

8*H*-Chromeno[2',3':4,5]imidazo[2,1-*a*]-isoquinolineSaifidin Safarov,<sup>a\*</sup> Leonid G. Voskressensky,<sup>b</sup> Oksana V. Bizhko,<sup>b</sup> Larisa N. Kulikova<sup>b</sup> and Victor N. Khrustalev<sup>c</sup>

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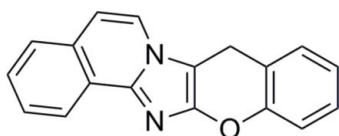
Received 19 February 2010; accepted 22 February 2010

Key indicators: single-crystal X-ray study; *T* = 100 K; mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$ ; *R* factor = 0.066; *wR* factor = 0.182; data-to-parameter ratio = 14.4.

The title compound,  $\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}$ , comprises two aromatic fragments, *viz.*, imidazo[2,1-*a*]isoquinoline and benzene, linked by oxygen and methylene bridges. Despite the absence of a common conjugative system within the molecule, it adopts an essentially planar conformation with an r.m.s. deviation of 0.036 Å. In the crystal, due to this structure, molecules form stacks along the *b* axis by  $\pi \cdots \pi$  stacking interactions, with shortest C $\cdots$ C distances in the range 3.340 (4)–3.510 (4) Å. The molecules are bound by intermolecular C–H $\cdots$ O interactions within the stacks and C–H $\cdots$  $\pi$  interactions between the stacks.

## Related literature

For background to cascade reactions, see: Bunce (1995); Tietze (1996); Parsons *et al.* (1996); Nicolaou *et al.* (2003, 2006); Wasilke *et al.* (2005); Pellissier (2006*a,b*); Parenty & Cronin (2008). For related compounds, see: Yadav *et al.* (2007); Kianmehr *et al.* (2009); Surpur *et al.* (2009).



## Experimental

## Crystal data

$\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}$   
 $M_r = 272.30$

Monoclinic,  $P2_1/n$   
 $a = 11.9717 (15) \text{ \AA}$

$b = 6.0580 (8) \text{ \AA}$   
 $c = 17.948 (2) \text{ \AA}$   
 $\beta = 102.682 (3)^\circ$   
 $V = 1269.9 (3) \text{ \AA}^3$   
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.09 \text{ mm}^{-1}$   
 $T = 100 \text{ K}$   
 $0.40 \times 0.12 \times 0.02 \text{ mm}$

## Data collection

Bruker APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)  
 $T_{\min} = 0.965$ ,  $T_{\max} = 0.998$

12413 measured reflections  
2734 independent reflections  
1821 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.056$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.066$   
 $wR(F^2) = 0.182$   
 $S = 1.00$   
2734 reflections

190 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.45 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.23 \text{ e \AA}^{-3}$

## Table 1

Hydrogen-bond geometry (Å, °).

Cg2 is the centroid of the O13, C12A, C8A, C8, C7A, C13A ring.

<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>
C8—H8A $\cdots$ O13 <sup>i</sup>	0.99	2.71	3.637 (4)	157
C8—H8B $\cdots$ Cg <sup>ii</sup>	0.99	2.63	3.547 (3)	154

Symmetry codes: (i)  $x, y + 1, z$ ; (ii)  $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$ .

Data collection: APEX2 (Bruker, 2005); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2193).

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**supplementary materials**

*Acta Cryst.* (2010). E66, o710 [ doi:10.1107/S1600536810006744 ]

## 8*H*-Chromeno[2',3':4,5]imidazo[2,1-*a*]isoquinoline

S. Safarov, L. G. Voskressensky, O. V. Bizhko, L. N. Kulikova and V. N. Khrustalev

### Comment

Cascade reactions have emerged as powerful tools to allow rapidly increasing molecular complexity (Tietze, 1996; Parsons *et al.*, 1996; Wasilke *et al.*, 2005). These processes avoid the excessive handling and isolation of synthetic intermediates generating less waste and thus contribute towards "Green Chemistry". Cascade reactions, in which multiple reactions are combined into one synthetic operation, have been reported extensively in the literature and have already become "state-of-the-art" in synthetic organic chemistry (Bunce, 1995; Nicolaou *et al.*, 2003, 2006; Pellissier, 2006*a*, 2006*b*; Parenty & Cronin, 2008).

