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## Key indicators

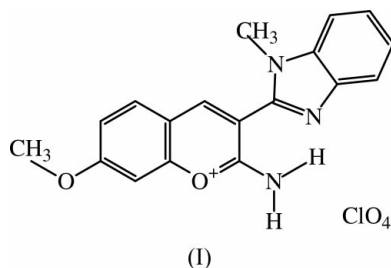
Single-crystal X-ray study  
*T* = 293 K  
Mean  $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$   
*R* factor = 0.047  
*wR* factor = 0.099  
Data-to-parameter ratio = 12.9For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.2-Amino-7-methoxy-3-(1-methyl-1*H*-benzimidazol-2-yl)chromenium perchlorate

In the title compound,  $\text{C}_{18}\text{H}_{16}\text{N}_3\text{O}_2^+\cdot\text{ClO}_4^-$ , the almost planar cation contains bicyclic chromenone and benzimidazole moieties, which are rotated slightly relative to each other. The positive charge of the cation is located on the pyrilium ring and causes noticeable aromatization of the O—C and C—C bonds. One of the H atoms of the amino group is involved in an intramolecular hydrogen bond which closes the six-membered pseudo-ring in the cation. The second H atom of the amino group participates in a hydrogen bond with one of the O atoms of the perchlorate anion.

## Comment

The title compound, (I), belongs to the class of iminocoumarin derivatives, which have hitherto received relatively little attention (Baumer *et al.*, 1993; Kovalenko *et al.*, 1999; O'Callaghan *et al.*, 1996).

The ionic crystals of (I) are composed of chromenium cations and perchlorate anions (Fig. 1). In the cation, two planar fragments (r.m.s. deviations of 0.016 and 0.007 Å for the coumarin and benzimidazole bicyclic systems, respectively) are rotated by 10.68 (10)° relative to each other (see also the list of torsion angles in Table 1). The positive charge of the cation causes noticeable changes in the bond lengths compared with those given by Bürgi & Dunitz (1994), especially in the pyrilium ring (Table 1). The corresponding values for the corresponding neutral molecule containing an iminocoumarin fragment, as given by Kovalenko *et al.* (1999), are as follows: O1—C2 1.379, C2—C3 1.449, C3—C4 1.347, C4—C9 1.427, C9—C10 1.361 and O1—C10 1.391 Å, with the same numbering as used in Table 1. Compared with these values, in (I), the O1—C2 bond is shorter, the C2—C3, C3—C4 and C9—C10 bonds are longer, and the O1—C10 and C4—C9 bonds are essentially the same.



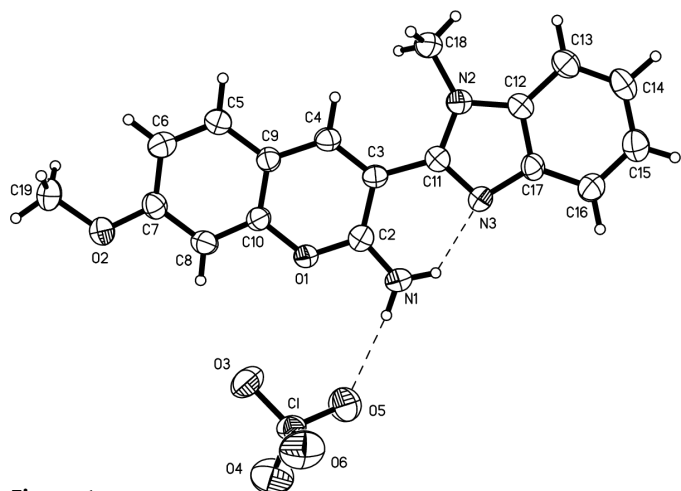
Both amino H atoms participate in hydrogen bonding; one is involved in an intramolecular hydrogen bond with the benzimidazole N atom, and the other is linked to one of the perchlorate O atoms (Table 2).

It should be noted that the observed configuration of the cation, in which the methyl and amino groups lie on opposite

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**Figure 1**  
The atom-umbering scheme and displacement ellipsoids (50% probability level) for the title compound.

sides with respect to the C3—C11 bond, explains the peculiarity in the absorption spectrum of (I), namely the fact that the long-wavelength band is up to  $1500\text{ cm}^{-1}$  blue-shifted with respect to its unmethylated analogue. This is probably a result of the observed arrangement of the two planar parts of the cation.

## Experimental

In accordance with previously described preparative methods (Karasev *et al.*, 1995, 1999), 1.52 g (0.01 M) of 4-methoxy-2-hydroxybenzaldehyde and 2.7 g (0.01 M) of 1-methyl-2-cyano-methylbenzimidazolium perchlorate in 20 ml of 2-propanol were refluxed for 10 min. After cooling, crystals were filtered off and recrystallized from acetonitrile. Yield 2.07 g (51%); m.p. 538 K.

