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2-[(2-Furylmethyl)sulfanyl]-1*H*-3,1-benzimidazol-3-ium chloride dihydrate

Sema Öztürk Yıldırım,[a] Mehmet Akkurt,[a]* Nihat Şireci,[b] Hasan Küçükbay[b] and Canan Kazak[c]

[a]Department of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, [b]Department of Chemistry, Faculty of Arts and Sciences, İnönü University, 44280 Malatya, Turkey, and [c]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey
Correspondence e-mail: akkurt@erciyes.edu.tr

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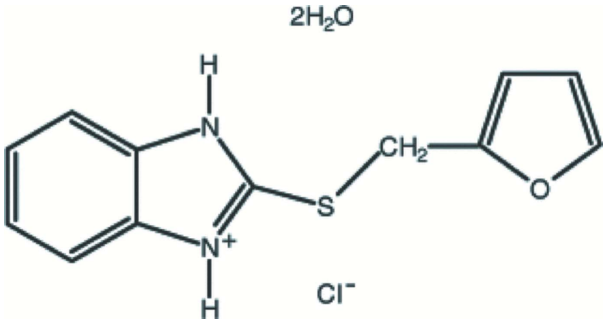
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.093; data-to-parameter ratio = 16.7.

The title compound, $C_{12}H_{11}N_2OS^+\cdot Cl^-\cdot 2H_2O$, was synthesized from the potassium salt of 2-mercaptobenzimidazole and 2-chloromethylfuran in ethanol. The molecule is not planar; the dihedral angle between the benzimidazole and furan ring systems is 83.2 (1)°. Cations, anions, and water molecules are extensively connected by hydrogen bonds.

Related literature

The crystal structures of some related benzimidazole derivatives have previously reported (Akkurt *et al.*, 2004; Akkurt *et al.*, 2005; Akkurt, Türktekin *et al.*, 2006; Akkurt, Yıldırım *et al.*, 2006; Yıldırım *et al.*, 2005).



Experimental

Crystal data

$C_{12}H_{11}N_2OS^+\cdot Cl^-\cdot 2H_2O$
M_r = 302.78
Monoclinic, $P2_1/c$
a = 7.0649 (6) Å
b = 21.5994 (17) Å
c = 9.5520 (7) Å
β = 97.925 (6)°
V = 1443.7 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.41 mm^{-1}
T = 296 K
0.51 × 0.42 × 0.32 mm

Data collection

Stoe IPDS-2 diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.817, T_{max} = 0.879
12197 measured reflections
3158 independent reflections
1882 reflections with $I > 2\sigma(I)$
R_{int} = 0.045

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.093
S = 0.84
3158 reflections
189 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.86	1.88	2.738 (2)	177
N2—H2A···Cl1	0.86	2.29	3.1032 (17)	159
O2—H21···Cl1^{ii}	0.93 (4)	2.25 (4)	3.178 (2)	177 (4)
O2—H22···O3^{iii}	0.77 (4)	2.11 (4)	2.850 (3)	162 (4)
O3—H31···Cl1	0.83 (3)	2.33 (3)	3.145 (2)	170 (3)
O3—H32···O2	0.93 (4)	1.87 (5)	2.763 (3)	160 (4)
C12—H12···Cl1^{iv}	0.93	2.82	3.673 (3)	152

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); 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: BT2335).

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supplementary materials

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2-[(2-Furylmethyl)sulfanyl]-1*H*-3,1-benzimidazol-3-ium chloride dihydrate

S. Ö. Yildirim, M. Akkurt, N. Sireci, H. Küçükbay and C. Kazak

Comment

In the molecule of (I) (Fig. 1), the C—N bond lengths (Table 1) in the benzimidazole ring system confirm the delocalization of the π electrons in this system. The title molecule is composed of a five-membered ring and a nine-membered bicyclic system linked by a thio and methylene group. The nine-membered benzimidazole ring and the five-membered furan ring (Fig. 1) are planar. The molecule, on the other hand, is not planar; the dihedral angle between the two ring systems is 83.2 (1)°. Geometric parameters are as expected (Table 1) and agree well with those reported for other structures (Akkurt *et al.*, 2004; Akkurt *et al.*, 2005; Akkurt, Türktekin *et al.*, 2006; Akkurt, Yıldırım *et al.*, 2006; Yıldırım *et al.*, 2005).

