Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 3-(4-chlorophenyl)-2-phenyl-3-(4-phenyl-1,2,3-selenadiazol-5-yl)propanoate

P. Sugumar,[a] S. Sankari,[b] P. Manisankar,[c] V. Thiruselvam[a] and M. N. Ponnuswamy[a]*

[a]Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600 025, India, [b]Department of Chemistry, Sri Sarada College for Women (Autonomous), Fairlands, Salem 636 016, India, and [c]Department of Industrial Chemistry, Alagappa University, Karaikudi 630 003, India
Correspondence e-mail: mnpsy2004@yahoo.com

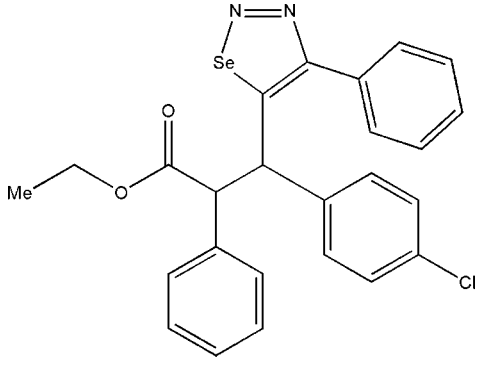
Received 14 June 2013; accepted 28 June 2013

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.107; data-to-parameter ratio = 20.6.

In the title compound, $C_{25}H_{21}ClN_2O_2Se$, the selenadiazole ring is almost planar [maximum deviation = 0.004 (2) Å], and the adjacent benzene ring is twisted by 50.6 (1)° with respect to this ring.

Related literature

For general background to selenadiazol derivatives, see: Khanna (2005). For related structures, see: Marx *et al.* (2008); Muthukumaran *et al.* (2011).



Experimental

Crystal data

$C_{25}H_{21}ClN_2O_2Se$
M_r = 495.85
Monoclinic, $P2_1/c$
a = 12.1337 (3) Å
b = 12.2267 (3) Å
c = 16.4423 (4) Å
β = 107.744 (1)°
V = 2323.26 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.76 mm^{-1}
T = 293 K
0.25 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.663, T_{max} = 0.729
22323 measured reflections
5764 independent reflections
3745 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.107
S = 1.02
5764 reflections
280 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

PS thanks the UGC, New Delhi, for financial support in the form of a Research Fellowship in Science for Meritorious Students. The authors thank the TBI Consultancy, University of Madras, India, for the data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5333).

References

Bruker (2008). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Khanna, P. K. (2005). *Phosphorus Sulfur Silicon Relat. Elem.* **180**, 951–955.
Marx, A., Saravanan, S., Muthusubramanian, S., Manivannan, V. & Rath, N. P. (2008). *Acta Cryst.* E**64**, o349.
Muthukumaran, J., Nachiappan, M., Chitra, S., Manisankar, P., Bhattacharya, S., Muthusubramanian, S., Krishna, R. & Jeyakanthan, J. (2011). *Acta Cryst.* E**67**, o2010–o2011.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2013). E**69**, o1239 [doi:10.1107/S1600536813017790]

Ethyl 3-(4-chlorophenyl)-2-phenyl-3-(4-phenyl-1,2,3-selenadiazol-5-yl)propanoate

P. Sugumar, S. Sankari, P. Manisankar, V. Thiruselvam and M. N. Ponnuswamy

S1. Comment

Selenadiazoles, having one selenium and two nitrogen atoms in a five membered ring, are the important class of organoselenium compounds utilized in the synthesis of semiconductor nanoparticles (Khanna, 2005). The crystal structure of the title compound is carried out to elucidate the conformational status of the molecule.

