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2,2,4-Trimethyl-7-nitro-2,3-dihydro-1*H*-1,5-benzodiazepin-5-ium perchlorateSayed Hasan Mehdi,^a Othman Sulaiman,^a Raza Murad Ghalib,^a Chin Sing Yeap^{b‡} and Hoong-Kun Fun^{b*§}^aSchool of Industrial Technology, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and ^bX-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: hkfun@usm.my

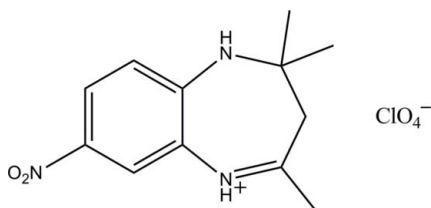
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Key indicators: single-crystal X-ray study; *T* = 100 K; mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$; *R* factor = 0.046; *wR* factor = 0.138; data-to-parameter ratio = 15.8.

In the title molecular salt, $\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_2^+\cdot\text{ClO}_4^-$, the nitro group is close to being coplanar with the benzene ring [dihedral angle = $8.1(3)^\circ$]. The seven-membered ring has a maximum deviation of $0.502(3) \text{ \AA}$ at the C atom between the dimethyl- and methyl-substituted C atoms. In the crystal, the components are linked into infinite sheets lying parallel to the *bc* plane by $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds. A short $\text{O}\cdots\text{N}$ contact of $2.896(4) \text{ \AA}$ occurs within the sheets and a short $\text{O}\cdots\text{O}$ contact of $2.608(4) \text{ \AA}$ occurs between the sheets.

Related literature

For general background and applications of benzimidazole derivatives, see: Landquist (1984); Insuasty *et al.* (2010); Balakrishna & Kaboudin (2001); Ballo *et al.* (2010). For the preparation of the title compound, see: Grech *et al.* (1994). For ring conformations, see Cremer & Pople (1975). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

 $\text{C}_{12}\text{H}_{16}\text{N}_3\text{O}_2^+\cdot\text{ClO}_4^-$ $M_r = 333.73$

Monoclinic, $C2/c$
 $a = 21.046(7) \text{ \AA}$
 $b = 11.818(3) \text{ \AA}$
 $c = 15.636(6) \text{ \AA}$
 $\beta = 132.176(9)^\circ$
 $V = 2882.0(16) \text{ \AA}^3$

$Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 0.30 \text{ mm}^{-1}$
 $T = 100 \text{ K}$
 $0.30 \times 0.17 \times 0.08 \text{ mm}$

Data collection

Bruker APEXII DUO CCD diffractometer
 Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
 $T_{\min} = 0.915$, $T_{\max} = 0.976$

24582 measured reflections
 3323 independent reflections
 2816 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.066$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.138$
 $S = 1.05$
 3323 reflections
 210 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 0.69 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.69 \text{ e \AA}^{-3}$

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

<i>D</i> — <i>H</i> ··· <i>A</i>	<i>D</i> — <i>H</i>	<i>H</i> ··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> — <i>H</i> ··· <i>A</i>
$\text{N1—H1N1}\cdots\text{O6}^i$	0.80 (3)	2.15 (3)	2.941 (3)	173 (3)
$\text{N2—H1N2}\cdots\text{O4}$	0.82 (5)	2.09 (4)	2.864 (4)	156 (4)
$\text{N2—H1N2}\cdots\text{O4}^{ii}$	0.82 (5)	2.46 (5)	3.000 (4)	124 (3)
$\text{C3—H3A}\cdots\text{O1}^i$	0.93	2.51	3.373 (3)	155
$\text{C11—H11A}\cdots\text{O5}^i$	0.96	2.58	3.524 (3)	169
$\text{C11—H11B}\cdots\text{O3}^{iii}$	0.96	2.45	3.396 (3)	168

Symmetry codes: (i) $x, -y + 2, z - \frac{1}{2}$; (ii) $-x, y, -z + \frac{1}{2}$; (iii) $x, -y + 1, z - \frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *S SAINT* (Bruker, 2009); data reduction: *S SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5507).

