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(*Z*)-3-[1-(4-Chlorobenzyl)-1*H*-indol-3-yl]-2-(3-thienyl)acrylonitrile

Vijayakumar N. Sonar,[a] Sean Parkin[b] and Peter A. Crooks[a]*

[a]Department of Pharmaceutical Sciences, College of Pharmacy, University of Kentucky, Lexington, KY 40536, USA, and [b]Department of Chemistry, University of Kentucky, Lexington, KY 40506, USA
Correspondence e-mail: pcrooks@email.uky.edu

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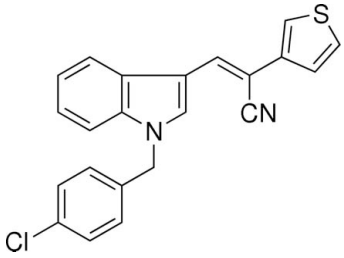
Key indicators: single-crystal X-ray study; T = 90 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.033; wR factor = 0.088; data-to-parameter ratio = 11.9.

The title compound, $C_{22}H_{15}ClN_2S$, was prepared by the base-catalyzed reaction of 1-(4-chlorobenzyl)indole-3-carboxaldehyde with thiophene-3-acetonitrile and recrystallization of the product from methanol. The double bond connecting the indole and thiophene units has *Z* geometry. The indole ring system is nearly planar and makes a dihedral angle of 79.81 (4)° with the plane of the 4-chlorophenyl ring. The molecule exhibits orientational disorder of the thienyl fragment, with occupancy factors of 0.65:0.35.

Related literature

For related literature, see: Allen (2002); Bacelo *et al.* (1997); Beddoes *et al.* (1986); Mason *et al.* (2003); Sonar *et al.* (2004); Wilson (1992); Zarza *et al.* (1988).



Experimental

Crystal data

$C_{22}H_{15}ClN_2S$
M_r = 374.87
Monoclinic, $P2_1/n$
a = 16.8531 (11) Å
b = 5.5629 (4) Å
c = 18.7889 (13) Å
β = 96.877 (2)°
V = 1748.8 (2) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 3.10 mm^{-1}
T = 90.0 (2) K
0.25 × 0.02 × 0.01 mm

Data collection

Bruker X8 Proteum diffractometer
Absorption correction: multi-scan (*SADABS* in *APEX2*; Bruker, 2006)
T_{min} = 0.657, T_{max} = 0.970
24522 measured reflections
3248 independent reflections
3020 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
S = 1.05
3248 reflections
273 parameters
162 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 1995); software used to prepare material for publication: *SHELXL97* and local procedures.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: OM2157).

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supplementary materials

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(*Z*)-3-[1-(4-Chlorobenzyl)-1*H*-indol-3-yl]-2-(3-thienyl)acrylonitrile

V. N. Sonar, S. Parkin and P. A. Crooks

Comment

We have synthesized a series of novel substituted aryl/heteroaryl-2-(thienyl) acrylonitriles and evaluated them for anticancer activity. The title compound was prepared by the base-catalyzed reaction of 1-(4-chlorobenzyl)indole-3- carboxaldehyde with thiophene-3-acetonitrile and recrystallization of the product from methanol to afford yellow needles. In order to confirm the double bond geometry in the title compound, and to obtain more detailed information of the structural conformation of the molecule, its X-ray structure determination has been carried out.

