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# 1,3-Bis(3-phenylpropyl)-1*H*-1,3-benzimidazole-2(3*H*)-selone

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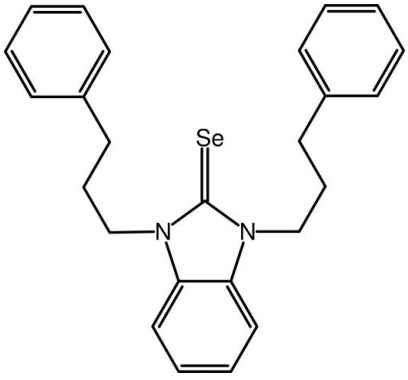
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.032; $wR$ factor = 0.066; data-to-parameter ratio = 19.8.

The title molecule, $C_{25}H_{26}N_2Se$, has mirror symmetry, with the mirror plane passing through the atoms of the C=Se bond and the mid-points of the two C—C bonds of the benzene ring of the benzimidazole group. The dihedral angle between the benzimidazole ring system and the phenyl ring is 71.62 (14)°.

## Related literature

For general background to benzimidazole derivatives, see: Aydın *et al.* (1998); Böhm & Herrmann (2000); Küçükbay *et al.* (1996, 1997); Lappert *et al.* (2009); Wanzlick & Schikora (1960); Yıldırım *et al.* (2006); Yılmaz & Küçükbay (2009); Çetinkaya *et al.* (1994, 1998). For related structures, see: Akkurt *et al.* (2004); Aydın *et al.* (1999); Yalçın *et al.* (2008).




## Experimental

### Crystal data

$C_{25}H_{26}N_2Se$
$M_r$ = 433.44
Tetragonal, $P4_12_12$
$a$ = 10.5150 (3) Å
$c$ = 19.8142 (8) Å
$V$ = 2190.76 (13) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.73 mm$^{-1}$
$T$ = 296 K
0.68 × 0.58 × 0.52 mm

### Data collection

Stowe IPDS 2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min}$ = 0.322, $T_{max}$ = 0.408
16780 measured reflections
2531 independent reflections
2225 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.066
$S$ = 1.07
2531 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$
Absolute structure: Flack (1983), 1003 Freidel pairs
Flack parameter: 0.004 (12)

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: QM2004).

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# supporting information

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## 1,3-Bis(3-phenylpropyl)-1*H*-1,3-benzimidazole-2(3*H*)-selone

**Mehmet Akkurt, Ülkü Yılmaz, Hasan Küçükbay and Orhan Büyükgüngör**

### S1. Comment

Electron-rich olefins (EROs) have been attracted considerable attention in both organic and inorganic preparative literature due to their unique properties as reagent and reaction intermediates since their first report by Wanzlick in 1960 (Wanzlick & Schikora, 1960; Böhm & Herrmann, 2000).

Benzimidazolium salts are convenient precursors for EROs through reacting with a strong base such as NaH comparing with other methods such as reacting a secondary amine (*N*,*N*′-disubstituted-1,2-diaminobenzene) with an acetal, chloral or triethyl orthoformate. We have synthesized and isolated first time the ERO, bis(1,3-dimethybenzimidazolidine-2-yl-idene) (Çetinkaya *et al.*, 1994). We have also synthesized a number of EROs using different synthesis methods and used them to synthesize many organic or organometallic compounds (Küçükbay *et al.*, 1996, Küçükbay *et al.*, 1997, Çetinkaya *et al.*, 1998; Aydın *et al.*, 1998 Yıldırım *et al.*, 2006; Yılmaz & Küçükbay, 2009). Their electron-richness confers on them a very high reactivity as strong nucleophiles, which assist in the preparation of numerous products by reaction, amongst others, with group 16 elements, transition metals, and many protic compounds (Lappert *et al.*, 2009). It is known that the ultimate oxidation product of EROs with air is urea; sulfur, selenium and tellurium react similarly to give the corresponding analogues. The objective of the present study was to elucidate the crystal structure of the title compound which is new ERO derivative.