The *ORTEP* plot of the molecule is shown in Fig.1. The selenadiazol ring is planar[with maximum deviation for the atom N2 is -0.004 (2) Å]. The attached phenyl ring is twisted away at an angle of 50.6 (1)° with respect to selenadiazol ring. The bond lengths [Se1—N2] 1.874 (2) Å, [Se1—C8] 1.838 (2) Å & [Cl1—C13] 1.736 (2)° are comparable with the values reported in the literature (Marx *et al.* 2008; Muthukumaran *et al.* 2011). The bond C9—C16 is slightly lengthened due to streic interaction between the phenyl and chlorophenyl rings.

The dihedral angle between the selenadiazol and chlorophenyl ring is 74.3 (1)°. The propanoate group assumes an extended conformation which can be seen from the torsion angle (C16—C23—O2—C24) value of -177.8 (2)°.

S2. Experimental

A mixture of ethyl 3-(4-chlorophenyl)-5-oxo-2,5-diphenylpentanoate (1 m*M*), semicarbazide hydrochloride(2 m*M*) and sodium acetate (3 m*M*) in ethanol (10 ml) was refluxed for 4 hrs. After completion of the reaction as monitored by TLC, the mixture was poured into ice cold water and the resulting semicarbazone was filtered off. Then, a mixture of semicarbazone (1 m*M*) and SeO_2 (2 m*M*) in tetrahydrofuran (10 ml) were refluxed on a water bath for 1hr. The selenium deposited on cooling was removed by filtration, and the filtrate was poured into crushed ice, extracted with dichloromethane, and purified by column chromatography using silica gel (60–120 mesh) with 97:3 petroleum ether: ethyl acetate as eluent to give ethyl-3-(4-chlorophenyl)-2-phenyl-3- (4-phenyl-1,2, 3-selenadiazol-5-yl)propanoate.

S3. Refinement

H atoms were positioned geometrically (C—H = 0.93–0.98 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H and 1.2U_{eq}(C) for other H atoms.

