

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2-(1-Propyl-2,6-distyryl-1,4-dihydropyridin-4-ylidene)malononitrile

Kwang Ha, Joon Heo and Hyung Jin Kim*

 School of Applied Chemical Engineering, Center for Functional Nano Fine Chemicals, Chonnam National University, Gwangju 500-757, Republic of Korea
 Correspondence e-mail: hyungkim@chonnam.ac.kr

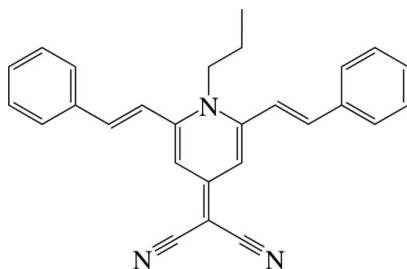
Received 16 November 2009; accepted 17 November 2009

 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.061; wR factor = 0.201; data-to-parameter ratio = 16.3.

In the title compound, $\text{C}_{27}\text{H}_{23}\text{N}_3$, the dihedral angles between the central pyridine ring and the two outer benzene rings are 32.6 (1) and 52.0 (1)°. The compound displays intermolecular π - π interactions between adjacent six-membered rings, the shortest centroid-centroid distance being 3.981 (3) Å.

Related literature

For the synthesis of the starting material, 2-(2,6-dimethylpyridin-4(1*H*)-ylidene)malononitrile, see: Kato *et al.* (1960). For an alternative synthesis of the title compound, see: Peng *et al.* (2006). For the uses and crystal structures of 4-(dicyanomethylene)-2-methyl-6-[(dimethylamino)styryl]-4*H*-pyran derivatives, see: Tang *et al.* (1989); Chen *et al.* (2000); Ju *et al.* (2006); Tong *et al.* (2006).



Experimental

Crystal data

 $\text{C}_{27}\text{H}_{23}\text{N}_3$
 $M_r = 389.48$
 Monoclinic, $P2_1/c$
 $a = 16.586$ (2) Å
 $b = 17.827$ (2) Å
 $c = 7.4543$ (9) Å
 $\beta = 99.790$ (3)°

 $V = 2171.9$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.07$ mm⁻¹
 $T = 293$ K
 $0.20 \times 0.20 \times 0.17$ mm

Data collection

 Bruker SMART 1000 CCD diffractometer
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.630$, $T_{\max} = 1.000$

 12600 measured reflections
 4433 independent reflections
 2084 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.201$
 $S = 1.01$
 4433 reflections

 272 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.14$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.16$ e Å⁻³

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

This study was supported financially by Chonnam National University, 2008.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2689).

References

- Bruker (2000). SADABS, SMART and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.
- Chen, C. H., Tang, C. W., Shi, J. & Klubek, K. P. (2000). *Thin Solid Films*, **363**, 327–331.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Ju, H., Wan, Y., Yu, W., Liu, A., Liu, Y., Ren, Y., Tao, X. & Zou, D. (2006). *Thin Solid Films*, **515**, 2403–2409.
- Kato, H., Ogawa, T. & Ohta, M. (1960). *Bull. Chem. Soc. Jpn.* **33**, 1468–1469.
- Peng, Q., Kang, E. T., Neoh, K. G., Xiao, D. & Zou, D. (2006). *J. Mater. Chem.* **16**, 376–383.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Tang, C. W., VanSlyke, S. A. & Chen, C. H. (1989). *J. Appl. Phys.* **65**, 3610–3616.
- Tong, H., Dong, Y., Häussler, M., Hong, Y., Lam, J. W. Y., Sung, H. H.-Y., Williams, I. D., Kwok, H. S. & Tang, B. Z. (2006). *Chem. Phys. Lett.* **428**, 326–330.

supporting information

Acta Cryst. (2009). E65, o3131 [doi:10.1107/S1600536809048892]

2-(1-Propyl-2,6-distyryl-1,4-dihydropyridin-4-ylidene)malononitrile**Kwang Ha, Joon Heo and Hyung Jin Kim****S1. Comment**