In the title molecule (I), Fig. 1, the Se═C bond length is 1.828 (2) Å, and this value is similar to those [1.829 (3) Å] found in 1-ethyl-3-(2-phenylethyl)benzimidazole-2-selone (Akkurt *et al.*, 2004) and [1.825 (7) Å] found in 1,3-dimethyl-benzimidazole-2-selone (Aydın *et al.*, 1999), and is shorter than that [2.058 (4) Å] found for the Te═ C bond length in 1,3-bis(3-phenylpropyl)1*H*-benzimidazole- 2(3*H*)-tellurone (Yalçın *et al.*, 2008).

The molecular structure is stabilized by a weak C—H···Se interaction (Table 1). The benzimidazole ring system (N1/C10/C11/C12/C13/N1a/C11*a*/C12*a*/C13*a*) of (I) is planar (r.m.s deviation of fitted atoms is 0.09 (3) Å). The dihedral angle between the phenyl ring (C1–C6) and the benzimidazole ring is 71.62 (14)°. The molecular packing in (I) is shown in Fig. 2.

### S2. Experimental

A mixture of bis(1,3-di(3-phenylpropyl)benzimidazolidine-2-ylidene) (0.68 g, 0.96 mmol) and selenium (0.15 g, 1.90 mmol) in dry toluene (10 ml) was heated under reflux for 2 h. Then the mixture was filtered to remove unreacted selenium and all volatiles were removed *in vacuo* (0.02 m mH g). The crude product was crystallized from alcohol upon cooling to 243 K. Yield: 0.63 g, 76%; m.p.: 439–441 K; $\nu_{(CSe)}$= 1480 cm$^{-1}$. Anal. found: C 69.58, H 5.98, N 6.38%. Calculated for $C_{25}H_{26}N_2Se$: C 69.27, H 6.05, N 6.46%. $^1$H-NMR ($\delta$, $CDCl_3$): 7.26–7.06 (m, 14H, Ar—H), 4.47 (t, 4H, N*CH*$_2$CH$_2$CH$_2$C$_6$H$_5$, $J$ = 7.8 Hz), 2.81 (t, 4H, NCH$_2$CH$_2$*CH*$_2$C$_6$H$_5$, $J$ = 7.8 Hz), 2.23 (quint, 4H, NCH$_2$*CH*$_2$CH$_2$C$_6$H$_5$, $J$ = 7.8 Hz). $^{13}$C-NMR ($\delta$, $CDCl_3$): 165.7 (C=Se), 140.8, 132.9, 128.5, 128.4, 126.2, 123.2 and 109.5 (Ar-*C*), 46.1 (N*CH*$_2$CH$_2$CH$_2$C$_6$H$_5$), 33.0 (NCH$_2$CH$_2$*CH*$_2$C$_6$H$_5$), 29.3 (NCH$_2$*CH*$_2$CH$_2$C$_6$H$_5$).

### S3. Refinement

All H atoms were positioned geometrically with C—H = 0.93–0.97 Å, and refined using a riding model with $U_{iso}$(H) = 1.2$U_{eq}$(C). The absolute configuration of the title compound was established by refinement of the Flack (1983) parameter.

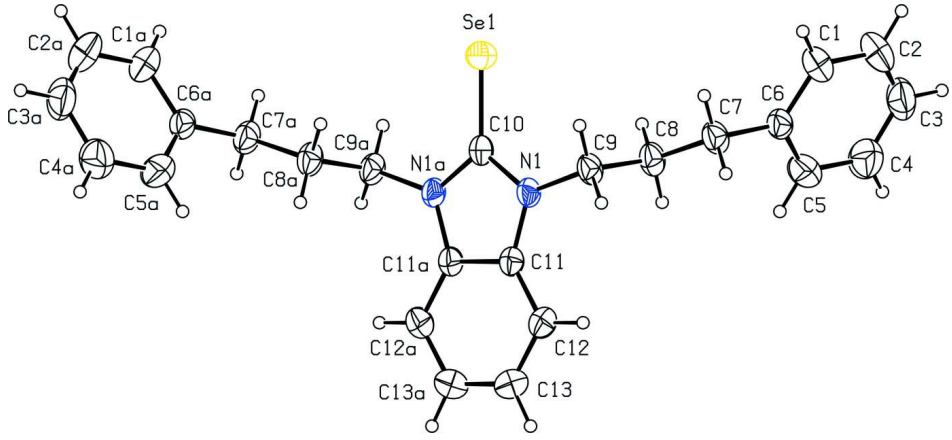


**Figure 1**

View of the title molecule, showing the atom labelling scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level. (Symmetry code: (*a*) *y*, *x*, 1 - *z*).

