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2-(4-Bromophenyl)-3-phenylbenzo[*f*]quinoline

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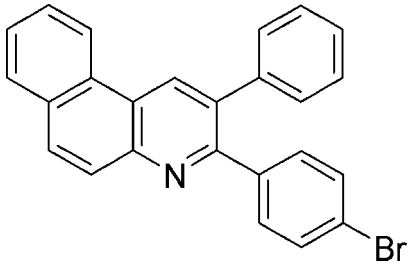
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.004 Å; R factor = 0.042; wR factor = 0.084; data-to-parameter ratio = 13.6.

The title compound, $C_{25}H_{16}BrN$, was synthesized by the reaction of *N*-arylidenenaphthalen-2-amine and phenylacetaldehyde in the presence of iodine. In the molecular structure, the benzoquinoline ring system makes dihedral angles of 61.1 (1) and 39.8 (1)°, respectively, with the phenyl and bromophenyl rings. The dihedral angle between these rings is 57.6 (1)°.

Related literature

For related literature, see: Brock *et al.* (1999); Fokialakis *et al.* (2002); Fossa *et al.* (2002); Sakata *et al.* (1988); Sawada *et al.* (2004).



Experimental

Crystal data

$C_{25}H_{16}BrN$
M_r = 410.30
Monoclinic, $P2_1/c$
a = 12.704 (2) Å
b = 9.4917 (14) Å
c = 15.142 (3) Å
β = 94.612 (4)°
V = 1819.9 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.27 mm^{-1}
T = 193 (2) K
0.78 × 0.55 × 0.17 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.298, T_{max} = 0.679
17280 measured reflections
3336 independent reflections
3034 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.084
S = 1.17
3336 reflections
245 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2196).

References

Brock, E. D., Lewis, D. M., Yousaf, T. I. & Harper, H. H. (1999). WO Patent 9 951 688.
Fokialakis, N., Magiatis, P., Chinou, L., Mitaku, S. & Tillequin, F. (2002). *Chem. Pharm. Bull.* **50**, 413–414.
Fossa, P., Mosti, L., Menozzi, G., Marzano, C., Baccichetti, F. & Bordin, F. (2002). *Bioorg. Med. Chem.* **10**, 743–751.
Jacobson, R. (1998). Private communication to the Rigaku Corporation, Tokyo, Japan.
Rigaku (1999). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2000). *CrystalStructure*. Rigaku/MSC, The Woodlands, Texas, USA.
Sakata, G., Makino, K. & Karasawa, Y. (1988). *Heterocycles*, **27**, 2481–2515.
Sawada, Y., Kayakiri, H., Abe, Y., Mizutani, T., Inamura, N., Asano, M., Hatori, C., Aramori, I., Oku, T. & Tanaka, H. (2004). *J. Med. Chem.* **47**, 2853–2863.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.

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supplementary materials

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2-(4-Bromophenyl)-3-phenylbenzo[*f*]quinoline

X.-S. Wang, Q. Li, M.-M. Zhang and S.-J. Tu

Comment

Quinoline and its derivatives represent an important class of nitrogen-containing heterocycles as they constitute useful intermediates in organic synthesis and are useful dyes (Brock *et al.*, 1999). They are well known in the pharmaceutical industry and have been shown to possess a broad spectrum of biological activities including antiasthmatic activity (Sawada *et al.*, 2004), anti-inflammatory activity (Fokialakis *et al.*, 2002), antimalarial activity (Fossa *et al.*, 2002) and anthelmintic agents (Sakata *et al.*, 1988). We report here the crystal structure of the title compound, (I).

In (I), the benzoquinoline ring system (C1—C5/N1/C18—C25) makes dihedral angles of 61.1 (1) and 39.8 (1)° with the phenyl (C12—C17) and benzene (C6—C11) rings, respectively. The dihedral angle between the phenyl (C12—C17) and benzene (C6—C11) rings is 57.6 (1)°. There is no intermolecular hydrogen bond in the crystal.

Experimental

The title compound was prepared by the reaction of *N*-arylidenenaphthalen-2-amine (0.62 g, 2 mmol) and phenylacetaldehyde (0.24 g, 2 mmol) in the presence of iodine (0.05 g) in THF at 340 K for 5 h (yield 72%; m.p. 478–480 K). Single crystals suitable for X-ray diffraction were obtained by slow evaporation of a DMF solution.