4-(Dicyanomethylene)-2-methyl-6-[(dimethylamino)styryl]-4*H*-pyran (DCM) and its analogs have been utilized as highly fluorescent dopants in organic light-emitting diodes (OLED) (Tang *et al.*, 1989; Chen *et al.*, 2000). In a recent year, a modified DCM, 2-[2,6-bis(2-arylviny)pyridin-4-ylidene]malononitrile (BPM), has been prepared from the corresponding (pyran-4-yliden)malononitrile derivative to obtain an efficient fluorescent material for OLED (Peng *et al.*, 2006). However, their yields were low. To improve the yields of BPM derivatives, we synthesized the title compound by Knoevenagel condensation of 2-(2,6-dimethyl-1-propylpyridin-4(1*H*)-ylidene)malononitrile with benzaldehyde and characterized its structure.

In the title compound, C₂₇H₂₃N₃, the dihedral angles between the central pyridine ring and the two outer benzene rings are 32.6 (1)° and 52.0 (1)°, respectively, and the dihedral angle between the benzene rings is 74.3 (1)° (Fig. 1). The dicyanomethylene group lies in the pyridine ring plane with the largest deviation of 0.212 (7) Å (N3) from the least-squares plane of the pyridine ring. The compound displays intermolecular π - π interactions between the adjacent six-membered rings (the symmetry operation for second plane $-x,-y,-z$), with a shortest centroid-centroid distance of 3.981 (3) Å, and the planes are parallel and shifted for 1.926 Å (Fig. 2).

S2. Experimental

A mixture of 2-(2,6-dimethyl-1-propylpyridin-4(1*H*)-ylidene)malononitrile (1.015 g, 4.76 mmol), benzaldehyde (1.111 g, 10.47 mmol) and piperidine (0.5 ml) in DMF (10 ml) was stirred and heated for 12 h at 100 °C under nitrogen. After cooling to room temperature the mixture was concentrated under vacuum to give the crude product, which was column chromatographed (SiO₂) by eluting with a mixture of acetone/CHCl₃ (1:20) to afford the title compound (1.290 g, 70%) as an orange solid. Crystals suitable for X-ray analysis were obtained by slow evaporation from a CHCl₃/EtOH solution. Mp 252–253 °C. ¹H NMR (300 MHz, CDCl₃): δ 7.55–7.40 (m, 10H, Ph), 7.23 (d, 2H, *J* = 15.6 Hz, $-\text{CH}=\text{CH}-\text{Ph}$), 7.01 (s, 2H, $\text{CH}=\text{C}$ of pyridine), 6.96 (d, 2H, *J* = 15.6 Hz, $-\text{CH}=\text{CH}-\text{Ph}$), 4.03 (t, 2H, *J* = 8.1 Hz, NCH₂CH₂), 1.87 (m, 2H, $-\text{CH}_2\text{CH}_2\text{CH}_3$), 1.02 (t, 3H, *J* = 7.2 Hz, $-\text{CH}_2\text{CH}_3$). ¹³C NMR (75 MHz, CDCl₃): δ 155.8, 148.0, 139.8, 134.8, 130.0, 129.1, 127.5, 118.7, 111.7, 51.4, 47.1, 23.3, 11.0.

S3. Refinement

H atoms were positioned geometrically and allowed to ride on their respective parent atoms [$\text{C}-\text{H} = 0.93$ (CH), 0.97 (CH₂) or 0.96 Å (CH₃) and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ or $1.5U_{\text{eq}}$ (methyl C)].