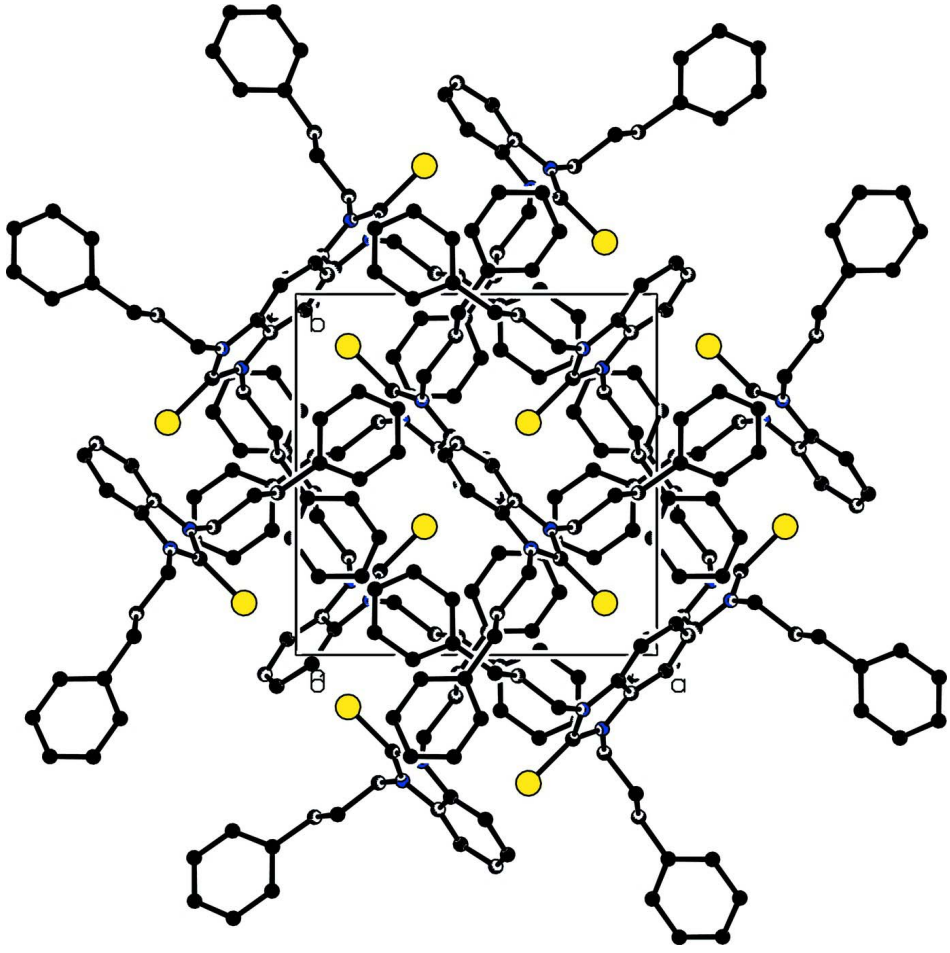


**Figure 2**

The packing diagram of (I) viewing down the *b* axis. All hydrogen atoms have been omitted for clarity.

