IUCrData

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N-[(1a*R*,5a*R*,8*R*,9a*R*)-1,1-Dichloro-1a,5,5,7-tetramethyl-1a,2,3,4,5,5a,8,9-octahydro-1*H*-benzo[*a*]cyclopropa[*b*][7]annulen-8-yl]acetamide

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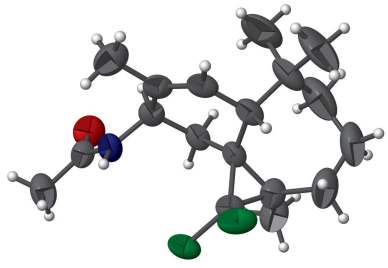
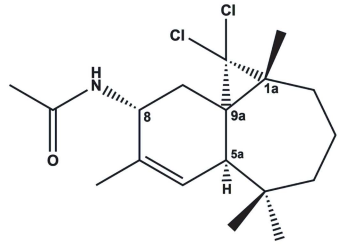
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{27}Cl_2NO$, the cyclohexene ring has an envelope conformation, with the C atom at the 9a position as the flap. The cycloheptane ring, to which it is fused, has a boat conformation. The dihedral angle between their mean planes is 60.7 (2)°. The 1,1-dichloro-cyclopropane ring is inclined to these two ring mean planes by 88.5 (3) and 28.3 (3)°, respectively. In the crystal, molecules are linked by N—H···O hydrogen bonds, forming 6_1 helices along the *c*-axis direction. The absolute configuration of the molecule in the crystal could be fully confirmed from anomalous dispersion effects [Flack parameter = 0.020 (15)].

3D view



Chemical scheme



Structure description

The bicyclic sesquiterpene β-himachalene is the main constituent of the essential oil of the Atlas cedar (*Cedrus Atlantica*) (El Haib *et al.*, 2010; Loubidi *et al.*, 2014). The reactivity of these sesquiterpenes and their derivatives has been studied extensively by our team (El Jamili *et al.*, 2002; El Haib *et al.*, 2011; Benharref *et al.*, 2015, 2016) in order to prepare new products with biological properties. Indeed, these compounds have been tested, using the food-poisoning technique, for their potential antifungal activity against the phytopathogen *Botrytis cinerea* (Daoubi *et al.*, 2004). Herein, we report on the synthesis and crystal structure of the title modified β-himachalene compound.

The structure of the title compound, Fig. 1, is built up from a cycloheptane ring (C1/C3–C8), which is fused to a cyclohexene ring (C1/C8–C12), and a cyclopropane ring (C1–

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.20	3.059 (4)	175

Symmetry code: (i) $y, -x+y, z-\frac{1}{6}$.

C3). The six-membered ring has an envelope conformation with atom C1 (position 9a) as the flap [puckering parameters are: Q_T = 0.456 (4) Å, θ = 125.3 (6)° and φ = 173.6 (7)°], whereas the seven-membered ring displays a boat conformation [puckering parameters are: Q_T = 1.1390 (53) Å, θ = 89.19 (30)°, $\varphi 2$ = 311.1 (3)°, $\varphi 3$ = 24 (2)°]. The dihedral angle between their mean planes is 60.7 (2)°. The cyclopropane ring is normal to the mean plane of the cyclohexene ring, making a dihedral angle of 88.5 (3)°.

In the crystal, molecules are linked by N—H···O hydrogen bonds, forming helices running along the *c*-axis direction (Fig. 2 and Table 1).

Synthesis and crystallization

3 g (10 mmol) of 2,2-dichloro-9,10-epoxy-3,7,7,10-tetramethyl-tricyclo[6.4.0.0^{1},^{3}]dodecane (Sbai *et al.*, 2002) was dissolved in 30 ml of CH_3CN and stirred at 273 K under argon. BF_3OEt (3% mmol) was added and the reaction mixture was stirred and monitored by TLC. After the completion of reaction, the solvent was removed and the residue obtained was chromatographed on silica, eluting with hexane–ethyl-acetate (90:10), which allowed the isolation of the title compound (yield 70%). It was recrystallized from ethyl acetate solution and yielded colourless prismatic crystals on slow evaporation of the solvent.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{27}Cl_2NO$
M_r	344.30
Crystal system, space group	Hexagonal, $P6_1$
Temperature (K)	296
a, c (Å)	10.5372 (4), 29.9710 (11)
V (Å^3)	2881.9 (2)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.34
Crystal size (mm)	0.24 × 0.2 × 0.15
Data collection	
Diffractometer	Bruker X8 *APEX* Diffractometer
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.666, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	53780, 3934, 3513
R_{int}	0.042
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.109, 1.08
No. of reflections	3934
No. of parameters	204
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.22
Absolute structure	Flack x determined using 1571 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.020 (15)