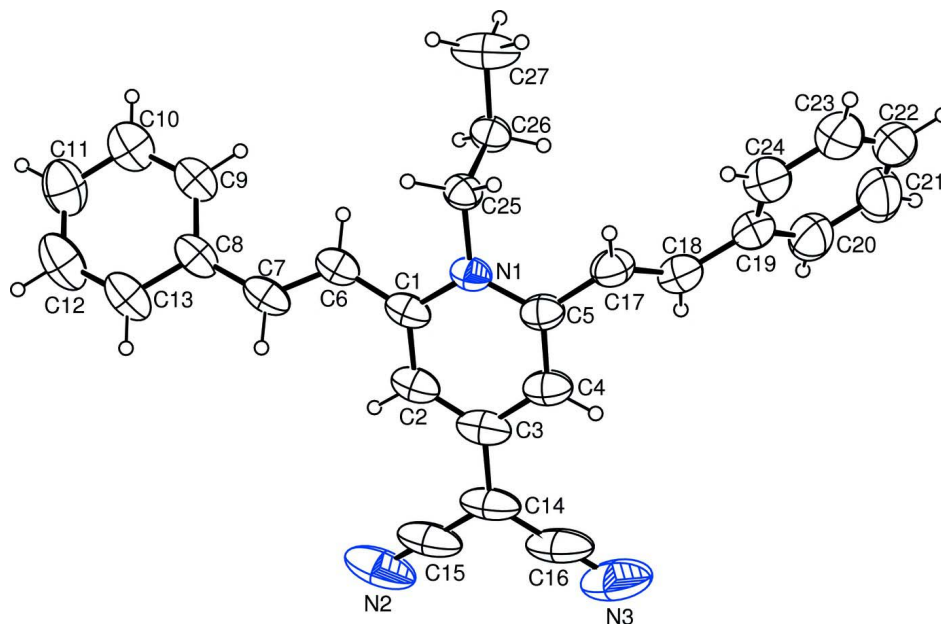


Figure 1

The structure of the title compound, with displacement ellipsoids drawn at the 30% probability level for non-H atoms.

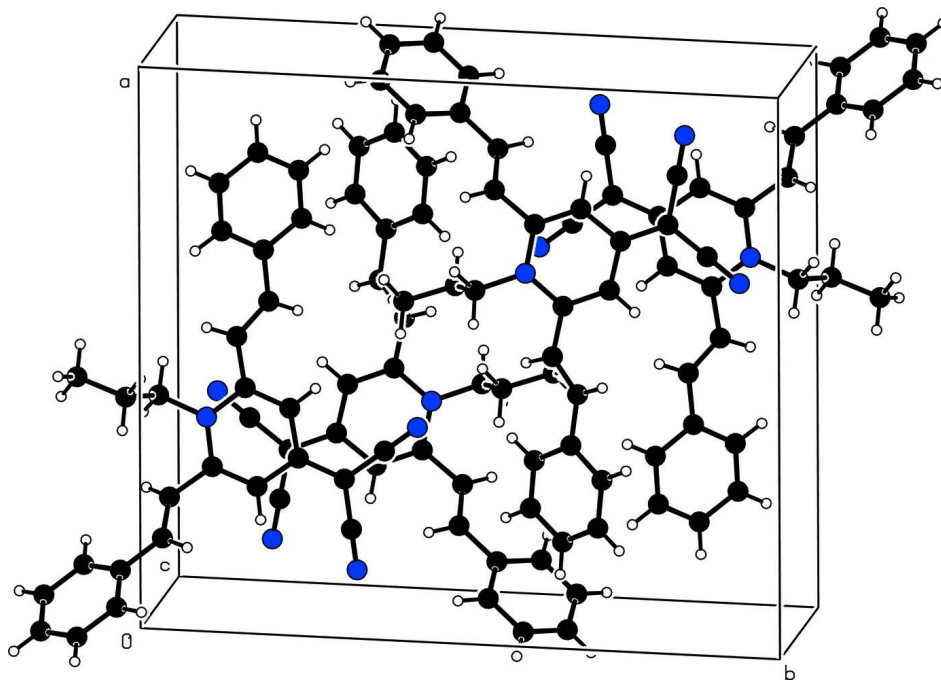


Figure 2

View of the unit-cell contents of the title compound.

2-(1-Propyl-2,6-distyryl-1,4-dihydropyridin-4-ylidene)malononitrile

Crystal data

$C_{27}H_{23}N_3$
 $M_r = 389.48$

Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc

$a = 16.586$ (2) Å
 $b = 17.827$ (2) Å
 $c = 7.4543$ (9) Å
 $\beta = 99.790$ (3)°
 $V = 2171.9$ (5) Å³
 $Z = 4$
 $F(000) = 824$
 $D_x = 1.191$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 690 reflections
 $\theta = 2.5$ – 19.1 °
 $\mu = 0.07$ mm⁻¹
 $T = 293$ K
 Stick, orange
 $0.20 \times 0.20 \times 0.17$ mm