X-ray crystallography confirmed the molecular structure and atom connectivity for the title compound. In the title molecule the double bond connecting the indole and thiophene moieties has the *Z*-geometry. The indole ring is nearly planar with bond distances and bond angles comparable with those reported for other indole derivatives (Mason *et al.*, 2003; Zarza *et al.*, 1988). In the molecule, atom N1 lies slightly [0.0640 (16) Å] out of the plane of connecting atoms C2, C9, and C19, the sum of the angles about N1 being 359.36 (13)°. In a previous study, 21 structurally related indole analogues were analyzed (Beddoes *et al.*, 1986) (available in the Cambridge Structural Database; Allen, 2002), and the sum of the three angles around the N atom were determined, to assess planarity. It was found that only two of the 21 compounds had values that were outside the range 359.0–360°, the farthest value from the perfectly planar situation being 357.2°. This is in general agreement with our current observation with the title compound. The plane of the 4-chlorophenyl group is twisted well out of the plane of the indole ring and makes a dihedral angle of 79.81 (4)°. There is an asymmetry of the exocyclic angles at C20 [C19—C20—C21 = 123.19 (14)° and C19—C20—C25 =117.73 (14)°].

Deviations from the ideal bond-angle geometry around the C_{sp}^2 atoms of the double bond are observed. The bond angles C2=C3—C10, C3—C10=C11, and C12—C11—C17 [129.95 (14), 129.61 (14), and 114.47 (13)°, respectively] are distorted because of strain induced by the double bond linking the indole and thiophene rings. The vinyl group bearing the three substituents has a double bond length of 1.352 (2)Å and is significantly longer than that observed in the disubstituted vinyl group of 2-styrylbenzimidazoles (1.304 (4) Å; Bacelo *et al.*, 1997). Furthermore, the C3—C10 bond length [1.431 (2) Å] is slightly shorter than a C_{ar}—C_{sp}^2 single bond (Wilson, 1992). The C2=C3—C10=C11, C3—C10=C11—C12, and C10=C11—C12=C16 torsion angles [4.7 (3), 178.75 (15), and −179.2 (8), respectively] show that the non-H atoms of the indole and thiophene rings are nearly coplanar. The 2-thienyl group exhibits rotational disorder over two sets of sites corresponding to 180° about the C11—C12 bond with occupancy factors of 0.65:0.35.

Experimental

The title compound was prepared according to the previously reported procedure of Sonar *et al.* (2004). Recrystallization from methanol afforded yellow colored needles. ^{1}H NMR (DMSO-d_6, p.p.m.): δ 7.22–7.30 (m, 4H), 7.41 (d, 2H), 7.55 (dd, 1H), 7.71 (s, 3H), 8.10 (dd, 1H), 8.15 (s, 1H), 8.45 (s, 1H). ^{13}C NMR (DMSO-d_6, p.p.m.): δ 48.90, 99.19, 110.27,

110.89, 119.09, 119.39, 120.82, 121.32, 122.93, 124.69, 127.66, 127.90, 128.55, 128.87, 129.34, 132.10, 132.45, 135.46, 136.18, 136.46.

Refinement

H atoms were found in difference Fourier maps and subsequently placed in idealized positions with contrained C—H distances of 0.95 Å and U_{iso}(H) values set to 1.2U_{eq} of the attached C atom. The thienyl group was disordered by a 180° rotation over two positions about the C11—C12 bond with occupancy factors of 0.65:0.35, as is common in this type of compound. Refinement of this disorder model required a number of restraints to maintain the similarity and the integrity of the thienyl groups. The restraints used in SHXLEL were:

SAME - helps to maintain similar bond lengths and angles between specified atoms.

SIMU - helps to ensure that the equivalent U_{iso} of the specified atoms remain similar.

DELU - restrains the components of anisotropic displacement parameters along bonds between specified atoms so that they do not change by any large amount from one atom to the next.

Figures

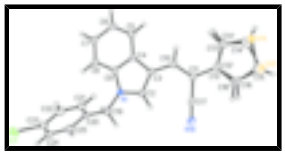


Fig. 1. A view of molecule (I), with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. The thienyl ring is disordered with occupancy factors of 0.65:0.35.

