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9-Methyl-2,3,4,9-tetrahydro-1*H*-carbazol-1-one

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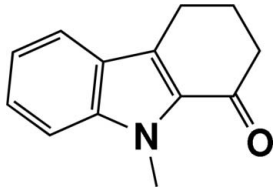
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.003 Å; R factor = 0.044; wR factor = 0.106; data-to-parameter ratio = 10.8.

The carbazole unit of the title molecule, $C_{13}H_{13}NO$, is not planar. The dihedral angle between the benzene ring and the fused pyrrole ring is 2.5 (1)°. The cyclohexene ring is in an envelope form. There is an intramolecular C—H···O hydrogen bond.

Related literature

For related literature, see: Chandrakantha *et al.* (1992); Rodriguez *et al.* (1985); Ebenezer Martin & Rajendra Prasad (2006); Balamurali & Rajendra Prasad (2001); Courseille *et al.* (1974); Govindasamy *et al.* (2003). Gunaseelan *et al.* (2007*a*,*b*) have reported crystal structures of substituted carbazole derivatives, wherein the carbazole units are not planar.



Experimental

Crystal data

$C_{13}H_{13}NO$
M_r = 199.24
Orthorhombic, $Pna2_1$
a = 7.4974 (5) Å
b = 14.9690 (11) Å
c = 8.9885 (10) Å
V = 1008.77 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 203 (2) K
0.39 × 0.37 × 0.28 mm

Data collection

Oxford Diffraction Gemini diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.798, T_{max} = 1.000
4884 measured reflections
1464 independent reflections
1056 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.106
S = 1.02
1464 reflections
136 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1	0.97	2.26	2.991 (4)	131

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2007); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WW2091).

References

Balamurali, R. & Rajendra Prasad, K. J. (2001). *Il Farmaco*, **56**, 229–232.
Chandrakantha, T. N., Puttaraja, & Nethaji, M. (1992). *Acta Cryst.* C**48**, 60–62.
Courseille, C., Busetta, B. & Hospital, M. (1974). *Acta Cryst.* B**30**, 2628–2631.
Ebenezer Martin, A. & Rajendra Prasad, K. J. (2006). *Acta Pharm.* **56**, 79–86.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Govindasamy, L., Rajakannan, V., Velmurugan, D., Mohanakrishnan, A. K. & Srinivasan, P. C. (2003). *Cryst. Res. Technol.* **38**, 182–192.
Gunaseelan, A. T., Thiruvalluvar, A., Martin, A. E. & Prasad, K. J. R. (2007*a*). *Acta Cryst.* E**63**, o2413–o2414.
Gunaseelan, A. T., Thiruvalluvar, A., Martin, A. E. & Prasad, K. J. R. (2007*b*). *Acta Cryst.* E**63**, o2729–o2730.
Oxford Diffraction (2007). *CrysAlis CCD* and *CrysAlis RED*. Versions 1.171.32. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Rodriguez, J. G., Temprano, F., Esteban-Calderon, C., Martinez-Ripoll, M. & Garcia-Blanco, S. (1985). *Tetrahedron*, **41**, 3813–3823.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.

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supplementary materials

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9-Methyl-2,3,4,9-tetrahydro-1*H*-carbazol-1-one

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Comment

Indole and its various substituted products have long been known for their interesting chemical and biological activities (Chandrakantha *et al.*, 1992). The indole ring system is present in a number of natural products, many of which are found to possess pharmacological properties like anti-microbial, anti-inflammatory and anti-implantation activities (Rodriguez *et al.*, 1985; Ebenezer Martin & Rajendra Prasad, 2006; Balamurali & Rajendra Prasad, 2001). Carbazoles formed by the fusion of indole ring with aromatic six-membered ring, are also widely used in many areas in biological sciences. The structures of these derivatives are analogous to that of ellipticine, a plant alkaloid having pronounced anti-tumour activity and are found to have DNA intercalating properties (Courseille *et al.*, 1974). Synthetic approaches to substituted carbazoles are of special interest and contemporary importance since the growing variety of carbazole alkaloids isolated show anti-microbial, anti-viral (Tubingensin A) and cytotoxic properties (Tubingensin B: a cytotoxic Carbazole alkaloid) against consumption of the sclerotia by insects (Govindasamy *et al.*, 2003). Benzo- and pyrido-annulated carbazoles are pharmacologically interesting since such compounds have potential for the development of compounds with anti-tumor activity. From the above findings it is concluded that the title compound can act as an important synthon to derive such active carbazoles.