Data collection

Bruker SMART 1000 CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2000)
 $T_{\min} = 0.630$, $T_{\max} = 1.000$

12600 measured reflections
 4433 independent reflections
 2084 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\max} = 26.4$ °, $\theta_{\min} = 2.3$ °
 $h = -17 \rightarrow 20$
 $k = -22 \rightarrow 22$
 $l = -9 \rightarrow 9$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.201$
 $S = 1.01$
 4433 reflections
 272 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
 $w = 1/[\sigma^2(F_o^2) + (0.0808P)^2 + 0.1288P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.14$ e Å⁻³
 $\Delta\rho_{\min} = -0.16$ e Å⁻³

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.35774 (14)	0.08906 (10)	0.2536 (3)	0.0713 (6)
N2	0.3616 (3)	0.42152 (17)	0.2101 (5)	0.1696 (17)
N3	0.1110 (3)	0.3314 (2)	0.1271 (6)	0.186 (2)
C1	0.4116 (2)	0.14869 (13)	0.2691 (3)	0.0772 (8)
C2	0.3815 (2)	0.21977 (15)	0.2438 (4)	0.0889 (9)
H2	0.4182	0.2596	0.2518	0.107*
C3	0.2971 (3)	0.23522 (16)	0.2060 (4)	0.0938 (10)
C4	0.2452 (2)	0.17187 (15)	0.1836 (4)	0.0900 (9)
H4	0.1889	0.1791	0.1539	0.108*