(*Z*)-3-[1-(4-Chlorobenzyl)-1*H*-indol-3-yl]-2-(3- thienyl)acrylonitrile

Crystal data

$C_{22}H_{15}ClN_2S$	F_{000} = 776
M_r = 374.87	D_x = 1.424 Mg m^{-3}
Monoclinic, $P2_1/n$	Cu $K\alpha$ radiation λ = 1.54178 Å
Hall symbol: -P 2yn	Cell parameters from 9856 reflections
a = 16.8531 (11) Å	θ = 3.3–69.6º
b = 5.5629 (4) Å	μ = 3.10 mm^{-1}
c = 18.7889 (13) Å	T = 90.0 (2) K
β = 96.877 (2)º	Needle, yellow
V = 1748.8 (2) Å^3	0.25 × 0.02 × 0.01 mm
Z = 4	

Data collection

Bruker X8 Proteum diffractometer	3248 independent reflections
Radiation source: fine-focus rotating anode	3020 reflections with $I > 2\sigma(I)$

Monochromator: graded multilayer optics
T = 90.0(2) K
φ and ω scans
Absorption correction: multi-scan (SADABS in APEX2; Bruker, 2006)
T_{min} = 0.657, T_{max} = 0.970
24522 measured reflections
R_{int} = 0.040
θ_{max} = 69.7º
θ_{min} = 3.3º
h = −20→20
k = −4→6
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
S = 1.05
3248 reflections
273 parameters
162 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
$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 1.6245P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.007
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00051 (14)

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 $F^2 > 2\sigma(F^2)$ 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}	Occ. (<1)
N1	0.60215 (8)	0.8954 (2)	0.37437 (7)	0.0171 (3)	
C2	0.55429 (9)	0.6994 (3)	0.37495 (8)	0.0170 (3)	
H2	0.5312	0.6435	0.4156	0.020*	
C3	0.54388 (9)	0.5928 (3)	0.30821 (8)	0.0164 (3)	
C4	0.58888 (9)	0.7374 (3)	0.26350 (8)	0.0168 (3)	
C5	0.60044 (9)	0.7306 (3)	0.19122 (8)	0.0203 (3)	
H5	0.5783	0.6044	0.1611	0.024*	
C6	0.64460 (10)	0.9105 (3)	0.16452 (9)	0.0229 (4)	
H6	0.6524	0.9082	0.1153	0.027*	