Gunaseelan *et al.* (2007*a*,b) have reported crystal structures of substituted carbazole derivatives, wherein the carbazole units are not planar. The molecular structure of the title compound, with atomic numbering scheme, is shown in Fig. 1. The carbazole unit is not planar. The dihedral angle between the benzene ring and the fused pyrrole ring is 2.5 (1)°. The cyclohexene ring is in envelope form. There is an intramolecular C9—H9A···O1 hydrogen bond.

Experimental

The mixture of 2,3,4,9-tetrahydro-1*H*-carbazol-1-one (185 mg, 0.001 mol), methyl iodide (1 ml) and ignited potassium carbonate (276 mg, 0.002 mol) in dry acetone (20 ml) was refluxed on a steam bath for 3 h. The reaction was monitored by TLC. After completion of the reaction, the solvent was removed by distillation and the mixture was poured into crushed ice. The solid obtained was filtered, washed with water and dried. It was purified by column chromatography over silica gel (60–120 mesh) using petroleum ether/ethyl acetate (98:2) as eluant to get the pure title compound (106 mg, 54%). It was recrystallized from petroleum ether/ethylacetate (90:10).

Refinement

Owing to the absence of any anomalous scatterers in the molecule, the Friedel pairs were merged. The absolute structure in the present model have been chosen arbitrarily. H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H = 0.94–0.98 Å and U_{iso}(H) = 1.2–1.5 times U_{eq}(C). The methyl group was treated as an idealized disordered methyl group over two positions; coordinates riding with C—H = 0.97 Å and U_{iso}(H) = 1.5times U_{eq}(C9).

Figures

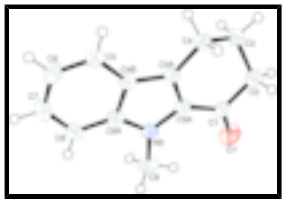

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and displacement ellipsoids drawn at the 50% probability level. Only one component of the disordered methyl group was shown.

9-Methyl-2,3,4,9-tetrahydro-*1H*-carbazol-1-one

Crystal data

$C_{13}H_{13}NO$	$D_x = 1.312$ Mg m^{-3}
$M_r = 199.24$	Melting point: 453(1) K
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: P 2c -2n	Cell parameters from 2548 reflections
$a = 7.4974$ (5) Å	$\theta = 4.7$–30.4º
$b = 14.9690$ (11) Å	$\mu = 0.08$ mm^{-1}
$c = 8.9885$ (10) Å	$T = 203$ (2) K
$V = 1008.77$ (15) Å^3	Block, light-brown
$Z = 4$	0.39 × 0.37 × 0.28 mm
$F_{000} = 424$	

Data collection

Oxford Diffraction Gemini diffractometer	1464 independent reflections
Radiation source: fine-focus sealed tube	1056 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.052$
$T = 203$(2) K	$\theta_{max} = 30.5$º
φ and ω scans	$\theta_{min} = 5.3$º
Absorption correction: multi-scan (CrysAlis CCD or RED?; Oxford Diffraction, 2007)	$h = 0\rightarrow10$
$T_{min} = 0.798$, $T_{max} = 1.000$	$k = 0\rightarrow19$
4884 measured reflections	$l = 0\rightarrow12$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.044$	$w = 1/[\sigma^2(F_o^2) + (0.0626P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.106$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.02$	$\Delta\rho_{max} = 0.21$ e Å^{-3}

1464 reflections	$\Delta\rho_{min} = -0.30$ e Å^{-3}
136 parameters	Extinction correction: none
1 restraint	Absolute structure: see Refinement section in supplementary materials
Primary atom site location: structure-invariant direct methods	Flack parameter: ?
Secondary atom site location: difference Fourier map	Rogers parameter: ?