Elemental analysis calculated: C 73.18, H 3.93, N, 3.41%; found: C 73.25, H 3.88, N 3.20%. ^{1}H NMR (DMSO-d$_6$): 7.38 (d, J = 8.4 Hz, 2H, ArH), 7.39 (s, 5H, ArH), 7.52 (d, J = 8.4 Hz, 2H, ArH), 7.74–7.76 (m, 2H, ArH), 7.99 (d, J = 8.8 Hz, 1H, ArH), 8.09–8.11 (m, 1H, ArH), 8.17 (d, J = 8.8 Hz, 1H, ArH), 9.19 (d, J = 7.6 Hz, 1H, ArH), 9.21 (s, 1H, ArH); IR (cm^{-1}): 3056(ArH), 1678(C=N), 1603, 1584, 1566, 1487, 1472, 1431(phenyl ring).

Refinement

The H atoms were calculated geometrically (C—H = 0.95 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C).

Figures

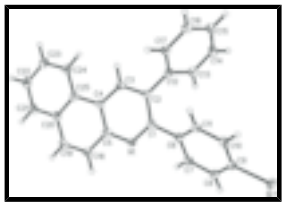


Fig. 1. The molecular structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

2-(4-Bromophenyl)-3-phenylbenzo[*f*]quinoline

Crystal data

$C_{25}H_{16}BrN$	F_{000} = 832
M_r = 410.30	D_x = 1.497 Mg m^{-3}
Monoclinic, $P2_1/c$	Melting point: 478-480 K
Hall symbol: -P 2ybc	Mo $K\alpha$ radiation λ = 0.71070 Å
a = 12.704 (2) Å	Cell parameters from 6717 reflections
b = 9.4917 (14) Å	θ = 3.0–25.3º
c = 15.142 (3) Å	μ = 2.27 mm^{-1}
β = 94.612 (4)º	T = 193 (2) K
V = 1819.9 (5) Å^3	Block, colorless
Z = 4	0.78 × 0.55 × 0.17 mm

Data collection

Rigaku Mercury CCD diffractometer	3336 independent reflections
Radiation source: fine-focus sealed tube	3034 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.042
Detector resolution: 7.31 pixels mm^{-1}	θ_{max} = 25.4º
T = 193(2) K	θ_{min} = 3.0º
ω scans	h = −15→13
Absorption correction: multi-scan (Jacobson, 1998)	k = −11→11
T_{min} = 0.298, T_{max} = 0.679	l = −18→17
17280 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.042	H-atom parameters constrained
$wR(F^2)$ = 0.084	$w = 1/[\sigma^2(F_o^2) + (0.0252P)^2 + 1.5016P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.17	$(\Delta/\sigma)_{max} < 0.001$
3336 reflections	$\Delta\rho_{max}$ = 0.36 e Å^{-3}
245 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.41136 (3)	−0.18517 (3)	0.83655 (2)	0.04218 (13)
N1	0.03956 (17)	0.1754 (2)	0.57827 (14)	0.0277 (5)
C1	0.1407 (2)	0.1676 (3)	0.56232 (17)	0.0257 (6)
C2	0.1811 (2)	0.2330 (3)	0.48741 (17)	0.0245 (6)
C3	0.1113 (2)	0.3102 (3)	0.43206 (17)	0.0270 (6)
H3	0.1367	0.3569	0.3825	0.032*
C4	0.0041 (2)	0.3215 (3)	0.44696 (17)	0.0247 (6)
C5	−0.0276 (2)	0.2501 (3)	0.52243 (17)	0.0268 (6)
C6	0.2081 (2)	0.0849 (3)	0.62874 (17)	0.0258 (6)
C7	0.1673 (2)	−0.0381 (3)	0.66346 (18)	0.0294 (6)
H7	0.0978	−0.0677	0.6438	0.035*
C8	0.2262 (2)	−0.1175 (3)	0.72588 (18)	0.0303 (6)
H8	0.1980	−0.2012	0.7491	0.036*
C9	0.3270 (2)	−0.0729 (3)	0.75395 (17)	0.0286 (6)
C10	0.3691 (2)	0.0492 (3)	0.72268 (18)	0.0304 (6)
H10	0.4378	0.0793	0.7438	0.036*
C11	0.3088 (2)	0.1277 (3)	0.65955 (17)	0.0271 (6)
H11	0.3371	0.2119	0.6372	0.033*
C12	0.2918 (2)	0.2181 (3)	0.46368 (17)	0.0251 (6)
C13	0.3338 (2)	0.0866 (3)	0.44567 (18)	0.0312 (7)
H13	0.2925	0.0041	0.4513	0.037*
C14	0.4349 (2)	0.0755 (3)	0.41985 (19)	0.0354 (7)
H14	0.4621	−0.0145	0.4063	0.042*
C15	0.4972 (2)	0.1933 (3)	0.41337 (19)	0.0339 (7)
H15	0.5674	0.1845	0.3966	0.041*
C16	0.4569 (2)	0.3239 (3)	0.43142 (19)	0.0331 (7)
H16	0.4994	0.4056	0.4275	0.040*
C17	0.3545 (2)	0.3359 (3)	0.45528 (18)	0.0294 (6)
H17	0.3266	0.4266	0.4661	0.035*
C18	−0.1360 (2)	0.2552 (3)	0.54188 (19)	0.0311 (7)
H18	−0.1573	0.2086	0.5930	0.037*
C19	−0.2081 (2)	0.3251 (3)	0.48871 (19)	0.0325 (7)
H19	−0.2794	0.3269	0.5031	0.039*

