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3-(5-Chloro-3-methyl-1-phenylpyrazol-4-yl)-1,5-di-2-thienylpentane-1,5-dione: centrosymmetric dimers formed by C—H···π(thiophene) hydrogen bonds

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.003 Å
Disorder in main residue
R factor = 0.046
wR factor = 0.117
Data-to-parameter ratio = 17.5

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

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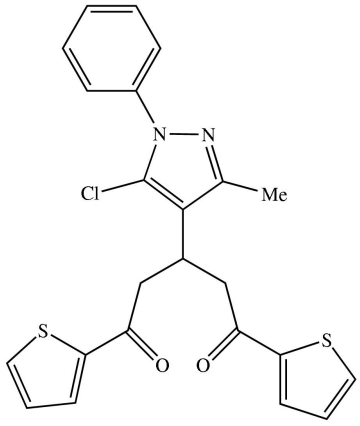
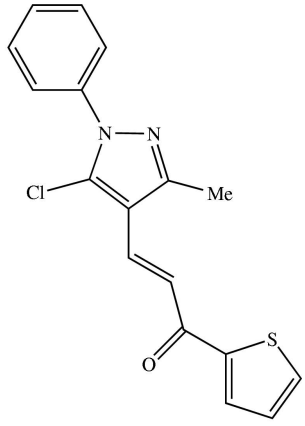
Molecules of the title compound, $C_{23}H_{19}ClN_2O_2S_2$, are linked into cyclic centrosymmetric dimers by paired C—H···π(thiophene) hydrogen bonds.

Comment

The title compound, (I), was obtained adventitiously during the attempted synthesis of the intermediate 3-(5-chloro-3-methyl-1-phenyl-4,5-dihydro-1*H*-pyrazol-4-yl)-1-thiophen-2-yl-propenone, (II), by base-catalysed condensation of 5-chloro-3-methyl-1-phenyl-1*H*-pyrazole-4-carbaldehyde with 2-aceylthiophene. Evidently, the expected product, (II), has undergone a Michael-type reaction with a further mole of 2-acetylthiophene to form the observed product, (I).



(I)



(II)

Within the molecule of (I), the thiophene ring containing S9 exhibits orientational disorder about the C9—C91 bond, with occupancies of 0.623 (3) and 0.377 (3): all bond distances and angles show normal values.

The supramolecular aggregation is determined by C—H···π(thiophene) hydrogen bonds (Table 1). Atom C8 in the molecule at (*x*, *y*, *z*) acts as a hydrogen-bond donor to the disordered thiophene ring of the molecule at (1 − *x*, 1 − *y*, 1 − *z*), so generating a centrosymmetric dimer (Fig. 2) whose formation is independent of the orientation of the thiophene acceptor (Table 1). The only other possible intermolecular interaction is a fairly short contact between atom Cl5 in the molecule at (*x*, *y*, *z*) and aryl atom C14 in the molecule at ($\frac{1}{2}+x$, *y*, $\frac{3}{2}-z$), with a Cl···C distance of 3.137 (2) Å and a C—Cl···C angle of 153.5 (2)°; this distance is not particularly short in terms of the polar flattening model for van der Waals contacts (Nyburg & Faerman, 1985) and is probably not structurally significant.

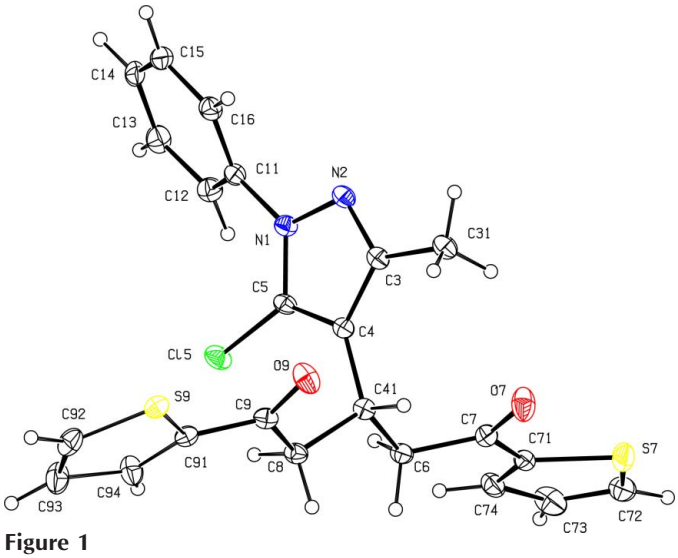


Figure 1
The molecular structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. For clarity, only the major orientation of the disordered thiophene ring is shown.