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 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
N9	0.2382 (2)	0.25379 (10)	0.0201 (2)	0.0289 (4)	
C4B	0.2697 (2)	0.39912 (14)	−0.0453 (3)	0.0260 (5)	
C4A	0.1978 (3)	0.39569 (13)	0.1011 (3)	0.0250 (5)	
C9A	0.1816 (3)	0.30606 (12)	0.1380 (3)	0.0259 (5)	
C5	0.3245 (3)	0.46894 (13)	−0.1400 (3)	0.0308 (6)	
H5	0.3115	0.5289	−0.1109	0.037*	
C8A	0.2933 (3)	0.30931 (14)	−0.0925 (3)	0.0283 (5)	
O1	0.1064 (2)	0.19597 (10)	0.3163 (2)	0.0496 (5)	
C1	0.1188 (3)	0.27520 (13)	0.2818 (3)	0.0310 (5)	
C4	0.1455 (3)	0.46920 (13)	0.2044 (3)	0.0300 (6)	
H4A	0.0222	0.4874	0.1846	0.036*	
H4B	0.2231	0.5211	0.1888	0.036*	
C8	0.3655 (3)	0.28846 (14)	−0.2314 (3)	0.0358 (6)	
H8	0.3780	0.2288	−0.2625	0.043*	
C7	0.4178 (3)	0.35812 (15)	−0.3211 (3)	0.0389 (6)	
H7	0.4681	0.3457	−0.4147	0.047*	
C6	0.3975 (3)	0.44756 (15)	−0.2758 (3)	0.0370 (6)	
H6	0.4346	0.4937	−0.3397	0.044*	
C9	0.2415 (3)	0.15656 (12)	0.0102 (4)	0.0390 (6)	
H9A	0.1977	0.1312	0.1026	0.058*	0.50
H9B	0.3628	0.1366	−0.0070	0.058*	0.50
H9C	0.1662	0.1373	−0.0714	0.058*	0.50
H9D	0.2867	0.1388	−0.0865	0.058*	0.50
H9E	0.1216	0.1334	0.0231	0.058*	0.50
H9F	0.3183	0.1327	0.0875	0.058*	0.50
C2	0.0641 (3)	0.34836 (14)	0.3883 (3)	0.0376 (6)	
H2A	0.0856	0.3279	0.4903	0.045*	

H2B	−0.0643	0.3589	0.3777	0.045*
C3	0.1626 (3)	0.43645 (15)	0.3643 (3)	0.0384 (6)
H3A	0.1139	0.4817	0.4318	0.046*
H3B	0.2890	0.4284	0.3885	0.046*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0612 (10)	0.0345 (8)	0.0532 (13)	−0.0010 (7)	0.0077 (11)	0.0149 (8)
N9	0.0321 (8)	0.0220 (7)	0.0327 (9)	−0.0002 (7)	−0.0026 (8)	0.0005 (9)
C1	0.0236 (9)	0.0336 (11)	0.0358 (15)	−0.0005 (8)	−0.0037 (10)	0.0056 (9)
C2	0.0394 (11)	0.0390 (11)	0.0345 (14)	−0.0025 (9)	0.0046 (11)	0.0026 (10)
C3	0.0478 (12)	0.0348 (12)	0.0327 (15)	−0.0042 (10)	−0.0016 (12)	−0.0029 (10)
C4	0.0314 (10)	0.0261 (10)	0.0326 (16)	−0.0001 (7)	0.0009 (11)	−0.0024 (9)
C4A	0.0230 (9)	0.0243 (9)	0.0277 (13)	0.0002 (8)	−0.0048 (10)	0.0011 (9)
C4B	0.0223 (8)	0.0253 (10)	0.0304 (12)	0.0017 (7)	−0.0043 (10)	0.0019 (9)
C5	0.0274 (9)	0.0273 (10)	0.0377 (16)	0.0027 (8)	−0.0016 (11)	0.0077 (10)
C6	0.0334 (10)	0.0410 (11)	0.0366 (16)	0.0035 (9)	0.0007 (12)	0.0140 (11)
C7	0.0355 (12)	0.0545 (14)	0.0267 (13)	0.0091 (9)	0.0027 (11)	0.0002 (11)
C8	0.0345 (10)	0.0374 (12)	0.0355 (16)	0.0041 (9)	−0.0041 (11)	−0.0101 (11)
C8A	0.0243 (9)	0.0283 (10)	0.0321 (15)	0.0018 (8)	−0.0059 (10)	−0.0016 (9)
C9	0.0431 (11)	0.0213 (9)	0.0526 (16)	0.0018 (9)	−0.0100 (12)	−0.0033 (11)
C9A	0.0219 (9)	0.0274 (10)	0.0285 (14)	0.0003 (8)	−0.0045 (9)	0.0013 (9)

