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7-Chloro-4-(2,5-dichlorophenyl)-1-phenyl-1*H*-thiochromeno[2,3-*b*]pyridine-2,5(3*H*,4*H*)-dione

Li-Rong Wen,* Chen Ji, Ji-Hui Sun and Huai-Yuan Xie

College of Chemistry and Molecular Engineering, Qingdao University of, Science and Technology, Qingdao 266042, People's Republic of China
Correspondence e-mail: wenlirong@qust.edu.cn

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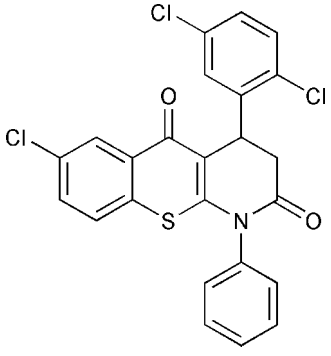
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.043; wR factor = 0.112; data-to-parameter ratio = 15.8.

In the crystal structure of the title compound, $C_{24}H_{14}Cl_3NO_2S$, the tetrahydropyridine ring adopts a half-chair conformation and both pendant benzene rings are oriented nearly perpendicular to the thiochromeno[2,3-*b*]pyridine system.

Related literature

For related literature, see: Ingall *et al.* (1996), Wang *et al.* (2006); Quaglia *et al.* (2002).



Experimental

Crystal data

$C_{24}H_{14}Cl_3NO_2S$
M_r = 486.77
Monoclinic, $P2_1/c$
a = 13.624 (5) Å
b = 13.474 (5) Å
c = 11.861 (4) Å
β = 95.042 (6)°
V = 2168.9 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.54 mm^{-1}
T = 294 (2) K
0.18 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.909, T_{max} = 0.948
12228 measured reflections
4426 independent reflections
2650 reflections with $I > 2\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.112
S = 0.99
4426 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2085).

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Li-Rong Wen, Chen Ji, Ji-Hui Sun and Huai-Yuan Xie

S1. Comment

N, S-containing heterocycles shows a wide range of biological activities Ingall *et al.*,1996). For example, the thiochromones (Wang *et al.*,2006) as important structural motifs exhibit interesting biological properties and have been tested and applied as drugs (Quaglia *et al.*, 2002). In a continuation of our study of structure-activity, we report here the crystal structure of the title compound,(I), which was synthesized from 3-(2,5- dichlorophenyl)-3-oxo-*N*-phenylpropanethioamide.

The thiopyran ring is almost planar and the 4*H*-pyridine ring adpots a half-chair conformation. Both benzene rings are oriented nearly perpendicular to the to the thiochromeno[2,3-*b*]pyridine ring. The bond length C11—O2(1.21 Å) is shorter than C7—O1(1.24 Å), which might be due to the strong electron withdrawing effect of the nitrogen atom in the pyridine ring.

The interest in the N, S-containing heterocycles has been significantly surged since a wide range of biological activities have been identified (Ingall *et al.*,1996). For example, the thiochromones (Wang *et al.*,2006) as important structural motifs exhibit interesting biological properties and have been tested and applied as drugs (Quaglia *et al.*, 2002). In a continuation of our study of structure-activity, we report here the crystal structure of the title compound.

S2. Experimental

3-(2,5-dichlorophenyl)-3-oxo-*N*-phenylpropanethioamide (1 mmol), 2,5-dichlorobenzaldehyde (1 mmol), (2,2-dimethyl-1,3-dioxane-4,6-dione) (1 mmol) and triethylamine (0.5 mmol)were refluxed in anhydrous alcohol for 8 h. The precipitate was filtered off and dissolved in THF. On slow evaporation of the solvent crystals of the title compound has formed (m.p.498 K).

S3. Refinement

All H atoms were placed in calculated positions, with C—H = 0.93, 0.97 or 0.98 A%, and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C).