C20	−0.1798 (2)	0.3970 (3)	0.41076 (18)	0.0293 (6)
C21	−0.2560 (2)	0.4670 (3)	0.35408 (19)	0.0360 (7)
H21	−0.3274	0.4687	0.3685	0.043*
C22	−0.2291 (3)	0.5324 (3)	0.2787 (2)	0.0408 (8)
H22	−0.2815	0.5799	0.2415	0.049*
C23	−0.1256 (3)	0.5294 (4)	0.2567 (2)	0.0435 (8)
H23	−0.1073	0.5736	0.2038	0.052*
C24	−0.0491 (2)	0.4632 (3)	0.3106 (2)	0.0389 (7)
H24	0.0217	0.4628	0.2946	0.047*
C25	−0.0736 (2)	0.3956 (3)	0.38919 (17)	0.0276 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0505 (2)	0.0406 (2)	0.03533 (19)	0.01776 (15)	0.00243 (14)	0.00900 (15)
N1	0.0279 (13)	0.0312 (13)	0.0238 (12)	−0.0001 (10)	0.0016 (10)	0.0020 (10)
C1	0.0287 (15)	0.0247 (14)	0.0237 (14)	−0.0015 (11)	0.0011 (12)	−0.0027 (12)
C2	0.0261 (14)	0.0255 (14)	0.0219 (14)	−0.0035 (11)	0.0015 (11)	−0.0030 (11)
C3	0.0311 (15)	0.0282 (14)	0.0216 (14)	−0.0030 (12)	0.0015 (12)	0.0012 (12)
C4	0.0249 (14)	0.0258 (14)	0.0230 (14)	−0.0012 (11)	0.0004 (11)	−0.0034 (12)
C5	0.0282 (15)	0.0282 (15)	0.0236 (14)	−0.0028 (12)	0.0002 (12)	−0.0031 (12)
C6	0.0305 (15)	0.0256 (14)	0.0217 (14)	0.0043 (12)	0.0045 (12)	−0.0017 (12)
C7	0.0334 (16)	0.0292 (15)	0.0260 (15)	−0.0020 (12)	0.0042 (12)	−0.0014 (12)
C8	0.0439 (18)	0.0227 (14)	0.0254 (15)	0.0043 (13)	0.0086 (13)	−0.0001 (12)
C9	0.0340 (16)	0.0309 (15)	0.0209 (14)	0.0113 (13)	0.0027 (12)	0.0005 (12)
C10	0.0299 (16)	0.0349 (16)	0.0264 (15)	0.0027 (12)	0.0025 (12)	−0.0009 (13)
C11	0.0320 (16)	0.0261 (14)	0.0233 (14)	−0.0017 (12)	0.0022 (12)	0.0021 (12)
C12	0.0252 (14)	0.0320 (15)	0.0175 (13)	−0.0002 (12)	−0.0012 (11)	0.0015 (12)
C13	0.0315 (16)	0.0310 (16)	0.0303 (15)	−0.0037 (13)	−0.0029 (13)	−0.0039 (13)
C14	0.0339 (17)	0.0361 (17)	0.0360 (17)	0.0065 (14)	0.0015 (14)	−0.0086 (14)
C15	0.0244 (15)	0.0477 (19)	0.0299 (15)	0.0039 (14)	0.0038 (12)	−0.0037 (14)
C16	0.0331 (16)	0.0351 (17)	0.0318 (16)	−0.0052 (13)	0.0070 (13)	0.0004 (13)
C17	0.0310 (16)	0.0284 (15)	0.0294 (15)	0.0019 (12)	0.0065 (13)	0.0007 (12)
C18	0.0293 (16)	0.0371 (16)	0.0272 (15)	−0.0006 (13)	0.0043 (13)	−0.0006 (13)
C19	0.0261 (15)	0.0397 (17)	0.0324 (16)	0.0007 (13)	0.0068 (13)	−0.0073 (14)
C20	0.0298 (15)	0.0301 (15)	0.0273 (15)	0.0039 (12)	−0.0016 (12)	−0.0083 (13)
C21	0.0328 (16)	0.0414 (18)	0.0332 (17)	0.0085 (14)	−0.0023 (13)	−0.0060 (14)
C22	0.0439 (19)	0.0441 (19)	0.0324 (17)	0.0140 (15)	−0.0098 (14)	−0.0032 (15)
C23	0.044 (2)	0.050 (2)	0.0352 (18)	0.0071 (16)	−0.0035 (15)	0.0135 (15)
C24	0.0341 (17)	0.0475 (19)	0.0349 (17)	−0.0005 (14)	0.0011 (14)	0.0095 (15)
C25	0.0286 (15)	0.0284 (15)	0.0252 (14)	−0.0003 (12)	−0.0022 (12)	−0.0023 (12)