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXT2014/7* (Sheldrick, 2015*a*), *Mercury* (Macrae *et al.*, 2008), *SHELXL2014/7* (Sheldrick, 2015*b*) and *publCIF* (Westrip, 2010).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Owing to the presence of the Cl

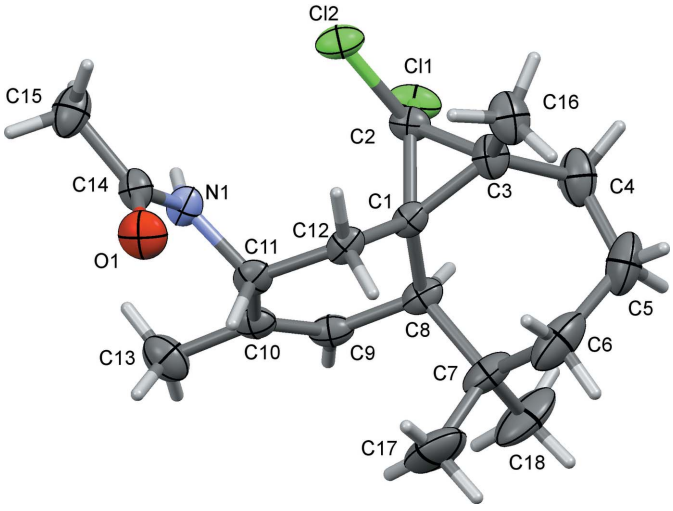


Figure 1
The molecular structure of the title compound, with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

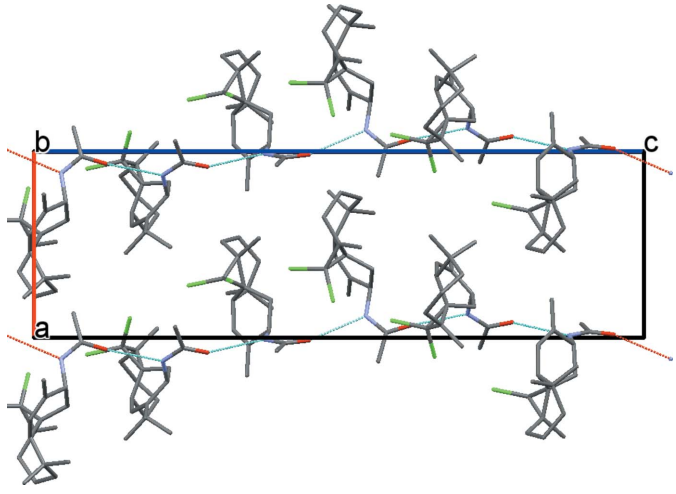


Figure 2
A view along the *a* axis of the crystal packing of the title compound, showing molecules linked by N—H···O hydrogen bonds (dashed lines; see Table 1). For clarity, C-bound H atoms have been omitted.

atoms, the absolute configuration could be fully confirmed from anomalous dispersion effects [Flack parameter = 0.020 (15)].

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170492 [https://doi.org/10.1107/S2414314617004928]

N-[(1a*R*,5a*R*,8*R*,9a*R*)-1,1-Dichloro-1a,5,5,7-tetramethyl-1a,2,3,4,5,5a,8,9-octahydro-1*H*-benzo[*a*]cyclopropa[*b*][7]annulen-8-yl]acetamide

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_N_-[(1a_R_,5a_R_,8_R_,9a_R_)-1,1-Dichloro-1a,5,5,7-tetramethyl-1a,2,3,4,5,5a,8,9-octahydro-1_H_-benzo[_a_]cyclopropa[_b_][7]annulen-8-yl]acetamide

Crystal data

$C_{18}H_{27}Cl_2NO$
M_r = 344.30
Hexagonal, $P6_1$
a = 10.5372 (4) Å
c = 29.9710 (11) Å
V = 2881.9 (2) Å^3
Z = 6
$F(000)$ = 1104
D_x = 1.190 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3934 reflections
θ = 2.3–26.4°
μ = 0.34 mm^{-1}
T = 296 K
Prismatic, colourless
0.24 × 0.2 × 0.15 mm