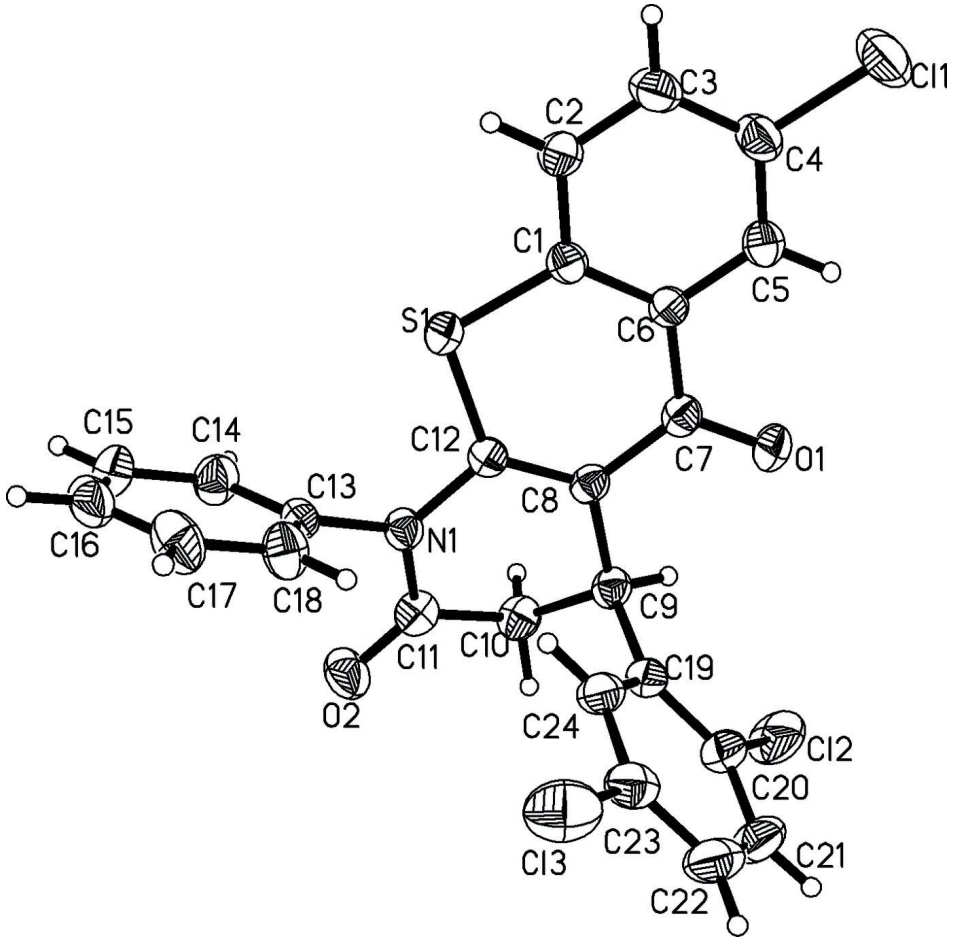

Figure 1

Crystal structure of the title compound (I) with labeling and displacement ellipsoids drawn at the 50% probability level.

7-Chloro-4-(2,5-dichlorophenyl)-1-phenyl-1*H*- thiochromeno[2,3-*b*]pyridine-2,5(3*H*,4*H*)-dione

Crystal data

$C_{24}H_{14}Cl_3NO_2S$
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$a = 13.624\ (5)$ Å
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$c = 11.861\ (4)$ Å
$\beta = 95.042\ (6)°$
$V = 2168.9\ (14)$ Å^3
$Z = 4$
$F(000) = 992$
$D_x = 1.491$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2857 reflections
$\theta = 2.3–23.4°$
$\mu = 0.54$ mm^{-1}
$T = 294$ K
Prism, yellow
0.18 × 0.12 × 0.10 mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.909$, $T_{max} = 0.948$
12228 measured reflections
4426 independent reflections
2650 reflections with $I > 2\sigma(I)$

