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1-Methoxy-3-*o*-tolylbicyclo[2.2.2]oct-5-ene-2,2-dicarbonitrile

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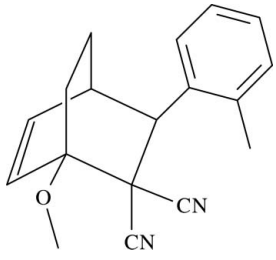
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.041; wR factor = 0.108; data-to-parameter ratio = 15.9.

In the title compound, $C_{18}H_{18}N_2O$, the cyclohexene and cyclohexane rings of the bicyclo[2.2.2]oct-5-ene unit adopt distorted boat conformations. In the crystal, molecules exist as C—H···N hydrogen-bonded centrosymmetric $R_2^2(14)$ dimers, which are further linked by C—H···π interactions.

Related literature

For general background, see: Çete *et al.* (2007); Corey (2002); Kurt & Anker (1998); Mamedov *et al.* (2007); Özkan *et al.*, (2007); Potapov (1988). For the synthesis, see: Zhang *et al.* (2006). For graph-set notation, see: Bernstein *et al.* (1995); Etter (1990). For ring conformations, see: Cremer & Pople (1975).



Experimental

Crystal data

$C_{18}H_{18}N_2O$
M_r = 278.34
Triclinic, $P\overline{1}$
a = 7.5922 (6) Å
b = 9.5026 (8) Å
c = 11.5584 (9) Å
α = 91.201 (7)°
β = 107.206 (6)°
γ = 110.856 (6)°
V = 736.89 (10) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 K
0.48 × 0.42 × 0.17 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.956, T_{max} = 0.989
8047 measured reflections
3057 independent reflections
2532 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.108
S = 1.05
3057 reflections
192 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···N1^{i}	0.93	2.70	3.509 (3)	146
C7—H7*C*···*Cg*1^{ii}	0.96	2.84	3.688 (2)	146

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y+1, -z+1$. *Cg*1 is the centroid of the C1–C6 ring.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); 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, 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: CI2877).

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supplementary materials

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1-Methoxy-3-*o*-tolylbicyclo[2.2.2]oct-5-ene-2,2-dicarbonitrile

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Comment

The Diels-Alder reactions are among the most useful of all synthetic processes for the construction of complex molecules and, for this reason, they have been studied extensively (Kurt & Anker, 1998). The reaction is easy, rapid and is a key reaction in fundamental organic synthesis. Cycloadducts of asymmetric Diels-Alder reactions have attracted attention owing to their utility in the synthesis of natural compounds (Corey, 2002).

In the conventional Diels-Alder reaction a double bond adds 1,4 to a conjugated diene. The title compound, (I), was prepared by a cycloaddiction reaction from 2-(2-methylbenzylidene) malononitrile and 1-methoxycyclohexa-1,3-diene. Bicyclo[2.2.2]octane and bicycle[2.2.2]octane moieties are essential fragment of many important natural and synthetic biologically active compounds (Potapov, 1988). Both this type bicyclo compounds and many cyano group containing compounds show biological activity (Özkan *et al.* 2007; Çete *et al.* 2007). Therefore, synthesis of these compounds in the practically active form is of practical interest (Mamedov *et al.* 2007).

The overall view and atom-labeling of the molecule of (I) are displayed in Fig. 1. The hydrogen-bonding parameters are given in Table 1 and the packing arrangement of the molecules is illustrated in Fig. 2. In the molecule, cyclohexene rings A(C8/C9/C10/C11/C12/C13) and B(C10/C11/C12/C13/C17/C16), and the cyclohexane ring C(C8/C9/C10/C16/C17/C13) of the bicyclo[2.2.2]oct-5-ene unit all adopt distorted boat conformations. The Cremer and Pople (1975) puckering parameters Q, θ and φ are 0.810 (2) Å, 84.8 (1)° and 111.8 (1)°, respectively for ring A, 0.788 (2) Å, 86.7 (1)° and 186.3 (1)°, respectively for ring B, and 0.906 (2) Å, 88.4 (1)° and 310.3 (1)°, respectively for ring C.

The crystal structure is stabilized by intermolecular C—H···N hydrogen bonds and C—H···π interactions (Table 1). As shown in Fig. 2, the molecules exist as C12—H12···N1 hydrogen-bonded centrosymmetric $R_2^2(14)$ dimers (Bernstein *et al.*, 1995; Etter, 1990). The dimers are linked through C7—H7C···π interactions.