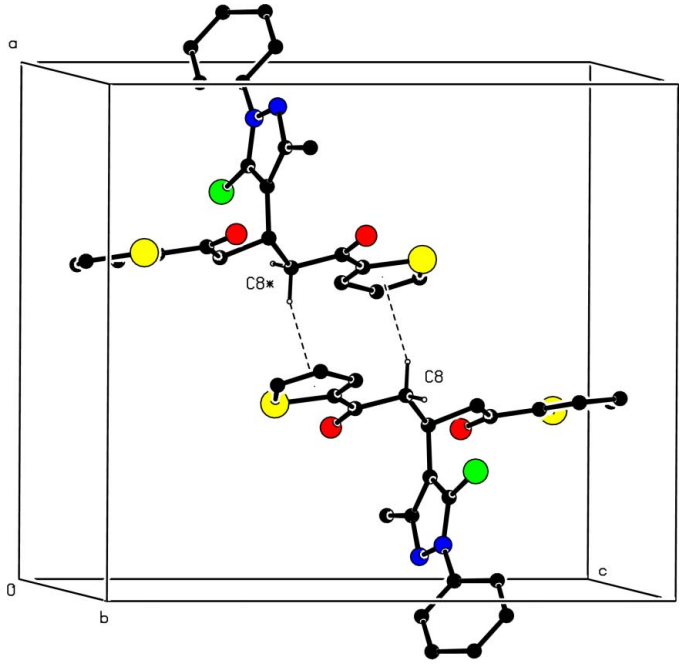


Figure 2
Part of the crystal structure of (I), showing the formation of a hydrogen-bonded dimer. For clarity, H atoms bonded to C atoms that are not involved in the motif shown have been omitted, and only the major orientation of the disordered thiophene ring is shown. Hydrogen bonds are shown as dashed lines. The atom marked with an asterisk (*) is at the symmetry position $(1-x, 1-y, 1-z)$.

Experimental

To a solution of 5-chloro-4-formyl-3-methyl-1-phenylpyrazole (0.5 mmol) and 2-acetylthiophene (1 mmol) in absolute ethanol (10 ml), a catalytic amount of sodium hydroxide (1 pellet) was added and the reaction mixture was stirred at room temperature for 2 h. The resulting precipitate was isolated by filtration, washed with ethanol, dried and finally recrystallized from dimethylformamide to give yellow crystals suitable for single-crystal X-ray diffraction. M.p. 573 K, yield 45%; MS (70 eV) *m*/*z* (%): 455 (2.6) (*M*+), 329 (42), 293 (20), 111 (100).

Crystal data

$C_{23}H_{19}ClN_2O_2S_2$
M_r = 454.99
Orthorhombic, *Pbca*
a = 14.6729 (5) Å
b = 17.8962 (6) Å
c = 16.2619 (3) Å
V = 4270.2 (2) Å^3
Z = 8
D_x = 1.416 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4887 reflections
θ = 3.0–27.5°
μ = 0.40 mm^{-1}
T = 120 (2) K
Lath, colourless
0.42 × 0.22 × 0.08 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.851, T_{max} = 0.969
35379 measured reflections
4887 independent reflections
3231 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 27.5°
$h = -19 \rightarrow 16$
$k = -23 \rightarrow 23$
$l = -17 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.117
S = 1.03
4887 reflections
279 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.8758P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids for the major and minor orientations of the disordered thiophene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8A···$Cg1^{i}$	0.99	2.67	3.628 (3)	162
C8—H8A···$Cg2^{i}$	0.99	2.67	3.614 (3)	159

Symmetry code: (i) $-x+1, -y+1, -z+1$.