R_{int} = 0.049
θ_{max} = 26.5°, θ_{min} = 1050°
h = −16→17
k = −13→16
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.112
S = 0.99
4426 reflections
280 parameters
0 restraints
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.2323P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 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}
S1	0.90221 (5)	0.18709 (5)	0.44648 (6)	0.04544 (19)
Cl1	1.15911 (7)	0.38600 (6)	0.09743 (8)	0.0852 (3)
Cl2	0.73863 (7)	0.67908 (6)	0.56211 (8)	0.0848 (3)
Cl3	0.48232 (6)	0.37484 (7)	0.27266 (7)	0.0859 (3)
O1	0.92297 (13)	0.51190 (12)	0.38778 (15)	0.0534 (5)
O2	0.66915 (15)	0.28572 (14)	0.71540 (16)	0.0633 (6)
N1	0.76934 (14)	0.25141 (14)	0.57736 (16)	0.0395 (5)
C1	0.97544 (16)	0.24922 (17)	0.3549 (2)	0.0388 (6)
C2	1.03240 (18)	0.18948 (19)	0.2898 (2)	0.0505 (7)
H2	1.0327	0.1211	0.3004	0.061*
C3	1.0880 (2)	0.2301 (2)	0.2103 (2)	0.0581 (8)
H3	1.1246	0.1896	0.1663	0.070*
C4	1.08877 (19)	0.3324 (2)	0.1967 (2)	0.0524 (7)
C5	1.03478 (18)	0.39236 (19)	0.2611 (2)	0.0464 (6)
H5	1.0366	0.4608	0.2511	0.056*
C6	0.97697 (16)	0.35243 (17)	0.3415 (2)	0.0370 (6)
C7	0.91855 (17)	0.42134 (18)	0.4054 (2)	0.0387 (6)
C8	0.85216 (17)	0.38283 (17)	0.4844 (2)	0.0362 (6)
C9	0.79469 (17)	0.45849 (17)	0.5447 (2)	0.0408 (6)
H9	0.8373	0.5166	0.5583	0.049*
C10	0.77372 (19)	0.41789 (18)	0.6606 (2)	0.0470 (7)
H10A	0.8346	0.4175	0.7097	0.056*
H10B	0.7281	0.4621	0.6940	0.056*
C11	0.73121 (19)	0.31487 (19)	0.6559 (2)	0.0450 (6)