In the crystal structure, there are N—H···O, N—H···Cl, O—H···Cl, O—H···O and C—H···Cl intra- and intermolecular hydrogen bonds (Table 2) (Fig. 2).

Experimental

A mixture of potassium salt of 2-mercaptobenzimidazole (1.0 g; 5.3 mmol) and 2-chloromethylfuran (0.65 g; 5.3 mmol) in ethanol (25 ml) was heated under reflux for 5 h. The mixture was cooled to room temperature and potassium chloride was then filtered off and washed a little EtOH. All volatiles were removed *in vacuo* (0.02 m mH g; 1 m mH g = 133.322 Pa) and HCl was added to convertsalt form before crystallization of crude product from EtOH. (yield:1.2 g, 75%;m.p. 424–425 (dec)K. ^{1}H-NMR (DMSO-d_6, p.p.m.): 4.96 (*s*, –S—CH_2–, 2H),6.36 (*t*, furan-H, 1H), 6.50 (*d*, furan-H,1*H*),7.44 (*t*, Ar—H, 2H), 7.48 (s, –NH–, 1H), 7.67 (s, =NH–, 1H), 7.71 (*m*, Ar—H, 2H). ^{13}C-NMR ($CDCl_3$): δ 29.89, 107.30, 110.07, 113.77, 114.90, 125.59, 126.55, 130.86, 133.37, 144.16, 149.25. Analytical calculated for $C_{12}H_{15}N_2SO_3Cl$: C 47.60, H 4.95, N 9.25, S 10.57%. Found: C 47.25, H 4.95, N 9.06, S 11.07%.

Refinement

The H atoms of the water molecules were found from a difference Fourier map and refined freely. The other H atoms were geometrically positioned with $C_{aromatic}$–H = 0.93 $C_{methylene}$–H = 0.97Å and N–H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C,*N*).

Figures

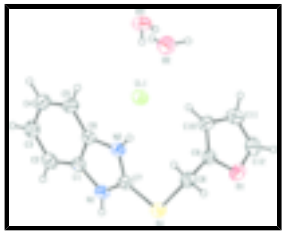

Fig. 1. An *ORTEP-3* view of (I), with the atom numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 30% probability level.

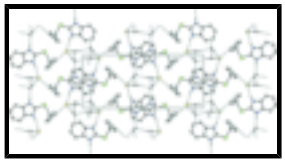

Fig. 2. A view of the crystal packing of (I), looking down the *a* axis; H atoms not involved in hydrogen bonds omitted; dashed lines indicate hydrogen contacts.

2-[(2-furylmethyl)sulfanyl]-1*H*-3,1-benzimidazol-3-ium chloride dihydrate

Crystal data

$C_{12}H_{11}N_2OS^+\cdot Cl^-\cdot 2H_2O$	F_{000} = 632
M_r = 302.78	D_x = 1.393 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 12416 reflections
a = 7.0649 (6) Å	θ = 1.9–27.1º
b = 21.5994 (17) Å	μ = 0.41 mm^{-1}
c = 9.5520 (7) Å	T = 296 K
β = 97.925 (6)º	Prism, colourless
V = 1443.7 (2) Å^3	0.51 × 0.42 × 0.32 mm
Z = 4	

Data collection

Stoe IPDS2 diffractometer	3158 independent reflections
Monochromator: plane graphite	1882 reflections with $I > 2\sigma(I)$
Detector resolution: 6.67 pixels mm^{-1}	R_{int} = 0.045
T = 296 K	θ_{max} = 27.1º
ω scans	θ_{min} = 1.9º
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	h = −9→9
T_{min} = 0.817, T_{max} = 0.879	k = −27→27
12197 measured reflections	l = −12→12

