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4,5-Bis(phthalimidomethyl)acridine

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The structure of the title symmetrically disubstituted acridine derivative [systematic name: *N*,*N*′-(acridine-4,5-diyldimethylene)bisphthalimide], $C_{31}H_{19}N_3O_4$, has been determined at 120 K using synchrotron radiation. The molecule contains a planar acridine and two planar phthalimide fragments. The pseudo-torsion angle N—C···C—N between the phthalimidomethyl groups, where C···C is an intramolecular contact between the methylene C atoms, is 95.9 (2)°; the phthalimide rings are almost parallel to each other.

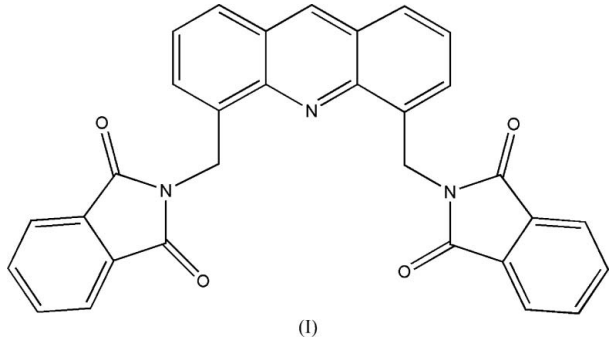
Key indicators

Single-crystal synchrotron study
T = 120 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.110
Data-to-parameter ratio = 10.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Certain acridine derivatives have been shown to have immunosuppresive properties (Farr *et al.*, 1965; Hess & Stewart, 1975; Hess *et al.*, 1971). Recently, acridine derivatives have been shown to exert toxicity towards *Plasmodium*, *Trypanosoma*, and *Leishmania* parasites (Di Giorgio *et al.*, 2005). Many of the compounds of interest are either 4-substituted or 4,5-disubstituted acridines. The title compound, (I), is a key starting material in the elaboration of the 4- and 5-positions of the acridine nucleus for the synthesis of novel hydrogen-bonding receptors. The single-crystal structure of 4-(phthalimidomethyl)acridine has been reported (Chiron & Galy, 2003) and a comparison of the relative arrangement of the planar systems in both this molecule and (I) was deemed to be of interest.



(I)

The structure of (I), is shown in Fig. 1. The two planar phthalimido groups are almost parallel to each other, the dihedral angle between the mean planes being 5.1 (2)°; these planes are inclined at 80.6 (2) and 81.5 (2)° with respect to the mean plane of the acridine system. The latter angle is 85.6 (2)° for the monosubstituted 4-(phthalimidomethyl)acridine. The pseudo-torsion angle N2—C14···C23—N3 is large [95.9 (2)°], resulting in one phthalimidomethyl group being approximately bisected by the plane of the acridine system and the other being nearly perpendicular to it.

Experimental

The title compound was prepared by a modification of the published method (Chiron & Galy, 2003) and spectroscopic data were in agreement with previous reports (Hess & Stewart, 1975). Crystals suitable for diffraction analysis were grown by slow cooling of a dimethylsulfoxide solution. Data were collected at the Daresbury SRS station 9.8 using a silicon 111 monochromator.

Crystal data

$C_{31}H_{19}N_3O_4$
$M_r = 497.49$
Orthorhombic, $Pna2_1$
$a = 40.462$ (12) Å
$b = 4.7732$ (14) Å
$c = 11.719$ (4) Å
$V = 2263.3$ (12) Å^3
$Z = 4$
$D_x = 1.460$ Mg m^{-3}
Synchrotron radiation
$\lambda = 0.6905$ Å
$\mu = 0.10$ mm^{-1}
$T = 120$ (2) K
Block, colourless
0.17 × 0.07 × 0.03 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
fine–slice ω scans
Absorption correction: none
15033 measured reflections
3485 independent reflections
3261 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 29.9°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.110$
$S = 1.11$
3485 reflections
343 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.0792P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Selected torsion angles (°).