Geometric parameters (Å, °)

O1—C1	1.229 (3)	C2—H2A	0.9800
N9—C8A	1.373 (3)	C2—H2B	0.9800
N9—C9	1.458 (2)	C3—H3A	0.9800
N9—C9A	1.384 (3)	C3—H3B	0.9800
C1—C2	1.511 (3)	C4—H4A	0.9800
C1—C9A	1.451 (4)	C4—H4B	0.9800
C2—C3	1.527 (3)	C5—H5	0.9400
C3—C4	1.524 (4)	C6—H6	0.9400
C4—C4A	1.492 (3)	C7—H7	0.9400
C4A—C4B	1.423 (4)	C8—H8	0.9400
C4A—C9A	1.387 (3)	C9—H9A	0.9700
C4B—C5	1.409 (3)	C9—H9B	0.9700
C4B—C8A	1.421 (3)	C9—H9C	0.9700
C5—C6	1.376 (4)	C9—H9D	0.9700
C6—C7	1.408 (3)	C9—H9E	0.9700
C7—C8	1.375 (3)	C9—H9F	0.9700
C8—C8A	1.396 (4)		
O1···N9	2.969 (3)	H3A···H9D^{v}	2.4700
O1···C9	2.991 (4)	H3B···C7^{x}	2.9800
O1···H9A	2.2600	H3B···C9A	3.0100
O1···H9E	2.8000	H3B···H7^{x}	2.5400
O1···H9F	2.7700	H4A···H3A^{xii}	2.5300