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0559P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.036	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.093	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
S = 0.84	$\Delta\rho_{min}$ = −0.25 e Å^{-3}
3158 reflections	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
189 parameters	Extinction coefficient: 0.0078 (13)

Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses 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 observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs 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}
S1	0.28109 (10)	0.18243 (3)	0.44205 (7)	0.0676 (2)
O1	−0.0559 (2)	0.26590 (7)	0.57648 (17)	0.0666 (6)
N1	0.2396 (2)	0.05992 (7)	0.41089 (17)	0.0508 (6)
N2	0.3027 (2)	0.08569 (7)	0.63196 (17)	0.0499 (5)
C1	0.2474 (3)	0.00497 (9)	0.4873 (2)	0.0463 (6)
C2	0.2215 (3)	−0.05649 (10)	0.4465 (2)	0.0563 (8)
C3	0.2386 (3)	−0.09954 (10)	0.5533 (3)	0.0616 (8)
C4	0.2792 (3)	−0.08243 (10)	0.6947 (2)	0.0649 (9)
C5	0.3050 (3)	−0.02185 (10)	0.7354 (2)	0.0578 (8)
C6	0.2875 (3)	0.02143 (9)	0.6287 (2)	0.0455 (6)
C7	0.2740 (3)	0.10729 (9)	0.4996 (2)	0.0494 (7)
C8	0.2646 (3)	0.22625 (9)	0.6037 (2)	0.0573 (8)
C9	0.0741 (3)	0.22686 (8)	0.6481 (2)	0.0480 (6)
C10	−0.0055 (3)	0.19611 (10)	0.7456 (2)	0.0545 (7)
C11	−0.1959 (3)	0.21770 (11)	0.7380 (2)	0.0630 (8)
C12	−0.2199 (3)	0.25924 (11)	0.6361 (3)	0.0681 (9)
O2	−0.1594 (3)	0.06471 (12)	0.9334 (2)	0.0775 (8)
O3	0.1745 (3)	0.06500 (8)	1.12185 (18)	0.0678 (6)
Cl1	0.44294 (7)	0.13331 (2)	0.93504 (6)	0.0562 (2)
H1	0.21620	0.06280	0.32040	0.0610*
H2	0.19410	−0.06790	0.35200	0.0680*
H2A	0.32680	0.10790	0.70700	0.0600*
H3	0.22270	−0.14130	0.53050	0.0740*
H4	0.28910	−0.11310	0.76370	0.0780*
H5	0.33270	−0.01060	0.83000	0.0690*
H8A	0.35430	0.20890	0.67950	0.0690*
H8B	0.30330	0.26860	0.58960	0.0690*
H10	0.05280	0.16620	0.80700	0.0650*

