

C3a	0.8420 (4)	-0.1649 (3)	0.6784 (3)	0.048 (1)
C4a	0.9295 (4)	-0.1401 (3)	0.7635 (3)	0.051 (1)
C5a	0.9348 (4)	0.0046 (3)	0.7470 (3)	0.050 (1)
C1b	0.6486 (3)	0.3854 (3)	0.1309 (3)	0.0314 (9)
C2b	0.7729 (4)	0.4708 (3)	0.0206 (3)	0.039 (1)
C3b	0.8705 (4)	0.4245 (3)	-0.0904 (3)	0.045 (1)
C4b	0.8437 (4)	0.2914 (3)	-0.0927 (3)	0.049 (1)
C5b	0.7195 (4)	0.2056 (3)	0.0160 (3)	0.051 (1)
C6b	0.6217 (4)	0.2515 (3)	0.1277 (3)	0.043 (1)

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Table 2. Geometric parameters (Å, °)

S—C1	1.762 (4)	N3—C5a	1.350 (4)
S—C3	1.749 (3)	C2—C3	1.332 (5)
O—C2a	1.364 (5)	C2—C5	1.492 (4)
N1—C1	1.363 (3)	C4—C1b	1.516 (4)
N1—C2	1.404 (4)	C1a—C2a	1.412 (5)
N1—C4	1.471 (5)	C2a—C3a	1.363 (4)
N2—C1	1.297 (4)	C3a—C4a	1.392 (6)
N2—C1a	1.383 (3)	C4a—C5a	1.366 (5)
N3—C1a	1.327 (5)		
C1—S—C3	90.3 (2)	S—C3—C2	112.8 (2)
C1—N1—C2	115.2 (3)	N1—C4—C1b	112.4 (2)
C1—N1—C4	119.2 (2)	N2—C1a—N3	123.6 (3)
C2—N1—C4	125.5 (2)	N2—C1a—C2a	114.8 (3)
C1—N2—C1a	121.0 (3)	N3—C1a—C2a	121.7 (2)
C1a—N3—C5a	117.7 (3)	O—C2a—C1a	118.9 (2)
S—C1—N1	109.3 (2)	O—C2a—C3a	121.2 (3)
S—C1—N2	129.3 (2)	C1a—C2a—C3a	119.9 (4)
N1—C1—N2	121.4 (3)	C2a—C3a—C4a	118.3 (3)
N1—C2—C3	112.3 (2)	C3a—C4a—C5a	118.7 (3)
N1—C2—C5	121.7 (3)	N3—C5a—C4a	123.8 (4)
C3—C2—C5	126.0 (3)		
C1—N1—C4—C1b	-74.8 (3)	C1—N2—C1a—C2a	-174.6 (3)
C2—N1—C4—C1b	104.0 (3)	N1—C4—C1b—C2b	-52.7 (4)
C1a—N2—C1—S	-0.1 (4)	N1—C4—C1b—C6b	129.0 (3)
C1a—N2—C1—N1	179.4 (3)	N2—C1a—C2a—O	-0.7 (4)
C1—N2—C1a—N3	4.8 (4)		

A mixture of 2-(2-oxopropylthio)oxazolo[4,5-*b*]pyridine, benzylamine and perchloric acid was warmed at 313 K for 1h. After neutralization with HCl it was left in a cool place overnight. The product was filtered, dried and recrystallized from EtOH/H₂O (2:1).

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71406 (12 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: NA1049]

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Structures of 1,1-Diphenyl-2-aza-1,3-butadienes. IV. 3-Cyano-4-(2,4-dichlorophenyl)-1,1-diphenyl-2-aza-1,3-butadiene (24CLPD) and 3-Cyano-4-(2,4-dimethoxyphenyl)-1,1-diphenyl-2-aza-1,3-butadiene (24MOPD)

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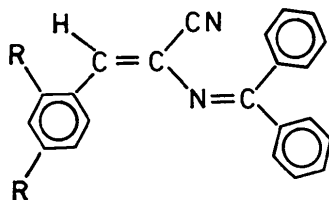
Abstract