Experimental

2-(2-Methylbenzylidene)malononitrile was prepared from 2-methyl benzaldehyde, malononitrile and potassium carbonate according to the literature method (Zhang *et al.* 2006). For the preparation of the title compound, 1-methoxycyclohexa-1,3-diene (330 mg, 3 mmol) and 2-(2-methylbenzylidene) malononitrile (459 mg, 3 mmol) were dissolved in benzene (20 ml). The reaction mixture was refluxed for 4 h, and monitored by TLC. After evaporation of the solvent, the reaction mixture was separated by column chromatography, using the mixture of hexane-ethyl acetate (1:2) as the eluant. The title compound was recrystallized from methanol in 3 d (m.p. 431–432 K).

Refinement

H atoms were positioned geometrically (C-H = 0.93–0.98 Å) and refined using a riding model with U_{iso}(H) = 1.2U_{eq}(C) and 1.5U_{eq}(methyl C). A rotating–group model was used for the methyl groups.

Figures

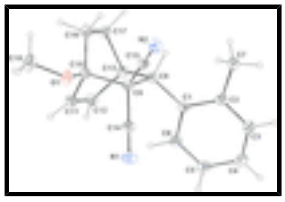


Fig. 1. The molecular structure of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 15% probability level.

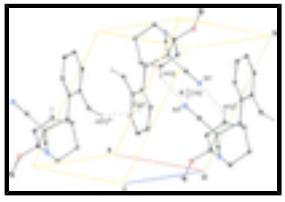


Fig. 2. Part of the crystal structure of (I), showing the formation of $R_2^2(14)$ dimers and a C—H···π interaction. H atoms not involved in the interactions have been omitted for clarity. The dashed lines indicate hydrogen bonds. [Symmetry code: (i) 1 - *x*, 1 - *y*, -*z*; (ii) 2- *x*, 1 - *y*, 1 - *z*]. Cg1 is the centroid of the C1-C6 ring.

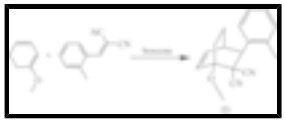


Fig. 3. Preparation of the title compound.

1-Methoxy-3-*o*-tolylbicyclo[2.2.2]oct-5-ene-2,2-dicarbonitrile

Crystal data

$C_{18}H_{18}N_2O$	$Z = 2$
$M_r = 278.34$	$F_{000} = 296$
Triclinic, $P\overline{1}$	$D_x = 1.254$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 7.5922$ (6) Å	Cell parameters from 8047 reflections
$b = 9.5026$ (8) Å	$\theta = 1.9$–28.1º
$c = 11.5584$ (9) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 91.201$ (7)º	$T = 296$ K
$\beta = 107.206$ (6)º	Prism, colourless
$\gamma = 110.856$ (6)º	0.48 × 0.42 × 0.17 mm
$V = 736.89$ (10) Å^3	

Data collection

Stoe IPDS II diffractometer	3057 independent reflections
Monochromator: plane graphite	2532 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	$R_{int} = 0.034$
$T = 296$ K	$\theta_{max} = 26.5$º
ω–scan rotation method	$\theta_{min} = 1.9$º
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$h = -9 \rightarrow 9$
$T_{min} = 0.956$, $T_{max} = 0.989$	$k = -11 \rightarrow 11$
8047 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.108$	$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.127P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} = 0.001$
3057 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
192 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.76186 (18)	0.53676 (14)	0.34535 (12)	0.0411 (3)
C2	0.75171 (19)	0.51461 (15)	0.46312 (12)	0.0434 (3)
C3	0.6500 (2)	0.36832 (17)	0.48325 (14)	0.0522 (4)
H3	0.6401	0.3530	0.5607	0.063*
C4	0.5636 (2)	0.24556 (17)	0.39194 (16)	0.0584 (4)
H4	0.4979	0.1488	0.4081	0.070*
C5	0.5753 (2)	0.26716 (17)	0.27703 (16)	0.0594 (4)
H5	0.5185	0.1848	0.2151	0.071*
C6	0.6717 (2)	0.41157 (16)	0.25353 (14)	0.0526 (4)
H6	0.6766	0.4256	0.1750	0.063*
C7	0.8491 (2)	0.64107 (17)	0.56952 (13)	0.0522 (3)
H7A	0.8152	0.6031	0.6396	0.078*
H7B	0.8031	0.7220	0.5486	0.078*
H7C	0.9911	0.6787	0.5882	0.078*
C8	0.87437 (18)	0.69280 (14)	0.31871 (11)	0.0390 (3)
H8	0.9680	0.7512	0.3977	0.047*
C9	0.74043 (18)	0.78601 (14)	0.26415 (11)	0.0398 (3)
C10	0.8251 (2)	0.88159 (16)	0.16893 (12)	0.0454 (3)