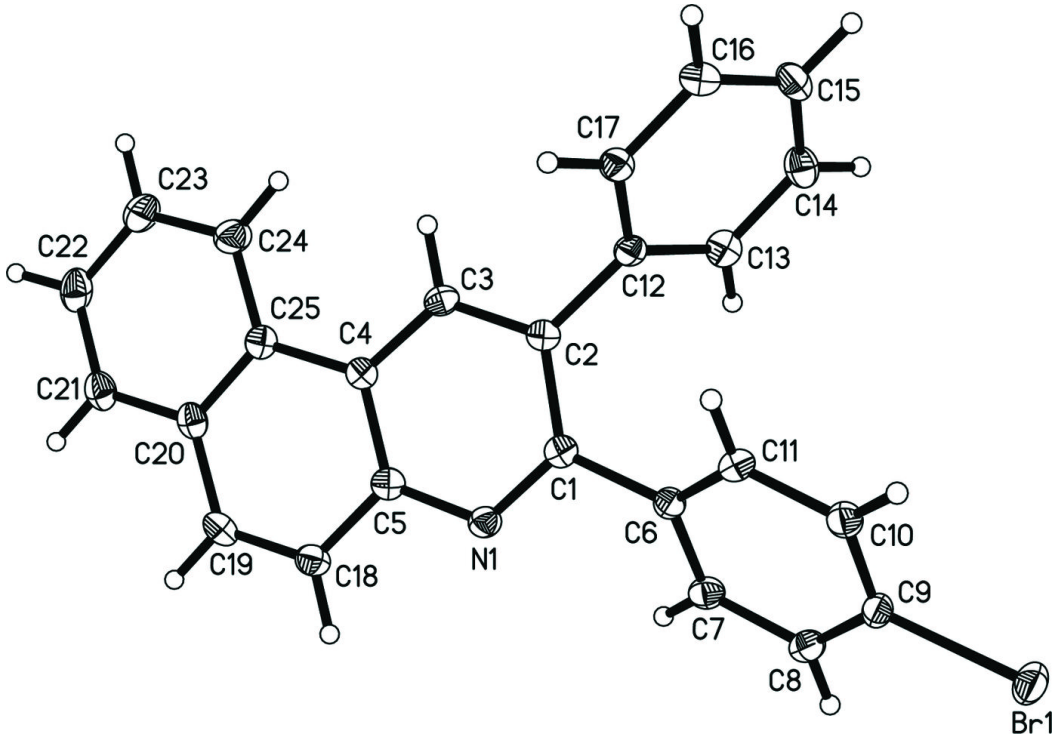
Geometric parameters (Å, °)