C4—C5—C14—N2	−114.29 (19)	C9—C8—C23—N3	−14.1 (3)
C6—C5—C14—N2	68.9 (2)	C7—C8—C23—N3	165.48 (16)

H atoms were included in calculated positions, C—H = 0.95–0.99 Å, and refined as riding on their respective C atoms, with $U_{iso}(H) = 1.2$ or 1.5 times $U_{eq}(C)$. In the absence of any significant anomalous scattering, Friedel equivalents were merged prior to the final refinements.

Data collection: *APEX2* (Bruker 2005); cell refinement: *SAINT* (Bruker 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *WinGX* (Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

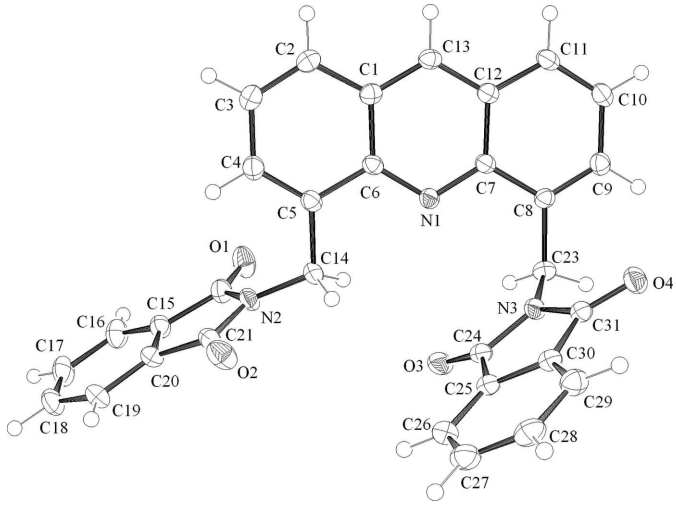


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level.

We acknowledge the use of the EPSRC's Chemical Database Service at Daresbury. The EPSRC National Crystallography Service is thanked for performing the data collection at Daresbury.