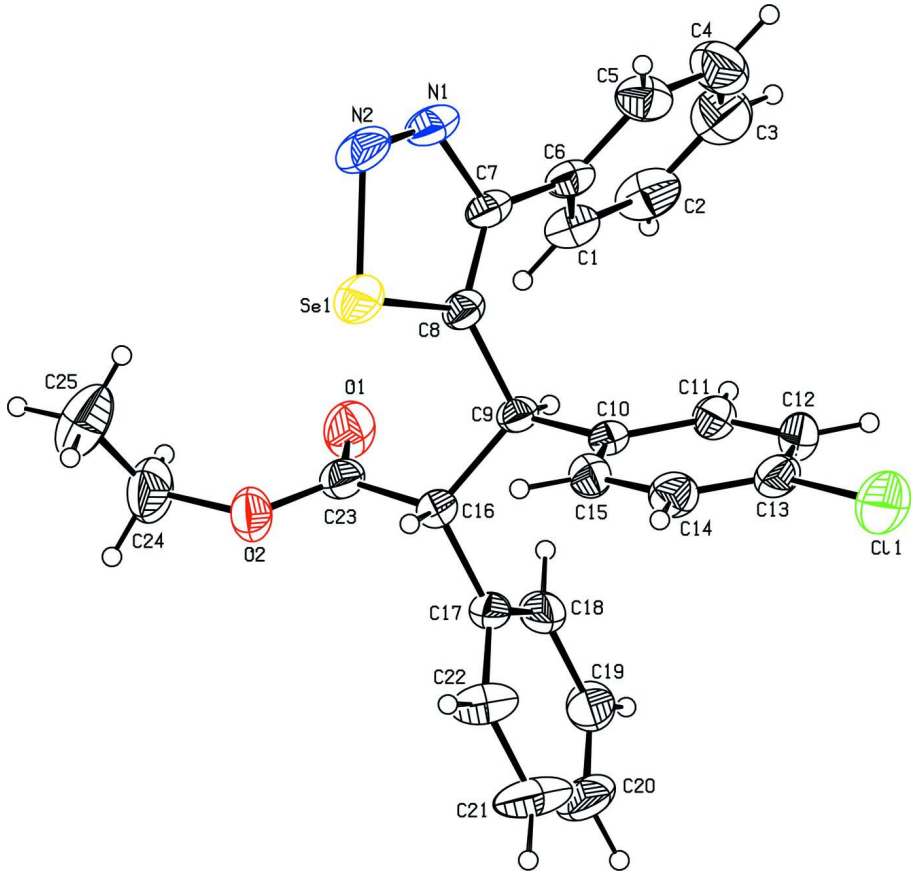


Figure 1

The molecular structure of the title compound with the displacement ellipsoids drawn at 30% probability level.

Ethyl 3-(4-chlorophenyl)-2-phenyl-3-(4-phenyl-1,2,3-selenadiazol-5-yl)propanoate

Crystal data

$C_{25}H_{21}ClN_2O_2Se$
$M_r = 495.85$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 12.1337\ (3)$ Å
$b = 12.2267\ (3)$ Å
$c = 16.4423\ (4)$ Å
$\beta = 107.744\ (1)°$
$V = 2323.26\ (10)$ Å^3
$Z = 4$
$F(000) = 1008$
$D_x = 1.418$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5764 reflections
$\theta = 1.8–28.4°$
$\mu = 1.76$ mm^{-1}
$T = 293$ K
Block, yellow
0.25 × 0.20 × 0.18 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min} = 0.663$, $T_{max} = 0.729$
22323 measured reflections
5764 independent reflections
3745 reflections with $I > 2\sigma(I)$
$R_{int} = 0.035$
$\theta_{max} = 28.4°$, $\theta_{min} = 1.8°$
$h = -12\rightarrow16$
$k = -16\rightarrow15$
$l = -21\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.107$
$S = 1.02$
5764 reflections
280 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
$w = 1/[\sigma^2(F_o^2) + (0.0471P)^2 + 0.6047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ 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}
C1	0.7760 (2)	0.5374 (2)	0.74986 (16)	0.0633 (6)
H1	0.7656	0.5310	0.6916	0.076*
C2	0.7134 (3)	0.6137 (2)	0.7793 (2)	0.0836 (9)
H2	0.6610	0.6588	0.7407	0.100*
C3	0.7278 (3)	0.6234 (3)	0.8652 (3)	0.0954 (10)
H3	0.6847	0.6744	0.8846	0.114*
C4	0.8054 (3)	0.5580 (3)	0.9219 (2)	0.0908 (10)
H4	0.8151	0.5647	0.9800	0.109*
C5	0.8696 (2)	0.4818 (2)	0.89387 (17)	0.0706 (7)
H5	0.9230	0.4381	0.9331	0.085*
C6	0.85467 (19)	0.47046 (18)	0.80734 (14)	0.0536 (5)
C7	0.92554 (18)	0.38995 (18)	0.77867 (13)	0.0502 (5)
C8	0.88943 (17)	0.31106 (18)	0.71769 (13)	0.0469 (5)
C9	0.76586 (16)	0.28344 (17)	0.66740 (12)	0.0428 (4)
H9	0.7191	0.3492	0.6659	0.051*
C10	0.72046 (16)	0.19519 (17)	0.71371 (12)	0.0426 (4)
C11	0.64815 (19)	0.2233 (2)	0.76108 (15)	0.0549 (5)
H11	0.6269	0.2960	0.7634	0.066*
C12	0.6070 (2)	0.1451 (2)	0.80495 (15)	0.0656 (7)
H12	0.5585	0.1648	0.8367	0.079*
C13	0.6383 (2)	0.0383 (2)	0.80109 (15)	0.0631 (7)
C14	0.7116 (2)	0.0082 (2)	0.75615 (15)	0.0622 (6)
H14	0.7338	−0.0644	0.7551	0.075*
C15	0.7521 (2)	0.08659 (19)	0.71257 (14)	0.0538 (5)
H15	0.8016	0.0663	0.6818	0.065*