C11	0.7944 (2)	0.76528 (19)	0.06747 (13)	0.0543 (4)
H11	0.7201	0.7619	−0.0133	0.065*
C12	0.8816 (2)	0.66815 (18)	0.10214 (13)	0.0528 (4)
H12	0.8691	0.5884	0.0483	0.063*
C13	1.00195 (19)	0.69628 (15)	0.23466 (12)	0.0440 (3)
H13	1.0670	0.6232	0.2537	0.053*
C14	0.5290 (2)	0.68754 (16)	0.20146 (13)	0.0473 (3)
C15	0.7433 (2)	0.88992 (15)	0.36219 (12)	0.0438 (3)
C16	1.0492 (2)	0.97044 (16)	0.23344 (14)	0.0487 (3)
H16A	1.1033	1.0413	0.1820	0.058*
H16B	1.0693	1.0283	0.3096	0.058*
C17	1.1581 (2)	0.86011 (16)	0.25968 (13)	0.0475 (3)
H17A	1.2439	0.8831	0.3443	0.057*
H17B	1.2402	0.8707	0.2076	0.057*
C18	0.7764 (3)	1.0878 (2)	0.0652 (2)	0.0806 (6)
H18A	0.8949	1.1689	0.1157	0.121*
H18B	0.6739	1.1264	0.0319	0.121*
H18C	0.8045	1.0458	−0.0004	0.121*
N1	0.3655 (2)	0.61425 (17)	0.15462 (14)	0.0698 (4)
N2	0.7485 (2)	0.96949 (16)	0.43909 (13)	0.0622 (4)
O1	0.71183 (17)	0.97361 (13)	0.13594 (10)	0.0617 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0353 (6)	0.0387 (7)	0.0463 (7)	0.0129 (5)	0.0108 (5)	0.0023 (5)
C2	0.0361 (6)	0.0444 (7)	0.0498 (7)	0.0165 (5)	0.0125 (5)	0.0072 (6)
C3	0.0439 (7)	0.0532 (8)	0.0595 (9)	0.0167 (6)	0.0181 (6)	0.0173 (7)
C4	0.0450 (8)	0.0424 (8)	0.0802 (11)	0.0101 (6)	0.0173 (7)	0.0138 (7)
C5	0.0509 (8)	0.0404 (7)	0.0717 (10)	0.0082 (6)	0.0106 (7)	−0.0054 (7)
C6	0.0512 (8)	0.0448 (7)	0.0531 (8)	0.0117 (6)	0.0133 (6)	−0.0010 (6)
C7	0.0558 (8)	0.0546 (8)	0.0455 (8)	0.0200 (7)	0.0165 (6)	0.0070 (6)
C8	0.0364 (6)	0.0384 (6)	0.0374 (6)	0.0114 (5)	0.0091 (5)	0.0003 (5)
C9	0.0366 (6)	0.0418 (7)	0.0387 (6)	0.0130 (5)	0.0115 (5)	0.0020 (5)
C10	0.0438 (7)	0.0520 (8)	0.0424 (7)	0.0192 (6)	0.0151 (6)	0.0116 (6)
C11	0.0471 (8)	0.0721 (10)	0.0357 (7)	0.0136 (7)	0.0132 (6)	0.0031 (7)
C12	0.0504 (8)	0.0570 (8)	0.0455 (8)	0.0110 (7)	0.0203 (6)	−0.0073 (6)
C13	0.0405 (7)	0.0437 (7)	0.0475 (7)	0.0141 (6)	0.0164 (6)	0.0002 (6)
C14	0.0415 (7)	0.0510 (8)	0.0486 (7)	0.0171 (6)	0.0143 (6)	0.0012 (6)
C15	0.0472 (7)	0.0431 (7)	0.0436 (7)	0.0189 (6)	0.0160 (6)	0.0070 (6)
C16	0.0452 (7)	0.0456 (7)	0.0518 (8)	0.0110 (6)	0.0184 (6)	0.0071 (6)
C17	0.0378 (7)	0.0513 (8)	0.0491 (7)	0.0111 (6)	0.0154 (6)	0.0038 (6)
C18	0.0877 (14)	0.0894 (13)	0.0880 (13)	0.0478 (11)	0.0411 (11)	0.0502 (11)
N1	0.0413 (7)	0.0762 (9)	0.0777 (10)	0.0141 (7)	0.0108 (6)	−0.0124 (8)
N2	0.0799 (9)	0.0595 (8)	0.0570 (8)	0.0357 (7)	0.0249 (7)	0.0036 (6)
O1	0.0616 (7)	0.0731 (7)	0.0663 (7)	0.0370 (6)	0.0273 (5)	0.0331 (6)