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supporting information

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$F(000) = 1032$
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Synchrotron radiation, $\lambda = 0.69050$ Å
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$\theta = 3.9$–$28.9°$
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$T = 120$ K
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Silicon 111 monochromator
fine–slice ω scans
15033 measured reflections
3485 independent reflections
3261 reflections with $I > 2\sigma(I)$
$R_{int} = 0.061$
$\theta_{max} = 29.9°$, $\theta_{min} = 2.9°$
$h = -41 \rightarrow 57$
$k = -6 \rightarrow 6$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.110$
$S = 1.11$
3485 reflections
343 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0613P)^2 + 0.0792P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.29$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ 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_{iso}*/U_{eq}
N1	0.83176 (4)	0.2925 (3)	0.78829 (13)	0.0183 (3)
N2	0.85102 (4)	0.0911 (3)	1.03501 (14)	0.0200 (3)
N3	0.92241 (4)	0.5471 (3)	0.63763 (14)	0.0215 (3)
O1	0.81187 (4)	0.1257 (3)	1.17883 (13)	0.0277 (3)
O2	0.90046 (3)	0.1223 (3)	0.93583 (13)	0.0279 (3)
O3	0.94365 (4)	0.8999 (3)	0.75155 (14)	0.0338 (4)
O4	0.91576 (4)	0.2316 (3)	0.48906 (15)	0.0344 (4)
C1	0.77150 (4)	0.2605 (4)	0.77479 (14)	0.0185 (3)
C2	0.74203 (4)	0.1222 (4)	0.81025 (17)	0.0223 (4)
H2	0.7214	0.1737	0.7779	0.027*
C3	0.74345 (5)	−0.0844 (4)	0.89074 (17)	0.0235 (4)
H3	0.7239	−0.1797	0.9129	0.028*
C4	0.77413 (4)	−0.1567 (4)	0.94126 (16)	0.0214 (3)
H4	0.7746	−0.2978	0.9984	0.026*
C5	0.80312 (4)	−0.0297 (4)	0.91040 (15)	0.0186 (3)
C6	0.80269 (4)	0.1822 (4)	0.82285 (15)	0.0177 (3)
C7	0.83094 (4)	0.4871 (4)	0.70479 (15)	0.0178 (3)
C8	0.86188 (4)	0.5955 (4)	0.66179 (15)	0.0197 (3)
C9	0.86127 (5)	0.8028 (4)	0.58156 (17)	0.0231 (4)
H9	0.8817	0.8753	0.5543	0.028*
C10	0.83127 (5)	0.9147 (4)	0.53718 (18)	0.0242 (4)
H10	0.8319	1.0620	0.4827	0.029*
C11	0.80172 (5)	0.8106 (4)	0.57279 (16)	0.0222 (4)
H11	0.7817	0.8829	0.5420	0.027*
C12	0.80068 (5)	0.5924 (4)	0.65653 (15)	0.0194 (3)
C13	0.77117 (4)	0.4729 (4)	0.69289 (16)	0.0199 (3)
H13	0.7508	0.5357	0.6620	0.024*
C14	0.83526 (5)	−0.1224 (4)	0.96340 (16)	0.0209 (3)
H14A	0.8311	−0.2912	1.0103	0.031*
H14B	0.8508	−0.1758	0.9018	0.031*
C15	0.83807 (4)	0.1954 (4)	1.13738 (16)	0.0208 (3)
C16	0.86271 (5)	0.4023 (4)	1.17980 (16)	0.0213 (4)
C17	0.86196 (5)	0.5752 (4)	1.27455 (17)	0.0267 (4)
H17	0.8439	0.5730	1.3262	0.032*
C18	0.88900 (6)	0.7534 (4)	1.29110 (19)	0.0296 (4)
H18	0.8892	0.8768	1.3547	0.035*
C19	0.91561 (5)	0.7531 (4)	1.2162 (2)	0.0301 (4)
H19	0.9336	0.8760	1.2298	0.036*
C20	0.91646 (5)	0.5767 (4)	1.12144 (19)	0.0269 (4)
H20	0.9347	0.5752	1.0706	0.032*
C21	0.88942 (5)	0.4038 (4)	1.10482 (16)	0.0211 (3)
C22	0.88282 (4)	0.1962 (4)	1.01334 (16)	0.0211 (3)
C23	0.89375 (4)	0.4725 (4)	0.70719 (17)	0.0227 (4)
H23A	0.8973	0.5399	0.7861	0.034*
H23B	0.8917	0.2659	0.7099	0.034*

