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## Structure Reports

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

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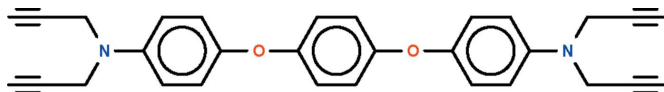
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 Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.063;  $wR$  factor = 0.172; data-to-parameter ratio = 15.9.

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  $61.4(2)^\circ$  with respect to the flanking aromatic ring [dihedral angle =  $70.7(3)^\circ$  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: Shemsi *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  
 $\alpha = 68.687(6)^\circ$   
 $\beta = 69.601(7)^\circ$   
 $\gamma = 88.529(5)^\circ$ 
 $V = 1162.19(13)$  Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.08$  mm<sup>-1</sup>  
 $T = 100$  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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.33$  e Å<sup>-3</sup>

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).

## References

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## supporting information

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

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

**Kiramat Shah, M. Raza Shah and Seik Weng Ng**

**S1. Comment**

1,4-Bis(4-aminophenoxy)benzene is a precursor for the synthesis of polyamides owing the functional amino  $\text{-NH}_2$  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).

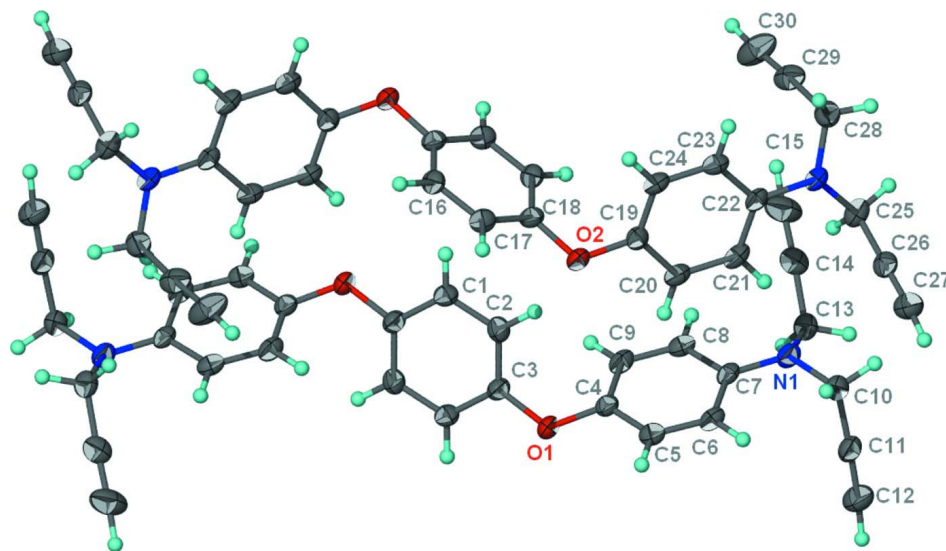
**S2. Experimental**

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%.

**S3. Refinement**

Carbon-bound H-atoms were placed in calculated positions [ $\text{C-H}$  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  $\text{C-H}$   $0.95 \pm 0.01$  Å; their temperature factors were refined.

**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of  $C_{30}H_{24}N_2O_2$  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

$C_{30}H_{24}N_2O_2$

$M_r = 444.51$

Triclinic,  $P\bar{1}$

Hall symbol: -P 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) Å<sup>3</sup>

$Z = 2$

$F(000) = 468$

$D_x = 1.270$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2448 reflections

$\theta = 2.2$ – $29.2$ °

$\mu = 0.08$  mm<sup>-1</sup>

$T = 100$  K

Prism, colorless

$0.30 \times 0.10 \times 0.05$  mm

#### Data collection

Agilent SuperNova Dual

diffractometer with an Atlas detector

Radiation source: SuperNova (Mo) X-ray

Source

Mirror monochromator

Detector resolution: 10.4041 pixels mm<sup>-1</sup>

$\omega$  scans

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  $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 2.2$ °

$h = -12 \rightarrow 12$

$k = -12 \rightarrow 14$

$l = -13 \rightarrow 15$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.172$

$S = 1.06$

5142 reflections

323 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

$$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2]$$

where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.33 \text{ e } \text{\AA}^{-3}$

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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)*
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 (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 (Å, °)*

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 <sup>ii</sup>	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 <sup>i</sup>	1.378 (3)	C18—C16 <sup>ii</sup>	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 <sup>i</sup>	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 <sup>ii</sup> —C16—C17	119.6 (2)
C22—N2—C28	117.61 (17)	C18 <sup>ii</sup> —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 <sup>i</sup> —C1—C2	119.6 (2)	C18—C17—H17	120.0
C3 <sup>i</sup> —C1—H1	120.2	C16—C17—H17	120.0
C2—C1—H1	120.2	C17—C18—C16 <sup>ii</sup>	120.50 (19)
C3—C2—C1	119.4 (2)	C17—C18—O2	117.25 (19)
C3—C2—H2	120.3	C16 <sup>ii</sup> —C18—O2	122.1 (2)
C1—C2—H2	120.3	C20—C19—C24	120.5 (2)
C1 <sup>i</sup> —C3—C2	121.0 (2)	C20—C19—O2	118.4 (2)
C1 <sup>i</sup> —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)
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 <sup>i</sup> —C1—C2—C3	0.5 (4)	C18 <sup>ii</sup> —C16—C17—C18	0.6 (4)
C1—C2—C3—C1 <sup>i</sup>	-0.5 (4)	C16—C17—C18—C16 <sup>ii</sup>	-0.6 (4)
C1—C2—C3—O1	-175.8 (2)	C16—C17—C18—O2	-176.80 (19)

C4—O1—C3—C1 <sup>i</sup>	146.9 (2)	C19—O2—C18—C17	-142.9 (2)
C4—O1—C3—C2	-37.5 (3)	C19—O2—C18—C16 <sup>ii</sup>	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 <sup>iii</sup>	0.96 (1)	2.66 (3)	3.263 (3)	121 (2)
C27—H27 $\cdots$ O2 <sup>iv</sup>	0.95 (1)	2.68 (2)	3.285 (3)	122 (2)

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