All H atoms were located in difference maps and then treated as riding atoms, with C—H distances of 0.95 Å (aromatic), 0.98 Å (CH_3), 0.99 Å (CH_2) or 1.00 Å (aliphatic CH), and with U_{iso}(H) = 1.2U_{eq}(C), or 1.5U_{eq}(C) for the methyl group.

Data collection: *COLLECT* (Hooft, 1999); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *WinGX* (Farrugia, 1999) and *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *OSCAIL* (McArdle, 2003) and *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England. JC thanks the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support. JQ and JT thank COLCIENCIAS and

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supporting information

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Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4887 reflections
$\theta = 3.0$–$27.5°$
$\mu = 0.40$ mm^{-1}
$T = 120$ K
Lath, colourless
0.42 × 0.22 × 0.08 mm

Data collection

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Radiation source: Bruker-Nonius FR91 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
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Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
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4887 independent reflections
3231 reflections with $I > 2\sigma(I)$
$R_{int} = 0.067$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -19\rightarrow16$
$k = -23\rightarrow23$
$l = -17\rightarrow21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.117$
$S = 1.03$
4887 reflections
279 parameters
0 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
$w = 1/[\sigma^2(F_o^2) + (0.0583P)^2 + 0.8758P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.31$ e Å^{-3}
$\Delta\rho_{min} = -0.45$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Cl5	0.23343 (4)	0.58885 (3)	0.71087 (3)	0.03435 (17)	

S7	0.33570 (5)	0.23047 (3)	0.90153 (4)	0.04035 (19)	
S9	0.36235 (11)	0.54448 (8)	0.36403 (6)	0.0250 (4)	0.623 (3)
S9A	0.4290 (3)	0.62233 (19)	0.5091 (2)	0.0371 (6)	0.377 (3)
O7	0.30212 (12)	0.28150 (9)	0.73188 (9)	0.0442 (4)	
O9	0.31145 (11)	0.42731 (9)	0.48101 (8)	0.0381 (4)	
N1	0.08746 (12)	0.50767 (10)	0.66660 (10)	0.0258 (4)	
N2	0.06214 (12)	0.43928 (10)	0.63595 (10)	0.0266 (4)	
C3	0.13963 (14)	0.40086 (12)	0.62814 (11)	0.0240 (5)	
C4	0.21663 (13)	0.44299 (11)	0.65326 (11)	0.0216 (4)	
C5	0.17983 (14)	0.51027 (12)	0.67661 (11)	0.0235 (5)	
C6	0.35290 (15)	0.40827 (11)	0.74088 (12)	0.0258 (5)	
C7	0.32864 (15)	0.33246 (12)	0.77585 (13)	0.0277 (5)	
C8	0.37538 (14)	0.47503 (12)	0.60526 (11)	0.0257 (5)	
C9	0.35033 (14)	0.47895 (12)	0.51536 (12)	0.0248 (5)	
C11	0.02046 (14)	0.56419 (12)	0.67820 (12)	0.0264 (5)	
C12	0.02307 (15)	0.61060 (12)	0.74644 (13)	0.0318 (5)	
C13	−0.04214 (16)	0.66648 (13)	0.75425 (14)	0.0360 (6)	
C14	−0.11037 (16)	0.67407 (13)	0.69671 (14)	0.0348 (6)	
C15	−0.11362 (16)	0.62629 (13)	0.62992 (14)	0.0352 (6)	
C16	−0.04802 (15)	0.57217 (13)	0.61962 (13)	0.0306 (5)	
C31	0.13661 (15)	0.32257 (13)	0.59625 (13)	0.0307 (5)	
C41	0.31553 (14)	0.42040 (12)	0.65328 (11)	0.0238 (5)	
C71	0.34196 (14)	0.32007 (12)	0.86398 (12)	0.0266 (5)	
C72	0.35368 (17)	0.26093 (16)	0.99922 (15)	0.0432 (7)	
C73	0.36350 (17)	0.33575 (16)	1.00332 (14)	0.0453 (7)	
C74	0.35713 (15)	0.37124 (14)	0.92627 (13)	0.0329 (6)	
C91	0.37737 (13)	0.54557 (12)	0.46840 (11)	0.0238 (5)	
C92	0.40182 (16)	0.62996 (13)	0.35551 (13)	0.0362 (6)	
C93	0.42986 (18)	0.66418 (13)	0.42573 (15)	0.0426 (6)	
C94	0.4101 (7)	0.6097 (5)	0.4957 (6)	0.0371 (6)	0.623 (3)
C94A	0.3664 (8)	0.5558 (7)	0.3839 (6)	0.0250 (4)	0.377 (3)
H6A	0.4201	0.4135	0.7399	0.031*	
H6B	0.3283	0.4476	0.7775	0.031*	
H8A	0.4399	0.4595	0.6103	0.031*	
H8B	0.3695	0.5254	0.6298	0.031*	
H12	0.0688	0.6043	0.7872	0.038*	
H13	−0.0396	0.6998	0.7997	0.043*	
H14	−0.1551	0.7120	0.7029	0.042*	
H15	−0.1615	0.6309	0.5909	0.042*	
H16	−0.0494	0.5404	0.5728	0.037*	
H31A	0.0736	0.3094	0.5825	0.046*	
H31B	0.1596	0.2883	0.6384	0.046*	
H31C	0.1747	0.3187	0.5469	0.046*	
H41	0.3194	0.3712	0.6244	0.029*	
H72	0.3565	0.2288	1.0457	0.052*	
H73	0.3737	0.3619	1.0533	0.054*	
H74	0.3626	0.4236	0.9181	0.039*	
H94A	0.3396	0.5198	0.3484	0.030*	0.377 (3)