C12	0.83881 (16)	0.28430 (17)	0.50370 (19)	0.0357 (6)
C13	0.73107 (17)	0.15033 (17)	0.56871 (19)	0.0365 (6)
C14	0.7620 (2)	0.0818 (2)	0.6502 (2)	0.0540 (7)
H14	0.8082	0.0993	0.7093	0.065*
C15	0.7234 (2)	−0.0139 (2)	0.6432 (3)	0.0646 (8)
H15	0.7440	−0.0608	0.6978	0.077*
C16	0.6561 (2)	−0.0390 (2)	0.5570 (3)	0.0654 (9)
H16	0.6301	−0.1029	0.5528	0.079*
C17	0.6263 (2)	0.0299 (2)	0.4760 (3)	0.0656 (9)
H17	0.5806	0.0121	0.4167	0.079*
C18	0.6631 (2)	0.1252 (2)	0.4812 (2)	0.0533 (7)
H18	0.6422	0.1716	0.4263	0.064*
C19	0.70135 (18)	0.49370 (19)	0.4760 (2)	0.0430 (6)
C20	0.6704 (2)	0.5922 (2)	0.4790 (2)	0.0545 (7)
C21	0.5847 (3)	0.6240 (2)	0.4178 (3)	0.0715 (9)
H21	0.5663	0.6904	0.4204	0.086*
C22	0.5269 (2)	0.5584 (3)	0.3538 (3)	0.0687 (9)
H22	0.4692	0.5796	0.3132	0.082*
C23	0.55580 (19)	0.4603 (2)	0.3506 (2)	0.0548 (7)
C24	0.64242 (18)	0.4289 (2)	0.4096 (2)	0.0480 (7)
H24	0.6614	0.3629	0.4045	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0490 (4)	0.0304 (3)	0.0585 (4)	−0.0002 (3)	0.0140 (3)	0.0006 (3)
Cl1	0.0958 (6)	0.0721 (6)	0.0966 (6)	−0.0206 (5)	0.0581 (5)	−0.0068 (5)
Cl2	0.0883 (6)	0.0413 (4)	0.1249 (8)	0.0078 (4)	0.0104 (6)	−0.0151 (5)
Cl3	0.0627 (5)	0.1131 (8)	0.0772 (6)	0.0090 (5)	−0.0198 (4)	−0.0077 (5)
O1	0.0648 (12)	0.0295 (10)	0.0678 (12)	0.0001 (8)	0.0161 (10)	0.0042 (9)
O2	0.0759 (14)	0.0576 (13)	0.0610 (12)	−0.0091 (10)	0.0315 (11)	−0.0065 (10)
N1	0.0441 (12)	0.0354 (11)	0.0394 (11)	−0.0040 (10)	0.0067 (10)	−0.0026 (9)
C1	0.0323 (13)	0.0371 (14)	0.0466 (15)	−0.0055 (11)	0.0021 (11)	−0.0025 (12)
C2	0.0500 (16)	0.0335 (14)	0.0698 (18)	−0.0063 (12)	0.0161 (14)	−0.0092 (14)
C3	0.0531 (17)	0.0519 (18)	0.073 (2)	−0.0066 (14)	0.0274 (15)	−0.0147 (15)
C4	0.0494 (17)	0.0490 (17)	0.0612 (18)	−0.0118 (13)	0.0181 (14)	−0.0051 (14)
C5	0.0436 (15)	0.0381 (14)	0.0581 (16)	−0.0082 (12)	0.0075 (13)	0.0000 (13)
C6	0.0302 (13)	0.0336 (13)	0.0465 (14)	−0.0036 (11)	−0.0005 (11)	−0.0006 (12)
C7	0.0369 (14)	0.0339 (14)	0.0444 (15)	−0.0034 (11)	−0.0022 (12)	−0.0012 (12)
C8	0.0353 (13)	0.0316 (13)	0.0408 (14)	0.0005 (11)	−0.0017 (11)	−0.0026 (11)
C9	0.0417 (14)	0.0347 (14)	0.0457 (15)	−0.0015 (11)	0.0024 (12)	−0.0029 (12)
C10	0.0558 (16)	0.0411 (15)	0.0438 (15)	−0.0003 (13)	0.0022 (13)	−0.0073 (12)
C11	0.0522 (16)	0.0462 (16)	0.0355 (14)	0.0019 (13)	−0.0014 (13)	−0.0021 (13)
C12	0.0336 (13)	0.0368 (13)	0.0360 (13)	−0.0020 (11)	−0.0004 (11)	−0.0014 (11)
C13	0.0360 (13)	0.0373 (13)	0.0372 (14)	−0.0044 (11)	0.0083 (11)	−0.0002 (11)
C14	0.0525 (17)	0.0521 (17)	0.0558 (17)	−0.0012 (14)	−0.0050 (14)	0.0090 (15)
C15	0.072 (2)	0.0414 (17)	0.082 (2)	0.0038 (15)	0.0182 (19)	0.0161 (16)
C16	0.069 (2)	0.0457 (18)	0.087 (2)	−0.0152 (16)	0.0352 (19)	−0.0166 (18)

C17	0.066 (2)	0.070 (2)	0.061 (2)	−0.0267 (17)	0.0071 (16)	−0.0144 (18)
C18	0.0604 (18)	0.0563 (18)	0.0424 (16)	−0.0108 (15)	−0.0004 (14)	0.0055 (14)
C19	0.0424 (15)	0.0423 (15)	0.0458 (15)	0.0057 (12)	0.0120 (13)	0.0036 (13)
C20	0.0566 (18)	0.0454 (16)	0.0632 (18)	0.0124 (14)	0.0155 (15)	0.0031 (14)
C21	0.079 (2)	0.057 (2)	0.081 (2)	0.0328 (18)	0.019 (2)	0.0087 (18)
C22	0.058 (2)	0.088 (3)	0.061 (2)	0.0302 (19)	0.0091 (16)	0.0115 (19)
C23	0.0449 (16)	0.073 (2)	0.0468 (16)	0.0085 (15)	0.0052 (13)	0.0046 (15)
C24	0.0444 (16)	0.0506 (16)	0.0495 (16)	0.0099 (13)	0.0063 (13)	0.0027 (14)

Geometric parameters (Å, º)