### 1,3-Bis(3-phenylpropyl)-1*H*-1,3-benzimidazole-2(3*H*)-selone

*Crystal data*

$C_{25}H_{26}N_2Se$
$M_r = 433.44$
Tetragonal, $P4_12_12$
Hall symbol: P 4abw 2nw
$a = 10.5150$ (3) Å
$c = 19.8142$ (8) Å
$V = 2190.76$ (13) Å$^3$
$Z = 4$
$F(000) = 896$
$D_x = 1.314$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 20954 reflections
$\theta = 1.9$–$28.0°$
$\mu = 1.73$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.68 × 0.58 × 0.52 mm

*Data collection*

Stowe IPDS 2 diffractometer
Radiation source: sealed X-ray tube, 12 x 0.4 mm long-fine focus
Plane graphite monochromator
Detector resolution: 6.67 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
$T_{min} = 0.322$, $T_{max} = 0.408$
16780 measured reflections
2531 independent reflections
2225 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$

$\theta_{max}$ = 27.5°, $\theta_{min}$ = 2.2°
$h$ = −13→13
$k$ = −13→13
$l$ = −25→25

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.066
$S$ = 1.07
2531 reflections
128 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
$w = 1/[\sigma^2(F_o^2) + (0.0285P)^2 + 0.3345P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$
Absolute structure: Flack (1983), 1003 Freidel pairs
Absolute structure parameter: 0.004 (12)

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**Refinement**. Refinement on $F^2$ for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Se1 | 0.35581 (2) | 0.35581 (2) | 0.50000 | 0.0563 (1) |
| N1 | 0.20501 (16) | 0.15139 (19) | 0.55133 (8) | 0.0486 (5) |
| C1 | 0.6763 (3) | 0.0124 (4) | 0.71439 (17) | 0.0933 (12) |
| C2 | 0.7825 (3) | −0.0624 (5) | 0.7188 (2) | 0.116 (2) |
| C3 | 0.7813 (3) | −0.1823 (4) | 0.69632 (19) | 0.0997 (16) |
| C4 | 0.6739 (4) | −0.2301 (4) | 0.6684 (2) | 0.1013 (16) |
| C5 | 0.5668 (3) | −0.1541 (3) | 0.66230 (17) | 0.0868 (11) |
| C6 | 0.5656 (2) | −0.0317 (3) | 0.68586 (12) | 0.0593 (8) |
| C7 | 0.4485 (2) | 0.0505 (3) | 0.68283 (11) | 0.0623 (9) |
| C8 | 0.3849 (2) | 0.0578 (3) | 0.61434 (11) | 0.0587 (8) |
| C9 | 0.2714 (2) | 0.1457 (3) | 0.61606 (10) | 0.0544 (7) |
| C10 | 0.2329 (2) | 0.2329 (2) | 0.50000 | 0.0474 (6) |
| C11 | 0.1061 (2) | 0.0716 (2) | 0.53275 (11) | 0.0508 (7) |
| C12 | 0.0438 (3) | −0.0248 (3) | 0.56674 (13) | 0.0675 (9) |
| C13 | −0.0536 (3) | −0.0863 (3) | 0.53297 (16) | 0.0813 (11) |
| H1 | 0.67910 | 0.09500 | 0.73110 | 0.1120* |
| H2 | 0.85650 | −0.02940 | 0.73770 | 0.1390* |
| H3 | 0.85380 | −0.23260 | 0.69990 | 0.1200* |
| H4 | 0.67210 | −0.31380 | 0.65320 | 0.1220* |
| H5 | 0.49430 | −0.18690 | 0.64180 | 0.1040* |
| H7A | 0.47150 | 0.13590 | 0.69670 | 0.0750* |