C16	0.75310 (17)	0.25174 (17)	0.57420 (13)	0.0456 (5)
H16	0.7931	0.1820	0.5747	0.055*
C17	0.62689 (19)	0.23681 (19)	0.52183 (13)	0.0497 (5)
C18	0.5471 (2)	0.3186 (2)	0.51442 (14)	0.0640 (6)
H18	0.5699	0.3853	0.5415	0.077*
C19	0.4325 (2)	0.3023 (3)	0.46674 (16)	0.0834 (9)
H19	0.3785	0.3579	0.4619	0.100*
C20	0.3993 (3)	0.2040 (4)	0.4268 (2)	0.0985 (12)
H20	0.3222	0.1923	0.3958	0.118*
C21	0.4772 (3)	0.1247 (3)	0.4322 (2)	0.1093 (13)
H21	0.4542	0.0589	0.4037	0.131*
C22	0.5919 (3)	0.1399 (2)	0.47981 (18)	0.0818 (8)
H22	0.6454	0.0842	0.4833	0.098*
C23	0.80904 (19)	0.3363 (2)	0.53277 (14)	0.0533 (5)
C24	0.9294 (3)	0.3559 (3)	0.4427 (2)	0.0910 (9)
H24A	0.9033	0.3406	0.3820	0.109*
H24B	0.9149	0.4325	0.4509	0.109*
C25	1.0522 (3)	0.3337 (3)	0.4767 (3)	0.1152 (13)
H25A	1.0935	0.3782	0.4477	0.173*
H25B	1.0663	0.2579	0.4683	0.173*
H25C	1.0781	0.3502	0.5366	0.173*
N1	1.04418 (17)	0.39168 (19)	0.81995 (13)	0.0663 (5)
N2	1.10574 (18)	0.3221 (2)	0.79702 (15)	0.0766 (6)
O1	0.80184 (17)	0.43304 (16)	0.54165 (12)	0.0777 (5)
O2	0.86582 (16)	0.28857 (15)	0.48558 (11)	0.0679 (5)
Cl1	0.58491 (9)	−0.06117 (8)	0.85433 (6)	0.1057 (3)
Se1	1.01461 (2)	0.23132 (3)	0.710678 (17)	0.06928 (12)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0524 (13)	0.0566 (14)	0.0712 (15)	−0.0052 (11)	0.0043 (11)	−0.0039 (12)
C2	0.0652 (17)	0.0621 (17)	0.109 (2)	0.0021 (14)	0.0058 (16)	−0.0044 (16)
C3	0.090 (2)	0.079 (2)	0.120 (3)	0.0026 (18)	0.036 (2)	−0.025 (2)
C4	0.119 (3)	0.079 (2)	0.080 (2)	−0.015 (2)	0.039 (2)	−0.0217 (17)
C5	0.0822 (19)	0.0585 (16)	0.0642 (16)	−0.0078 (13)	0.0121 (13)	−0.0058 (12)
C6	0.0494 (12)	0.0467 (12)	0.0576 (13)	−0.0146 (10)	0.0057 (10)	−0.0040 (10)
C7	0.0385 (11)	0.0530 (13)	0.0515 (12)	−0.0106 (9)	0.0025 (9)	0.0027 (10)
C8	0.0350 (10)	0.0535 (12)	0.0485 (11)	−0.0031 (9)	0.0071 (8)	0.0028 (9)
C9	0.0331 (9)	0.0476 (12)	0.0437 (11)	−0.0031 (8)	0.0056 (8)	−0.0046 (8)
C10	0.0336 (9)	0.0515 (12)	0.0391 (10)	−0.0046 (8)	0.0058 (8)	−0.0060 (8)
C11	0.0436 (11)	0.0644 (14)	0.0559 (13)	0.0018 (10)	0.0142 (10)	−0.0053 (11)
C12	0.0503 (13)	0.093 (2)	0.0591 (14)	−0.0091 (13)	0.0247 (11)	−0.0038 (13)
C13	0.0588 (14)	0.0749 (18)	0.0536 (13)	−0.0249 (13)	0.0141 (11)	0.0025 (12)
C14	0.0702 (16)	0.0545 (14)	0.0609 (14)	−0.0117 (12)	0.0185 (12)	−0.0019 (11)
C15	0.0561 (13)	0.0543 (14)	0.0546 (13)	−0.0043 (10)	0.0222 (10)	−0.0054 (10)
C16	0.0383 (10)	0.0516 (13)	0.0451 (11)	−0.0037 (9)	0.0098 (8)	−0.0024 (9)
C17	0.0447 (11)	0.0649 (14)	0.0365 (10)	−0.0117 (10)	0.0082 (8)	−0.0027 (9)