The title compound **I**, C<sub>18</sub>H<sub>12</sub>N<sub>2</sub>O, is the product of a novel cascade reaction (Fig. 1) (Yadav *et al.*, 2007; Kianmehr *et al.*, 2009; Surpur *et al.*, 2009) starting with the Kroehnke condensation of salicylic aldehyde and isoquinolinium salt to afford the styryl derivative **A**, which forms zwitterion **B** upon thermally-induced cleavage of acetyl chloride. Then zwitterion **B** undergoes two consecutive nucleophilic cyclizations followed by [1,4]-proton shift to give the pentacycle **I** (Fig. 2). The single crystals of **I** suitable for X-ray diffraction analysis were obtained by slow crystallization from ethyl acetate solution.

Compound **I** comprises two aromatic fragments - imidazo[2,1-*a*]isoquinoline and benzene linked by the oxygen and methylene bridges (Fig. 3). Despite the absence of common conjugative system within the molecule, it adopts practically planar conformation, with the r.m.s. deviation of 0.036 Å. In the crystal, due to this structure, molecules form stacks along the *b* axis by the stacking interactions [C1<sup>i</sup>...C7A<sup>i</sup> = 3.340 (4) Å, C2<sup>i</sup>...C8<sup>i</sup> = 3.510 Å, C2<sup>i</sup>...C8A<sup>i</sup> = 3.451 (4) Å, C3<sup>i</sup>...C12A<sup>i</sup> = 3.394 (4) Å, C13A<sup>i</sup>...C14B<sup>i</sup> = 3.496 (4) Å and C14A<sup>i</sup>...C14A<sup>i</sup> = 3.426 (4) Å] (Fig. 4). The molecules are also bound by the C8—H8A...O13<sup>ii</sup> [H...O = 2.71 Å, C—H...O 157°] interactions within the stacks and the C8—H8B...π (C12A<sup>iii</sup>—O13<sup>iii</sup>—C13A<sup>iii</sup>) [H...C12A = 2.94 Å, H...O13 = 2.80 Å and H...C13A 2.81 Å, C—H...O 175°] interactions between the stacks. Symmetry codes: (i) 1-*x*, 1-*y*, *z*; (ii) *x*, 1+*y*, *z*; (iii) 1.5-*x*, 0.5+*y*, 0.5-*z*.

### Experimental

A water solution of K<sub>2</sub>CO<sub>3</sub> (0.4 g in 1 ml of H<sub>2</sub>O) was added to a solution of freshly distilled salicylic aldehyde (0.18 g, 1.47 mmol) and 2-(cyanomethyl)isoquinolinium chloride (0.30 g, 1.47 mmol) in H<sub>2</sub>O (5 ml). The resulting mixture was stirred for 3 hours at 293 K. The precipitate formed was filtered-off and recrystallized from ethyl acetate / hexane mixture to give product **I** as colourless needles. Yield is 32%. M.p. = 444 K. Found (%): C 79.13, H 4.58, N 10.53. Calcd. for C<sub>18</sub>H<sub>12</sub>N<sub>2</sub>O (%): C 79.39, H 4.44, N 10.29. <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>): δ = 4.25 (s, 2H, CH<sub>2</sub>), 6.98 (dd, 1H, H12, *J*<sub>11,12</sub> = 8.1, *J*<sub>10,12</sub> = 1.2), 7.01 (d, 1H, H5, *J*<sub>5,6</sub> = 7.5), 7.07–7.12 (m, 2H, H9+H10), 7.16 (dd, 1H, H11, *J*<sub>11,12</sub> = 8.1, *J*<sub>9,11</sub> = 1.2), 7.40–7.45 (m, 1H, H3), 7.48–7.53 (m, 1H, H2), 7.55 (d, 1H, H4, *J*<sub>3,4</sub> = 7.5), 7.58 (d, 1H, H6, *J*<sub>5,6</sub> = 7.5), 8.47 (d, 1H, H1, *J*<sub>1,2</sub> = 8.1). <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>): δ = 23.2 (CH<sub>2</sub>), 112.9 (CH), 117.8 (C<sub>q</sub>), 118.1 (C<sub>q</sub>), 118.3 (CH), 120.3 (CH), 123.1 (CH), 123.2 (C<sub>q</sub>), 123.5 (CH), 127.1 (CH), 127.8 (CH), 128.2 (2xCH), 129.1 (C<sub>q</sub>), 130.3 (CH), 138.0 (C<sub>q</sub>), 152.0 (C<sub>q</sub>), 161.1 (C<sub>q</sub>). Mass spectrum (EI MS), *m/z* (I<sub>r</sub>, %): 272 (70) [*M*<sup>+</sup>], 136 (11), 128 (10).