S1—C12	1.739 (2)	C9—H9	0.9800
S1—C1	1.751 (2)	C10—C11	1.503 (3)
Cl1—C4	1.739 (3)	C10—H10A	0.9700
Cl2—C20	1.744 (3)	C10—H10B	0.9700
Cl3—C23	1.737 (3)	C13—C18	1.371 (3)
O1—C7	1.240 (3)	C13—C14	1.376 (3)
O2—C11	1.213 (3)	C14—C15	1.393 (4)
N1—C11	1.398 (3)	C14—H14	0.9300
N1—C12	1.414 (3)	C15—C16	1.355 (4)
N1—C13	1.459 (3)	C15—H15	0.9300
C1—C2	1.397 (3)	C16—C17	1.372 (4)
C1—C6	1.400 (3)	C16—H16	0.9300
C2—C3	1.374 (3)	C17—C18	1.377 (4)
C2—H2	0.9300	C17—H17	0.9300
C3—C4	1.389 (4)	C18—H18	0.9300
C3—H3	0.9300	C19—C24	1.384 (3)
C4—C5	1.370 (3)	C19—C20	1.395 (3)
C5—C6	1.397 (3)	C20—C21	1.387 (4)
C5—H5	0.9300	C21—C22	1.368 (4)
C6—C7	1.475 (3)	C21—H21	0.9300
C7—C8	1.454 (3)	C22—C23	1.382 (4)
C8—C12	1.362 (3)	C22—H22	0.9300
C8—C9	1.504 (3)	C23—C24	1.384 (3)
C9—C19	1.525 (3)	C24—H24	0.9300
C9—C10	1.530 (3)		

C12—S1—C1	102.22 (11)	O2—C11—C10	124.3 (2)
C11—N1—C12	121.9 (2)	N1—C11—C10	115.2 (2)
C11—N1—C13	117.80 (19)	C8—C12—N1	121.0 (2)
C12—N1—C13	120.23 (19)	C8—C12—S1	126.18 (19)
C2—C1—C6	119.7 (2)	N1—C12—S1	112.79 (16)
C2—C1—S1	116.23 (18)	C18—C13—C14	120.7 (2)
C6—C1—S1	124.06 (19)	C18—C13—N1	119.8 (2)
C3—C2—C1	121.1 (2)	C14—C13—N1	119.4 (2)
C3—C2—H2	119.4	C13—C14—C15	119.2 (3)
C1—C2—H2	119.4	C13—C14—H14	120.4
C2—C3—C4	119.0 (3)	C15—C14—H14	120.4

C2—C3—H3	120.5	C16—C15—C14	120.2 (3)
C4—C3—H3	120.5	C16—C15—H15	119.9
C5—C4—C3	120.7 (2)	C14—C15—H15	119.9
C5—C4—Cl1	119.2 (2)	C15—C16—C17	119.8 (3)
C3—C4—Cl1	120.1 (2)	C15—C16—H16	120.1
C4—C5—C6	121.1 (2)	C17—C16—H16	120.1
C4—C5—H5	119.5	C16—C17—C18	121.1 (3)
C6—C5—H5	119.4	C16—C17—H17	119.5
C5—C6—C1	118.3 (2)	C18—C17—H17	119.5
C5—C6—C7	118.1 (2)	C13—C18—C17	118.9 (3)
C1—C6—C7	123.6 (2)	C13—C18—H18	120.6
O1—C7—C8	120.1 (2)	C17—C18—H18	120.6
O1—C7—C6	119.8 (2)	C24—C19—C20	117.0 (2)
C8—C7—C6	120.0 (2)	C24—C19—C9	121.5 (2)
C12—C8—C7	123.8 (2)	C20—C19—C9	121.5 (2)
C12—C8—C9	119.9 (2)	C21—C20—C19	121.5 (3)
C7—C8—C9	116.4 (2)	C21—C20—Cl2	118.1 (2)
C8—C9—C19	113.64 (19)	C19—C20—Cl2	120.4 (2)
C8—C9—C10	109.34 (19)	C22—C21—C20	120.5 (3)
C19—C9—C10	112.3 (2)	C22—C21—H21	119.8
C8—C9—H9	107.1	C20—C21—H21	119.8
C19—C9—H9	107.1	C21—C22—C23	118.9 (3)
C10—C9—H9	107.1	C21—C22—H22	120.6
C11—C10—C9	113.5 (2)	C23—C22—H22	120.6
C11—C10—H10A	108.9	C22—C23—C24	120.7 (3)
C9—C10—H10A	108.9	C22—C23—Cl3	119.8 (2)
C11—C10—H10B	108.9	C24—C23—Cl3	119.5 (2)
C9—C10—H10B	108.9	C23—C24—C19	121.4 (3)
H10A—C10—H10B	107.7	C23—C24—H24	119.3
O2—C11—N1	120.6 (2)	C19—C24—H24	119.3