C24	0.94534 (5)	0.7539 (4)	0.66824 (16)	0.0228 (4)
C25	0.97115 (5)	0.7509 (4)	0.57742 (17)	0.0226 (4)
C26	0.99967 (5)	0.9096 (4)	0.5676 (2)	0.0284 (4)
H26	1.0057	1.0433	0.6239	0.034*
C27	1.01919 (5)	0.8640 (5)	0.4710 (2)	0.0322 (5)
H27	1.0388	0.9705	0.4607	0.039*
C28	1.01049 (6)	0.6664 (5)	0.3899 (2)	0.0339 (5)
H28	1.0243	0.6399	0.3251	0.041*
C29	0.98168 (6)	0.5042 (5)	0.4015 (2)	0.0308 (4)
H29	0.9757	0.3675	0.3463	0.037*
C30	0.96241 (5)	0.5526 (4)	0.49682 (17)	0.0232 (4)
C31	0.93105 (5)	0.4174 (4)	0.53474 (17)	0.0238 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0173 (7)	0.0224 (7)	0.0153 (6)	−0.0011 (5)	0.0008 (5)	−0.0004 (5)
N2	0.0175 (7)	0.0252 (7)	0.0172 (6)	−0.0011 (5)	0.0007 (6)	−0.0014 (5)
N3	0.0169 (7)	0.0281 (7)	0.0196 (7)	−0.0044 (6)	0.0034 (6)	−0.0013 (6)
O1	0.0224 (7)	0.0370 (8)	0.0237 (7)	−0.0034 (6)	0.0048 (5)	−0.0017 (6)
O2	0.0190 (7)	0.0426 (9)	0.0222 (7)	0.0031 (5)	0.0017 (5)	−0.0015 (6)
O3	0.0277 (8)	0.0442 (9)	0.0295 (8)	−0.0079 (6)	0.0027 (6)	−0.0120 (7)
O4	0.0405 (9)	0.0342 (8)	0.0284 (7)	−0.0145 (6)	0.0076 (7)	−0.0072 (6)
C1	0.0173 (8)	0.0214 (8)	0.0168 (8)	0.0002 (6)	0.0002 (6)	−0.0028 (6)
C2	0.0153 (8)	0.0283 (9)	0.0235 (9)	−0.0003 (6)	−0.0004 (7)	−0.0024 (7)
C3	0.0188 (8)	0.0274 (9)	0.0244 (9)	−0.0034 (7)	0.0033 (7)	−0.0010 (7)
C4	0.0216 (8)	0.0241 (8)	0.0186 (7)	−0.0018 (6)	0.0022 (7)	−0.0004 (7)
C5	0.0184 (8)	0.0212 (8)	0.0162 (7)	0.0005 (6)	−0.0012 (6)	−0.0009 (6)
C6	0.0159 (8)	0.0220 (8)	0.0153 (7)	−0.0001 (6)	0.0001 (6)	−0.0022 (6)
C7	0.0164 (8)	0.0205 (8)	0.0166 (7)	−0.0008 (6)	−0.0002 (6)	−0.0021 (6)
C8	0.0172 (8)	0.0232 (8)	0.0187 (8)	−0.0029 (6)	0.0000 (6)	−0.0019 (6)
C9	0.0236 (9)	0.0252 (9)	0.0204 (8)	−0.0041 (6)	0.0013 (7)	0.0006 (7)
C10	0.0287 (10)	0.0230 (9)	0.0209 (8)	−0.0013 (7)	−0.0003 (7)	0.0023 (7)
C11	0.0254 (9)	0.0222 (8)	0.0191 (8)	0.0021 (6)	−0.0028 (7)	0.0000 (6)
C12	0.0204 (8)	0.0209 (8)	0.0168 (7)	0.0011 (6)	−0.0010 (6)	−0.0018 (6)
C13	0.0185 (8)	0.0240 (9)	0.0171 (7)	0.0024 (6)	−0.0018 (6)	−0.0026 (6)
C14	0.0208 (8)	0.0221 (8)	0.0198 (8)	0.0008 (6)	−0.0028 (6)	−0.0011 (6)
C15	0.0186 (8)	0.0266 (8)	0.0171 (8)	0.0012 (6)	−0.0007 (6)	0.0009 (6)
C16	0.0204 (8)	0.0248 (9)	0.0185 (8)	0.0006 (6)	−0.0027 (7)	0.0010 (6)
C17	0.0284 (10)	0.0297 (10)	0.0220 (9)	0.0016 (7)	−0.0016 (7)	−0.0026 (7)
C18	0.0368 (11)	0.0281 (10)	0.0237 (9)	−0.0008 (8)	−0.0087 (8)	−0.0025 (7)
C19	0.0297 (10)	0.0290 (10)	0.0317 (11)	−0.0053 (7)	−0.0097 (8)	0.0013 (8)
C20	0.0217 (9)	0.0313 (9)	0.0277 (10)	−0.0024 (7)	−0.0028 (7)	0.0033 (8)
C21	0.0196 (8)	0.0256 (9)	0.0182 (8)	0.0003 (6)	−0.0028 (6)	0.0013 (6)
C22	0.0174 (8)	0.0271 (9)	0.0186 (8)	0.0016 (6)	−0.0025 (6)	0.0020 (6)
C23	0.0168 (8)	0.0301 (9)	0.0211 (8)	−0.0024 (7)	0.0028 (6)	0.0029 (7)
C24	0.0171 (8)	0.0275 (9)	0.0239 (9)	−0.0025 (6)	0.0001 (7)	−0.0003 (7)
C25	0.0162 (8)	0.0261 (9)	0.0256 (8)	0.0006 (6)	0.0013 (7)	0.0015 (7)