## Refinement

The hydrogen atoms were placed in calculated positions with C—H = 0.95–0.99 Å and refined in the riding model with fixed isotropic displacement parameters [ $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ ].

## Figures



Fig. 1. Synthesis of compound **I**.

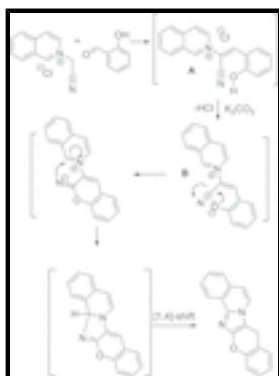


Fig. 2. The plausible formation mechanism of **I**.

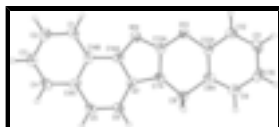


Fig. 3. Molecular structure of **I** with the atom numbering scheme. Displacement ellipsoids are shown at the 50% probability level. H atoms are presented as a small spheres of arbitrary radius.

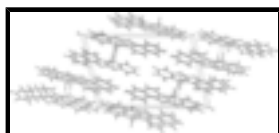


Fig. 4. Crystal packing of **I** viewed down the *b* axis. Dashed lines indicate the C—H...O and C—H... $\pi$  interactions.

## 8*H*-Chromeno[2',3':4,5]imidazo[2,1-*a*]isoquinoline

### Crystal data

$\text{C}_{18}\text{H}_{12}\text{N}_2\text{O}$

$M_r = 272.30$

Monoclinic,  $P2_1/n$

Hall symbol:  $-P\ 2_1n$

$a = 11.9717(15)\ \text{\AA}$

$b = 6.0580(8)\ \text{\AA}$

$c = 17.948(2)\ \text{\AA}$

$\beta = 102.682(3)^\circ$

$V = 1269.9(3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 568$

$D_x = 1.424\ \text{Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 1700 reflections

$\theta = 2.3\text{--}26.3^\circ$

$\mu = 0.09\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Needle, colourless

$0.40 \times 0.12 \times 0.02\ \text{mm}$

*Data collection*

Bruker APEXII CCD diffractometer	2734 independent reflections
Radiation source: fine-focus sealed tube graphite	1821 reflections with $I > 2\sigma(I)$
$\varphi$ and $\omega$ scans	$R_{\text{int}} = 0.056$
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	$\theta_{\text{max}} = 27.0^\circ$ , $\theta_{\text{min}} = 1.9^\circ$
$T_{\text{min}} = 0.965$ , $T_{\text{max}} = 0.998$	$h = -15 \rightarrow 15$
12413 measured reflections	$k = -7 \rightarrow 7$
	$l = -22 \rightarrow 22$