H92	0.4049	0.6544	0.3038	0.043*	
H93	0.4565	0.7124	0.4303	0.051*	
H94	0.4202	0.6206	0.5522	0.044*	0.623 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl5	0.0311 (3)	0.0303 (3)	0.0417 (3)	−0.0071 (2)	−0.0016 (2)	−0.0110 (2)
S7	0.0467 (4)	0.0321 (4)	0.0422 (4)	−0.0021 (3)	−0.0082 (3)	0.0117 (3)
S9	0.0278 (5)	0.0314 (7)	0.0157 (7)	0.0035 (4)	−0.0035 (5)	−0.0017 (5)
S9A	0.0480 (19)	0.0264 (14)	0.0368 (15)	−0.0057 (10)	−0.0015 (10)	−0.0003 (9)
O7	0.0690 (13)	0.0272 (9)	0.0365 (9)	−0.0060 (8)	−0.0146 (9)	−0.0009 (7)
O9	0.0521 (11)	0.0372 (10)	0.0249 (8)	−0.0152 (8)	−0.0008 (7)	−0.0042 (7)
N1	0.0236 (11)	0.0268 (10)	0.0269 (9)	−0.0019 (8)	−0.0012 (7)	−0.0022 (7)
N2	0.0270 (11)	0.0264 (10)	0.0264 (9)	−0.0057 (8)	−0.0012 (7)	−0.0029 (7)
C3	0.0262 (13)	0.0273 (12)	0.0185 (10)	−0.0042 (9)	0.0010 (8)	−0.0003 (8)
C4	0.0227 (12)	0.0256 (11)	0.0163 (9)	−0.0031 (9)	−0.0005 (8)	0.0008 (8)
C5	0.0231 (12)	0.0282 (12)	0.0192 (10)	−0.0060 (9)	−0.0021 (8)	−0.0021 (8)
C6	0.0221 (12)	0.0300 (12)	0.0252 (10)	−0.0034 (9)	−0.0008 (9)	0.0020 (9)
C7	0.0265 (13)	0.0261 (12)	0.0305 (11)	0.0005 (10)	−0.0027 (9)	0.0006 (9)
C8	0.0228 (12)	0.0320 (13)	0.0223 (10)	−0.0025 (9)	0.0009 (8)	0.0018 (9)
C9	0.0219 (12)	0.0297 (13)	0.0229 (10)	0.0009 (9)	0.0033 (8)	−0.0053 (9)
C11	0.0229 (12)	0.0272 (12)	0.0293 (11)	−0.0012 (9)	0.0044 (9)	0.0048 (9)
C12	0.0305 (14)	0.0348 (13)	0.0302 (12)	0.0002 (10)	0.0012 (10)	0.0002 (10)
C13	0.0384 (14)	0.0307 (13)	0.0389 (13)	0.0012 (11)	0.0088 (11)	−0.0014 (10)
C14	0.0295 (14)	0.0264 (13)	0.0484 (14)	0.0016 (10)	0.0074 (11)	0.0141 (11)
C15	0.0269 (13)	0.0374 (14)	0.0414 (13)	−0.0012 (11)	−0.0004 (10)	0.0167 (11)
C16	0.0298 (13)	0.0322 (13)	0.0298 (11)	−0.0047 (10)	−0.0003 (10)	0.0056 (9)
C31	0.0315 (14)	0.0298 (13)	0.0310 (12)	−0.0062 (10)	−0.0012 (10)	−0.0038 (9)
C41	0.0242 (12)	0.0261 (12)	0.0209 (10)	−0.0012 (9)	0.0006 (8)	−0.0012 (8)
C71	0.0227 (12)	0.0277 (12)	0.0295 (11)	−0.0037 (9)	−0.0015 (9)	0.0058 (9)
C72	0.0357 (15)	0.0562 (18)	0.0377 (13)	−0.0107 (13)	−0.0104 (11)	0.0240 (12)
C73	0.0475 (17)	0.062 (2)	0.0264 (12)	−0.0181 (14)	−0.0055 (11)	0.0043 (12)
C74	0.0323 (14)	0.0343 (14)	0.0319 (12)	−0.0100 (10)	−0.0008 (10)	0.0059 (10)
C91	0.0224 (12)	0.0275 (12)	0.0216 (10)	0.0038 (9)	0.0005 (8)	−0.0024 (9)
C92	0.0404 (15)	0.0390 (14)	0.0292 (12)	0.0102 (12)	−0.0003 (10)	0.0082 (10)
C93	0.0568 (18)	0.0261 (13)	0.0448 (15)	0.0002 (12)	−0.0087 (12)	0.0017 (11)
C94	0.0480 (19)	0.0264 (14)	0.0368 (15)	−0.0057 (10)	−0.0015 (10)	−0.0003 (9)
C94A	0.0278 (5)	0.0314 (7)	0.0157 (7)	0.0035 (4)	−0.0035 (5)	−0.0017 (5)

