

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

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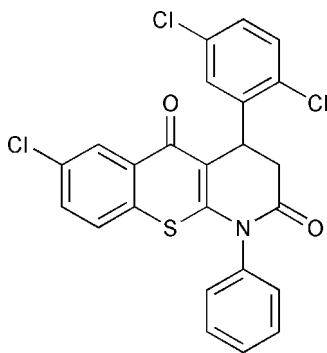
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Key indicators: single-crystal X-ray study;  $T = 294$  K; mean  $\sigma(\text{C}-\text{C}) = 0.004$  Å;  $R$  factor = 0.043;  $wR$  factor = 0.112; data-to-parameter ratio = 15.8.

In the crystal structure of the title compound,  $\text{C}_{24}\text{H}_{14}\text{Cl}_3\text{NO}_2\text{S}$ , 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

$\text{C}_{24}\text{H}_{14}\text{Cl}_3\text{NO}_2\text{S}$   
 $M_r = 486.77$   
 Monoclinic,  $P2_1/c$   
 $a = 13.624$  (5) Å  
 $b = 13.474$  (5) Å  
 $c = 11.861$  (4) Å  
 $\beta = 95.042$  (6)°

$V = 2168.9$  (14) Å<sup>3</sup>  
 $Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.54$  mm<sup>-1</sup>  
 $T = 294$  (2) K  
 $0.18 \times 0.12 \times 0.10$  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  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.049$

#### 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<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.26$  e Å<sup>-3</sup>

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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**supplementary materials**

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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

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### 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 adopts a half-chair conformation. Both benzene rings are oriented nearly perpendicular 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.

### 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).

### Refinement

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

### Figures

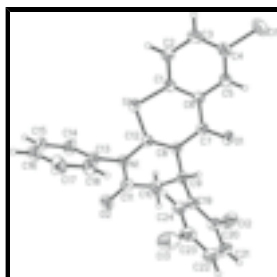


Fig. 1. Crystal structure of the title compound (I) with labeling and displacement ellipsoids drawn at the 50% probability level.

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

### Crystal data

$C_{24}H_{14}Cl_3NO_2S$	$F_{000} = 992$
$M_r = 486.77$	$D_x = 1.491 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 13.624 (5) \text{ \AA}$	Cell parameters from 2857 reflections
$b = 13.474 (5) \text{ \AA}$	$\theta = 2.3\text{--}23.4^\circ$
$c = 11.861 (4) \text{ \AA}$	$\mu = 0.54 \text{ mm}^{-1}$
$\beta = 95.042 (6)^\circ$	$T = 294 (2) \text{ K}$
$V = 2168.9 (14) \text{ \AA}^3$	Prism, yellow
$Z = 4$	$0.18 \times 0.12 \times 0.10 \text{ mm}$

### Data collection

Bruker SMART 1000 CCD area-detector diffractometer	4426 independent reflections
Radiation source: fine-focus sealed tube	2650 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.049$
$T = 294(2) \text{ K}$	$\theta_{\text{max}} = 26.5^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\text{min}} = 1050^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -16 \rightarrow 17$
$T_{\text{min}} = 0.909$ , $T_{\text{max}} = 0.948$	$k = -13 \rightarrow 16$
12228 measured reflections	$l = -14 \rightarrow 14$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 0.2323P]$
$R[F^2 > 2\sigma(F^2)] = 0.043$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.112$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 0.99$	$\Delta\rho_{\text{max}} = 0.28 \text{ e \AA}^{-3}$
4426 reflections	$\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$
280 parameters	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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
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*

## supplementary materials

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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 ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0490 (4)	0.0304 (3)	0.0585 (4)	-0.0002 (3)	0.0140 (3)	0.0006 (3)
C11	0.0958 (6)	0.0721 (6)	0.0966 (6)	-0.0206 (5)	0.0581 (5)	-0.0068 (5)
C12	0.0883 (6)	0.0413 (4)	0.1249 (8)	0.0078 (4)	0.0104 (6)	-0.0151 (5)
C13	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 ( $\text{\AA}$ , $^\circ$ )

S1—C12	1.739 (2)	C9—H9	0.9800
S1—C1	1.751 (2)	C10—C11	1.503 (3)
C11—C4	1.739 (3)	C10—H10A	0.9700
C12—C20	1.744 (3)	C10—H10B	0.9700
C13—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—C11	119.2 (2)	C15—C16—C17	119.8 (3)
C3—C4—C11	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—C12	118.1 (2)
C8—C9—C19	113.64 (19)	C19—C20—C12	120.4 (2)
C8—C9—C10	109.34 (19)	C22—C21—C20	120.5 (3)

## supplementary materials

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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—C11	179.6 (2)	C1—S1—C12—C8	-4.3 (2)
C3—C4—C5—C6	-0.5 (4)	C1—S1—C12—N1	176.67 (16)
C11—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—C12	178.93 (19)
C8—C9—C10—C11	-49.6 (3)	C9—C19—C20—C12	0.3 (3)
C19—C9—C10—C11	77.5 (3)	C19—C20—C21—C22	1.1 (4)
C12—N1—C11—O2	177.4 (2)	C12—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)



Fig. 1