The 2,4-disubstituted derivatives [24CLPD: 3-(2,4-dichlorophenyl)-2-(diphenylmethyleamino)propenenitrile, C₂₂H₁₄Cl₂N₂; 24MOPD: 3-(2,4-dimethoxyphenyl)-2-(diphenylmethyleamino)propenenitrile, C₂₄H₂₀N₂O₂] have the *Z* configuration, as in the previously described monosubstituted representatives from this series. The C1c—C3 bond length [in Phc—C3=C2(CN)—N1=C1(Pha)(Phb)] is 1.459 (5) Å in 24CLPD, which is slightly longer than in 24MOPD, 1.448 (3) Å, while the C3—C2 bond in 24CLPD, 1.337 (5) Å, is shorter than in 24MOPD, 1.357 (4) Å. The *c* ring is twisted out of the C1c—C3=C2(N1)—C4 plane by 10.9 (2) and 21.8 (2)° for 24CLPD and 24MOPD, respectively. The C1=N1—C2—C3 torsion angle in 24MOPD, 151.6 (3)°, is the largest among those determined so far. In 24CLPD, this angle has the mean value 135.9 (3)°. The dihedral angles between the N1=C1(C1a)—C1b plane and the *a* and *b* phenyl rings are 15.0 (1)/20.4 (3) and 58.3 (1)/62.3 (1)° for 24CLPD/24MOPD, respectively. Correspondingly, the C1a—C1 bond distances, 1.481 (4)/1.488 (5) Å, are shorter than C1b—C1, 1.488 (4)/1.490 (3) Å. The molecules are held together only by dispersion forces and both compounds obey the close-

packing principle. The structure of 24MOPD can be described as layers of centrosymmetric dimers, related by inversion centers and parallel to the *ac* face of the unit cell. In the structure of 24CLPD, the layers are parallel to the *ab* face and are related by a system of 2 and 2₁ axes; in the layer, the centrosymmetric dimers are ordered in chains extended along the *ab* face diagonals and related only by inversion centers.

Comment

In previous papers of this series, only monosubstituted-phenyl-3-cyano-1,1-diphenyl-2-azabutadienes have been described (Angelova, Maciček & Dryanska, 1993*a,b*; Maciček, Angelova & Dryanska, 1993). It has not been possible to note any direct correlation between the type of substituent and the geometry of the molecule. By investigating disubstituted derivatives (I), it was expected that the influence of the substituents on the π -conjugation in the system would become better understood.



(I) $R = \text{Cl}, \text{OCH}_3$

Interatomic distances and angles found for both compounds are in good agreement with previously reported values. Bond length variations in the C1c—C3—C2 fragment are worth consideration as they should be most influenced by the presence of substituents. The C1c—C3 bond in 24CLPD is longer than in 24MOPD by more than 2σ and the C3—C2 bond in 24CLPD is shorter than in 24MOPD by more than 4σ . This is consistent with the recently proposed bond polarity indexes, related to the group electronegativity of Cl⁻ and MeO⁻ groups [MeO approximated by OH since it is not included in the list (Reed & Allen, 1992)]. Because of its higher electronegativity, the Cl atom is expected to disturb the π -conjugated system in the Phc—C=C fragment to a greater extent than the methoxy group. Moreover, a comparison of the above values with the statistically calculated mean bond lengths in conjugated C=C—C_{ar} systems [1.339 (11), 1.470 (15) Å; Allen *et al.*, 1987] indicates that the conjugation in 24MOPD is enhanced, most likely by the mesomeric effect of the methoxy group. Similar bond variations to 24CLPD were also observed in 3-cyano-4-(4-cyanophenyl)-1,1-diphenyl-2-aza-1,3-butadiene (4CNPD; Angelova *et al.*, 1993*b*), where the corresponding C1c—C3—C2 bond lengths are 1.466 (9) and 1.336 (9) Å, but the large e.s.d.'s prevent any further conclusions.