C5	0.27456 (19)	0.10081 (14)	0.2040 (4)	0.0780 (7)
C6	0.49940 (19)	0.13383 (15)	0.3018 (4)	0.0803 (8)
H6	0.5171	0.0897	0.2545	0.096*
C7	0.5559 (2)	0.17842 (14)	0.3937 (4)	0.0843 (8)
H7	0.5369	0.2203	0.4483	0.101*
C8	0.6446 (2)	0.16912 (15)	0.4189 (4)	0.0828 (8)
C9	0.6811 (2)	0.10774 (16)	0.3513 (4)	0.0902 (9)
H9	0.6487	0.0697	0.2918	0.108*
C10	0.7643 (3)	0.1027 (2)	0.3714 (5)	0.1122 (11)
H10	0.7879	0.0614	0.3243	0.135*
C11	0.8137 (2)	0.1581 (2)	0.4608 (5)	0.1264 (13)
H11	0.8703	0.1547	0.4722	0.152*
C12	0.7787 (3)	0.2177 (2)	0.5321 (5)	0.1301 (14)
H12	0.8116	0.2549	0.5942	0.156*
C13	0.6951 (2)	0.22324 (18)	0.5128 (4)	0.1046 (11)
H13	0.6720	0.2639	0.5635	0.125*
C14	0.2655 (3)	0.30813 (17)	0.1869 (4)	0.1153 (13)
C15	0.3178 (3)	0.3705 (2)	0.2000 (5)	0.1326 (16)
C16	0.1804 (4)	0.3210 (2)	0.1529 (6)	0.143 (2)
C17	0.22033 (18)	0.03589 (15)	0.1665 (4)	0.0869 (8)
H17	0.2284	-0.0049	0.2451	0.104*
C18	0.1602 (2)	0.03298 (17)	0.0248 (5)	0.0929 (9)
H18	0.1523	0.0759	-0.0471	0.111*
C19	0.1048 (2)	-0.0295 (2)	-0.0320 (6)	0.1017 (10)
C20	0.0541 (2)	-0.0257 (2)	-0.1978 (6)	0.1274 (13)
H20	0.0540	0.0172	-0.2686	0.153*
C21	0.0036 (3)	-0.0844 (3)	-0.2604 (8)	0.166 (2)
H21	-0.0296	-0.0811	-0.3740	0.199*
C22	0.0015 (3)	-0.1471 (3)	-0.1589 (12)	0.167 (3)
H22	-0.0327	-0.1867	-0.2026	0.200*
C23	0.0501 (3)	-0.1516 (3)	0.0085 (10)	0.171 (2)
H23	0.0485	-0.1942	0.0800	0.206*
C24	0.1018 (2)	-0.0927 (2)	0.0712 (7)	0.1312 (13)
H24	0.1348	-0.0960	0.1849	0.157*
C25	0.38929 (15)	0.01206 (12)	0.2886 (3)	0.0690 (7)
H25A	0.3520	-0.0159	0.3506	0.083*
H25B	0.4418	0.0142	0.3687	0.083*
C26	0.39921 (16)	-0.02907 (13)	0.1163 (3)	0.0744 (7)
H26A	0.3472	-0.0299	0.0341	0.089*
H26B	0.4382	-0.0024	0.0565	0.089*
C27	0.4281 (3)	-0.10736 (17)	0.1544 (5)	0.1335 (14)
H27A	0.4785	-0.1069	0.2395	0.200*
H27B	0.4368	-0.1307	0.0432	0.200*
H27C	0.3876	-0.1350	0.2049	0.200*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0922 (16)	0.0552 (12)	0.0665 (13)	0.0047 (11)	0.0136 (11)	0.0026 (10)
N2	0.326 (5)	0.0653 (18)	0.119 (3)	0.013 (3)	0.043 (3)	0.0021 (19)
N3	0.238 (5)	0.138 (3)	0.175 (4)	0.105 (3)	0.018 (3)	0.009 (2)
C1	0.118 (2)	0.0539 (15)	0.0615 (16)	-0.0031 (15)	0.0220 (15)	-0.0006 (12)
C2	0.137 (3)	0.0596 (17)	0.0723 (18)	0.0013 (17)	0.0248 (18)	-0.0003 (13)
C3	0.164 (3)	0.0635 (18)	0.0571 (16)	0.023 (2)	0.0264 (18)	0.0057 (13)
C4	0.123 (2)	0.0749 (19)	0.0732 (18)	0.0276 (17)	0.0181 (16)	0.0061 (14)
C5	0.095 (2)	0.0701 (17)	0.0693 (17)	0.0147 (15)	0.0158 (15)	0.0058 (13)
C6	0.109 (2)	0.0616 (16)	0.0746 (17)	-0.0105 (16)	0.0265 (16)	-0.0036 (14)
C7	0.131 (3)	0.0583 (16)	0.0676 (17)	-0.0189 (16)	0.0293 (17)	-0.0045 (13)
C8	0.117 (3)	0.0737 (18)	0.0625 (16)	-0.0325 (17)	0.0299 (16)	-0.0055 (13)
C9	0.114 (3)	0.083 (2)	0.0746 (19)	-0.0237 (17)	0.0218 (18)	-0.0060 (15)
C10	0.124 (3)	0.122 (3)	0.096 (2)	-0.021 (2)	0.032 (2)	-0.010 (2)
C11	0.115 (3)	0.159 (4)	0.110 (3)	-0.042 (3)	0.033 (2)	-0.014 (3)
C12	0.149 (4)	0.143 (4)	0.106 (3)	-0.068 (3)	0.040 (3)	-0.028 (2)
C13	0.138 (3)	0.095 (2)	0.087 (2)	-0.047 (2)	0.037 (2)	-0.0206 (17)
C14	0.202 (4)	0.064 (2)	0.079 (2)	0.044 (2)	0.021 (2)	0.0034 (16)
C15	0.254 (5)	0.062 (2)	0.084 (2)	0.039 (3)	0.032 (3)	0.0040 (19)
C16	0.237 (6)	0.086 (3)	0.103 (3)	0.077 (3)	0.021 (4)	0.0076 (19)
C17	0.086 (2)	0.0750 (19)	0.101 (2)	0.0131 (15)	0.0182 (18)	0.0124 (16)
C18	0.092 (2)	0.088 (2)	0.099 (2)	0.0194 (17)	0.0166 (19)	0.0030 (17)
C19	0.080 (2)	0.095 (3)	0.131 (3)	0.0138 (18)	0.022 (2)	-0.020 (2)
C20	0.098 (3)	0.147 (4)	0.136 (3)	0.009 (2)	0.014 (3)	-0.037 (3)
C21	0.106 (3)	0.189 (5)	0.196 (6)	-0.006 (4)	0.012 (3)	-0.087 (5)
C22	0.086 (3)	0.123 (4)	0.298 (9)	-0.004 (3)	0.049 (4)	-0.076 (5)
C23	0.102 (4)	0.111 (4)	0.302 (8)	0.000 (3)	0.036 (4)	-0.021 (4)
C24	0.102 (3)	0.099 (3)	0.192 (4)	0.001 (2)	0.023 (3)	-0.001 (3)
C25	0.0808 (17)	0.0565 (14)	0.0680 (16)	-0.0001 (11)	0.0082 (13)	0.0074 (12)
C26	0.0885 (18)	0.0652 (15)	0.0711 (16)	-0.0002 (13)	0.0181 (14)	0.0013 (12)
C27	0.231 (4)	0.079 (2)	0.102 (3)	0.049 (2)	0.062 (3)	0.0116 (18)

