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

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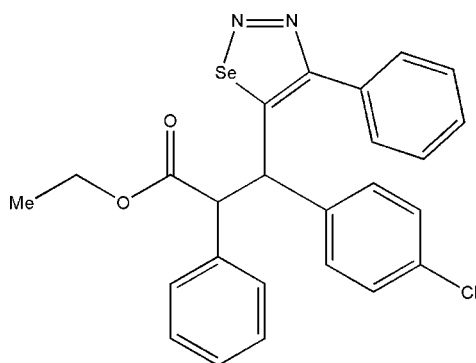
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.037; wR factor = 0.107; data-to-parameter ratio = 20.6.

In the title compound, $\text{C}_{25}\text{H}_{21}\text{ClN}_2\text{O}_2\text{Se}$, 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); Muthukumar *et al.* (2011).



Experimental

Crystal data

$\text{C}_{25}\text{H}_{21}\text{ClN}_2\text{O}_2\text{Se}$
 $M_r = 495.85$
 Monoclinic, $P2_1/c$
 $a = 12.1337$ (3) Å
 $b = 12.2267$ (3) Å
 $c = 16.4423$ (4) Å
 $\beta = 107.744$ (1)°

$V = 2323.26$ (10) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.76$ mm⁻¹
 $T = 293$ K
 $0.25 \times 0.20 \times 0.18$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$

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).

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

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supplementary materials

Acta Cryst. (2013). E69, o1239 [doi:10.1107/S1600536813017790]

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

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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 $50.6(1)^\circ$ with respect to selenadiazol ring. The bond lengths [Se1—N2] $1.874(2)$ Å, [Se1—C8] $1.838(2)$ Å & [C11—C13] $1.736(2)^\circ$ 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 steric interaction between the phenyl and chlorophenyl rings.

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

Experimental

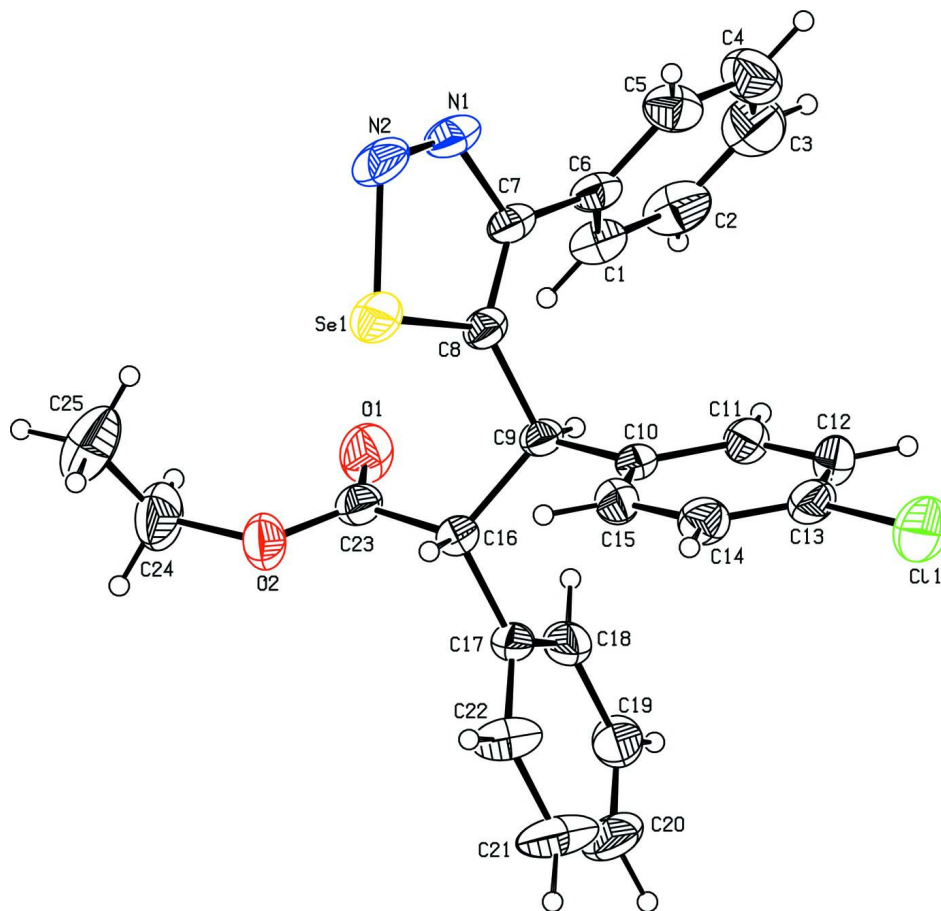
A mixture of ethyl 3-(4-chlorophenyl)-5-oxo-2,5-diphenylpentanoate (1 mM), semicarbazide hydrochloride (2 mM) and sodium acetate (3 mM) in ethanol (10 ml) was refluxed for 4 hrs. After completion of the reaction as monitored by TLC, the mixture was poured into ice cold water and the resulting semicarbazone was filtered off. Then, a mixture of semicarbazone (1 mM) and SeO₂ (2 mM) 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.

Refinement

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

Computing details

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINTE* (Bruker, 2008); data reduction: *SAINTE* (Bruker, 2008); 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* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

**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: $-P\ 2_1/c$

$a = 12.1337\ (3)\ \text{\AA}$

$b = 12.2267\ (3)\ \text{\AA}$

$c = 16.4423\ (4)\ \text{\AA}$

$\beta = 107.744\ (1)^\circ$

$V = 2323.26\ (10)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1008$

$D_x = 1.418\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5764 reflections

$\theta = 1.8\text{--}28.4^\circ$

$\mu = 1.76\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Block, yellow

$0.25 \times 0.20 \times 0.18\ \text{mm}$

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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.035$
 $\theta_{\text{max}} = 28.4^\circ$, $\theta_{\text{min}} = 1.8^\circ$
 $h = -12 \rightarrow 16$

$k = -16 \rightarrow 15$
 $l = -21 \rightarrow 19$

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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.002$
 $\Delta\rho_{\text{max}} = 0.42 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.27 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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 (\AA^2)

	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, °)

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—C11	119.2 (2)	H25B—C25—H25C	109.5
C12—C13—C11	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—C11	-178.78 (18)	C7—C8—Se1—N2	-0.22 (17)
C12—C13—C14—C15	-1.5 (4)	C9—C8—Se1—N2	-175.37 (18)
C11—C13—C14—C15	178.69 (18)	N1—N2—Se1—C8	0.5 (2)
C13—C14—C15—C10	0.3 (3)		