The *c* ring is twisted out of the C1c—C3=C2(N1)—C4 plane by angles of 10.9 (2) and 21.8 (2)° for 24CLPD and 24MOPD, respectively. As mentioned earlier by Angelova *et al.* (1993*a*), this rotation could be caused by the H3...Cl/O—C2c intramolecular interactions. The relevant H...Cl/O distances are 2.586 (1) and 2.335 (2) Å. The orientation of the methoxy groups toward the ring is identical to 3-cyano-1,1-diphenyl-4-(2-methoxyphenyl)-2-aza-1,3-butadiene (2MOPD) and 3-cyano-1,1-diphenyl-4-(4-methoxyphenyl)-2-aza-1,3-butadiene (4MOPD; Angelova *et al.*, 1993*a*). The C5—O1—C2c—C3c torsion angles are -3.1 (5) and -9.8 (3)° and C6—O2—C4c—C5c are -0.7 (5) and -3.5 (3)° for 24MOPD and 4MOPD, respectively. The C1—N1—C2—C3 torsion angle in 24MOPD, 151.6 (3)°, is the largest among those determined so far, varying in the range 129.2 (4)–139.5 (3)° (Angelova *et al.*, 1993*a,b*; Maciček *et al.*, 1993). In 24CLPD, this angle has the mean value 135.9 (5)°. The dihedral angles between the non-substituted phenyl rings are 70.0 (1) and 74.7 (1)° for 24CLPD and 24MOPD, respectively. The dihedral angles between the N1=C1(C1a)—C1b plane and the *a* and *b* rings are 15.0 (1)/20.4 (3) and 58.3 (1)/62.3 (1)°, respectively. Hence, slightly greater conjugation is expected between the *a* ring and the azene part of the molecule. Indeed, in both compounds the C1a—C1 bond distance [1.481 (4) and 1.488 (5) Å] is shorter than C1b—C1 [1.488 (4) and 1.490 (3) Å]. This trend in bond length differences persists throughout the whole series. The corresponding mean values are 1.484 (4) and 1.490 (8) Å. ORTEP drawings of 24CLPD and 24MOPD are shown in Figs. 1 and 2.

The molecules are held together only by dispersion forces and both compounds obey the close-packing principle (Kitaigorodskii, 1961). The number of neighbors calculated according to Zefirov & Zorkii (1978) is 11 + 1 and 13 for 24CLPD and 24MOPD, respectively. Intermolecular distances slightly shorter than the sums of

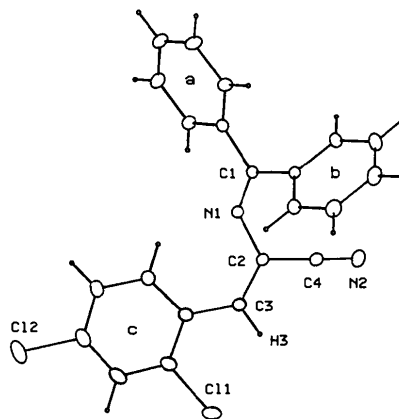


Fig. 1. ORTEP (Johnson, 1976) drawing of the 24CLPD molecule with the atom-numbering scheme and 10% probability thermal ellipsoids; H atom spheres are arbitrarily reduced.

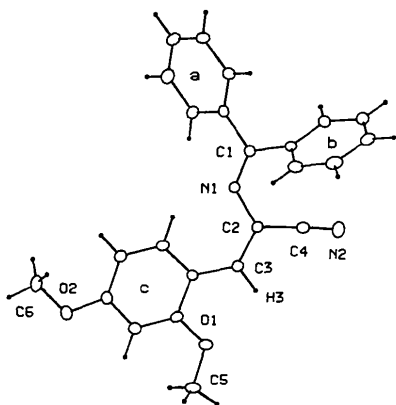


Fig. 2. ORTEP (Johnson, 1976) drawing of the 24MOPD molecule with the atom-numbering scheme and 10% probability thermal ellipsoids; H atom spheres are arbitrarily reduced.

the van der Waals radii occur for $\text{Cl2} \cdots \text{H3}(\frac{1}{2} - x, -\frac{1}{2} + y, \frac{1}{2} - z)$, 2.960 (1) Å [van der Waals radii sum 3.06 Å (Zefirov & Zorkii, 1978)], in 24CLPD, and $\text{C4b} \cdots \text{H5c}(1 - x, 1 - y, 1 - z)$, 2.780 (3) Å (van der Waals radii sum 2.87 Å), in 24MOPD.

A three-dimensional structure could be sliced into layers, which could be further cut into chains, groups, rings, etc. (Kitaigorodskii, 1961). Since the criterion for six