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supplementary materials

Acta Cryst. (2010). E66, o1845 [doi:10.1107/S1600536810024475]

2,2,4-Trimethyl-7-nitro-2,3-dihydro-1*H*-1,5-benzodiazepin-5-ium perchlorate

S. H. Mehdi, O. Sulaiman, R. M. Ghalib, C. S. Yeap and H.-K. Fun

Comment

Benzodiazepines are interesting compounds due to their wide range of biological activities (Landquist, 1984). Recently many methods have been employed for the synthesis of benzodiazepines derivatives (Insuasty *et al.*, 2010; Balakrishna & Kaboudin, 2001; Ballo *et al.*, 2010). Here we report the synthesis and the crystal structure of title compound.

The asymmetric unit of title compound (Fig. 1) consists of one the benzodiazepinium cation and one perchlorate anion. The nitro group is coplanar with the benzene ring with the dihedral angle of 8.1 (3)°. The seven-membered ring (N1/C1/C6/N2/C7–C9) have a maximum deviation of 0.502 (3) Å at atom C8. In the crystal structure, the molecules are linked into infinite two-dimensional planes parallel to *bc* plane by the intermolecular N—H···O, C—H···O hydrogen bonds (Table 1) and short O6···N3 interaction of 2.896 (4) Å. Short O2···O3 interaction of 2.608 (4) Å linked these planes into a three-dimensional framework (Fig. 2).

Experimental

A mixture of 4-nitro *o*-phenylenediamine (0.153 g m) and 4-hydroxy coumarin (0.162 g m) in molar ratio 1:1 was refluxed in a mixture of acetic acid-ethanol (1:1 *v/v*) for 3 h (Grech *et al.*, 1994). The solid settled in the reaction mixture was filtered and crystallized from ethanol to furnish brownish plates of the unexpected title compound, (I) (55%, m.p. 458 K).

Refinement

The N-bound hydrogen atoms were located from the difference Fourier map and were refined freely. The rest of hydrogen atoms were positioned geometrically [C—H = 0.93–0.97 Å] and refined using a riding model, with $U_{\text{iso}}(\text{H}) = 1.2$ or $1.5U_{\text{eq}}(\text{C})$. Rotating-group model was applied for methyl groups.

Figures

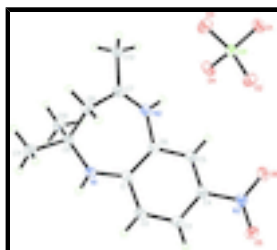


Fig. 1. The molecular structure of (I) with 50% probability ellipsoids for non-H atoms.

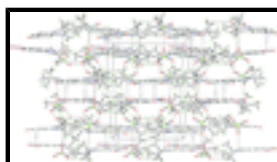


Fig. 2. The crystal packing of (I), viewed down the *c* axis, showing the components linked into a 3-D network. Intermolecular hydrogen bonds are shown as dashed lines.

2,2,4-Trimethyl-7-nitro-2,3-dihydro-1H-1,5-benzodiazepin-5-ium perchlorate

Crystal data

$C_{12}H_{16}N_3O_2^+ \cdot ClO_4^-$	$F(000) = 1392$
$M_r = 333.73$	$D_x = 1.538 \text{ Mg m}^{-3}$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: $-C 2yc$	Cell parameters from 7331 reflections
$a = 21.046 (7) \text{ \AA}$	$\theta = 2.2\text{--}29.8^\circ$
$b = 11.818 (3) \text{ \AA}$	$\mu = 0.30 \text{ mm}^{-1}$
$c = 15.636 (6) \text{ \AA}$	$T = 100 \text{ K}$
$\beta = 132.176 (9)^\circ$	Plate, brown
$V = 2882.0 (16) \text{ \AA}^3$	$0.30 \times 0.17 \times 0.08 \text{ mm}$
$Z = 8$	