C7	0.67814 (10)	1.0960 (3)	0.20821 (9)	0.0223 (3)	
H7	0.7082	1.2176	0.1881	0.027*	
C8	0.66845 (9)	1.1062 (3)	0.27981 (9)	0.0200 (3)	
H8	0.6915	1.2314	0.3098	0.024*	
C9	0.62347 (9)	0.9253 (3)	0.30613 (8)	0.0168 (3)	
C10	0.49692 (9)	0.3884 (3)	0.28348 (8)	0.0171 (3)	
H10	0.5021	0.3391	0.2358	0.021*	
C11	0.44630 (9)	0.2549 (3)	0.31782 (8)	0.0168 (3)	
C12	0.39941 (9)	0.0499 (3)	0.28704 (8)	0.0181 (3)	0.652 (2)
C13	0.4007 (10)	−0.034 (2)	0.2194 (7)	0.0193 (13)	0.652 (2)
H13	0.4324	0.0366	0.1864	0.023*	0.652 (2)
S14	0.33986 (9)	−0.2784 (3)	0.19900 (6)	0.0198 (3)	0.652 (2)
C15	0.3100 (7)	−0.266 (2)	0.2821 (6)	0.0279 (18)	0.652 (2)
H15	0.2722	−0.3744	0.2979	0.034*	0.652 (2)
C16	0.3446 (8)	−0.0911 (19)	0.3232 (6)	0.0187 (12)	0.652 (2)
H16	0.3343	−0.0623	0.3711	0.022*	0.652 (2)
C12'	0.39941 (9)	0.0499 (3)	0.28704 (8)	0.0181 (3)	0.348 (2)
C13'	0.4009 (19)	−0.059 (4)	0.2181 (13)	0.020 (2)	0.348 (2)
H13'	0.4334	−0.0094	0.1827	0.024*	0.348 (2)
C14'	0.3494 (8)	−0.239 (2)	0.2119 (6)	0.029 (2)	0.348 (2)
H14'	0.3407	−0.3328	0.1695	0.034*	0.348 (2)
S15'	0.2997 (3)	−0.2935 (10)	0.2838 (2)	0.0211 (7)	0.348 (2)
C16'	0.3492 (16)	−0.058 (4)	0.3271 (11)	0.020 (2)	0.348 (2)
H16'	0.3420	−0.0087	0.3743	0.024*	0.348 (2)
C17	0.43384 (9)	0.3125 (3)	0.38978 (8)	0.0189 (3)	
N18	0.42323 (8)	0.3528 (3)	0.44772 (7)	0.0243 (3)	
C19	0.61814 (9)	1.0662 (3)	0.43239 (8)	0.0185 (3)	
H19A	0.5852	1.0225	0.4707	0.022*	
H19B	0.6006	1.2273	0.4144	0.022*	
C20	0.70410 (9)	1.0828 (3)	0.46485 (8)	0.0171 (3)	
C21	0.75987 (10)	0.9063 (3)	0.45686 (8)	0.0207 (3)	
H21	0.7445	0.7671	0.4293	0.025*	
C22	0.83803 (10)	0.9300 (3)	0.48858 (9)	0.0245 (4)	
H22	0.8764	0.8087	0.4828	0.029*	
C23	0.85917 (10)	1.1319 (3)	0.52860 (8)	0.0240 (4)	
C24	0.80456 (10)	1.3088 (3)	0.53802 (9)	0.0244 (4)	
H24	0.8199	1.4461	0.5665	0.029*	
C25	0.72715 (10)	1.2843 (3)	0.50554 (8)	0.0211 (3)	
H25	0.6892	1.4070	0.5111	0.025*	
Cl1	0.95722 (3)	1.16827 (10)	0.56800 (2)	0.03730 (15)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0194 (7)	0.0150 (6)	0.0176 (6)	−0.0007 (5)	0.0048 (5)	0.0005 (5)
C2	0.0160 (7)	0.0160 (7)	0.0197 (7)	0.0016 (6)	0.0048 (6)	0.0040 (6)
C3	0.0159 (7)	0.0166 (7)	0.0172 (7)	0.0013 (6)	0.0033 (6)	0.0033 (6)
C4	0.0147 (7)	0.0156 (7)	0.0206 (8)	0.0024 (6)	0.0037 (6)	0.0032 (6)