Geometric parameters (Å, °)

N1—C1	1.381 (3)	C13—H13	0.9300
N1—C5	1.382 (3)	C14—C15	1.402 (6)
N1—C25	1.476 (3)	C14—C16	1.411 (6)
N2—C15	1.160 (5)	C17—C18	1.324 (4)
N3—C16	1.148 (6)	C17—H17	0.9300
C1—C2	1.363 (4)	C18—C19	1.460 (4)
C1—C6	1.459 (4)	C18—H18	0.9300
C2—C3	1.408 (4)	C19—C24	1.369 (5)
C2—H2	0.9300	C19—C20	1.373 (5)
C3—C14	1.399 (4)	C20—C21	1.372 (5)
C3—C4	1.413 (4)	C20—H20	0.9300
C4—C5	1.357 (3)	C21—C22	1.353 (7)

C4—H4	0.9300	C21—H21	0.9300
C5—C17	1.463 (4)	C22—C23	1.367 (8)
C6—C7	1.327 (4)	C22—H22	0.9300
C6—H6	0.9300	C23—C24	1.386 (6)
C7—C8	1.461 (4)	C23—H23	0.9300
C7—H7	0.9300	C24—H24	0.9300
C8—C9	1.386 (4)	C25—C26	1.512 (3)
C8—C13	1.387 (4)	C25—H25A	0.9700
C9—C10	1.364 (4)	C25—H25B	0.9700
C9—H9	0.9300	C26—C27	1.487 (3)
C10—C11	1.380 (4)	C26—H26A	0.9700
C10—H10	0.9300	C26—H26B	0.9700
C11—C12	1.362 (5)	C27—H27A	0.9600
C11—H11	0.9300	C27—H27B	0.9600
C12—C13	1.373 (5)	C27—H27C	0.9600
C12—H12	0.9300		
C1—N1—C5	120.5 (2)	N2—C15—C14	179.2 (5)
C1—N1—C25	119.7 (2)	N3—C16—C14	179.3 (5)
C5—N1—C25	119.7 (2)	C18—C17—C5	122.6 (3)
C2—C1—N1	119.1 (3)	C18—C17—H17	118.7
C2—C1—C6	121.6 (3)	C5—C17—H17	118.7
N1—C1—C6	119.2 (2)	C17—C18—C19	127.8 (3)
C1—C2—C3	122.6 (3)	C17—C18—H18	116.1
C1—C2—H2	118.7	C19—C18—H18	116.1
C3—C2—H2	118.7	C24—C19—C20	118.1 (4)
C14—C3—C2	123.0 (4)	C24—C19—C18	123.1 (4)
C14—C3—C4	121.4 (4)	C20—C19—C18	118.8 (4)
C2—C3—C4	115.6 (3)	C21—C20—C19	120.9 (5)
C5—C4—C3	122.2 (3)	C21—C20—H20	119.5
C5—C4—H4	118.9	C19—C20—H20	119.5
C3—C4—H4	118.9	C22—C21—C20	120.7 (6)
C4—C5—N1	119.7 (3)	C22—C21—H21	119.6
C4—C5—C17	121.3 (3)	C20—C21—H21	119.6
N1—C5—C17	119.0 (2)	C21—C22—C23	119.5 (5)
C7—C6—C1	125.1 (3)	C21—C22—H22	120.2
C7—C6—H6	117.5	C23—C22—H22	120.2
C1—C6—H6	117.5	C22—C23—C24	119.8 (6)
C6—C7—C8	127.3 (3)	C22—C23—H23	120.1
C6—C7—H7	116.4	C24—C23—H23	120.1
C8—C7—H7	116.4	C19—C24—C23	120.9 (5)
C9—C8—C13	118.0 (3)	C19—C24—H24	119.5
C9—C8—C7	122.4 (3)	C23—C24—H24	119.5
C13—C8—C7	119.6 (3)	N1—C25—C26	112.79 (19)
C10—C9—C8	120.5 (3)	N1—C25—H25A	109.0
C10—C9—H9	119.7	C26—C25—H25A	109.0
C8—C9—H9	119.7	N1—C25—H25B	109.0
C9—C10—C11	120.8 (4)	C26—C25—H25B	109.0