Geometric parameters (Å, °)

C1—C6	1.3955 (19)	C10—O1	1.4160 (17)
C1—C2	1.4019 (19)	C10—C11	1.501 (2)
C1—C8	1.5153 (17)	C10—C16	1.5372 (19)
C2—C3	1.3923 (19)	C11—C12	1.321 (2)
C2—C7	1.5068 (19)	C11—H11	0.93
C3—C4	1.378 (2)	C12—C13	1.494 (2)
C3—H3	0.93	C12—H12	0.93
C4—C5	1.372 (2)	C13—C17	1.5417 (19)
C4—H4	0.93	C13—H13	0.98
C5—C6	1.382 (2)	C14—N1	1.1355 (19)
C5—H5	0.93	C15—N2	1.1371 (18)
C6—H6	0.93	C16—C17	1.535 (2)
C7—H7A	0.96	C16—H16A	0.97
C7—H7B	0.96	C16—H16B	0.97
C7—H7C	0.96	C17—H17A	0.97
C8—C13	1.5551 (18)	C17—H17B	0.97
C8—C9	1.5816 (17)	C18—O1	1.408 (2)
C8—H8	0.98	C18—H18A	0.96
C9—C15	1.4776 (18)	C18—H18B	0.96
C9—C14	1.4804 (18)	C18—H18C	0.96
C9—C10	1.5794 (18)		
C6—C1—C2	118.87 (12)	C11—C10—C16	109.89 (12)
C6—C1—C8	120.32 (12)	O1—C10—C9	104.47 (10)
C2—C1—C8	120.77 (11)	C11—C10—C9	104.90 (11)
C3—C2—C1	118.44 (13)	C16—C10—C9	107.10 (11)
C3—C2—C7	118.43 (13)	C12—C11—C10	114.56 (12)
C1—C2—C7	123.11 (12)	C12—C11—H11	122.7
C4—C3—C2	121.98 (14)	C10—C11—H11	122.7
C4—C3—H3	119.0	C11—C12—C13	114.81 (13)
C2—C3—H3	119.0	C11—C12—H12	122.6
C5—C4—C3	119.50 (14)	C13—C12—H12	122.6
C5—C4—H4	120.3	C12—C13—C17	106.54 (12)
C3—C4—H4	120.3	C12—C13—C8	111.97 (11)
C4—C5—C6	119.87 (14)	C17—C13—C8	105.91 (10)
C4—C5—H5	120.1	C12—C13—H13	110.7
C6—C5—H5	120.1	C17—C13—H13	110.7
C5—C6—C1	121.31 (15)	C8—C13—H13	110.7
C5—C6—H6	119.3	N1—C14—C9	178.43 (15)
C1—C6—H6	119.3	N2—C15—C9	178.70 (15)
C2—C7—H7A	109.5	C17—C16—C10	110.08 (11)
C2—C7—H7B	109.5	C17—C16—H16A	109.6
H7A—C7—H7B	109.5	C10—C16—H16A	109.6
C2—C7—H7C	109.5	C17—C16—H16B	109.6
H7A—C7—H7C	109.5	C10—C16—H16B	109.6
H7B—C7—H7C	109.5	H16A—C16—H16B	108.2
C1—C8—C13	115.60 (10)	C16—C17—C13	108.74 (11)