Br1—C9	1.906 (3)	C13—C14	1.376 (4)
N1—C1	1.328 (3)	C13—H13	0.9500
N1—C5	1.353 (3)	C14—C15	1.379 (4)
C1—C2	1.424 (4)	C14—H14	0.9500
C1—C6	1.491 (4)	C15—C16	1.376 (4)

C2—C3	1.380 (4)	C15—H15	0.9500
C2—C12	1.485 (4)	C16—C17	1.383 (4)
C3—C4	1.403 (4)	C16—H16	0.9500
C3—H3	0.9500	C17—H17	0.9500
C4—C5	1.415 (4)	C18—C19	1.344 (4)
C4—C25	1.448 (4)	C18—H18	0.9500
C5—C18	1.432 (4)	C19—C20	1.434 (4)
C6—C11	1.387 (4)	C19—H19	0.9500
C6—C7	1.398 (4)	C20—C21	1.407 (4)
C7—C8	1.381 (4)	C20—C25	1.414 (4)
C7—H7	0.9500	C21—C22	1.366 (4)
C8—C9	1.383 (4)	C21—H21	0.9500
C8—H8	0.9500	C22—C23	1.383 (4)
C9—C10	1.376 (4)	C22—H22	0.9500
C10—C11	1.392 (4)	C23—C24	1.370 (4)
C10—H10	0.9500	C23—H23	0.9500
C11—H11	0.9500	C24—C25	1.409 (4)
C12—C17	1.385 (4)	C24—H24	0.9500
C12—C13	1.393 (4)		
C1—N1—C5	119.1 (2)	C14—C13—H13	119.8
N1—C1—C2	122.5 (2)	C12—C13—H13	119.8
N1—C1—C6	114.7 (2)	C13—C14—C15	120.8 (3)
C2—C1—C6	122.8 (2)	C13—C14—H14	119.6
C3—C2—C1	117.4 (2)	C15—C14—H14	119.6
C3—C2—C12	118.5 (2)	C16—C15—C14	119.4 (3)
C1—C2—C12	124.1 (2)	C16—C15—H15	120.3
C2—C3—C4	121.8 (2)	C14—C15—H15	120.3
C2—C3—H3	119.1	C15—C16—C17	119.9 (3)
C4—C3—H3	119.1	C15—C16—H16	120.0
C3—C4—C5	115.9 (2)	C17—C16—H16	120.0
C3—C4—C25	124.3 (2)	C16—C17—C12	121.2 (3)
C5—C4—C25	119.7 (2)	C16—C17—H17	119.4
N1—C5—C4	123.3 (2)	C12—C17—H17	119.4
N1—C5—C18	117.3 (2)	C19—C18—C5	120.9 (3)
C4—C5—C18	119.4 (2)	C19—C18—H18	119.6
C11—C6—C7	118.6 (3)	C5—C18—H18	119.6
C11—C6—C1	122.5 (2)	C18—C19—C20	121.6 (3)
C7—C6—C1	118.9 (2)	C18—C19—H19	119.2
C8—C7—C6	121.0 (3)	C20—C19—H19	119.2
C8—C7—H7	119.5	C21—C20—C25	119.1 (3)
C6—C7—H7	119.5	C21—C20—C19	121.4 (3)
C7—C8—C9	118.8 (3)	C25—C20—C19	119.5 (3)
C7—C8—H8	120.6	C22—C21—C20	121.2 (3)
C9—C8—H8	120.6	C22—C21—H21	119.4
C10—C9—C8	121.8 (3)	C20—C21—H21	119.4
C10—C9—Br1	118.9 (2)	C21—C22—C23	119.8 (3)
C8—C9—Br1	119.3 (2)	C21—C22—H22	120.1
C9—C10—C11	118.7 (3)	C23—C22—H22	120.1
C9—C10—H10	120.7	C24—C23—C22	120.6 (3)