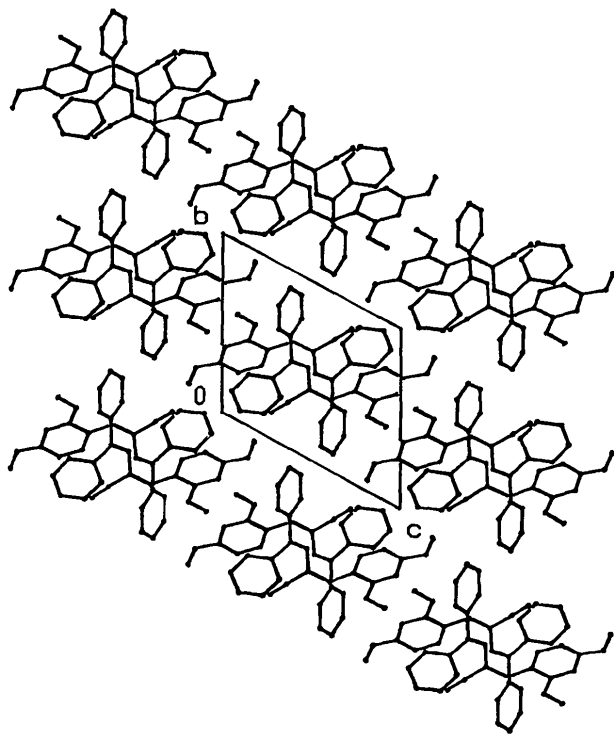


Fig. 3. Molecular packing in the structure of 24MOPD viewed down the *a* axis. (A view of a separated *ac* layer is available as supplementary material.) H atoms are omitted for clarity.

neighbors in a layer allows more than one choice for such irregular molecules, the ultimate choice has to be accomplished by symmetry considerations. The structure of 24MOPD can be described as layers related by inversion centers and parallel to the *ac* face of the unit cell (Fig. 3). Each layer is composed of centrosymmetric dimers also related by inversion centers (an additional packing diagram is available as supplementary material). In the structure of 24CLPD, the layers are parallel to the *ab* face and are related by the system of 2 and 2_1 axes intrinsic for the $C2/c$ (No. 15) space group (Fig. 4). The centrosymmetric dimers in each layer are only related by inversion centers and are ordered in chains extended along the *ab* face diagonals (an additional packing diagram is available as supplementary material).

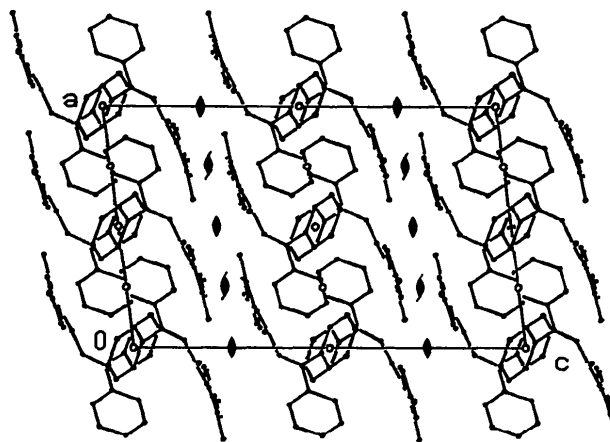


Fig. 4. Molecular packing in the structure of 24CLPD viewed down the *b* axis with the space group symmetry operations denoted. (A view of an *ab* layer with the chains clearly separated is available as supplementary material.) H atoms are omitted for clarity.

Experimental

24CLPD

Crystal data

$\text{C}_{22}\text{H}_{14}\text{Cl}_2\text{N}_2$
 $M_r = 377.27$
 Monoclinic
 $C2/c$
 $a = 11.956$ (3) Å
 $b = 16.275$ (3) Å
 $c = 19.501$ (4) Å
 $\beta = 97.03$ (1)°
 $V = 3766$ (2) Å³
 $Z = 8$
 $D_x = 1.330$ Mg m⁻³

Mo $K\alpha$ radiation
 $\lambda = 0.71073$ Å
 Cell parameters from 22 reflections
 $\theta = 20 - 21.08^\circ$
 $\mu = 0.35$ mm⁻¹
 $T = 292$ K
 Prismatic
 $0.46 \times 0.26 \times 0.13$ mm
 Yellow

Data collection

Enraf-Nonius CAD-4 diffractometer

$R_{\text{int}} = 0.020$
 $\theta_{\text{max}} = 25^\circ$

Continuous scan profile $h = 0 \rightarrow 14$
 Absorption correction: $k = 0 \rightarrow 19$
 none $l = -23 \rightarrow 22$
 3473 measured reflections 3 standard reflections
 3305 independent reflections frequency: 120 min
 1831 observed reflections intensity variation: -0.3%
 $[I > 3.0\sigma(I)]$