C5	0.0205 (8)	0.0209 (8)	0.0199 (8)	−0.0004 (6)	0.0045 (6)	0.0003 (6)
C6	0.0237 (8)	0.0262 (9)	0.0201 (8)	0.0006 (7)	0.0084 (6)	0.0032 (7)
C7	0.0216 (8)	0.0190 (8)	0.0280 (8)	−0.0007 (6)	0.0102 (6)	0.0056 (7)
C8	0.0181 (8)	0.0165 (8)	0.0261 (8)	−0.0002 (6)	0.0059 (6)	0.0006 (6)
C9	0.0157 (7)	0.0158 (7)	0.0194 (7)	0.0030 (6)	0.0045 (6)	0.0027 (6)
C10	0.0176 (7)	0.0174 (8)	0.0166 (7)	0.0024 (6)	0.0027 (6)	0.0021 (6)
C11	0.0163 (7)	0.0175 (8)	0.0165 (7)	0.0024 (6)	0.0020 (6)	0.0034 (6)
C12	0.0159 (7)	0.0159 (7)	0.0220 (8)	0.0019 (6)	0.0007 (6)	0.0049 (6)
C13	0.020 (2)	0.013 (3)	0.024 (2)	−0.002 (2)	0.0019 (17)	0.0015 (17)
S14	0.0220 (5)	0.0171 (5)	0.0203 (5)	−0.0011 (3)	0.0023 (4)	−0.0002 (3)
C15	0.026 (3)	0.021 (3)	0.037 (3)	−0.001 (2)	0.006 (2)	0.0089 (19)
C16	0.017 (2)	0.017 (3)	0.023 (2)	−0.0039 (18)	0.0053 (18)	0.0060 (17)
C12'	0.0159 (7)	0.0159 (7)	0.0220 (8)	0.0019 (6)	0.0007 (6)	0.0049 (6)
C13'	0.021 (3)	0.020 (4)	0.020 (3)	0.007 (3)	0.004 (3)	−0.002 (3)
C14'	0.027 (3)	0.026 (4)	0.030 (3)	0.008 (3)	−0.004 (3)	−0.006 (3)
S15'	0.0206 (12)	0.0173 (12)	0.0253 (10)	−0.0030 (9)	0.0021 (7)	0.0016 (8)
C16'	0.019 (4)	0.015 (4)	0.026 (3)	−0.002 (3)	−0.004 (3)	0.003 (3)
C17	0.0153 (7)	0.0180 (8)	0.0236 (9)	−0.0007 (6)	0.0035 (6)	0.0052 (6)
N18	0.0234 (7)	0.0283 (8)	0.0223 (7)	−0.0017 (6)	0.0064 (6)	0.0031 (6)
C19	0.0205 (8)	0.0154 (7)	0.0203 (8)	0.0012 (6)	0.0056 (6)	−0.0010 (6)
C20	0.0215 (8)	0.0157 (7)	0.0149 (7)	0.0005 (6)	0.0059 (6)	0.0030 (6)
C21	0.0239 (8)	0.0181 (8)	0.0205 (8)	0.0023 (6)	0.0046 (6)	−0.0013 (6)
C22	0.0246 (9)	0.0265 (9)	0.0231 (8)	0.0092 (7)	0.0059 (6)	0.0003 (7)
C23	0.0212 (8)	0.0346 (10)	0.0165 (7)	0.0019 (7)	0.0032 (6)	−0.0002 (7)
C24	0.0277 (9)	0.0253 (9)	0.0203 (8)	−0.0006 (7)	0.0036 (7)	−0.0057 (7)
C25	0.0231 (8)	0.0194 (8)	0.0217 (8)	0.0032 (6)	0.0057 (6)	−0.0010 (6)
Cl1	0.0219 (2)	0.0607 (3)	0.0282 (2)	0.0056 (2)	−0.00151 (16)	−0.0154 (2)

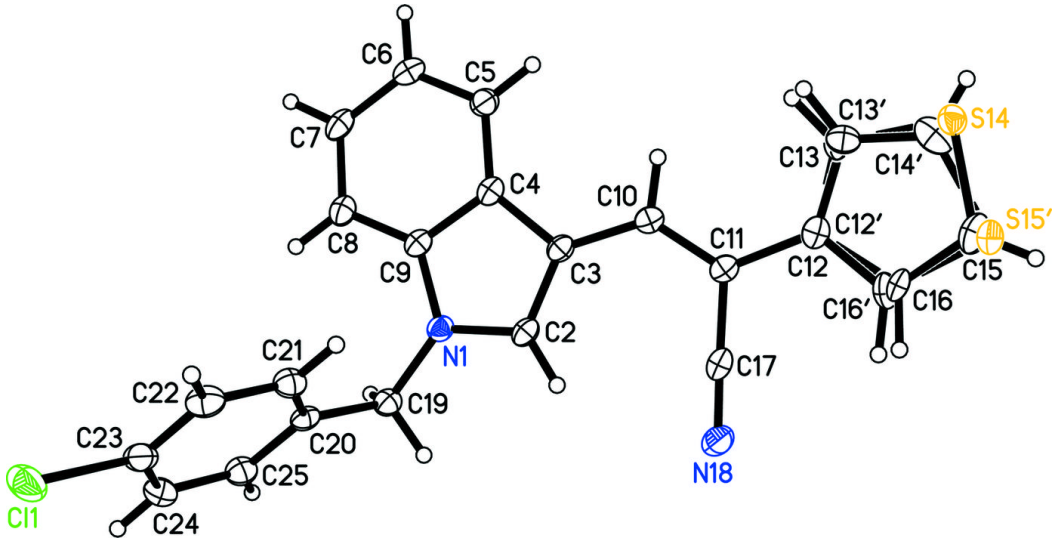
Geometric parameters (Å, °)