Geometric parameters (Å, º)

N1—C5	1.366 (3)	C7—O7	1.222 (2)
N1—N2	1.373 (2)	C7—C71	1.463 (3)
N1—C11	1.423 (3)	C71—C74	1.384 (3)
C11—C12	1.387 (3)	C71—S7	1.718 (2)
C11—C16	1.392 (3)	S7—C72	1.700 (3)
C12—C13	1.390 (3)	C72—C73	1.348 (4)

C12—H12	0.95	C72—H72	0.95
C13—C14	1.377 (3)	C73—C74	1.408 (3)
C13—H13	0.95	C73—H73	0.95
C14—C15	1.383 (3)	C74—H74	0.95
C14—H14	0.95	C8—C9	1.509 (3)
C15—C16	1.376 (3)	C8—H8A	0.99
C15—H15	0.95	C8—H8B	0.99
C16—H16	0.95	C9—O9	1.221 (3)
N2—C3	1.335 (3)	C9—C91	1.470 (3)
C3—C4	1.418 (3)	C91—C94	1.321 (8)
C3—C31	1.495 (3)	C91—C94A	1.396 (10)
C31—H31A	0.98	C91—S9A	1.703 (3)
C31—H31B	0.98	C91—S9	1.712 (2)
C31—H31C	0.98	S9—C92	1.642 (3)
C4—C5	1.373 (3)	C94A—C92	1.498 (13)
C4—C41	1.506 (3)	C94A—H94A	0.95
C41—C8	1.529 (3)	C92—C93	1.360 (3)
C41—C6	1.542 (3)	C92—H92	0.95
C41—H41	1.00	C93—C94	1.526 (11)
C5—Cl5	1.705 (2)	C93—S9A	1.549 (5)
C6—C7	1.514 (3)	C93—H93	0.95
C6—H6A	0.99	C94—H94	0.95
C6—H6B	0.99		