C18	0.0468 (13)	0.0940 (19)	0.0471 (13)	0.0022 (13)	0.0082 (10)	−0.0126 (12)
C19	0.0429 (13)	0.148 (3)	0.0523 (14)	0.0061 (16)	0.0045 (11)	−0.0008 (16)
C20	0.0558 (18)	0.154 (4)	0.0665 (18)	−0.038 (2)	−0.0093 (14)	0.011 (2)
C21	0.097 (3)	0.095 (3)	0.101 (2)	−0.043 (2)	−0.024 (2)	−0.007 (2)
C22	0.0739 (18)	0.0680 (18)	0.0809 (18)	−0.0149 (14)	−0.0103 (14)	−0.0079 (14)
C23	0.0448 (12)	0.0626 (16)	0.0478 (12)	−0.0083 (10)	0.0073 (9)	0.0007 (10)
C24	0.085 (2)	0.114 (3)	0.086 (2)	−0.0062 (19)	0.0439 (17)	0.0262 (18)
C25	0.087 (3)	0.094 (3)	0.179 (4)	−0.016 (2)	0.062 (3)	0.019 (2)
N1	0.0416 (11)	0.0765 (14)	0.0671 (13)	−0.0124 (10)	−0.0039 (9)	−0.0003 (10)
N2	0.0349 (10)	0.0998 (18)	0.0827 (15)	−0.0066 (11)	−0.0002 (10)	−0.0018 (13)
O1	0.0910 (14)	0.0613 (12)	0.0898 (13)	−0.0124 (10)	0.0409 (11)	0.0029 (9)
O2	0.0688 (11)	0.0807 (12)	0.0641 (10)	−0.0032 (9)	0.0352 (9)	0.0054 (9)
Cl1	0.1182 (7)	0.1091 (7)	0.1002 (6)	−0.0457 (5)	0.0485 (5)	0.0149 (5)
Se1	0.03892 (14)	0.0867 (2)	0.0777 (2)	0.00811 (12)	0.01107 (11)	−0.00725 (13)

Geometric parameters (Å, º)