Data collection

Bruker APEXII DUO CCD diffractometer	3323 independent reflections
Radiation source: fine-focus sealed tube graphite	2816 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{\text{int}} = 0.066$
Absorption correction: multi-scan (SADABS; Bruker, 2009)	$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 2.2^\circ$
$T_{\text{min}} = 0.915$, $T_{\text{max}} = 0.976$	$h = -27 \rightarrow 27$
24582 measured reflections	$k = -15 \rightarrow 15$
	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.138$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0714P)^2 + 7.0069P]$
3323 reflections	where $P = (F_o^2 + 2F_c^2)/3$
210 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.69 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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>	$U_{\text{iso}}^*/U_{\text{eq}}$
C11	0.15021 (3)	0.71202 (4)	0.49658 (4)	0.01923 (16)
O1	0.13150 (11)	0.68718 (14)	0.56727 (14)	0.0259 (4)
O2	0.19403 (11)	0.82394 (13)	0.52807 (14)	0.0245 (4)
O3	0.21587 (10)	0.62367 (14)	0.52533 (14)	0.0256 (4)
O4	0.07604 (10)	0.70691 (14)	0.37336 (13)	0.0234 (4)
O5	0.08273 (11)	1.21240 (13)	0.25797 (14)	0.0249 (4)
O6	0.09384 (11)	1.07773 (14)	0.36195 (13)	0.0246 (4)
N1	0.11724 (12)	0.79665 (15)	0.04379 (16)	0.0183 (4)
N2	0.10204 (12)	0.72103 (15)	0.21588 (15)	0.0176 (4)
N3	0.08881 (11)	1.11171 (16)	0.28211 (15)	0.0194 (4)
C1	0.10956 (12)	0.86625 (17)	0.10449 (16)	0.0152 (4)
C2	0.10763 (13)	0.98440 (18)	0.08478 (17)	0.0166 (4)
H2A	0.1127	1.0079	0.0328	0.020*
C3	0.09866 (12)	1.06450 (17)	0.13882 (17)	0.0166 (4)
H3A	0.0967	1.1410	0.1232	0.020*
C4	0.09241 (12)	1.02892 (18)	0.21822 (17)	0.0172 (4)
C5	0.09300 (13)	0.91616 (18)	0.24014 (17)	0.0172 (4)
H5A	0.0872	0.8945	0.2918	0.021*
C6	0.10220 (12)	0.83451 (17)	0.18541 (17)	0.0155 (4)
C7	0.14051 (13)	0.63366 (18)	0.21973 (17)	0.0180 (4)
C8	0.19130 (13)	0.64237 (19)	0.18564 (18)	0.0191 (4)
H8A	0.2184	0.5700	0.1991	0.023*
H8B	0.2364	0.6978	0.2347	0.023*
C9	0.13798 (13)	0.67632 (17)	0.05830 (17)	0.0165 (4)
C10	0.05645 (14)	0.60604 (19)	-0.02308 (18)	0.0216 (4)
H10A	0.0269	0.6260	-0.1015	0.032*
H10B	0.0200	0.6207	-0.0077	0.032*
H10C	0.0710	0.5271	-0.0113	0.032*
C11	0.19389 (15)	0.6604 (2)	0.0295 (2)	0.0234 (5)
H11A	0.1627	0.6841	-0.0485	0.035*
H11B	0.2091	0.5821	0.0377	0.035*
H11C	0.2450	0.7051	0.0813	0.035*
C12	0.13540 (15)	0.52362 (18)	0.26078 (19)	0.0222 (4)
H12A	0.0970	0.5305	0.2738	0.033*
H12B	0.1914	0.5028	0.3315	0.033*