N1—C2	1.357 (2)	S14—C15	1.698 (10)
N1—C9	1.3823 (19)	C15—C16	1.334 (15)
N1—C19	1.447 (2)	C15—H15	0.9500
C2—C3	1.379 (2)	C16—H16	0.9500
C2—H2	0.9500	C13'—C14'	1.32 (2)
C3—C10	1.431 (2)	C13'—H13'	0.9500
C3—C4	1.442 (2)	C14'—S15'	1.701 (11)
C4—C5	1.395 (2)	C14'—H14'	0.9500
C4—C9	1.401 (2)	S15'—C16'	1.707 (17)
C5—C6	1.377 (2)	C16'—H16'	0.9500
C5—H5	0.9500	C17—N18	1.146 (2)
C6—C7	1.396 (2)	C19—C20	1.506 (2)
C6—H6	0.9500	C19—H19A	0.9900
C7—C8	1.375 (2)	C19—H19B	0.9900
C7—H7	0.9500	C20—C21	1.380 (2)
C8—C9	1.386 (2)	C20—C25	1.386 (2)
C8—H8	0.9500	C21—C22	1.385 (2)
C10—C11	1.352 (2)	C21—H21	0.9500
C10—H10	0.9500	C22—C23	1.375 (3)

C11—C17	1.429 (2)	C22—H22	0.9500
C11—C12	1.466 (2)	C23—C24	1.373 (2)
C12—C13	1.355 (11)	C23—Cl1	1.7397 (17)
C12—C16	1.442 (9)	C24—C25	1.379 (2)
C13—S14	1.721 (10)	C24—H24	0.9500
C13—H13	0.9500	C25—H25	0.9500
C2—N1—C9	108.95 (13)	C15—S14—C13	89.9 (5)
C2—N1—C19	125.38 (13)	C16—C15—S14	113.8 (8)
C9—N1—C19	125.03 (13)	C16—C15—H15	123.1
N1—C2—C3	110.44 (13)	S14—C15—H15	123.1
N1—C2—H2	124.8	C15—C16—C12	112.7 (8)
C3—C2—H2	124.8	C15—C16—H16	123.7
C2—C3—C10	129.95 (14)	C12—C16—H16	123.7
C2—C3—C4	105.73 (13)	C14'—C13'—H13'	125.8
C10—C3—C4	124.27 (14)	C13'—C14'—S15'	116.6 (11)
C5—C4—C9	118.68 (14)	C13'—C14'—H14'	121.7
C5—C4—C3	134.10 (15)	S15'—C14'—H14'	121.7
C9—C4—C3	107.15 (13)	C14'—S15'—C16'	88.9 (8)
C6—C5—C4	118.64 (15)	S15'—C16'—H16'	123.8
C6—C5—H5	120.7	N18—C17—C11	178.23 (17)
C4—C5—H5	120.7	N1—C19—C20	115.37 (13)
C5—C6—C7	121.44 (15)	N1—C19—H19A	108.4
C5—C6—H6	119.3	C20—C19—H19A	108.4
C7—C6—H6	119.3	N1—C19—H19B	108.4
C8—C7—C6	121.23 (15)	C20—C19—H19B	108.4
C8—C7—H7	119.4	H19A—C19—H19B	107.5
C6—C7—H7	119.4	C21—C20—C25	119.08 (15)
C7—C8—C9	116.95 (15)	C21—C20—C19	123.19 (14)
C7—C8—H8	121.5	C25—C20—C19	117.73 (14)
C9—C8—H8	121.5	C20—C21—C22	120.70 (15)
N1—C9—C8	129.21 (15)	C20—C21—H21	119.7
N1—C9—C4	107.71 (13)	C22—C21—H21	119.7
C8—C9—C4	123.06 (14)	C23—C22—C21	118.93 (15)
C11—C10—C3	129.61 (14)	C23—C22—H22	120.5
C11—C10—H10	115.2	C21—C22—H22	120.5
C3—C10—H10	115.2	C24—C23—C22	121.48 (16)
C10—C11—C17	120.07 (14)	C24—C23—Cl1	118.61 (14)
C10—C11—C12	125.45 (14)	C22—C23—Cl1	119.90 (13)
C17—C11—C12	114.47 (13)	C23—C24—C25	119.02 (16)
C13—C12—C16	109.8 (4)	C23—C24—H24	120.5
C13—C12—C11	124.6 (4)	C25—C24—H24	120.5
C16—C12—C11	125.6 (4)	C24—C25—C20	120.78 (15)
C12—C13—S14	113.8 (7)	C24—C25—H25	119.6
C12—C13—H13	123.1	C20—C25—H25	119.6
S14—C13—H13	123.1		
C9—N1—C2—C3	1.06 (17)	C10—C11—C12—C13	0.1 (10)
C19—N1—C2—C3	172.28 (14)	C17—C11—C12—C13	178.9 (10)
N1—C2—C3—C10	−177.97 (15)	C10—C11—C12—C16	−179.2 (8)