C1—C8—C9	114.62 (10)	C16—C17—H17A	109.9
C13—C8—C9	107.25 (10)	C13—C17—H17A	109.9
C1—C8—H8	106.2	C16—C17—H17B	109.9
C13—C8—H8	106.2	C13—C17—H17B	109.9
C9—C8—H8	106.2	H17A—C17—H17B	108.3
C15—C9—C14	106.69 (11)	O1—C18—H18A	109.5
C15—C9—C10	109.45 (11)	O1—C18—H18B	109.5
C14—C9—C10	108.55 (11)	H18A—C18—H18B	109.5
C15—C9—C8	110.69 (10)	O1—C18—H18C	109.5
C14—C9—C8	112.91 (11)	H18A—C18—H18C	109.5
C10—C9—C8	108.49 (10)	H18B—C18—H18C	109.5
O1—C10—C11	114.96 (12)	C18—O1—C10	116.48 (12)
O1—C10—C16	114.58 (12)		
C6—C1—C2—C3	−0.63 (19)	C14—C9—C10—C11	−57.83 (14)
C8—C1—C2—C3	−178.64 (12)	C8—C9—C10—C11	65.22 (13)
C6—C1—C2—C7	178.11 (13)	C15—C9—C10—C16	69.33 (14)
C8—C1—C2—C7	0.10 (19)	C14—C9—C10—C16	−174.58 (11)
C1—C2—C3—C4	1.4 (2)	C8—C9—C10—C16	−51.54 (13)
C7—C2—C3—C4	−177.44 (13)	O1—C10—C11—C12	−172.24 (12)
C2—C3—C4—C5	−0.8 (2)	C16—C10—C11—C12	56.73 (16)
C3—C4—C5—C6	−0.6 (2)	C9—C10—C11—C12	−58.09 (15)
C4—C5—C6—C1	1.3 (2)	C10—C11—C12—C13	−2.60 (18)
C2—C1—C6—C5	−0.7 (2)	C11—C12—C13—C17	−57.14 (16)
C8—C1—C6—C5	177.32 (13)	C11—C12—C13—C8	58.22 (17)
C6—C1—C8—C13	−39.45 (17)	C1—C8—C13—C12	85.22 (14)
C2—C1—C8—C13	138.53 (12)	C9—C8—C13—C12	−44.02 (14)
C6—C1—C8—C9	86.10 (15)	C1—C8—C13—C17	−159.04 (11)
C2—C1—C8—C9	−95.92 (14)	C9—C8—C13—C17	71.72 (12)
C1—C8—C9—C15	95.40 (13)	O1—C10—C16—C17	−177.48 (11)
C13—C8—C9—C15	−134.81 (11)	C11—C10—C16—C17	−46.25 (15)
C1—C8—C9—C14	−24.13 (15)	C9—C10—C16—C17	67.16 (14)
C13—C8—C9—C14	105.66 (12)	C10—C16—C17—C13	−10.53 (15)
C1—C8—C9—C10	−144.50 (11)	C12—C13—C17—C16	61.71 (14)
C13—C8—C9—C10	−14.70 (13)	C8—C13—C17—C16	−57.67 (14)
C15—C9—C10—O1	−52.60 (13)	C11—C10—O1—C18	−74.84 (18)
C14—C9—C10—O1	63.49 (13)	C16—C10—O1—C18	53.89 (18)
C8—C9—C10—O1	−173.47 (10)	C9—C10—O1—C18	170.76 (14)
C15—C9—C10—C11	−173.91 (11)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···N1^{i}	0.93	2.70	3.509 (3)	146
C7—H7C···Cg1^{ii}	0.96	2.84	3.688 (2)	146

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+2, −*y*+1, −*z*+1.