Data collection

Bruker X8 APEX Diffractometer
Radiation source: fine-focus sealed tube
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.666, T_{max} = 0.746
53780 measured reflections
3934 independent reflections
3513 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 26.4°, θ_{min} = 2.3°
h = −13→13
k = −13→13
l = −37→37

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
S = 1.08
3934 reflections
204 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + (0.0665P)^2 + 0.3403P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack x determined using 1571 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.020 (15)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C18	0.5450 (7)	0.7825 (6)	0.1505 (3)	0.128 (3)
H18A	0.5000	0.7884	0.1233	0.192*
H18B	0.6077	0.7429	0.1443	0.192*
H18C	0.6019	0.8787	0.1631	0.192*
C17	0.5129 (8)	0.6699 (7)	0.2229 (2)	0.123 (3)
H17A	0.5735	0.6318	0.2126	0.184*
H17B	0.4447	0.6044	0.2447	0.184*
H17C	0.5732	0.7644	0.2362	0.184*
Cl1	0.09118 (10)	0.37089 (13)	0.08694 (3)	0.0641 (3)
Cl2	−0.10316 (9)	0.19825 (11)	0.15688 (3)	0.0607 (3)
N1	0.1265 (4)	0.1158 (3)	0.21087 (9)	0.0511 (7)
H1	0.1080	0.0828	0.1840	0.061*
C2	0.0507 (4)	0.3694 (4)	0.14440 (11)	0.0469 (7)
C10	0.3586 (4)	0.3202 (4)	0.18513 (12)	0.0530 (8)
C9	0.3998 (4)	0.4388 (4)	0.16039 (12)	0.0520 (8)
H9	0.4794	0.4661	0.1415	0.062*
C1	0.1732 (4)	0.4450 (3)	0.17758 (10)	0.0430 (7)
C11	0.2348 (4)	0.2701 (4)	0.21848 (11)	0.0498 (8)
H11	0.2777	0.2748	0.2479	0.060*
O1	0.0812 (4)	0.0650 (4)	0.28373 (10)	0.0747 (9)
C12	0.1652 (4)	0.3679 (4)	0.22130 (10)	0.0466 (7)
H12A	0.0634	0.3083	0.2300	0.056*
H12B	0.2148	0.4410	0.2443	0.056*
C8	0.3304 (4)	0.5331 (4)	0.15991 (11)	0.0494 (8)
H8	0.3227	0.5542	0.1285	0.059*
C3	0.0687 (4)	0.5032 (4)	0.16756 (12)	0.0565 (9)
C14	0.0566 (4)	0.0260 (4)	0.24435 (12)	0.0510 (8)
C13	0.4342 (6)	0.2307 (7)	0.18241 (17)	0.0803 (13)
H13A	0.3695	0.1377	0.1689	0.120*
H13B	0.4596	0.2155	0.2119	0.120*
H13C	0.5214	0.2821	0.1647	0.120*
C15	−0.0558 (6)	−0.1280 (5)	0.23115 (18)	0.0775 (13)
H15A	−0.0320	−0.1959	0.2448	0.116*
H15B	−0.0558	−0.1376	0.1993	0.116*
H15C	−0.1510	−0.1487	0.2409	0.116*
C4	0.1314 (7)	0.6467 (6)	0.14176 (18)	0.0827 (15)
H4A	0.0515	0.6616	0.1325	0.099*
H4B	0.1795	0.6396	0.1151	0.099*
C16	−0.0474 (6)	0.4854 (6)	0.20148 (16)	0.0751 (12)