supplementary materials

H12C	0.1145	0.4665	0.2035	0.033*
H1N1	0.1130 (16)	0.826 (2)	-0.006 (2)	0.016 (6)*
H1N2	0.0798 (19)	0.715 (2)	0.243 (3)	0.030 (8)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0193 (3)	0.0214 (3)	0.0170 (3)	-0.00116 (18)	0.0122 (2)	-0.00003 (18)
O1	0.0328 (9)	0.0283 (9)	0.0249 (8)	-0.0029 (7)	0.0228 (8)	0.0002 (7)
O2	0.0298 (8)	0.0167 (8)	0.0277 (8)	-0.0057 (6)	0.0195 (7)	-0.0039 (6)
O3	0.0230 (8)	0.0219 (8)	0.0289 (9)	0.0046 (6)	0.0162 (7)	0.0013 (7)
O4	0.0169 (7)	0.0350 (9)	0.0147 (8)	-0.0018 (6)	0.0091 (7)	-0.0003 (6)
O5	0.0305 (9)	0.0176 (8)	0.0253 (8)	0.0029 (6)	0.0183 (7)	0.0006 (6)
O6	0.0319 (9)	0.0267 (8)	0.0192 (8)	0.0026 (7)	0.0188 (7)	0.0002 (6)
N1	0.0239 (9)	0.0180 (9)	0.0167 (9)	0.0012 (7)	0.0152 (8)	0.0019 (7)
N2	0.0186 (8)	0.0192 (9)	0.0156 (8)	-0.0018 (7)	0.0118 (7)	0.0008 (7)
N3	0.0185 (8)	0.0213 (9)	0.0169 (8)	0.0015 (7)	0.0113 (7)	-0.0003 (7)
C1	0.0108 (8)	0.0192 (10)	0.0122 (9)	-0.0005 (7)	0.0064 (7)	-0.0002 (7)
C2	0.0147 (9)	0.0202 (10)	0.0134 (9)	-0.0019 (8)	0.0088 (8)	0.0006 (7)
C3	0.0132 (9)	0.0174 (10)	0.0136 (9)	-0.0013 (7)	0.0067 (8)	0.0001 (7)
C4	0.0146 (9)	0.0204 (10)	0.0141 (9)	0.0014 (8)	0.0087 (8)	-0.0008 (8)
C5	0.0144 (9)	0.0234 (10)	0.0127 (9)	0.0004 (8)	0.0086 (8)	0.0012 (8)
C6	0.0128 (9)	0.0179 (10)	0.0138 (9)	-0.0011 (7)	0.0082 (8)	0.0003 (7)
C7	0.0164 (9)	0.0205 (10)	0.0113 (9)	-0.0025 (8)	0.0069 (8)	0.0003 (7)
C8	0.0159 (9)	0.0220 (10)	0.0172 (10)	0.0016 (8)	0.0102 (8)	0.0027 (8)
C9	0.0162 (9)	0.0164 (9)	0.0174 (10)	0.0013 (8)	0.0115 (8)	0.0018 (8)
C10	0.0209 (10)	0.0231 (11)	0.0182 (10)	-0.0032 (8)	0.0121 (9)	-0.0019 (8)
C11	0.0254 (11)	0.0241 (11)	0.0289 (12)	0.0026 (9)	0.0215 (10)	0.0029 (9)
C12	0.0278 (11)	0.0181 (10)	0.0207 (10)	-0.0013 (9)	0.0163 (9)	0.0017 (8)

Geometric parameters (\AA , $^\circ$)

Cl1—O1	1.4310 (16)	C4—C5	1.374 (3)
Cl1—O4	1.4538 (16)	C5—C6	1.387 (3)
Cl1—O2	1.4941 (16)	C5—H5A	0.9300
Cl1—O3	1.5388 (17)	C7—C8	1.484 (3)
O5—N3	1.229 (2)	C7—C12	1.486 (3)
O6—N3	1.246 (2)	C8—C9	1.544 (3)
N1—C1	1.345 (3)	C8—H8A	0.9700
N1—C9	1.460 (3)	C8—H8B	0.9700
N1—H1N1	0.79 (3)	C9—C10	1.524 (3)
N2—C7	1.288 (3)	C9—C11	1.528 (3)
N2—C6	1.424 (3)	C10—H10A	0.9600
N2—H1N2	0.81 (3)	C10—H10B	0.9600
N3—C4	1.436 (3)	C10—H10C	0.9600
C1—C6	1.425 (3)	C11—H11A	0.9600
C1—C2	1.425 (3)	C11—H11B	0.9600
C2—C3	1.364 (3)	C11—H11C	0.9600
C2—H2A	0.9300	C12—H12A	0.9600