C26	0.0175 (8)	0.0341 (10)	0.0335 (10)	−0.0039 (7)	0.0012 (8)	0.0022 (8)
C27	0.0182 (9)	0.0349 (11)	0.0436 (12)	−0.0002 (7)	0.0086 (8)	0.0088 (9)
C28	0.0283 (11)	0.0344 (11)	0.0390 (12)	0.0047 (8)	0.0178 (9)	0.0077 (9)
C29	0.0329 (11)	0.0297 (10)	0.0299 (10)	0.0007 (8)	0.0112 (8)	0.0008 (8)
C30	0.0209 (8)	0.0238 (8)	0.0247 (9)	−0.0003 (6)	0.0042 (7)	0.0022 (7)
C31	0.0244 (9)	0.0254 (9)	0.0217 (8)	−0.0028 (7)	0.0033 (7)	−0.0003 (7)

Geometric parameters (Å, º)

N1—C7	1.350 (2)	C11—H11	0.9500
N1—C6	1.351 (2)	C12—C13	1.390 (3)
N2—C15	1.401 (2)	C13—H13	0.9500
N2—C22	1.404 (2)	C14—H14A	0.9900
N2—C14	1.466 (2)	C14—H14B	0.9900
N3—C31	1.400 (2)	C15—C16	1.489 (3)
N3—C24	1.401 (2)	C16—C17	1.384 (3)
N3—C23	1.461 (2)	C16—C21	1.393 (3)
O1—C15	1.213 (2)	C17—C18	1.399 (3)
O2—C22	1.208 (2)	C17—H17	0.9500
O3—C24	1.201 (2)	C18—C19	1.389 (3)
O4—C31	1.207 (2)	C18—H18	0.9500
C1—C13	1.396 (3)	C19—C20	1.393 (3)
C1—C2	1.425 (3)	C19—H19	0.9500
C1—C6	1.432 (2)	C20—C21	1.384 (3)
C2—C3	1.366 (3)	C20—H20	0.9500
C2—H2	0.9500	C21—C22	1.484 (3)
C3—C4	1.418 (3)	C23—H23A	0.9900
C3—H3	0.9500	C23—H23B	0.9900
C4—C5	1.369 (2)	C24—C25	1.491 (3)
C4—H4	0.9500	C25—C30	1.383 (3)
C5—C6	1.441 (2)	C25—C26	1.385 (3)
C5—C14	1.507 (3)	C26—C27	1.398 (3)
C7—C12	1.439 (2)	C26—H26	0.9500
C7—C8	1.446 (2)	C27—C28	1.384 (4)
C8—C9	1.365 (3)	C27—H27	0.9500
C8—C23	1.513 (3)	C28—C29	1.406 (3)
C9—C10	1.425 (3)	C28—H28	0.9500
C9—H9	0.9500	C29—C30	1.382 (3)
C10—C11	1.360 (3)	C29—H29	0.9500
C10—H10	0.9500	C30—C31	1.491 (3)
C11—C12	1.432 (3)		

C7—N1—C6	117.65 (15)	O1—C15—C16	129.32 (18)
C15—N2—C22	111.76 (16)	N2—C15—C16	105.73 (16)
C15—N2—C14	125.08 (16)	C17—C16—C21	121.34 (18)
C22—N2—C14	122.92 (16)	C17—C16—C15	130.45 (18)
C31—N3—C24	111.51 (15)	C21—C16—C15	108.21 (16)
C31—N3—C23	124.81 (17)	C16—C17—C18	117.2 (2)