*Refinement*

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.066$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.182$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.077P)^2 + 1.7P]$
2734 reflections	where $P = (F_o^2 + 2F_c^2)/3$
190 parameters	$(\Delta/\sigma)_{\text{max}} < 0.001$
0 restraints	$\Delta\rho_{\text{max}} = 0.45 \text{ e } \text{\AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$

*Special details*

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.6165 (2)	0.1766 (5)	-0.07577 (16)	0.0290 (6)
H1	0.5719	0.0665	-0.0583	0.035*
C2	0.6436 (2)	0.1563 (5)	-0.14599 (17)	0.0349 (7)
H2	0.6185	0.0302	-0.1766	0.042*
C3	0.7068 (2)	0.3167 (6)	-0.17271 (17)	0.0372 (7)
H3	0.7237	0.3008	-0.2217	0.045*

## supplementary materials

C4	0.7447 (2)	0.4957 (5)	-0.12988 (17)	0.0349 (7)
H4	0.7885	0.6033	-0.1494	0.042*
C4A	0.7213 (2)	0.5276 (5)	-0.05755 (16)	0.0309 (6)
C5	0.7591 (2)	0.7182 (5)	-0.01180 (16)	0.0332 (7)
H5	0.8052	0.8253	-0.0295	0.040*
C6	0.7306 (2)	0.7478 (5)	0.05559 (16)	0.0310 (6)
H6	0.7538	0.8777	0.0845	0.037*
N7	0.66701 (19)	0.5884 (4)	0.08314 (13)	0.0269 (5)
C7A	0.6332 (2)	0.5823 (4)	0.15238 (15)	0.0251 (6)
C8	0.6498 (2)	0.7432 (5)	0.21381 (16)	0.0326 (7)
H8A	0.6141	0.8858	0.1950	0.039*
H8B	0.7325	0.7676	0.2349	0.039*
C8A	0.5921 (2)	0.6458 (5)	0.27520 (16)	0.0301 (6)
C9	0.5902 (2)	0.7644 (5)	0.34032 (18)	0.0347 (7)
H9	0.6261	0.9050	0.3466	0.042*
C10	0.5385 (3)	0.6886 (5)	0.39654 (18)	0.0382 (7)
H10	0.5390	0.7752	0.4407	0.046*
C11	0.4851 (2)	0.4809 (6)	0.38774 (18)	0.0387 (8)
H11	0.4483	0.4261	0.4258	0.046*
C12	0.4864 (2)	0.3558 (5)	0.32275 (16)	0.0304 (6)
H12	0.4516	0.2141	0.3163	0.037*
C12A	0.5393 (2)	0.4417 (5)	0.26757 (15)	0.0264 (6)
O13	0.53167 (16)	0.2981 (3)	0.20489 (11)	0.0319 (5)
C13A	0.5786 (2)	0.3795 (5)	0.14856 (15)	0.0297 (6)
N14	0.57698 (19)	0.2676 (4)	0.08385 (13)	0.0297 (5)
C14A	0.6311 (2)	0.3960 (5)	0.04379 (16)	0.0291 (6)
C14B	0.6554 (2)	0.3618 (5)	-0.02983 (14)	0.0278 (6)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0230 (13)	0.0287 (15)	0.0340 (15)	-0.0002 (11)	0.0032 (11)	0.0065 (12)
C2	0.0304 (15)	0.0366 (16)	0.0339 (16)	0.0086 (13)	-0.0012 (12)	-0.0084 (13)
C3	0.0285 (15)	0.056 (2)	0.0270 (15)	0.0063 (14)	0.0051 (12)	0.0020 (14)
C4	0.0300 (15)	0.0386 (17)	0.0360 (17)	0.0009 (13)	0.0072 (12)	0.0117 (13)
C4A	0.0256 (13)	0.0281 (15)	0.0354 (16)	0.0053 (11)	-0.0012 (12)	-0.0019 (12)
C5	0.0312 (15)	0.0325 (15)	0.0360 (16)	-0.0054 (12)	0.0080 (12)	0.0073 (13)
C6	0.0333 (15)	0.0264 (14)	0.0335 (15)	0.0002 (12)	0.0078 (12)	0.0053 (12)
N7	0.0261 (11)	0.0246 (12)	0.0282 (12)	0.0025 (9)	0.0021 (9)	0.0000 (10)
C7A	0.0187 (12)	0.0265 (14)	0.0297 (14)	-0.0019 (10)	0.0045 (10)	0.0056 (11)
C8	0.0258 (14)	0.0372 (16)	0.0350 (16)	-0.0040 (12)	0.0072 (12)	-0.0058 (13)
C8A	0.0209 (13)	0.0325 (15)	0.0350 (15)	0.0021 (11)	0.0020 (11)	0.0023 (13)
C9	0.0278 (14)	0.0313 (15)	0.0440 (17)	0.0019 (12)	0.0055 (12)	0.0008 (13)
C10	0.0365 (16)	0.0407 (18)	0.0362 (16)	0.0091 (14)	0.0054 (13)	-0.0132 (14)
C11	0.0304 (15)	0.051 (2)	0.0388 (17)	0.0089 (14)	0.0175 (13)	0.0082 (15)
C12	0.0239 (13)	0.0275 (14)	0.0397 (16)	0.0001 (11)	0.0067 (12)	0.0026 (13)
C12A	0.0214 (12)	0.0294 (14)	0.0283 (14)	0.0068 (11)	0.0055 (11)	-0.0016 (11)
O13	0.0344 (11)	0.0285 (10)	0.0352 (11)	-0.0058 (8)	0.0130 (9)	-0.0022 (9)