C3—C4	1.398 (3)	C12—H12B	0.9600
C3—H3A	0.9300	C12—H12C	0.9600
O1—C11—O4	114.06 (10)	N2—C7—C8	120.61 (19)
O1—C11—O2	110.86 (10)	N2—C7—C12	119.75 (19)
O4—C11—O2	110.46 (10)	C8—C7—C12	119.63 (19)
O1—C11—O3	107.10 (10)	C7—C8—C9	113.96 (17)
O4—C11—O3	108.27 (10)	C7—C8—H8A	108.8
O2—C11—O3	105.65 (10)	C9—C8—H8A	108.8
C1—N1—C9	130.62 (18)	C7—C8—H8B	108.8
C1—N1—H1N1	115.8 (19)	C9—C8—H8B	108.8
C9—N1—H1N1	113.4 (19)	H8A—C8—H8B	107.7
C7—N2—C6	128.90 (19)	N1—C9—C10	110.47 (17)
C7—N2—H1N2	118 (2)	N1—C9—C11	106.44 (17)
C6—N2—H1N2	113 (2)	C10—C9—C11	110.21 (18)
O5—N3—O6	122.75 (18)	N1—C9—C8	109.64 (17)
O5—N3—C4	119.30 (18)	C10—C9—C8	111.79 (17)
O6—N3—C4	117.94 (18)	C11—C9—C8	108.13 (17)
N1—C1—C6	127.01 (19)	C9—C10—H10A	109.5
N1—C1—C2	116.50 (18)	C9—C10—H10B	109.5
C6—C1—C2	116.48 (18)	H10A—C10—H10B	109.5
C3—C2—C1	122.82 (19)	C9—C10—H10C	109.5
C3—C2—H2A	118.6	H10A—C10—H10C	109.5
C1—C2—H2A	118.6	H10B—C10—H10C	109.5
C2—C3—C4	118.43 (19)	C9—C11—H11A	109.5
C2—C3—H3A	120.8	C9—C11—H11B	109.5
C4—C3—H3A	120.8	H11A—C11—H11B	109.5
C5—C4—C3	121.52 (19)	C9—C11—H11C	109.5
C5—C4—N3	118.88 (18)	H11A—C11—H11C	109.5
C3—C4—N3	119.55 (19)	H11B—C11—H11C	109.5
C4—C5—C6	120.17 (19)	C7—C12—H12A	109.5
C4—C5—H5A	119.9	C7—C12—H12B	109.5
C6—C5—H5A	119.9	H12A—C12—H12B	109.5
C5—C6—N2	114.60 (18)	C7—C12—H12C	109.5
C5—C6—C1	120.55 (19)	H12A—C12—H12C	109.5
N2—C6—C1	124.83 (18)	H12B—C12—H12C	109.5
C9—N1—C1—C6	-14.5 (3)	C7—N2—C6—C1	31.3 (3)
C9—N1—C1—C2	166.30 (19)	N1—C1—C6—C5	-178.74 (19)
N1—C1—C2—C3	178.87 (18)	C2—C1—C6—C5	0.5 (3)
C6—C1—C2—C3	-0.5 (3)	N1—C1—C6—N2	0.2 (3)
C1—C2—C3—C4	1.0 (3)	C2—C1—C6—N2	179.44 (18)
C2—C3—C4—C5	-1.6 (3)	C6—N2—C7—C8	-2.4 (3)
C2—C3—C4—N3	175.77 (18)	C6—N2—C7—C12	176.47 (19)
O5—N3—C4—C5	-175.37 (19)	N2—C7—C8—C9	-62.3 (3)
O6—N3—C4—C5	6.1 (3)	C12—C7—C8—C9	118.8 (2)
O5—N3—C4—C3	7.1 (3)	C1—N1—C9—C10	97.6 (2)
O6—N3—C4—C3	-171.40 (18)	C1—N1—C9—C11	-142.8 (2)
C3—C4—C5—C6	1.7 (3)	C1—N1—C9—C8	-26.1 (3)
N3—C4—C5—C6	-175.70 (18)	C7—C8—C9—N1	74.8 (2)