C11—C10—H10	120.7	C24—C23—H23	119.7
C6—C11—C10	121.1 (3)	C22—C23—H23	119.7
C6—C11—H11	119.5	C23—C24—C25	121.2 (3)
C10—C11—H11	119.5	C23—C24—H24	119.4
C17—C12—C13	118.2 (2)	C25—C24—H24	119.4
C17—C12—C2	120.5 (2)	C24—C25—C20	118.1 (3)
C13—C12—C2	121.2 (2)	C24—C25—C4	123.1 (3)
C14—C13—C12	120.4 (3)	C20—C25—C4	118.8 (2)
C5—N1—C1—C2	−1.2 (4)	C1—C2—C12—C17	−122.9 (3)
C5—N1—C1—C6	179.0 (2)	C3—C2—C12—C13	−117.5 (3)
N1—C1—C2—C3	2.1 (4)	C1—C2—C12—C13	59.9 (4)
C6—C1—C2—C3	−178.2 (2)	C17—C12—C13—C14	−0.3 (4)
N1—C1—C2—C12	−175.3 (2)	C2—C12—C13—C14	177.0 (3)
C6—C1—C2—C12	4.4 (4)	C12—C13—C14—C15	1.6 (4)
C1—C2—C3—C4	−1.7 (4)	C13—C14—C15—C16	−1.2 (4)
C12—C2—C3—C4	175.9 (2)	C14—C15—C16—C17	−0.4 (4)
C2—C3—C4—C5	0.5 (4)	C15—C16—C17—C12	1.7 (4)
C2—C3—C4—C25	−177.1 (3)	C13—C12—C17—C16	−1.3 (4)
C1—N1—C5—C4	0.0 (4)	C2—C12—C17—C16	−178.6 (2)
C1—N1—C5—C18	179.7 (2)	N1—C5—C18—C19	−178.8 (3)
C3—C4—C5—N1	0.4 (4)	C4—C5—C18—C19	1.0 (4)
C25—C4—C5—N1	178.2 (2)	C5—C18—C19—C20	0.1 (4)
C3—C4—C5—C18	−179.4 (2)	C18—C19—C20—C21	178.3 (3)
C25—C4—C5—C18	−1.6 (4)	C18—C19—C20—C25	−0.4 (4)
N1—C1—C6—C11	−138.9 (3)	C25—C20—C21—C22	0.4 (4)
C2—C1—C6—C11	41.3 (4)	C19—C20—C21—C22	−178.4 (3)
N1—C1—C6—C7	39.0 (3)	C20—C21—C22—C23	0.6 (5)
C2—C1—C6—C7	−140.8 (3)	C21—C22—C23—C24	−1.1 (5)
C11—C6—C7—C8	−1.2 (4)	C22—C23—C24—C25	0.5 (5)
C1—C6—C7—C8	−179.3 (2)	C23—C24—C25—C20	0.5 (4)
C6—C7—C8—C9	0.2 (4)	C23—C24—C25—C4	178.5 (3)
C7—C8—C9—C10	1.2 (4)	C21—C20—C25—C24	−0.9 (4)
C7—C8—C9—Br1	−177.56 (19)	C19—C20—C25—C24	177.9 (3)
C8—C9—C10—C11	−1.5 (4)	C21—C20—C25—C4	−179.0 (2)
Br1—C9—C10—C11	177.3 (2)	C19—C20—C25—C4	−0.2 (4)
C7—C6—C11—C10	1.0 (4)	C3—C4—C25—C24	0.8 (4)
C1—C6—C11—C10	178.9 (2)	C5—C4—C25—C24	−176.8 (3)
C9—C10—C11—C6	0.4 (4)	C3—C4—C25—C20	178.8 (3)
C3—C2—C12—C17	59.8 (3)	C5—C4—C25—C20	1.2 (4)

Fig. 1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