H16A	−0.1333	0.4713	0.1860	0.113*
H16B	−0.0095	0.5718	0.2196	0.113*
H16C	−0.0723	0.4020	0.2201	0.113*
C7	0.4279 (5)	0.6846 (5)	0.18313 (17)	0.0756 (13)
C5	0.2408 (8)	0.7790 (6)	0.1690 (2)	0.1000 (19)
H5A	0.1872	0.8152	0.1860	0.120*
H5B	0.3049	0.8560	0.1486	0.120*
C6	0.3382 (8)	0.7484 (6)	0.2021 (3)	0.113 (2)
H6A	0.4051	0.8399	0.2167	0.136*
H6B	0.2744	0.6820	0.2250	0.136*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C18	0.098 (4)	0.062 (3)	0.151 (6)	−0.014 (3)	0.053 (4)	−0.003 (4)
C17	0.117 (5)	0.088 (4)	0.106 (5)	0.008 (3)	−0.042 (4)	−0.035 (4)
Cl1	0.0514 (5)	0.1048 (8)	0.0286 (4)	0.0334 (5)	0.0005 (3)	−0.0010 (4)
Cl2	0.0445 (4)	0.0679 (6)	0.0495 (5)	0.0128 (4)	0.0036 (4)	−0.0046 (4)
N1	0.0697 (19)	0.0473 (15)	0.0320 (13)	0.0262 (14)	−0.0014 (12)	0.0003 (11)
C2	0.0447 (16)	0.061 (2)	0.0299 (15)	0.0226 (15)	0.0048 (13)	0.0045 (13)
C10	0.0502 (18)	0.062 (2)	0.0375 (16)	0.0212 (16)	−0.0087 (14)	−0.0015 (15)
C9	0.0430 (16)	0.062 (2)	0.0359 (17)	0.0150 (15)	−0.0008 (13)	−0.0028 (15)
C1	0.0501 (17)	0.0399 (15)	0.0299 (14)	0.0157 (14)	0.0044 (13)	0.0001 (12)
C11	0.062 (2)	0.0530 (18)	0.0273 (14)	0.0233 (16)	−0.0061 (13)	0.0004 (13)
O1	0.091 (2)	0.093 (2)	0.0381 (14)	0.0438 (18)	0.0096 (13)	0.0121 (13)
C12	0.059 (2)	0.0438 (16)	0.0258 (13)	0.0172 (15)	0.0029 (13)	−0.0016 (12)
C8	0.0501 (17)	0.0469 (17)	0.0328 (15)	0.0105 (14)	0.0066 (14)	0.0014 (13)
C3	0.070 (2)	0.062 (2)	0.043 (2)	0.0369 (19)	0.0142 (16)	0.0122 (16)
C14	0.062 (2)	0.055 (2)	0.0431 (19)	0.0338 (17)	0.0100 (15)	0.0097 (15)
C13	0.089 (3)	0.106 (4)	0.061 (3)	0.060 (3)	−0.001 (2)	0.012 (2)
C15	0.089 (3)	0.056 (2)	0.080 (3)	0.031 (2)	0.027 (2)	0.013 (2)
C4	0.117 (4)	0.078 (3)	0.069 (3)	0.061 (3)	0.027 (3)	0.029 (2)
C16	0.095 (3)	0.086 (3)	0.064 (3)	0.059 (3)	0.024 (2)	0.010 (2)
C7	0.068 (3)	0.047 (2)	0.072 (3)	−0.0012 (19)	0.010 (2)	−0.0086 (19)
C5	0.139 (5)	0.057 (3)	0.106 (4)	0.050 (3)	0.030 (4)	0.021 (3)
C6	0.121 (5)	0.060 (3)	0.121 (5)	0.016 (3)	0.033 (4)	−0.022 (3)

Geometric parameters (Å, º)

C18—C7	1.506 (7)	C12—H12A	0.9700
C18—H18A	0.9600	C12—H12B	0.9700
C18—H18B	0.9600	C8—C7	1.565 (5)
C18—H18C	0.9600	C8—H8	0.9800
C17—C7	1.544 (9)	C3—C4	1.524 (6)
C17—H17A	0.9600	C3—C16	1.529 (5)
C17—H17B	0.9600	C14—C15	1.506 (6)
C17—H17C	0.9600	C13—H13A	0.9600
Cl1—C2	1.772 (3)	C13—H13B	0.9600

Cl2—C2	1.760 (4)	C13—H13C	0.9600
N1—C14	1.322 (5)	C15—H15A	0.9600
N1—C11	1.464 (5)	C15—H15B	0.9600
N1—H1	0.8600	C15—H15C	0.9600
C2—C3	1.495 (5)	C4—C5	1.528 (9)
C2—C1	1.504 (5)	C4—H4A	0.9700
C10—C9	1.326 (6)	C4—H4B	0.9700
C10—C13	1.510 (7)	C16—H16A	0.9600
C10—C11	1.514 (5)	C16—H16B	0.9600
C9—C8	1.500 (6)	C16—H16C	0.9600
C9—H9	0.9300	C7—C6	1.518 (9)
C1—C12	1.522 (4)	C5—C6	1.572 (11)
C1—C8	1.532 (4)	C5—H5A	0.9700
C1—C3	1.533 (5)	C5—H5B	0.9700
C11—C12	1.537 (5)	C6—H6A	0.9700
C11—H11	0.9800	C6—H6B	0.9700
O1—C14	1.234 (5)		