supplementary materials

C4—C5—C6—N2	179.81 (18)	C7—C8—C9—C10	-48.0 (2)
C4—C5—C6—C1	-1.2 (3)	C7—C8—C9—C11	-169.51 (18)
C7—N2—C6—C5	-149.7 (2)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H \cdots <i>A</i>	<i>D</i> —H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> —H \cdots <i>A</i>
N1—H1N1 \cdots O6 ⁱ	0.80 (3)	2.15 (3)	2.941 (3)	173 (3)
N2—H1N2 \cdots O4	0.82 (5)	2.09 (4)	2.864 (4)	156 (4)
N2—H1N2 \cdots O4 ⁱⁱ	0.82 (5)	2.46 (5)	3.000 (4)	124 (3)
C3—H3A \cdots O1 ⁱ	0.93	2.51	3.373 (3)	155
C11—H11A \cdots O5 ⁱ	0.96	2.58	3.524 (3)	169
C11—H11B \cdots O3 ⁱⁱⁱ	0.96	2.45	3.396 (3)	168

Symmetry codes: (i) $x, -y+2, z-1/2$; (ii) $-x, y, -z+1/2$; (iii) $x, -y+1, z-1/2$.

Fig. 1

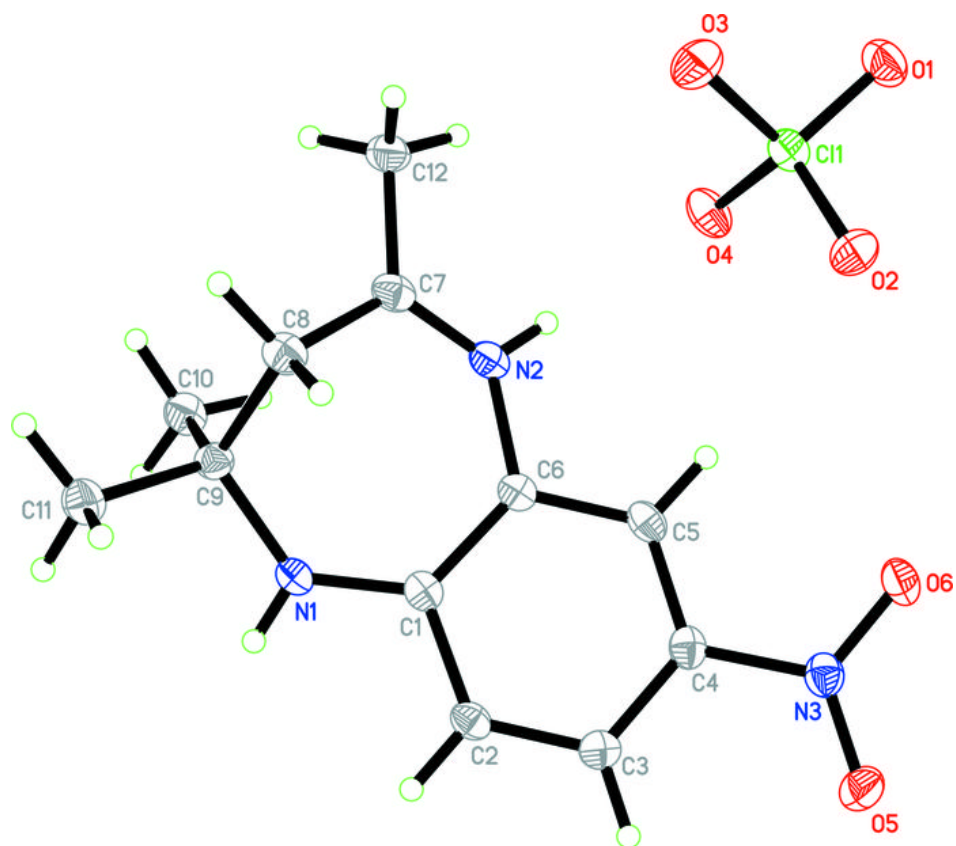


Fig. 2