C5—N1—N2	110.01 (16)	O7—C7—C71	120.2 (2)
C5—N1—C11	130.20 (18)	O7—C7—C6	121.59 (19)
N2—N1—C11	119.66 (17)	C71—C7—C6	118.19 (18)
C12—C11—C16	120.4 (2)	C74—C71—C7	129.7 (2)
C12—C11—N1	120.85 (19)	C74—C71—S7	111.47 (16)
C16—C11—N1	118.74 (19)	C7—C71—S7	118.84 (16)
C11—C12—C13	119.0 (2)	C72—S7—C71	91.41 (12)
C11—C12—H12	120.5	C73—C72—S7	112.41 (18)
C13—C12—H12	120.5	C73—C72—H72	123.8
C14—C13—C12	120.6 (2)	S7—C72—H72	123.8
C14—C13—H13	119.7	C72—C73—C74	113.4 (2)
C12—C13—H13	119.7	C72—C73—H73	123.3
C13—C14—C15	119.8 (2)	C74—C73—H73	123.3
C13—C14—H14	120.1	C71—C74—C73	111.3 (2)
C15—C14—H14	120.1	C71—C74—H74	124.3
C16—C15—C14	120.4 (2)	C73—C74—H74	124.3
C16—C15—H15	119.8	C9—C8—C41	112.62 (17)
C14—C15—H15	119.8	C9—C8—H8A	109.1
C15—C16—C11	119.6 (2)	C41—C8—H8A	109.1
C15—C16—H16	120.2	C9—C8—H8B	109.1
C11—C16—H16	120.2	C41—C8—H8B	109.1
C3—N2—N1	105.27 (16)	H8A—C8—H8B	107.8
N2—C3—C4	112.16 (18)	O9—C9—C91	120.14 (18)
N2—C3—C31	119.38 (18)	O9—C9—C8	121.45 (19)

C4—C3—C31	128.46 (19)	C91—C9—C8	118.37 (18)
C3—C31—H31A	109.5	C94—C91—C9	128.9 (5)
C3—C31—H31B	109.5	C94A—C91—C9	125.9 (5)
H31A—C31—H31B	109.5	C94A—C91—S9A	109.2 (5)
C3—C31—H31C	109.5	C9—C91—S9A	124.91 (19)
H31A—C31—H31C	109.5	C94—C91—S9	113.0 (5)
H31B—C31—H31C	109.5	C9—C91—S9	118.10 (16)
C5—C4—C3	103.45 (18)	C92—S9—C91	91.59 (11)
C5—C4—C41	127.89 (18)	C91—C94A—C92	112.3 (7)
C3—C4—C41	128.66 (18)	C91—C94A—H94A	123.9
C4—C41—C8	112.44 (17)	C92—C94A—H94A	123.9
C4—C41—C6	112.38 (16)	C93—C92—C94A	104.2 (4)
C8—C41—C6	110.96 (17)	C93—C92—S9	117.10 (18)
C4—C41—H41	106.9	C93—C92—H92	121.4
C8—C41—H41	106.9	C94A—C92—H92	134.3
C6—C41—H41	106.9	S9—C92—H92	121.4
N1—C5—C4	109.11 (17)	C92—C93—C94	106.3 (3)
N1—C5—Cl5	121.65 (16)	C92—C93—S9A	121.0 (2)
C4—C5—Cl5	129.22 (16)	C92—C93—H93	126.8
C7—C6—C41	112.93 (17)	C94—C93—H93	126.8
C7—C6—H6A	109.0	S9A—C93—H93	112.0
C41—C6—H6A	109.0	C91—C94—C93	111.9 (7)
C7—C6—H6B	109.0	C91—C94—H94	124.0
C41—C6—H6B	109.0	C93—C94—H94	124.0
H6A—C6—H6B	107.8	C93—S9A—C91	93.06 (18)