C7—C18—H18A	109.5	C2—C3—C4	119.2 (3)
C7—C18—H18B	109.5	C2—C3—C16	118.5 (3)
H18A—C18—H18B	109.5	C4—C3—C16	112.4 (4)
C7—C18—H18C	109.5	C2—C3—C1	59.5 (2)
H18A—C18—H18C	109.5	C4—C3—C1	117.1 (3)
H18B—C18—H18C	109.5	C16—C3—C1	120.7 (3)
C7—C17—H17A	109.5	O1—C14—N1	122.6 (4)
C7—C17—H17B	109.5	O1—C14—C15	122.1 (4)
H17A—C17—H17B	109.5	N1—C14—C15	115.4 (4)
C7—C17—H17C	109.5	C10—C13—H13A	109.5
H17A—C17—H17C	109.5	C10—C13—H13B	109.5
H17B—C17—H17C	109.5	H13A—C13—H13B	109.5
C14—N1—C11	121.5 (3)	C10—C13—H13C	109.5
C14—N1—H1	119.2	H13A—C13—H13C	109.5
C11—N1—H1	119.2	H13B—C13—H13C	109.5
C3—C2—C1	61.5 (2)	C14—C15—H15A	109.5
C3—C2—Cl2	119.0 (2)	C14—C15—H15B	109.5
C1—C2—Cl2	120.6 (2)	H15A—C15—H15B	109.5
C3—C2—Cl1	121.7 (3)	C14—C15—H15C	109.5
C1—C2—Cl1	119.9 (2)	H15A—C15—H15C	109.5
Cl2—C2—Cl1	108.06 (19)	H15B—C15—H15C	109.5
C9—C10—C13	122.2 (4)	C3—C4—C5	112.9 (4)
C9—C10—C11	121.1 (4)	C3—C4—H4A	109.0
C13—C10—C11	116.7 (4)	C5—C4—H4A	109.0
C10—C9—C8	126.3 (3)	C3—C4—H4B	109.0
C10—C9—H9	116.9	C5—C4—H4B	109.0
C8—C9—H9	116.9	H4A—C4—H4B	107.8
C2—C1—C12	118.9 (3)	C3—C16—H16A	109.5
C2—C1—C8	118.3 (3)	C3—C16—H16B	109.5
C12—C1—C8	112.0 (3)	H16A—C16—H16B	109.5

C2—C1—C3	59.0 (2)	C3—C16—H16C	109.5
C12—C1—C3	121.5 (3)	H16A—C16—H16C	109.5
C8—C1—C3	117.7 (3)	H16B—C16—H16C	109.5
N1—C11—C10	110.0 (3)	C18—C7—C6	114.7 (5)
N1—C11—C12	112.7 (3)	C18—C7—C17	104.6 (6)
C10—C11—C12	114.8 (3)	C6—C7—C17	106.0 (5)
N1—C11—H11	106.2	C18—C7—C8	107.8 (4)
C10—C11—H11	106.2	C6—C7—C8	112.4 (4)
C12—C11—H11	106.2	C17—C7—C8	111.1 (4)
C1—C12—C11	113.2 (3)	C4—C5—C6	115.0 (4)
C1—C12—H12A	108.9	C4—C5—H5A	108.5
C11—C12—H12A	108.9	C6—C5—H5A	108.5
C1—C12—H12B	108.9	C4—C5—H5B	108.5
C11—C12—H12B	108.9	C6—C5—H5B	108.5
H12A—C12—H12B	107.8	H5A—C5—H5B	107.5
C9—C8—C1	109.5 (3)	C7—C6—C5	118.0 (5)
C9—C8—C7	112.5 (3)	C7—C6—H6A	107.8
C1—C8—C7	115.1 (3)	C5—C6—H6A	107.8
C9—C8—H8	106.4	C7—C6—H6B	107.8
C1—C8—H8	106.4	C5—C6—H6B	107.8
C7—C8—H8	106.4	H6A—C6—H6B	107.1

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.86	2.20	3.059 (4)	175

Symmetry code: (i) $y, -x+y, z-1/6$.