Refinement

Refinement on F $w = 1/[\sigma^2(F) + (0.040F)^2]$
 $R = 0.041$ $(\Delta/\sigma)_{\max} = 0.001$
 $wR = 0.061$ $\Delta\rho_{\max} = 0.301 \text{ e } \text{\AA}^{-3}$
 $S = 1.109$ $\Delta\rho_{\min} = -0.254 \text{ e } \text{\AA}^{-3}$
 1831 reflections Atomic scattering factors
 235 parameters from *SDP/PDP* (Enraf-
 H atoms refined as riding Nonius, 1985)

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2) for 24CLPD

$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U_{eq}
Cl1	0.11484 (7)	0.02633 (7)	0.19955 (5)	0.0745 (3)
Cl2	0.2765 (1)	-0.27924 (7)	0.19722 (7)	0.1118 (5)
N1	0.5301 (2)	0.0864 (2)	0.1325 (1)	0.0461 (7)
N2	0.4351 (3)	0.2828 (2)	0.1609 (2)	0.079 (1)
C1	0.5745 (2)	0.1066 (2)	0.0780 (2)	0.0399 (8)
C2	0.4340 (2)	0.1246 (2)	0.1531 (2)	0.0449 (9)
C3	0.3488 (3)	0.0833 (2)	0.1754 (2)	0.0479 (9)
C4	0.4327 (3)	0.2133 (2)	0.1563 (2)	0.055 (1)
C1a	0.6793 (2)	0.0624 (2)	0.0672 (2)	0.0387 (8)
C2a	0.7366 (3)	0.0178 (2)	0.1212 (2)	0.0516 (9)
C3a	0.8300 (3)	-0.0285 (2)	0.1114 (2)	0.058 (1)
C4a	0.8682 (3)	-0.0304 (2)	0.0470 (2)	0.060 (1)
C5a	0.8137 (3)	0.0142 (2)	-0.0061 (2)	0.061 (1)
C6a	0.7188 (3)	0.0611 (2)	0.0030 (2)	0.0492 (9)
C1b	0.5236 (2)	0.1665 (2)	0.0256 (2)	0.0409 (8)
C2b	0.5832 (3)	0.2353 (2)	0.0084 (2)	0.054 (1)
C3b	0.5339 (3)	0.2908 (2)	-0.0392 (2)	0.071 (1)
C4b	0.4248 (3)	0.2784 (2)	-0.0706 (2)	0.075 (1)
C5b	0.3660 (3)	0.2102 (2)	-0.0542 (2)	0.072 (1)
C6b	0.4153 (3)	0.1547 (2)	-0.0067 (2)	0.055 (1)
C1c	0.3327 (2)	-0.0053 (2)	0.1795 (2)	0.0446 (8)
C2c	0.2288 (3)	-0.0382 (2)	0.1923 (2)	0.055 (1)
C3c	0.2103 (3)	-0.1214 (2)	0.1982 (2)	0.068 (1)
C4c	0.2978 (3)	-0.1738 (2)	0.1910 (2)	0.068 (1)
C5c	0.4025 (3)	-0.1460 (2)	0.1784 (2)	0.064 (1)
C6c	0.4184 (3)	-0.0625 (2)	0.1727 (2)	0.053 (1)

Table 2. Geometric parameters (\AA , $^\circ$) for 24CLPD

Cl1—C2c	1.740 (4)	C1—C1a	1.481 (4)
Cl2—C4c	1.742 (4)	C1—C1b	1.488 (4)
N1—C1	1.288 (4)	C2—C3	1.337 (5)
N1—C2	1.407 (4)	C2—C4	1.446 (5)
N2—C4	1.134 (5)	C3—C1c	1.459 (5)
C1—N1—C2	123.8 (3)	C2—C3—C1c	128.7 (3)
N1—C1—C1a	115.7 (3)	N2—C4—C2	177.3 (4)
N1—C1—C1b	124.0 (3)	C11—C2c—C1c	120.2 (3)
C1a—C1—C1b	120.2 (3)	C11—C2c—C3c	116.8 (3)
N1—C2—C3	123.6 (3)	C12—C4c—C3c	119.1 (3)
N1—C2—C4	117.8 (3)	C12—C4c—C5c	118.6 (3)
C3—C2—C4	118.3 (3)		
C2—N1—C1—C1a	176.7 (3)	N1—C1—C1b—C2b	123.4 (3)
C2—N1—C1—C1b	-6.8 (5)	N1—C2—C3—C1c	-3.9 (5)
C1—N1—C2—C3	135.9 (3)	C4—C2—C3—C1c	-177.9 (3)
C1—N1—C2—C4	-50.1 (4)	C2—C3—C1c—C2c	-168.3 (3)
N1—C1—C1a—C2a	-14.4 (4)	C3—C1c—C2c—C11	3.0 (4)