O1···H5^{i}	2.6600	H4A···H9F^{iv}	2.5200
O1···H2B^{ii}	2.6600	H4B···C6^{xiii}	2.9000
O1···H7^{iii}	2.7000	H4B···H6^{xiii}	2.5900
N9···O1	2.969 (3)	H5···H2B^{xii}	2.5000
C8A···C9^{ii}	3.522 (3)	H5···O1^{vi}	2.6600
C9···O1	2.991 (4)	H6···H4B^{vii}	2.5900
C9···C9A^{ii}	3.538 (3)	H6···C9^{vi}	3.0800
C9···C8A^{iv}	3.522 (3)	H6···H9A^{vi}	2.3400
C9A···C9^{iv}	3.538 (3)	H6···H9E^{vi}	2.4700
C1···H9A	2.7600	H7···H3B^{viii}	2.5400
C3···H9D^{v}	3.0900	H7···O1^{xiv}	2.7000
C4···H9F^{iv}	3.0700	H8···C9	2.8700
C4A···H9B^{iv}	2.7400	H8···H9D	2.1900
C4A···H9F^{iv}	2.8800	H9A···O1	2.2600
C4B···H9E^{ii}	2.7500	H9A···C1	2.7600
C4B···H9C^{ii}	3.0300	H9A···C6^{i}	3.0400
C5···H9C^{ii}	3.0800	H9A···H6^{i}	2.3400
C5···H9E^{ii}	3.0800	H9B···C8	3.0400
C6···H9A^{vi}	3.0400	H9B···H3A^{ix}	2.3900
C6···H4B^{vii}	2.9000	H9B···C4A^{ii}	2.7400
C6···H9C^{ii}	3.0100	H9B···C9A^{ii}	2.8500
C7···H3B^{viii}	2.9800	H9C···C8	3.0700
C7···H9C^{ii}	2.9200	H9C···C4B^{iv}	3.0300
C7···H2A^{viii}	3.0500	H9C···C5^{iv}	3.0800
C8···H9C^{ii}	2.9000	H9C···C6^{iv}	3.0100
C8···H9C	3.0700	H9C···C7^{iv}	2.9200
C8···H9D	2.6600	H9C···C8^{iv}	2.9000
C8···H9B	3.0400	H9C···C8A^{iv}	2.9100
C8A···H9E^{ii}	2.8100	H9D···C8	2.6600
C8A···H9C^{ii}	2.9100	H9D···H8	2.1900
C9···H6^{i}	3.0800	H9D···C3^{ix}	3.0900
C9···H3A^{ix}	2.9200	H9D···H3A^{ix}	2.4700
C9···H8	2.8700	H9E···O1	2.8000
C9A···H3B	3.0100	H9E···H6^{i}	2.4700
C9A···H9B^{iv}	2.8500	H9E···C4B^{iv}	2.7500
C9A···H9F^{iv}	2.9100	H9E···C5^{iv}	3.0800
H2A···C7^{x}	3.0500	H9E···C8A^{iv}	2.8100
H2B···H5^{xi}	2.5000	H9F···O1	2.7700
H2B···O1^{iv}	2.6600	H9F···C4^{ii}	3.0700
H3A···H4A^{xi}	2.5300	H9F···C4A^{ii}	2.8800
H3A···C9^{v}	2.9200	H9F···C9A^{ii}	2.9100