### Crystal data

$\text{C}_{18}\text{H}_{16}\text{N}_3\text{O}_2^+\cdot\text{ClO}_4^-$	$D_x = 1.520\text{ Mg m}^{-3}$
$M_r = 405.79$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 24 reflections
$a = 8.6272(17)\text{ \AA}$	$\theta = 11.0\text{--}12.0^\circ$
$b = 10.979(3)\text{ \AA}$	$\mu = 0.26\text{ mm}^{-1}$
$c = 18.788(7)\text{ \AA}$	$T = 293(2)\text{ K}$
$\beta = 94.71(3)^\circ$	Irregular polyhedron, red
$V = 1773.5(9)\text{ \AA}^3$	$0.4 \times 0.3 \times 0.2\text{ mm}$
$Z = 4$	

### Data collection

Siemens P3/PC diffractometer	$h = 0 \rightarrow 10$
$2\theta/\theta$ scans	$k = 0 \rightarrow 13$
3526 measured reflections	$l = -22 \rightarrow 22$
3297 independent reflections	2 standard reflections
1992 reflections with $I > 2\sigma(I)$	every 98 reflections
$R_{\text{int}} = 0.043$	intensity decay: 1%
$\theta_{\text{max}} = 25.5^\circ$	

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.03P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.047$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.099$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.01$	$\Delta\rho_{\text{max}} = 0.23\text{ e \AA}^{-3}$
3297 reflections	$\Delta\rho_{\text{min}} = -0.28\text{ e \AA}^{-3}$
256 parameters	Extinction correction: SHELXL97
H-atom parameters constrained	Extinction coefficient: 0.0017(5)

**Table 1**  
Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

O1—C2	1.351 (3)	C5—C9	1.427 (4)
O1—C10	1.397 (3)	C6—C7	1.420 (4)
O2—C7	1.364 (3)	C7—C8	1.422 (4)
O2—C19	1.457 (3)	C8—C10	1.378 (4)
N1—C2	1.310 (3)	C9—C10	1.403 (4)
N2—C11	1.392 (3)	C12—C17	1.410 (4)
N2—C12	1.406 (3)	C12—C13	1.407 (4)
N2—C18	1.488 (3)	C13—C14	1.384 (4)
N3—C11	1.343 (3)	C14—C15	1.419 (4)
N3—C17	1.399 (4)	C15—C16	1.389 (4)
C2—C3	1.467 (4)	C16—C17	1.421 (4)
C3—C4	1.385 (4)	Cl—O4	1.428 (2)
C3—C11	1.483 (4)	Cl—O3	1.440 (2)
C4—C9	1.426 (4)	Cl—O5	1.446 (2)
C5—C6	1.384 (4)	Cl—O6	1.450 (3)
C2—O1—C10	122.2 (2)	C8—C10—O1	116.9 (2)
C7—O2—C19	118.3 (2)	C8—C10—C9	124.0 (3)
C11—N2—C12	106.5 (2)	O1—C10—C9	119.2 (2)
C11—N2—C18	130.9 (2)	N3—C11—N2	112.3 (3)
C12—N2—C18	122.4 (2)	N3—C11—C3	121.5 (2)
C11—N3—C17	105.5 (2)	N2—C11—C3	126.2 (3)
N1—C2—O1	113.1 (3)	N2—C12—C17	105.7 (2)
N1—C2—C3	125.7 (3)	N2—C12—C13	132.7 (3)
O1—C2—C3	121.2 (2)	C13—C12—C17	121.6 (3)
C4—C3—C2	115.5 (3)	C14—C13—C12	117.1 (3)
C4—C3—C11	126.2 (3)	C13—C14—C15	122.1 (3)
C2—C3—C11	118.2 (2)	C16—C15—C14	121.3 (3)
C3—C4—C9	123.1 (3)	C15—C16—C17	117.2 (3)
C6—C5—C9	120.4 (3)	N3—C17—C12	110.1 (3)
C5—C6—C7	120.8 (3)	N3—C17—C16	129.1 (3)
O2—C7—C8	116.2 (3)	C12—C17—C16	120.7 (3)
O2—C7—C6	124.4 (3)	O4—Cl—O3	110.78 (17)
C6—C7—C8	119.4 (3)	O4—Cl—O5	110.15 (19)
C10—C8—C7	118.1 (3)	O3—Cl—O5	109.83 (15)
C10—C9—C4	118.6 (2)	O4—Cl—O6	107.82 (18)
C10—C9—C5	117.2 (3)	O3—Cl—O6	108.98 (16)
C4—C9—C5	124.2 (3)	O5—Cl—O6	109.2 (2)
C10—O1—C2—N1	175.7 (2)	C12—N2—C11—C3	−179.3 (3)
O1—O1—C2—C3	−4.1 (4)	C18—N2—C11—C3	−5.0 (5)
O1—C2—C3—C4	5.3 (4)	C4—C3—C11—N3	169.0 (3)
N1—C2—C3—C11	3.1 (4)	C2—C3—C11—N3	−8.3 (4)
C2—C3—C4—C9	−3.6 (4)	C4—C3—C11—N2	−11.6 (5)
C11—C3—C4—C9	179.0 (3)	C2—C3—C11—N2	171.1 (3)
C19—O2—C7—C8	−178.5 (3)	C11—N2—C12—C17	−0.5 (3)
C17—N3—C11—N2	0.2 (3)	C18—N2—C12—C17	−175.4 (2)
C17—N3—C11—C3	179.7 (2)	C11—N2—C12—C13	−179.8 (3)
C12—N2—C11—N3	0.2 (3)	C18—N2—C12—C13	5.4 (5)
C18—N2—C11—N3	174.5 (3)		

**Table 2**  
Hydrogen-bonding geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D\cdots H\cdots A$	$D\cdots H$	$H\cdots A$	$D\cdots A$	$D\cdots H\cdots A$
N1—H1A $\cdots$ O5	0.86	2.30	3.130 (4)	163
N1—H1B $\cdots$ N3	0.86	2.01	2.665 (4)	132

Data collection: P3 (Siemens, 1989); cell refinement: P3; data reduction: XDISK and XPREP (Siemens, 1991); program(s) used to solve structure: SHELXS (Sheldrick, 1990); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: XP (Siemens, 1991); software used to prepare material for publication: WinGX (Farrugia, 1999).

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