C9—C10—H10	119.6	H25A—C25—H25B	107.8
C11—C10—H10	119.6	C27—C26—C25	111.8 (2)
C12—C11—C10	119.3 (4)	C27—C26—H26A	109.3
C12—C11—H11	120.3	C25—C26—H26A	109.3
C10—C11—H11	120.3	C27—C26—H26B	109.3
C11—C12—C13	120.3 (3)	C25—C26—H26B	109.3
C11—C12—H12	119.9	H26A—C26—H26B	107.9
C13—C12—H12	119.9	C26—C27—H27A	109.5
C12—C13—C8	121.0 (3)	C26—C27—H27B	109.5
C12—C13—H13	119.5	H27A—C27—H27B	109.5
C8—C13—H13	119.5	C26—C27—H27C	109.5
C3—C14—C15	120.9 (4)	H27A—C27—H27C	109.5
C3—C14—C16	121.0 (4)	H27B—C27—H27C	109.5
C15—C14—C16	118.1 (3)		
C5—N1—C1—C2	3.2 (3)	C10—C11—C12—C13	-1.0 (6)
C25—N1—C1—C2	-177.3 (2)	C11—C12—C13—C8	-0.8 (5)
C5—N1—C1—C6	-173.3 (2)	C9—C8—C13—C12	2.5 (4)
C25—N1—C1—C6	6.2 (3)	C7—C8—C13—C12	-177.2 (3)
N1—C1—C2—C3	1.4 (4)	C2—C3—C14—C15	1.7 (4)
C6—C1—C2—C3	177.8 (2)	C4—C3—C14—C15	-176.7 (3)
C1—C2—C3—C14	177.4 (3)	C2—C3—C14—C16	-178.6 (3)
C1—C2—C3—C4	-4.1 (4)	C4—C3—C14—C16	3.0 (4)
C14—C3—C4—C5	-179.1 (3)	C4—C5—C17—C18	41.4 (4)
C2—C3—C4—C5	2.4 (4)	N1—C5—C17—C18	-135.8 (3)
C3—C4—C5—N1	2.0 (4)	C5—C17—C18—C19	176.8 (3)
C3—C4—C5—C17	-175.2 (3)	C17—C18—C19—C24	8.4 (5)
C1—N1—C5—C4	-4.9 (4)	C17—C18—C19—C20	-170.6 (3)
C25—N1—C5—C4	175.7 (2)	C24—C19—C20—C21	-1.8 (5)
C1—N1—C5—C17	172.3 (2)	C18—C19—C20—C21	177.2 (3)
C25—N1—C5—C17	-7.1 (3)	C19—C20—C21—C22	1.1 (7)
C2—C1—C6—C7	34.3 (4)	C20—C21—C22—C23	0.4 (8)
N1—C1—C6—C7	-149.3 (2)	C21—C22—C23—C24	-1.0 (8)
C1—C6—C7—C8	-175.1 (2)	C20—C19—C24—C23	1.2 (5)
C6—C7—C8—C9	-2.6 (4)	C18—C19—C24—C23	-177.8 (3)
C6—C7—C8—C13	177.1 (3)	C22—C23—C24—C19	0.2 (7)
C13—C8—C9—C10	-2.4 (4)	C1—N1—C25—C26	-96.4 (3)
C7—C8—C9—C10	177.3 (3)	C5—N1—C25—C26	83.0 (3)
C8—C9—C10—C11	0.6 (5)	N1—C25—C26—C27	-177.9 (3)
C9—C10—C11—C12	1.1 (6)		