.80 (19)
C4—O1—C3—C1 ⁱ	146.9 (2)	C19—O2—C18—C17	-142.9 (2)
C4—O1—C3—C2	-37.5 (3)	C19—O2—C18—C16 ⁱⁱ	41.0 (3)
C3—O1—C4—C5	151.1 (2)	C18—O2—C19—C20	-138.0 (2)
C3—O1—C4—C9	-35.0 (3)	C18—O2—C19—C24	45.9 (3)
C9—C4—C5—C6	0.6 (3)	C24—C19—C20—C21	-2.3 (3)
O1—C4—C5—C6	174.64 (18)	O2—C19—C20—C21	-178.41 (18)
C4—C5—C6—C7	0.8 (3)	C19—C20—C21—C22	-0.4 (3)
C5—C6—C7—C8	-1.3 (3)	C28—N2—C22—C23	-23.4 (3)
C5—C6—C7—N1	177.5 (2)	C25—N2—C22—C23	-173.04 (19)
C10—N1—C7—C6	5.2 (3)	C28—N2—C22—C21	158.4 (2)
C13—N1—C7—C6	157.2 (2)	C25—N2—C22—C21	8.8 (3)
C10—N1—C7—C8	-176.13 (19)	C20—C21—C22—C23	2.4 (3)
C13—N1—C7—C8	-24.1 (3)	C20—C21—C22—N2	-179.4 (2)
C6—C7—C8—C9	0.5 (3)	N2—C22—C23—C24	179.92 (19)
N1—C7—C8—C9	-178.26 (19)	C21—C22—C23—C24	-1.8 (3)
C5—C4—C9—C8	-1.3 (3)	C22—C23—C24—C19	-0.8 (3)
O1—C4—C9—C8	-174.98 (19)	C20—C19—C24—C23	2.9 (3)
C7—C8—C9—C4	0.8 (3)	O2—C19—C24—C23	178.92 (18)

C7—N1—C10—C11	72.2 (3)	C22—N2—C25—C26	-82.9 (2)
C13—N1—C10—C11	-80.6 (3)	C28—N2—C25—C26	127.0 (2)
C7—N1—C13—C14	85.2 (2)	C22—N2—C28—C29	-56.4 (3)
C10—N1—C13—C14	-121.7 (2)	C25—N2—C28—C29	94.1 (2)

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12 \cdots O1 ⁱⁱⁱ	0.96 (1)	2.66 (3)	3.263 (3)	121 (2)
C27—H27 \cdots O2 ^{iv}	0.95 (1)	2.68 (2)	3.285 (3)	122 (2)

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

Fig. 1