C24—N3—C23	123.65 (16)	C16—C17—H17	121.4
C13—C1—C2	121.95 (17)	C18—C17—H17	121.4
C13—C1—C6	117.93 (16)	C19—C18—C17	121.17 (19)
C2—C1—C6	120.12 (16)	C19—C18—H18	119.4
C3—C2—C1	120.07 (17)	C17—C18—H18	119.4
C3—C2—H2	120.0	C18—C19—C20	121.55 (19)
C1—C2—H2	120.0	C18—C19—H19	119.2
C2—C3—C4	120.05 (17)	C20—C19—H19	119.2
C2—C3—H3	120.0	C21—C20—C19	116.92 (19)
C4—C3—H3	120.0	C21—C20—H20	121.5
C5—C4—C3	122.16 (17)	C19—C20—H20	121.5
C5—C4—H4	118.9	C20—C21—C16	121.85 (18)
C3—C4—H4	118.9	C20—C21—C22	129.94 (18)
C4—C5—C6	119.23 (16)	C16—C21—C22	108.21 (16)
C4—C5—C14	120.04 (16)	O2—C22—N2	124.97 (18)
C6—C5—C14	120.65 (15)	O2—C22—C21	129.18 (18)
N1—C6—C1	123.22 (16)	N2—C22—C21	105.84 (15)
N1—C6—C5	118.46 (15)	N3—C23—C8	112.66 (16)
C1—C6—C5	118.30 (15)	N3—C23—H23A	109.1
N1—C7—C12	123.11 (16)	C8—C23—H23A	109.1
N1—C7—C8	118.53 (16)	N3—C23—H23B	109.1
C12—C7—C8	118.36 (16)	C8—C23—H23B	109.1
C9—C8—C7	118.93 (17)	H23A—C23—H23B	107.8
C9—C8—C23	122.60 (17)	O3—C24—N3	125.37 (18)
C7—C8—C23	118.47 (16)	O3—C24—C25	128.72 (18)
C8—C9—C10	122.59 (17)	N3—C24—C25	105.91 (16)
C8—C9—H9	118.7	C30—C25—C26	122.03 (19)
C10—C9—H9	118.7	C30—C25—C24	108.37 (16)
C11—C10—C9	120.00 (18)	C26—C25—C24	129.61 (19)
C11—C10—H10	120.0	C25—C26—C27	116.9 (2)
C9—C10—H10	120.0	C25—C26—H26	121.5
C10—C11—C12	120.12 (17)	C27—C26—H26	121.5
C10—C11—H11	119.9	C28—C27—C26	121.24 (19)
C12—C11—H11	119.9	C28—C27—H27	119.4
C13—C12—C11	122.27 (17)	C26—C27—H27	119.4
C13—C12—C7	117.83 (16)	C27—C28—C29	121.3 (2)
C11—C12—C7	119.89 (16)	C27—C28—H28	119.3
C12—C13—C1	120.04 (16)	C29—C28—H28	119.3
C12—C13—H13	120.0	C30—C29—C28	117.0 (2)
C1—C13—H13	120.0	C30—C29—H29	121.5
N2—C14—C5	114.04 (15)	C28—C29—H29	121.5
N2—C14—H14A	108.7	C29—C30—C25	121.50 (18)
C5—C14—H14A	108.7	C29—C30—C31	130.43 (19)
N2—C14—H14B	108.7	C25—C30—C31	108.06 (17)
C5—C14—H14B	108.7	O4—C31—N3	125.39 (19)
H14A—C14—H14B	107.6	O4—C31—C30	128.47 (19)
O1—C15—N2	124.94 (18)	N3—C31—C30	106.13 (16)