Fig. 1

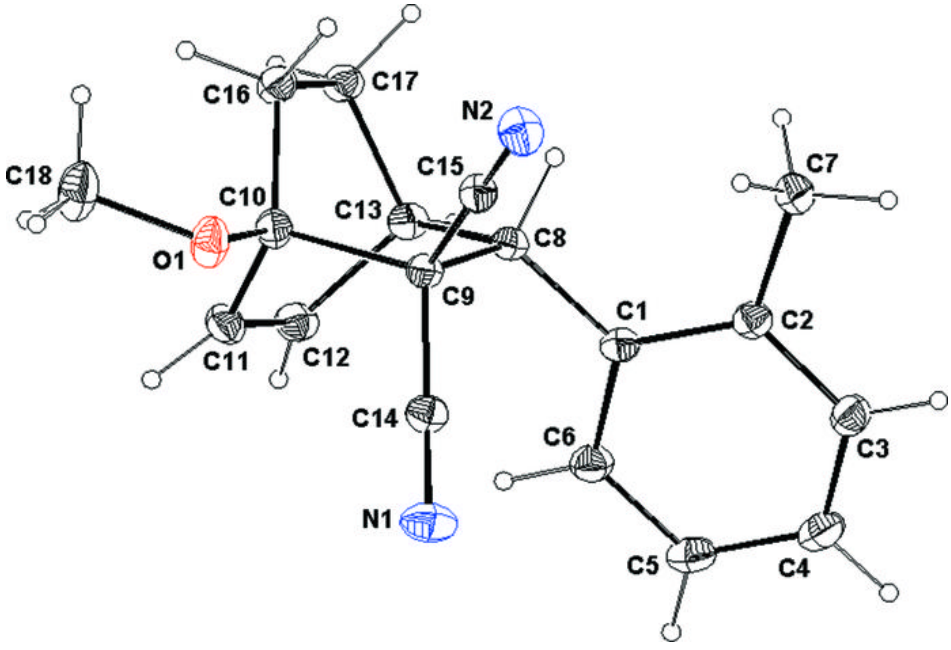

C16
C17
N2
C18
C15
C7
C10
C13
C8
O1
C9
C1
C2
C11
C12
C14
C6
C3
N1
C5
C4

Fig. 2

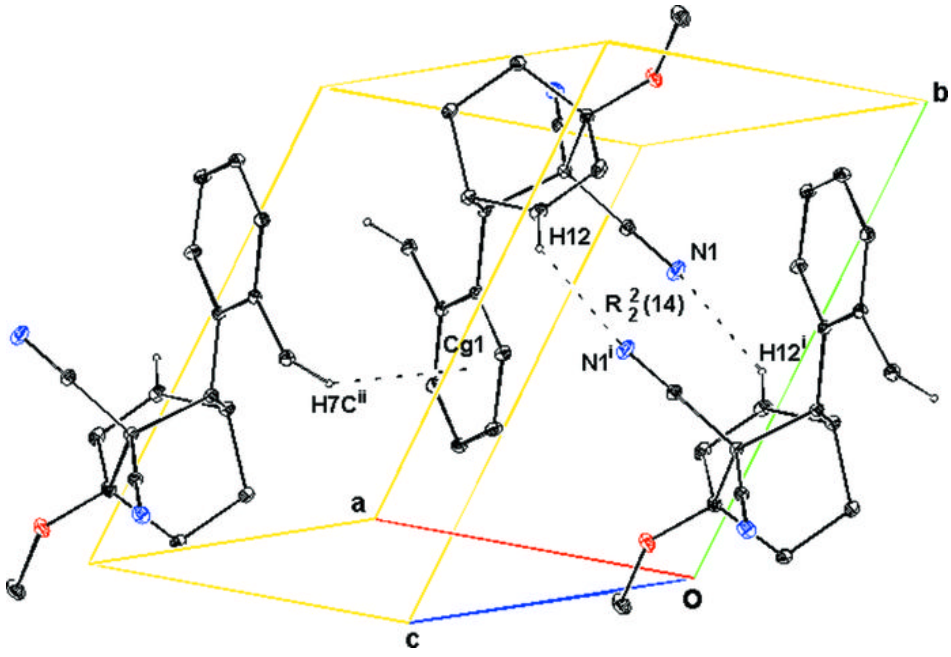
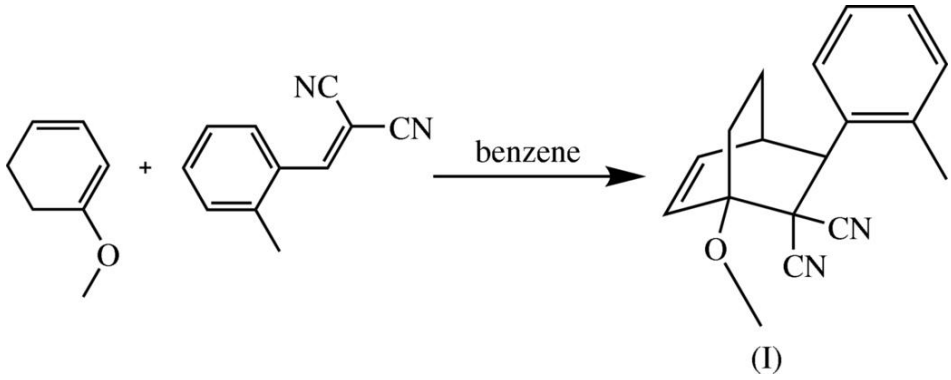


Fig. 3



(I)