C5—N1—C11—C12	−43.7 (3)	C7—C71—C74—C73	178.2 (2)
N2—N1—C11—C12	140.8 (2)	S7—C71—C74—C73	0.1 (2)
C5—N1—C11—C16	136.3 (2)	C72—C73—C74—C71	0.1 (3)
N2—N1—C11—C16	−39.2 (3)	C4—C41—C8—C9	−62.5 (2)
C16—C11—C12—C13	−1.8 (3)	C6—C41—C8—C9	170.71 (17)
N1—C11—C12—C13	178.18 (19)	C41—C8—C9—O9	−24.0 (3)
C11—C12—C13—C14	2.3 (3)	C41—C8—C9—C91	158.58 (18)
C12—C13—C14—C15	−0.8 (3)	O9—C9—C91—C94	171.5 (7)
C13—C14—C15—C16	−1.4 (3)	C8—C9—C91—C94	−11.0 (7)
C14—C15—C16—C11	1.9 (3)	O9—C9—C91—C94A	−3.0 (7)
C12—C11—C16—C15	−0.3 (3)	C8—C9—C91—C94A	174.5 (6)
N1—C11—C16—C15	179.73 (19)	O9—C9—C91—S9A	178.1 (2)
C5—N1—N2—C3	0.4 (2)	C8—C9—C91—S9A	−4.5 (3)
C11—N1—N2—C3	176.69 (16)	O9—C9—C91—S9	−5.9 (3)
N1—N2—C3—C4	0.0 (2)	C8—C9—C91—S9	171.50 (16)
N1—N2—C3—C31	179.65 (17)	C94—C91—S9—C92	1.0 (6)
N2—C3—C4—C5	−0.3 (2)	C94A—C91—S9—C92	16 (4)
C31—C3—C4—C5	−179.93 (19)	C9—C91—S9—C92	178.87 (17)
N2—C3—C4—C41	−179.39 (17)	S9A—C91—S9—C92	−4.8 (2)
C31—C3—C4—C41	1.0 (3)	C94—C91—C94A—C92	4.7 (10)
C5—C4—C41—C8	−54.1 (3)	C9—C91—C94A—C92	−179.7 (4)
C3—C4—C41—C8	124.8 (2)	S9A—C91—C94A—C92	−0.6 (9)

C5—C4—C41—C6	72.0 (3)	S9—C91—C94A—C92	−161 (4)
C3—C4—C41—C6	−109.1 (2)	C91—C94A—C92—C93	−2.6 (9)
N2—N1—C5—C4	−0.6 (2)	C91—C94A—C92—S9	168 (3)
C11—N1—C5—C4	−176.38 (18)	C91—S9—C92—C93	1.3 (2)
N2—N1—C5—Cl5	178.01 (13)	C91—S9—C92—C94A	−9 (2)
C11—N1—C5—Cl5	2.2 (3)	C94A—C92—C93—C94	−0.4 (7)
C3—C4—C5—N1	0.5 (2)	S9—C92—C93—C94	−2.8 (5)
C41—C4—C5—N1	179.61 (17)	C94A—C92—C93—S9A	5.5 (6)
C3—C4—C5—Cl5	−177.93 (15)	S9—C92—C93—S9A	3.1 (4)
C41—C4—C5—Cl5	1.2 (3)	C94A—C91—C94—C93	−4.9 (10)
C4—C41—C6—C7	80.9 (2)	C9—C91—C94—C93	179.7 (3)
C8—C41—C6—C7	−152.22 (18)	S9A—C91—C94—C93	125 (6)
C41—C6—C7—O7	16.3 (3)	S9—C91—C94—C93	−2.7 (9)
C41—C6—C7—C71	−166.61 (18)	C92—C93—C94—C91	3.5 (9)
O7—C7—C71—C74	−168.6 (2)	S9A—C93—C94—C91	−157 (3)
C6—C7—C71—C74	14.3 (3)	C92—C93—S9A—C91	−5.5 (3)
O7—C7—C71—S7	9.3 (3)	C94—C93—S9A—C91	16 (2)
C6—C7—C71—S7	−167.84 (16)	C94—C91—S9A—C93	−49 (6)
C74—C71—S7—C72	−0.27 (18)	C94A—C91—S9A—C93	3.1 (6)
C7—C71—S7—C72	−178.53 (18)	C9—C91—S9A—C93	−177.8 (2)
C71—S7—C72—C73	0.3 (2)	S9—C91—S9A—C93	6.2 (3)
S7—C72—C73—C74	−0.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8*A*···*Cg*1^{i}	0.99	2.67	3.628 (3)	162
C8—H8*A*···*Cg*2^{i}	0.99	2.67	3.614 (3)	159

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.