C12—S1—C1—C2	−176.43 (19)	C7—C8—C12—S1	4.3 (3)
C12—S1—C1—C6	1.4 (2)	C9—C8—C12—S1	−177.11 (17)
C6—C1—C2—C3	−1.8 (4)	C11—N1—C12—C8	−17.6 (3)
S1—C1—C2—C3	176.1 (2)	C13—N1—C12—C8	158.9 (2)
C1—C2—C3—C4	1.3 (4)	C11—N1—C12—S1	161.51 (17)
C2—C3—C4—C5	−0.2 (4)	C13—N1—C12—S1	−22.0 (3)
C2—C3—C4—Cl1	179.6 (2)	C1—S1—C12—C8	−4.3 (2)
C3—C4—C5—C6	−0.5 (4)	C1—S1—C12—N1	176.67 (16)
Cl1—C4—C5—C6	179.76 (19)	C11—N1—C13—C18	101.9 (3)
C4—C5—C6—C1	0.0 (4)	C12—N1—C13—C18	−74.8 (3)
C4—C5—C6—C7	−178.2 (2)	C11—N1—C13—C14	−76.6 (3)
C2—C1—C6—C5	1.1 (3)	C12—N1—C13—C14	106.7 (3)
S1—C1—C6—C5	−176.60 (18)	C18—C13—C14—C15	−0.1 (4)
C2—C1—C6—C7	179.3 (2)	N1—C13—C14—C15	178.4 (2)
S1—C1—C6—C7	1.5 (3)	C13—C14—C15—C16	−0.1 (4)
C5—C6—C7—O1	−1.0 (3)	C14—C15—C16—C17	0.5 (4)
C1—C6—C7—O1	−179.1 (2)	C15—C16—C17—C18	−0.7 (4)

C5—C6—C7—C8	175.8 (2)	C14—C13—C18—C17	−0.1 (4)
C1—C6—C7—C8	−2.3 (3)	N1—C13—C18—C17	−178.6 (2)
O1—C7—C8—C12	176.1 (2)	C16—C17—C18—C13	0.5 (4)
C6—C7—C8—C12	−0.7 (3)	C8—C9—C19—C24	38.9 (3)
O1—C7—C8—C9	−2.5 (3)	C10—C9—C19—C24	−85.8 (3)
C6—C7—C8—C9	−179.3 (2)	C8—C9—C19—C20	−142.5 (2)
C12—C8—C9—C19	−95.5 (3)	C10—C9—C19—C20	92.8 (3)
C7—C8—C9—C19	83.2 (3)	C24—C19—C20—C21	−0.3 (4)
C12—C8—C9—C10	30.8 (3)	C9—C19—C20—C21	−179.0 (2)
C7—C8—C9—C10	−150.5 (2)	C24—C19—C20—Cl2	178.93 (19)
C8—C9—C10—C11	−49.6 (3)	C9—C19—C20—Cl2	0.3 (3)
C19—C9—C10—C11	77.5 (3)	C19—C20—C21—C22	1.1 (4)
C12—N1—C11—O2	177.4 (2)	Cl2—C20—C21—C22	−178.2 (2)
C13—N1—C11—O2	0.8 (3)	C20—C21—C22—C23	−0.5 (5)
C12—N1—C11—C10	−3.4 (3)	C21—C22—C23—C24	−1.0 (4)
C13—N1—C11—C10	180.0 (2)	C21—C22—C23—Cl3	178.5 (2)
C9—C10—C11—O2	−143.4 (3)	C22—C23—C24—C19	1.8 (4)
C9—C10—C11—N1	37.4 (3)	Cl3—C23—C24—C19	−177.65 (19)
C7—C8—C12—N1	−176.7 (2)	C20—C19—C24—C23	−1.1 (4)
C9—C8—C12—N1	1.9 (3)	C9—C19—C24—C23	177.5 (2)