C13A	0.0256 (14)	0.0345 (15)	0.0290 (14)	0.0048 (12)	0.0059 (11)	0.0012 (12)
N14	0.0254 (11)	0.0327 (13)	0.0314 (13)	0.0016 (10)	0.0070 (9)	0.0015 (10)
C14A	0.0252 (13)	0.0257 (14)	0.0347 (15)	0.0004 (11)	0.0029 (11)	-0.0018 (12)
C14B	0.0227 (13)	0.0376 (16)	0.0214 (13)	0.0105 (11)	0.0014 (10)	0.0021 (12)

*Geometric parameters (Å, °)*

C1—C2	1.374 (4)	C8—C8A	1.540 (4)
C1—C14B	1.410 (4)	C8—H8A	0.9900
C1—H1	0.9500	C8—H8B	0.9900
C2—C3	1.380 (5)	C8A—C9	1.377 (4)
C2—H2	0.9500	C8A—C12A	1.382 (4)
C3—C4	1.349 (5)	C9—C10	1.373 (4)
C3—H3	0.9500	C9—H9	0.9500
C4—C4A	1.400 (4)	C10—C11	1.405 (5)
C4—H4	0.9500	C10—H10	0.9500
C4A—C5	1.432 (4)	C11—C12	1.394 (4)
C4A—C14B	1.432 (4)	C11—H11	0.9500
C5—C6	1.339 (4)	C12—C12A	1.389 (4)
C5—H5	0.9500	C12—H12	0.9500
C6—N7	1.386 (4)	C12A—O13	1.409 (3)
C6—H6	0.9500	O13—C13A	1.353 (3)
N7—C14A	1.382 (4)	C13A—N14	1.341 (4)
N7—C7A	1.390 (4)	N14—C14A	1.321 (4)
C7A—C13A	1.386 (4)	C14A—C14B	1.429 (4)
C7A—C8	1.452 (4)		
C2—C1—C14B	119.6 (3)	C8A—C8—H8B	110.5
C2—C1—H1	120.2	H8A—C8—H8B	108.7
C14B—C1—H1	120.2	C9—C8A—C12A	117.3 (3)
C1—C2—C3	120.9 (3)	C9—C8A—C8	120.1 (3)
C1—C2—H2	119.6	C12A—C8A—C8	122.6 (3)
C3—C2—H2	119.6	C10—C9—C8A	122.9 (3)
C4—C3—C2	120.6 (3)	C10—C9—H9	118.5
C4—C3—H3	119.7	C8A—C9—H9	118.5
C2—C3—H3	119.7	C9—C10—C11	119.0 (3)
C3—C4—C4A	121.9 (3)	C9—C10—H10	120.5
C3—C4—H4	119.0	C11—C10—H10	120.5
C4A—C4—H4	119.0	C12—C11—C10	119.5 (3)
C4—C4A—C5	122.7 (3)	C12—C11—H11	120.2
C4—C4A—C14B	117.6 (3)	C10—C11—H11	120.2
C5—C4A—C14B	119.7 (3)	C12A—C12—C11	118.9 (3)
C6—C5—C4A	121.0 (3)	C12A—C12—H12	120.5
C6—C5—H5	119.5	C11—C12—H12	120.5
C4A—C5—H5	119.5	C8A—C12A—C12	122.4 (3)
C5—C6—N7	119.9 (3)	C8A—C12A—O13	125.4 (2)
C5—C6—H6	120.1	C12—C12A—O13	112.2 (2)
N7—C6—H6	120.1	C13A—O13—C12A	114.0 (2)
C14A—N7—C6	122.6 (2)	N14—C13A—O13	122.2 (3)
C14A—N7—C7A	108.4 (2)	N14—C13A—C7A	114.1 (2)