24MOPD*Crystal data*

$\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}_2$
 $M_r = 368.43$
 Triclinic
 $P\bar{1}$
 $a = 9.991 (4) \text{ \AA}$
 $b = 10.012 (3) \text{ \AA}$
 $c = 11.763 (2) \text{ \AA}$
 $\alpha = 113.46 (2)^\circ$
 $\beta = 108.65 (2)^\circ$
 $\gamma = 96.59 (3)^\circ$
 $V = 982 (1) \text{ \AA}^3$
 $Z = 2$

$D_x = 1.245 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\lambda = 0.71073 \text{ \AA}$
 Cell parameters from 22 reflections
 $\theta = 20.09\text{--}21.50^\circ$
 $\mu = 0.07 \text{ mm}^{-1}$
 $T = 292 \text{ K}$
 Plate
 $0.29 \times 0.26 \times 0.06 \text{ mm}$
 Yellow, transparent

Data collection

Enraf-Nonius CAD-4 diffractometer

Continuous scan profile

Absorption correction: none

4087 measured reflections

3852 independent reflections

1592 observed reflections

$[I > 2.0\sigma(I)]$

$R_{\text{int}} = 0.023$

$\theta_{\text{max}} = 26^\circ$

$h = 0 \rightarrow 12$

$k = -12 \rightarrow 12$

$l = -14 \rightarrow 13$

3 standard reflections

frequency: 120 min

intensity variation: -0.3%

Refinement

Refinement on F

$R = 0.058$

$wR = 0.029$

$S = 1.573$

1592 reflections

254 parameters

H atoms refined as riding

$w = 1/[\sigma^2(F) + (0.001F)^2]$

$(\Delta/\sigma)_{\max} = 0.373$

$\Delta\rho_{\max} = 0.213 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.220 \text{ e } \text{\AA}^{-3}$

Extinction correction: Stout & Jensen (1968) formula
 17.16

Extinction coefficient:
 6.918×10^7

Atomic scattering factors from *SDP/PDP* (Enraf-Nonius, 1985)

Table 3. Fractional atomic coordinates and equivalent isotropic thermal parameters (\AA^2) for 24MOPD

$$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U_{eq}
O1	-0.1558 (2)	0.5890 (2)	0.1858 (2)	0.0662 (8)
O2	-0.0918 (2)	0.1719 (2)	-0.1470 (2)	0.0714 (9)
N1	0.2116 (2)	0.4929 (2)	0.5199 (2)	0.0514 (9)
N2	0.1905 (3)	0.8526 (3)	0.7242 (3)	0.094 (1)
C1	0.3319 (3)	0.5100 (3)	0.6144 (2)	0.046 (1)
C2	0.1618 (3)	0.6146 (3)	0.5105 (3)	0.048 (1)
C3	0.0767 (3)	0.6073 (3)	0.3910 (3)	0.052 (1)
C4	0.1813 (3)	0.7483 (3)	0.6315 (3)	0.060 (1)
C5	-0.2756 (3)	0.5940 (3)	0.0831 (3)	0.069 (1)
C6	-0.0121 (3)	0.0628 (3)	-0.1847 (3)	0.085 (2)
C1a	0.3612 (3)	0.3694 (3)	0.6190 (3)	0.053 (1)
C2a	0.2456 (4)	0.2394 (3)	0.5559 (3)	0.071 (1)
C3a	0.2709 (4)	0.1072 (3)	0.5576 (3)	0.103 (2)
C4a	0.4110 (4)	0.1044 (4)	0.6217 (3)	0.121 (2)
C5a	0.5270 (4)	0.2307 (3)	0.6829 (3)	0.105 (2)
C6a	0.5026 (3)	0.3650 (3)	0.6839 (3)	0.072 (1)
C1b	0.4435 (3)	0.6578 (3)	0.7157 (3)	0.045 (1)
C2b	0.4770 (3)	0.7116 (3)	0.8529 (3)	0.058 (1)
C3b	0.5777 (3)	0.8525 (3)	0.9450 (3)	0.069 (1)
C4b	0.6461 (3)	0.9377 (3)	0.9014 (3)	0.077 (2)
C5b	0.6151 (3)	0.8831 (3)	0.7656 (3)	0.077 (1)
C6b	0.5127 (3)	0.7432 (3)	0.6717 (3)	0.062 (1)
C1c	0.0357 (3)	0.4873 (3)	0.2555 (3)	0.046 (1)