N1—C2—C3—C4	−0.34 (17)	C17—C11—C12—C16	−0.4 (8)
C2—C3—C4—C5	−177.53 (17)	C16—C12—C13—S14	−1.1 (15)
C10—C3—C4—C5	0.3 (3)	C11—C12—C13—S14	179.5 (5)
C2—C3—C4—C9	−0.48 (17)	C12—C13—S14—C15	1.2 (13)
C10—C3—C4—C9	177.32 (14)	C13—S14—C15—C16	−0.9 (14)
C9—C4—C5—C6	−0.8 (2)	S14—C15—C16—C12	0.4 (17)
C3—C4—C5—C6	176.00 (16)	C13—C12—C16—C15	0.5 (17)
C4—C5—C6—C7	0.6 (2)	C11—C12—C16—C15	179.8 (9)
C5—C6—C7—C8	0.1 (3)	C13'—C14'—S15'—C16'	1(2)
C6—C7—C8—C9	−0.5 (2)	C2—N1—C19—C20	117.63 (16)
C2—N1—C9—C8	176.85 (15)	C9—N1—C19—C20	−72.53 (19)
C19—N1—C9—C8	5.6 (3)	N1—C19—C20—C21	−18.7 (2)
C2—N1—C9—C4	−1.35 (17)	N1—C19—C20—C25	162.34 (13)
C19—N1—C9—C4	−172.60 (13)	C25—C20—C21—C22	−0.4 (2)
C7—C8—C9—N1	−177.66 (15)	C19—C20—C21—C22	−179.32 (14)
C7—C8—C9—C4	0.3 (2)	C20—C21—C22—C23	0.4 (2)
C5—C4—C9—N1	178.70 (13)	C21—C22—C23—C24	0.4 (3)
C3—C4—C9—N1	1.11 (17)	C21—C22—C23—Cl1	−179.11 (13)
C5—C4—C9—C8	0.4 (2)	C22—C23—C24—C25	−1.0 (3)
C3—C4—C9—C8	−177.21 (14)	Cl1—C23—C24—C25	178.44 (13)
C2—C3—C10—C11	4.7 (3)	C23—C24—C25—C20	1.0 (2)
C4—C3—C10—C11	−172.51 (15)	C21—C20—C25—C24	−0.3 (2)
C3—C10—C11—C17	0.0 (3)	C19—C20—C25—C24	178.69 (14)
C3—C10—C11—C12	178.75 (15)		

Fig. 1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