## supplementary materials

C6—N7—C7A	129.0 (2)	O13—C13A—C7A	123.7 (2)
C13A—C7A—N7	101.9 (2)	C14A—N14—C13A	104.9 (2)
C13A—C7A—C8	128.1 (2)	N14—C14A—N7	110.7 (2)
N7—C7A—C8	130.0 (2)	N14—C14A—C14B	129.9 (3)
C7A—C8—C8A	106.1 (2)	N7—C14A—C14B	119.4 (3)
C7A—C8—H8A	110.5	C1—C14B—C14A	123.3 (3)
C8A—C8—H8A	110.5	C1—C14B—C4A	119.4 (2)
C7A—C8—H8B	110.5	C14A—C14B—C4A	117.3 (3)
C14B—C1—C2—C3	-1.1 (4)	C11—C12—C12A—O13	-178.9 (2)
C1—C2—C3—C4	0.9 (4)	C8A—C12A—O13—C13A	-2.1 (4)
C2—C3—C4—C4A	-0.5 (4)	C12—C12A—O13—C13A	177.7 (2)
C3—C4—C4A—C5	-178.9 (3)	C12A—O13—C13A—N14	-178.5 (2)
C3—C4—C4A—C14B	0.2 (4)	C12A—O13—C13A—C7A	2.1 (4)
C4—C4A—C5—C6	176.9 (3)	N7—C7A—C13A—N14	-0.3 (3)
C14B—C4A—C5—C6	-2.3 (4)	C8—C7A—C13A—N14	180.0 (3)
C4A—C5—C6—N7	2.4 (4)	N7—C7A—C13A—O13	179.1 (2)
C5—C6—N7—C14A	0.2 (4)	C8—C7A—C13A—O13	-0.6 (4)
C5—C6—N7—C7A	176.8 (3)	O13—C13A—N14—C14A	-179.3 (2)
C14A—N7—C7A—C13A	0.3 (3)	C7A—C13A—N14—C14A	0.1 (3)
C6—N7—C7A—C13A	-176.7 (3)	C13A—N14—C14A—N7	0.1 (3)
C14A—N7—C7A—C8	-179.9 (3)	C13A—N14—C14A—C14B	179.9 (3)
C6—N7—C7A—C8	3.1 (5)	C6—N7—C14A—N14	177.0 (2)
C13A—C7A—C8—C8A	-1.0 (4)	C7A—N7—C14A—N14	-0.3 (3)
N7—C7A—C8—C8A	179.3 (2)	C6—N7—C14A—C14B	-2.8 (4)
C7A—C8—C8A—C9	-177.9 (2)	C7A—N7—C14A—C14B	179.9 (2)
C7A—C8—C8A—C12A	1.0 (4)	C2—C1—C14B—C14A	179.9 (3)
C12A—C8A—C9—C10	-0.1 (4)	C2—C1—C14B—C4A	0.8 (4)
C8—C8A—C9—C10	178.9 (3)	N14—C14A—C14B—C1	3.9 (4)
C8A—C9—C10—C11	0.0 (4)	N7—C14A—C14B—C1	-176.3 (2)
C9—C10—C11—C12	0.6 (4)	N14—C14A—C14B—C4A	-176.9 (3)
C10—C11—C12—C12A	-1.0 (4)	N7—C14A—C14B—C4A	2.8 (4)
C9—C8A—C12A—C12	-0.4 (4)	C4—C4A—C14B—C1	-0.4 (4)
C8—C8A—C12A—C12	-179.3 (2)	C5—C4A—C14B—C1	178.8 (2)
C9—C8A—C12A—O13	179.4 (2)	C4—C4A—C14B—C14A	-179.5 (2)
C8—C8A—C12A—O13	0.5 (4)	C5—C4A—C14B—C14A	-0.4 (4)
C11—C12—C12A—C8A	0.9 (4)		