C2c	-0.0827 (3)	0.4824 (3)	0.1481 (3)	0.050 (1)
C3c	-0.1241 (3)	0.3758 (3)	0.0163 (3)	0.054 (1)
C4c	-0.0455 (3)	0.2702 (3)	-0.0119 (3)	0.052 (1)
C5c	0.0722 (3)	0.2694 (3)	0.0900 (3)	0.056 (1)
C6c	0.1107 (3)	0.3779 (3)	0.2215 (3)	0.054 (1)

Table 4. Geometric parameters (Å, °) for 24MOPD

O1—C5	1.425 (4)	N2—C4	1.138 (4)
O1—C2c	1.370 (4)	C1—C1a	1.488 (5)
O2—C6	1.437 (4)	C1—C1b	1.490 (3)
O2—C4c	1.374 (3)	C2—C3	1.357 (4)
N1—C1	1.287 (3)	C2—C4	1.450 (4)
N1—C2	1.399 (4)	C3—C1c	1.448 (3)
C5—O1—C2c	118.6 (2)	C3—C2—C4	116.2 (3)
C6—O2—C4c	117.7 (2)	C2—C3—C1c	128.3 (3)
C1—N1—C2	123.1 (2)	N2—C4—C2	177.1 (3)
N1—C1—C1a	116.5 (2)	O1—C2c—C1c	114.9 (2)
N1—C1—C1b	125.1 (3)	O1—C2c—C3c	122.8 (3)
C1a—C1—C1b	118.4 (2)	O2—C4c—C5c	124.1 (3)
N1—C2—C3	122.8 (2)	C3c—C4c—C5c	121.4 (2)
N1—C2—C4	120.4 (3)		
C2—N1—C1—C1a	173.5 (3)	N1—C1—C1b—C2b	118.2 (4)
C2—N1—C1—C1b	-7.9 (5)	N1—C2—C3—C1c	-7.4 (5)
C1—N1—C2—C3	151.6 (3)	C4—C2—C3—C1c	-178.6 (3)
C1—N1—C2—C4	-37.6 (4)	C2—C3—C1c—C2c	163.5 (3)
N1—C1—C1a—C2a	-20.3 (4)		

24CLPD and 24MOPD were synthesized according to a previously described procedure (Dryanska, 1990). 24CLPD: m.p. 436–437 K (from ethanol/ethylacetate); ^1H NMR (80 MHz, CDCl_3) δ 6.94 (s, 1H, CH=), 7.00–8.00 (m, 13H, H_{phenyl}); elemental analysis found/calculated C 70.16/70.04, H 3.78/3.74, N 7.20/7.43%. 24MOPD: m.p. 410–411 K (from ethanol); ^1H NMR (80 MHz, CDCl_3) δ 3.72, 3.78 (ss, 6H, $2\text{CH}_3\text{O}$), 7.01 (s, 1H, CH=), 6.90–7.90 (m, 13H, H_{phenyl}); elemental analysis found/calculated C 78.49/78.24, H 5.77/5.47, N 7.90/7.60%.

Data collection: CAD-4 (Enraf–Nonius, 1988). Data reduction: SDP/PDP (Enraf–Nonius, 1985). Program(s) used to solve structure: MULTAN11/82 (Main *et al.*, 1982). Program(s) used to refine structure: SDP/PDP. Molecular graphics: ORTEPII (Johnson, 1976). Software used to prepare material for publication: KAPPA (Maciček, 1992).

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry, along with additional packing diagrams, have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 71423 (28 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: KA1045]

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Structure of *N*-Acetyl-L-prolylglycinamide

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Abstract

In the crystal, two *N*-acetyl-L-prolylglycinamide molecules form the asymmetric unit and are linked as a dimer by two hydrogen bonds between the N—H groups and amidic O atoms. Each molecule shares six hydrogen bonds with three translated conformers. All the hydrogen bonds lie approximately in planes, which separate the apolar regions. In both independent molecules, the puckering of the proline rings can be described as slightly distorted C_2 – C^β -*exo* conformations.