| | | | | |
|---|---|---|---|---|
| H7B | 0.38720 | 0.01830 | 0.71520 | 0.0750* |
| H8A | 0.44560 | 0.08840 | 0.58120 | 0.0700* |
| H8B | 0.35770 | −0.02650 | 0.60080 | 0.0700* |
| H9A | 0.21270 | 0.11680 | 0.65050 | 0.0650* |
| H9B | 0.29950 | 0.23050 | 0.62830 | 0.0650* |
| H12 | 0.06640 | −0.04730 | 0.61050 | 0.0810* |
| H13 | −0.09810 | −0.15080 | 0.55470 | 0.0980* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Se1 | 0.0586 (1) | 0.0586 (1) | 0.0515 (2) | −0.0076 (2) | 0.0010 (1) | −0.0010 (1) |
| N1 | 0.0503 (9) | 0.0574 (10) | 0.0382 (8) | 0.0010 (9) | −0.0077 (7) | 0.0101 (8) |
| C1 | 0.070 (2) | 0.097 (2) | 0.113 (2) | −0.0031 (16) | −0.0375 (17) | 0.0133 (19) |
| C2 | 0.063 (2) | 0.135 (4) | 0.151 (4) | 0.003 (2) | −0.040 (2) | 0.024 (3) |
| C3 | 0.064 (2) | 0.127 (3) | 0.108 (3) | 0.021 (2) | −0.0043 (18) | 0.044 (2) |
| C4 | 0.086 (3) | 0.088 (2) | 0.130 (3) | 0.0157 (19) | −0.001 (2) | 0.018 (2) |
| C5 | 0.0574 (16) | 0.087 (2) | 0.116 (2) | −0.0015 (16) | −0.0133 (16) | 0.005 (2) |
| C6 | 0.0501 (13) | 0.0737 (17) | 0.0540 (13) | −0.0025 (12) | −0.0056 (11) | 0.0214 (12) |
| C7 | 0.0573 (14) | 0.0798 (18) | 0.0498 (12) | 0.0021 (13) | −0.0118 (11) | 0.0089 (12) |
| C8 | 0.0570 (15) | 0.0762 (16) | 0.0429 (11) | 0.0077 (12) | −0.0055 (9) | 0.0103 (10) |
| C9 | 0.0543 (12) | 0.0730 (15) | 0.0358 (9) | 0.0014 (13) | −0.0081 (9) | 0.0081 (12) |
| C10 | 0.0517 (10) | 0.0517 (10) | 0.0389 (13) | 0.0066 (13) | −0.0040 (10) | 0.0040 (10) |
| C11 | 0.0520 (14) | 0.0536 (13) | 0.0467 (11) | 0.0019 (11) | −0.0064 (9) | 0.0096 (10) |
| C12 | 0.0673 (16) | 0.0664 (16) | 0.0689 (15) | −0.0040 (12) | −0.0058 (13) | 0.0236 (13) |
| C13 | 0.075 (2) | 0.0690 (19) | 0.100 (2) | −0.0168 (17) | −0.0071 (16) | 0.0207 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Se1—C10 | 1.828 (2) | C12—C13 | 1.384 (4) |
| N1—C9 | 1.462 (3) | C13—C13$^{i}$ | 1.394 (4) |
| N1—C10 | 1.362 (2) | C1—H1 | 0.9300 |
| N1—C11 | 1.386 (3) | C2—H2 | 0.9300 |
| C1—C2 | 1.369 (5) | C3—H3 | 0.9300 |
| C1—C6 | 1.375 (4) | C4—H4 | 0.9300 |
| C2—C3 | 1.337 (7) | C5—H5 | 0.9300 |
| C3—C4 | 1.354 (5) | C7—H7A | 0.9700 |
| C4—C5 | 1.386 (5) | C7—H7B | 0.9700 |
| C5—C6 | 1.369 (4) | C8—H8A | 0.9700 |
| C6—C7 | 1.506 (4) | C8—H8B | 0.9700 |
| C7—C8 | 1.515 (3) | C9—H9A | 0.9700 |
| C8—C9 | 1.510 (4) | C9—H9B | 0.9700 |
| C11—C12 | 1.382 (4) | C12—H12 | 0.9300 |
| C11—C11$^{i}$ | 1.396 (3) | C13—H13 | 0.9300 |
| | | | |
| C9—N1—C10 | 125.33 (18) | C2—C3—H3 | 120.00 |
| C9—N1—C11 | 124.52 (19) | C4—C3—H3 | 120.00 |
| C10—N1—C11 | 110.13 (16) | C3—C4—H4 | 120.00 |