C1—C2	1.380 (4)	C14—H14	0.9300
C1—C6	1.387 (3)	C15—H15	0.9300
C1—H1	0.9300	C16—C23	1.509 (3)
C2—C3	1.374 (4)	C16—C17	1.522 (3)
C2—H2	0.9300	C16—H16	0.9800
C3—C4	1.364 (5)	C17—C18	1.372 (3)
C3—H3	0.9300	C17—C22	1.372 (3)
C4—C5	1.381 (4)	C18—C19	1.386 (3)
C4—H4	0.9300	C18—H18	0.9300
C5—C6	1.385 (3)	C19—C20	1.371 (5)
C5—H5	0.9300	C19—H19	0.9300
C6—C7	1.476 (3)	C20—C21	1.338 (5)
C7—C8	1.364 (3)	C20—H20	0.9300
C7—N1	1.392 (3)	C21—C22	1.386 (4)
C8—C9	1.513 (3)	C21—H21	0.9300
C8—Se1	1.838 (2)	C22—H22	0.9300
C9—C10	1.518 (3)	C23—O1	1.198 (3)
C9—C16	1.542 (3)	C23—O2	1.320 (3)
C9—H9	0.9800	C24—C25	1.448 (5)
C10—C11	1.382 (3)	C24—O2	1.449 (3)
C10—C15	1.384 (3)	C24—H24A	0.9700
C11—C12	1.379 (3)	C24—H24B	0.9700
C11—H11	0.9300	C25—H25A	0.9600
C12—C13	1.367 (4)	C25—H25B	0.9600
C12—H12	0.9300	C25—H25C	0.9600
C13—C14	1.368 (3)	N1—N2	1.263 (3)
C13—Cl1	1.736 (2)	N2—Se1	1.874 (2)
C14—C15	1.374 (3)		
C2—C1—C6	119.8 (3)	C14—C15—H15	119.4
C2—C1—H1	120.1	C10—C15—H15	119.4

C6—C1—H1	120.1	C23—C16—C17	109.90 (17)
C3—C2—C1	120.5 (3)	C23—C16—C9	110.70 (17)
C3—C2—H2	119.7	C17—C16—C9	111.81 (17)
C1—C2—H2	119.7	C23—C16—H16	108.1
C4—C3—C2	119.8 (3)	C17—C16—H16	108.1
C4—C3—H3	120.1	C9—C16—H16	108.1
C2—C3—H3	120.1	C18—C17—C22	118.9 (2)
C3—C4—C5	120.6 (3)	C18—C17—C16	121.6 (2)
C3—C4—H4	119.7	C22—C17—C16	119.5 (2)
C5—C4—H4	119.7	C17—C18—C19	120.3 (3)
C4—C5—C6	120.0 (3)	C17—C18—H18	119.8
C4—C5—H5	120.0	C19—C18—H18	119.8
C6—C5—H5	120.0	C20—C19—C18	119.7 (3)
C5—C6—C1	119.2 (2)	C20—C19—H19	120.2
C5—C6—C7	119.2 (2)	C18—C19—H19	120.2
C1—C6—C7	121.5 (2)	C21—C20—C19	120.3 (3)
C8—C7—N1	115.0 (2)	C21—C20—H20	119.8
C8—C7—C6	128.22 (19)	C19—C20—H20	119.8
N1—C7—C6	116.80 (19)	C20—C21—C22	120.6 (3)
C7—C8—C9	127.0 (2)	C20—C21—H21	119.7
C7—C8—Se1	109.56 (15)	C22—C21—H21	119.7
C9—C8—Se1	123.19 (16)	C17—C22—C21	120.2 (3)
C8—C9—C10	109.59 (16)	C17—C22—H22	119.9
C8—C9—C16	112.45 (17)	C21—C22—H22	119.9
C10—C9—C16	112.21 (16)	O1—C23—O2	125.4 (2)
C8—C9—H9	107.4	O1—C23—C16	124.2 (2)
C10—C9—H9	107.4	O2—C23—C16	110.4 (2)
C16—C9—H9	107.4	C25—C24—O2	110.1 (3)
C11—C10—C15	118.2 (2)	C25—C24—H24A	109.6
C11—C10—C9	119.7 (2)	O2—C24—H24A	109.6
C15—C10—C9	122.06 (19)	C25—C24—H24B	109.6
C12—C11—C10	121.1 (2)	O2—C24—H24B	109.6
C12—C11—H11	119.5	H24A—C24—H24B	108.2
C10—C11—H11	119.5	C24—C25—H25A	109.5
C13—C12—C11	119.1 (2)	C24—C25—H25B	109.5
C13—C12—H12	120.4	H25A—C25—H25B	109.5
C11—C12—H12	120.4	C24—C25—H25C	109.5
C14—C13—C12	121.2 (2)	H25A—C25—H25C	109.5
C14—C13—Cl1	119.2 (2)	H25B—C25—H25C	109.5
C12—C13—Cl1	119.6 (2)	N2—N1—C7	117.5 (2)
C13—C14—C15	119.3 (2)	N1—N2—Se1	111.03 (15)
C13—C14—H14	120.4	C23—O2—C24	119.0 (2)
C15—C14—H14	120.4	C8—Se1—N2	86.93 (10)
C14—C15—C10	121.2 (2)		