H3A···H9B^{v}	2.3900	H9F···H4A^{ii}	2.5200
C8A—N9—C9	123.7 (2)	C3—C4—H4A	110.00
C8A—N9—C9A	108.33 (16)	C3—C4—H4B	110.00
C9—N9—C9A	128.0 (2)	C4A—C4—H4A	110.00
O1—C1—C2	121.3 (2)	C4A—C4—H4B	110.00
O1—C1—C9A	123.8 (2)	H4A—C4—H4B	108.00
C2—C1—C9A	114.93 (18)	C4B—C5—H5	121.00
C1—C2—C3	113.9 (2)	C6—C5—H5	121.00
C2—C3—C4	111.7 (2)	C5—C6—H6	119.00
C3—C4—C4A	109.12 (18)	C7—C6—H6	119.00
C4—C4A—C4B	130.42 (19)	C6—C7—H7	119.00
C4—C4A—C9A	122.8 (2)	C8—C7—H7	119.00
C4B—C4A—C9A	106.8 (2)	C7—C8—H8	121.00
C4A—C4B—C5	134.1 (2)	C8A—C8—H8	121.00
C4A—C4B—C8A	106.8 (2)	N9—C9—H9A	109.00
C5—C4B—C8A	119.0 (2)	N9—C9—H9B	109.00
C4B—C5—C6	118.7 (2)	N9—C9—H9C	109.00
C5—C6—C7	121.4 (2)	N9—C9—H9D	109.00
C6—C7—C8	121.4 (2)	N9—C9—H9E	109.00
C7—C8—C8A	117.7 (2)	N9—C9—H9F	109.00
N9—C8A—C4B	108.4 (2)	H9A—C9—H9B	109.00
N9—C8A—C8	129.8 (2)	H9A—C9—H9C	109.00
C4B—C8A—C8	121.8 (2)	H9A—C9—H9D	141.00
N9—C9A—C1	126.99 (17)	H9A—C9—H9E	56.00
N9—C9A—C4A	109.7 (2)	H9A—C9—H9F	56.00
C1—C9A—C4A	123.3 (2)	H9B—C9—H9C	109.00
C1—C2—H2A	109.00	H9B—C9—H9D	56.00
C1—C2—H2B	109.00	H9B—C9—H9E	141.00
C3—C2—H2A	109.00	H9B—C9—H9F	56.00
C3—C2—H2B	109.00	H9C—C9—H9D	56.00
H2A—C2—H2B	108.00	H9C—C9—H9E	56.00
C2—C3—H3A	109.00	H9C—C9—H9F	141.00
C2—C3—H3B	109.00	H9D—C9—H9E	109.00
C4—C3—H3A	109.00	H9D—C9—H9F	109.00
C4—C3—H3B	109.00	H9E—C9—H9F	109.00
H3A—C3—H3B	108.00		
C9—N9—C8A—C4B	179.30 (19)	C4—C4A—C4B—C8A	−179.6 (2)
C9—N9—C8A—C8	−2.2 (4)	C9A—C4A—C4B—C5	−176.2 (2)
C9A—N9—C8A—C4B	−0.4 (2)	C9A—C4A—C4B—C8A	0.5 (2)
C9A—N9—C8A—C8	178.1 (2)	C4—C4A—C9A—N9	179.3 (2)
C8A—N9—C9A—C1	−177.6 (2)	C4—C4A—C9A—C1	−2.4 (4)
C8A—N9—C9A—C4A	0.7 (3)	C4B—C4A—C9A—N9	−0.7 (3)
C9—N9—C9A—C1	2.7 (4)	C4B—C4A—C9A—C1	177.6 (2)
C9—N9—C9A—C4A	−179.0 (2)	C4A—C4B—C5—C6	176.9 (2)
O1—C1—C2—C3	152.8 (2)	C8A—C4B—C5—C6	0.6 (3)
C9A—C1—C2—C3	−28.5 (3)	C4A—C4B—C8A—N9	0.0 (2)
O1—C1—C9A—N9	−0.9 (4)	C4A—C4B—C8A—C8	−178.7 (2)
O1—C1—C9A—C4A	−178.9 (2)	C5—C4B—C8A—N9	177.21 (18)

C2—C1—C9A—N9	−179.5 (2)	C5—C4B—C8A—C8	−1.5 (3)
C2—C1—C9A—C4A	2.4 (3)	C4B—C5—C6—C7	0.1 (3)
C1—C2—C3—C4	54.6 (3)	C5—C6—C7—C8	0.0 (4)
C2—C3—C4—C4A	−51.8 (2)	C6—C7—C8—C8A	−0.8 (3)
C3—C4—C4A—C4B	−152.8 (2)	C7—C8—C8A—N9	−176.8 (2)
C3—C4—C4A—C9A	27.2 (3)	C7—C8—C8A—C4B	1.5 (3)
C4—C4A—C4B—C5	3.8 (4)		

Symmetry codes: (i) −*x*+1/2, *y*−1/2, *z*+1/2; (ii) *x*+1/2, −*y*+1/2, *z*; (iii) *x*−1/2, −*y*+1/2, *z*+1; (iv) *x*−1/2, −*y*+1/2, *z*; (v) −*x*+1/2, *y*+1/2, *z*+1/2; (vi) −*x*+1/2, *y*+1/2, *z*−1/2; (vii) −*x*+1, −*y*+1, *z*−1/2; (viii) *x*, *y*, *z*−1; (ix) −*x*+1/2, *y*−1/2, *z*−1/2; (x) *x*, *y*, *z*+1; (xi) −*x*, −*y*+1, *z*+1/2; (xii) −*x*, −*y*+1, *z*−1/2; (xiii) −*x*+1, −*y*+1, *z*+1/2; (xiv) *x*+1/2, −*y*+1/2, *z*−1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9A···O1	0.97	2.26	2.991 (4)	131

Fig. 1