| | | | |
|---|---|---|---|
| C2—C1—C6 | 121.6 (4) | C5—C4—H4 | 120.00 |
| C1—C2—C3 | 120.9 (3) | C4—C5—H5 | 119.00 |
| C2—C3—C4 | 119.6 (3) | C6—C5—H5 | 119.00 |
| C3—C4—C5 | 119.9 (4) | C6—C7—H7A | 108.00 |
| C4—C5—C6 | 121.3 (3) | C6—C7—H7B | 108.00 |
| C1—C6—C5 | 116.7 (3) | C8—C7—H7A | 108.00 |
| C1—C6—C7 | 121.0 (3) | C8—C7—H7B | 108.00 |
| C5—C6—C7 | 122.3 (2) | H7A—C7—H7B | 108.00 |
| C6—C7—C8 | 115.2 (2) | C7—C8—H8A | 109.00 |
| C7—C8—C9 | 111.1 (2) | C7—C8—H8B | 109.00 |
| N1—C9—C8 | 112.51 (19) | C9—C8—H8A | 109.00 |
| Se1—C10—N1 | 126.67 (11) | C9—C8—H8B | 109.00 |
| Se1—C10—N1$^{i}$ | 126.67 (11) | H8A—C8—H8B | 108.00 |
| N1—C10—N1$^{i}$ | 106.66 (17) | N1—C9—H9A | 109.00 |
| N1—C11—C12 | 132.1 (2) | N1—C9—H9B | 109.00 |
| N1—C11—C11$^{i}$ | 106.54 (18) | C8—C9—H9A | 109.00 |
| C11$^{i}$—C11—C12 | 121.4 (2) | C8—C9—H9B | 109.00 |
| C11—C12—C13 | 117.3 (2) | H9A—C9—H9B | 108.00 |
| C12—C13—C13$^{i}$ | 121.4 (3) | C11—C12—H12 | 121.00 |
| C2—C1—H1 | 119.00 | C13—C12—H12 | 121.00 |
| C6—C1—H1 | 119.00 | C12—C13—H13 | 119.00 |
| C1—C2—H2 | 120.00 | C13$^{i}$—C13—H13 | 119.00 |
| C3—C2—H2 | 120.00 | | |

| | | | |
|---|---|---|---|
| C11—N1—C10—Se1 | −179.91 (16) | C3—C4—C5—C6 | −2.0 (6) |
| C9—N1—C10—N1$^{i}$ | 178.5 (2) | C4—C5—C6—C1 | 1.3 (5) |
| C11—N1—C10—N1$^{i}$ | 0.1 (2) | C4—C5—C6—C7 | −177.0 (3) |
| C9—N1—C11—C12 | 2.2 (4) | C1—C6—C7—C8 | 130.7 (3) |
| C10—N1—C11—C12 | −179.4 (3) | C5—C6—C7—C8 | −51.1 (4) |
| C9—N1—C11—C11$^{i}$ | −178.7 (2) | C6—C7—C8—C9 | −178.1 (2) |
| C10—N1—C11—C11$^{i}$ | −0.2 (2) | C7—C8—C9—N1 | −177.9 (2) |
| C9—N1—C10—Se1 | −1.5 (3) | N1—C11—C12—C13 | 179.5 (3) |
| C10—N1—C9—C8 | −88.2 (3) | C11$^{i}$—C11—C12—C13 | 0.5 (4) |
| C11—N1—C9—C8 | 90.0 (3) | N1—C11—C11$^{i}$—N1$^{i}$ | 0.3 (2) |
| C6—C1—C2—C3 | −1.1 (6) | N1—C11—C11$^{i}$—C12$^{i}$ | 179.6 (2) |
| C2—C1—C6—C5 | 0.2 (5) | C12—C11—C11$^{i}$—N1$^{i}$ | 179.6 (2) |
| C2—C1—C6—C7 | 178.5 (3) | C12—C11—C11$^{i}$—C12$^{i}$ | −1.2 (4) |
| C1—C2—C3—C4 | 0.5 (6) | C11—C12—C13—C13$^{i}$ | 0.9 (5) |
| C2—C3—C4—C5 | 1.0 (6) | C12—C13—C13$^{i}$—C12$^{i}$ | −1.6 (5) |

Symmetry code: (i) *y*, *x*, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C9—H9*B*···Se1 | 0.97 | 2.92 | 3.310 (3) | 105 |