### Hydrogen-bond geometry (Å, °)

Cg2 is the centroid of the O13,C12A,C8A,C8,C7A,C13A ring.

<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>
C8—H8A $\cdots$ O13 <sup>i</sup>	0.99	2.71	3.637 (4)	157
C8—H8B $\cdots$ Cg <sup>ii</sup>	0.99	2.63	3.547 (3)	154

Symmetry codes: (i)  $x, y+1, z$ ; (ii)  $-x+3/2, y+1/2, -z+1/2$ .



Fig. 1

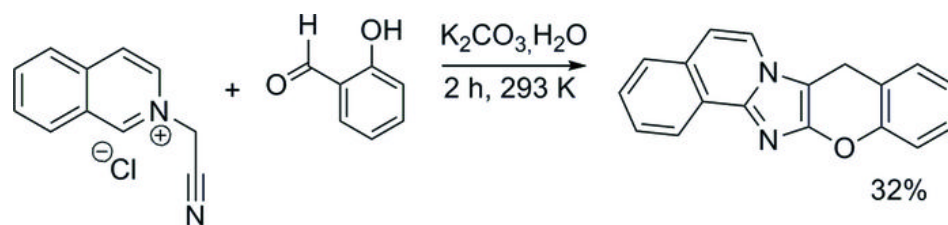


Fig. 2

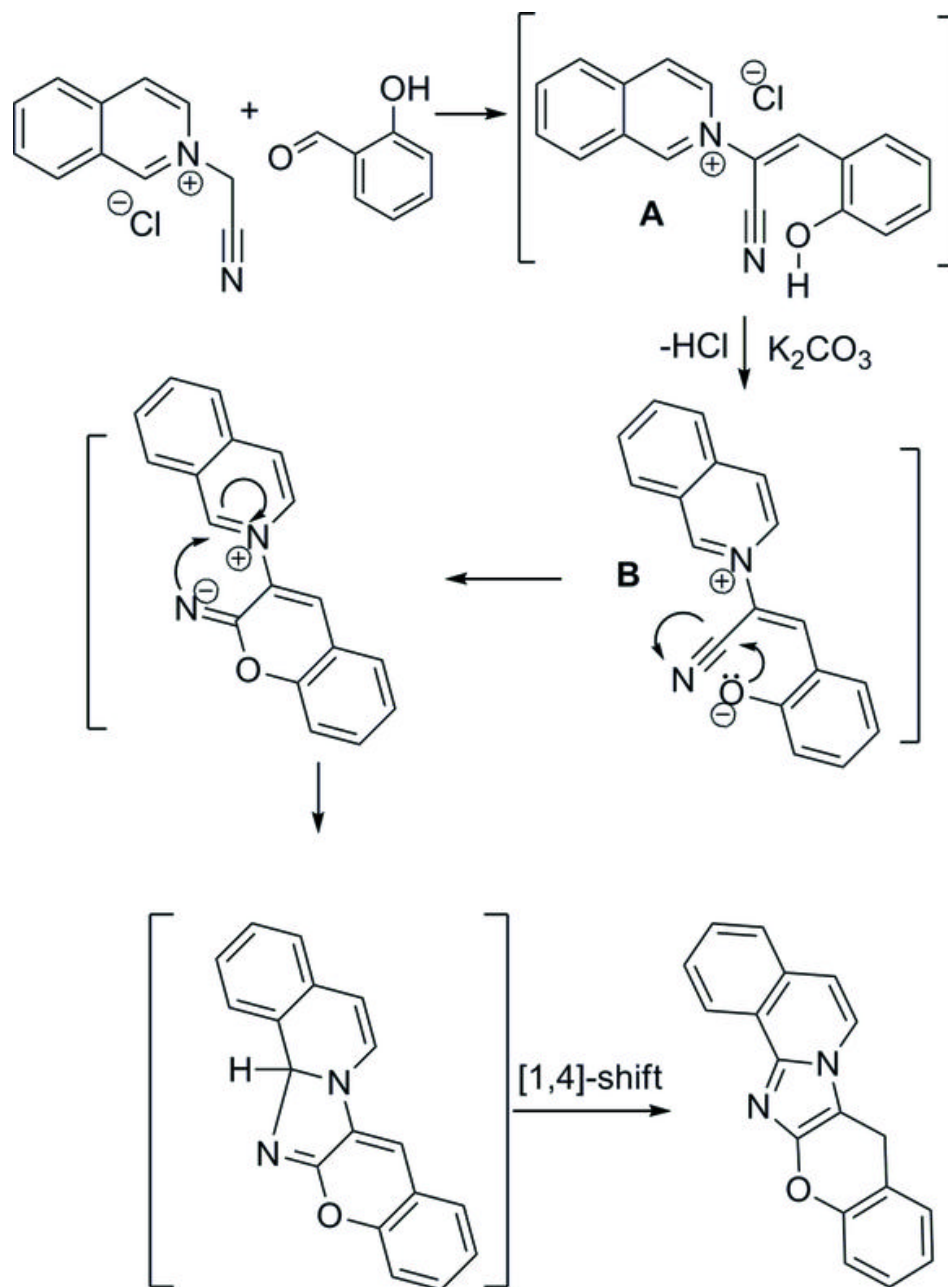


Fig. 3

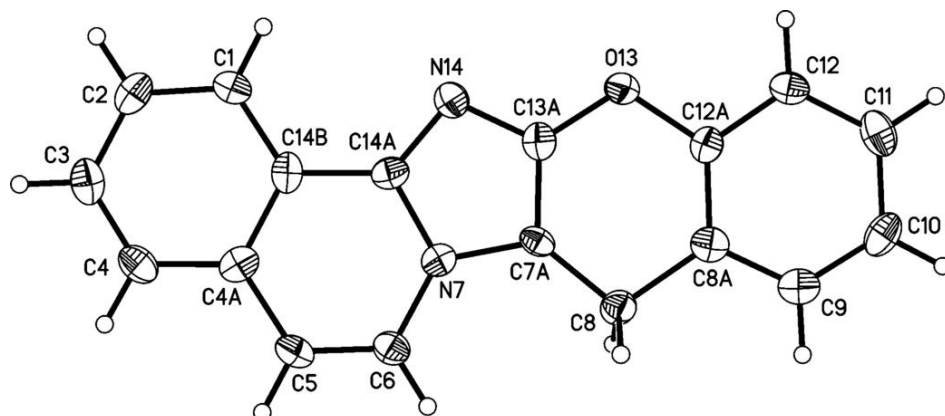


Fig. 4