C6—C1—C2—C3	−0.4 (4)	C11—C10—C15—C14	1.0 (3)
C1—C2—C3—C4	0.7 (5)	C9—C10—C15—C14	178.84 (19)
C2—C3—C4—C5	−0.1 (5)	C8—C9—C16—C23	−50.6 (2)

C3—C4—C5—C6	−0.7 (5)	C10—C9—C16—C23	−174.72 (17)
C4—C5—C6—C1	1.0 (4)	C8—C9—C16—C17	−173.52 (18)
C4—C5—C6—C7	179.0 (2)	C10—C9—C16—C17	62.4 (2)
C2—C1—C6—C5	−0.5 (4)	C23—C16—C17—C18	−66.8 (3)
C2—C1—C6—C7	−178.4 (2)	C9—C16—C17—C18	56.6 (3)
C5—C6—C7—C8	129.5 (3)	C23—C16—C17—C22	112.2 (3)
C1—C6—C7—C8	−52.6 (3)	C9—C16—C17—C22	−124.4 (2)
C5—C6—C7—N1	−48.6 (3)	C22—C17—C18—C19	1.4 (4)
C1—C6—C7—N1	129.3 (2)	C16—C17—C18—C19	−179.6 (2)
N1—C7—C8—C9	174.8 (2)	C17—C18—C19—C20	−0.1 (4)
C6—C7—C8—C9	−3.3 (4)	C18—C19—C20—C21	−1.4 (5)
N1—C7—C8—Se1	−0.1 (2)	C19—C20—C21—C22	1.6 (6)
C6—C7—C8—Se1	−178.24 (18)	C18—C17—C22—C21	−1.3 (4)
C7—C8—C9—C10	−91.3 (3)	C16—C17—C22—C21	179.7 (3)
Se1—C8—C9—C10	83.0 (2)	C20—C21—C22—C17	−0.2 (6)
C7—C8—C9—C16	143.2 (2)	C17—C16—C23—O1	82.5 (3)
Se1—C8—C9—C16	−42.5 (2)	C9—C16—C23—O1	−41.5 (3)
C8—C9—C10—C11	101.5 (2)	C17—C16—C23—O2	−97.2 (2)
C16—C9—C10—C11	−132.8 (2)	C9—C16—C23—O2	138.78 (19)
C8—C9—C10—C15	−76.3 (2)	C8—C7—N1—N2	0.5 (3)
C16—C9—C10—C15	49.4 (2)	C6—C7—N1—N2	178.9 (2)
C15—C10—C11—C12	−1.1 (3)	C7—N1—N2—Se1	−0.7 (3)
C9—C10—C11—C12	−178.98 (19)	O1—C23—O2—C24	2.6 (4)
C10—C11—C12—C13	−0.1 (4)	C16—C23—O2—C24	−177.8 (2)
C11—C12—C13—C14	1.5 (4)	C25—C24—O2—C23	115.2 (3)
C11—C12—C13—Cl1	−178.78 (18)	C7—C8—Se1—N2	−0.22 (17)
C12—C13—C14—C15	−1.5 (4)	C9—C8—Se1—N2	−175.37 (18)
Cl1—C13—C14—C15	178.69 (18)	N1—N2—Se1—C8	0.5 (2)
C13—C14—C15—C10	0.3 (3)		