C13—C1—C2—C3	−179.93 (17)	C15—C16—C17—C18	−178.88 (19)
C6—C1—C2—C3	0.4 (3)	C16—C17—C18—C19	−0.8 (3)
C1—C2—C3—C4	1.6 (3)	C17—C18—C19—C20	0.2 (3)
C2—C3—C4—C5	−1.4 (3)	C18—C19—C20—C21	0.6 (3)
C3—C4—C5—C6	−0.7 (3)	C19—C20—C21—C16	−0.9 (3)
C3—C4—C5—C14	−177.57 (17)	C19—C20—C21—C22	179.74 (19)
C7—N1—C6—C1	0.4 (3)	C17—C16—C21—C20	0.2 (3)
C7—N1—C6—C5	178.85 (16)	C15—C16—C21—C20	179.83 (18)
C13—C1—C6—N1	−3.8 (3)	C17—C16—C21—C22	179.75 (17)
C2—C1—C6—N1	175.88 (17)	C15—C16—C21—C22	−0.6 (2)
C13—C1—C6—C5	177.80 (16)	C15—N2—C22—O2	173.75 (18)
C2—C1—C6—C5	−2.5 (2)	C14—N2—C22—O2	−0.8 (3)
C4—C5—C6—N1	−175.82 (17)	C15—N2—C22—C21	−5.2 (2)
C14—C5—C6—N1	1.0 (2)	C14—N2—C22—C21	−179.70 (15)
C4—C5—C6—C1	2.7 (3)	C20—C21—C22—O2	4.1 (3)
C14—C5—C6—C1	179.48 (16)	C16—C21—C22—O2	−175.39 (19)
C6—N1—C7—C12	3.7 (3)	C20—C21—C22—N2	−177.08 (19)
C6—N1—C7—C8	−176.34 (16)	C16—C21—C22—N2	3.4 (2)
N1—C7—C8—C9	−176.64 (17)	C31—N3—C23—C8	−79.5 (2)
C12—C7—C8—C9	3.3 (3)	C24—N3—C23—C8	102.6 (2)
N1—C7—C8—C23	3.8 (2)	C9—C8—C23—N3	−14.1 (3)
C12—C7—C8—C23	−176.31 (15)	C7—C8—C23—N3	165.48 (16)
C7—C8—C9—C10	−0.8 (3)	C31—N3—C24—O3	178.9 (2)
C23—C8—C9—C10	178.72 (19)	C23—N3—C24—O3	−3.0 (3)
C8—C9—C10—C11	−1.5 (3)	C31—N3—C24—C25	−1.1 (2)
C9—C10—C11—C12	1.2 (3)	C23—N3—C24—C25	177.07 (17)
C10—C11—C12—C13	−177.84 (18)	O3—C24—C25—C30	−178.5 (2)
C10—C11—C12—C7	1.3 (3)	N3—C24—C25—C30	1.5 (2)
N1—C7—C12—C13	−4.4 (3)	O3—C24—C25—C26	1.5 (4)
C8—C7—C12—C13	175.64 (16)	N3—C24—C25—C26	−178.6 (2)
N1—C7—C12—C11	176.39 (16)	C30—C25—C26—C27	1.0 (3)
C8—C7—C12—C11	−3.5 (2)	C24—C25—C26—C27	−178.97 (19)
C11—C12—C13—C1	179.99 (16)	C25—C26—C27—C28	−0.8 (3)
C7—C12—C13—C1	0.8 (3)	C26—C27—C28—C29	0.1 (3)
C2—C1—C13—C12	−176.71 (17)	C27—C28—C29—C30	0.5 (3)
C6—C1—C13—C12	2.9 (3)	C28—C29—C30—C25	−0.2 (3)
C15—N2—C14—C5	65.6 (2)	C28—C29—C30—C31	−179.4 (2)
C22—N2—C14—C5	−120.55 (18)	C26—C25—C30—C29	−0.5 (3)
C4—C5—C14—N2	−114.29 (19)	C24—C25—C30—C29	179.48 (19)
C6—C5—C14—N2	68.9 (2)	C26—C25—C30—C31	178.77 (18)
C22—N2—C15—O1	−175.73 (18)	C24—C25—C30—C31	−1.2 (2)
C14—N2—C15—O1	−1.3 (3)	C24—N3—C31—O4	179.6 (2)
C22—N2—C15—C16	4.8 (2)	C23—N3—C31—O4	1.5 (3)
C14—N2—C15—C16	179.16 (16)	C24—N3—C31—C30	0.4 (2)
O1—C15—C16—C17	−2.3 (3)	C23—N3—C31—C30	−177.78 (17)
N2—C15—C16—C17	177.15 (19)	C29—C30—C31—O4	0.6 (4)
O1—C15—C16—C21	178.12 (19)	C25—C30—C31—O4	−178.6 (2)
N2—C15—C16—C21	−2.4 (2)	C29—C30—C31—N3	179.8 (2)

C21—C16—C17—C18	0.6 (3)	C25—C30—C31—N3	0.6 (2)