H11	−0.28650	0.20500	0.79400	0.0760*
H12	−0.33250	0.28100	0.60870	0.0820*
H21	−0.274 (6)	0.0857 (18)	0.937 (4)	0.152 (15)*
H22	−0.182 (6)	0.0299 (19)	0.929 (4)	0.138 (18)*
H31	0.252 (4)	0.0849 (12)	1.082 (3)	0.084 (9)*
H32	0.055 (6)	0.073 (2)	1.070 (5)	0.176 (18)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0905 (5)	0.0574 (3)	0.0611 (4)	0.0132 (3)	0.0330 (3)	0.0147 (3)
O1	0.0700 (10)	0.0607 (9)	0.0695 (11)	0.0096 (8)	0.0112 (8)	0.0167 (8)
N1	0.0570 (10)	0.0601 (10)	0.0360 (9)	0.0062 (8)	0.0094 (7)	0.0019 (8)
N2	0.0623 (10)	0.0496 (9)	0.0387 (9)	0.0012 (8)	0.0104 (8)	−0.0020 (7)
C1	0.0454 (10)	0.0544 (11)	0.0401 (11)	0.0048 (9)	0.0090 (8)	0.0007 (9)
C2	0.0559 (13)	0.0628 (13)	0.0508 (13)	−0.0004 (10)	0.0091 (10)	−0.0120 (10)
C3	0.0666 (14)	0.0517 (12)	0.0667 (16)	−0.0010 (10)	0.0103 (11)	−0.0067 (11)
C4	0.0845 (17)	0.0529 (12)	0.0575 (15)	0.0010 (11)	0.0107 (12)	0.0077 (11)
C5	0.0730 (15)	0.0573 (12)	0.0430 (12)	0.0007 (10)	0.0081 (10)	0.0039 (9)
C6	0.0488 (11)	0.0464 (10)	0.0421 (11)	0.0023 (8)	0.0092 (8)	−0.0008 (8)
C7	0.0515 (12)	0.0556 (11)	0.0430 (12)	0.0068 (9)	0.0137 (9)	0.0049 (9)
C8	0.0591 (13)	0.0468 (11)	0.0677 (15)	−0.0030 (9)	0.0152 (11)	0.0052 (10)
C9	0.0534 (11)	0.0415 (10)	0.0487 (12)	0.0012 (9)	0.0053 (9)	−0.0025 (9)
C10	0.0541 (12)	0.0555 (12)	0.0535 (13)	0.0005 (9)	0.0057 (10)	0.0112 (10)
C11	0.0580 (13)	0.0800 (16)	0.0527 (13)	−0.0050 (12)	0.0136 (10)	0.0011 (12)
C12	0.0545 (14)	0.0699 (14)	0.0804 (18)	0.0128 (11)	0.0107 (12)	−0.0016 (13)
O2	0.0754 (13)	0.0817 (14)	0.0744 (13)	0.0137 (11)	0.0066 (9)	0.0059 (10)
O3	0.0687 (11)	0.0866 (12)	0.0487 (10)	−0.0051 (9)	0.0100 (8)	0.0097 (8)
Cl1	0.0560 (3)	0.0628 (3)	0.0493 (3)	−0.0030 (2)	0.0055 (2)	−0.0033 (2)

Geometric parameters (Å, °)

S1—C7	1.717 (2)	C3—C4	1.392 (3)
S1—C8	1.828 (2)	C4—C5	1.370 (3)
O1—C9	1.360 (2)	C5—C6	1.376 (3)
O1—C12	1.367 (3)	C8—C9	1.466 (3)
O2—H21	0.93 (4)	C9—C10	1.330 (3)
O2—H22	0.77 (4)	C10—C11	1.416 (3)
O3—H31	0.83 (3)	C11—C12	1.318 (3)
O3—H32	0.93 (4)	C2—H2	0.9300
N1—C7	1.329 (2)	C3—H3	0.9300
N1—C1	1.391 (2)	C4—H4	0.9300
N2—C6	1.392 (2)	C5—H5	0.9300
N2—C7	1.337 (2)	C8—H8A	0.9700
N1—H1	0.8600	C8—H8B	0.9700
N2—H2A	0.8600	C10—H10	0.9300
C1—C6	1.388 (3)	C11—H11	0.9300
C1—C2	1.389 (3)	C12—H12	0.9300
C2—C3	1.373 (3)		

Cl1···N2	3.1032 (17)	C10···H3^{viii}	3.1000
Cl1···O2^{i}	3.178 (2)	C10···H2A	3.0800
Cl1···O3	3.145 (2)	C11···H3^{viii}	3.0300
Cl1···H11^{i}	2.9300	C12···H3^{viii}	3.0000
Cl1···H2A	2.2900	C12···H4^{xi}	2.9800
Cl1···H8A	2.9300	H1···O3^{ix}	1.8800
Cl1···H10	2.9400	H1···H31^{ix}	2.3700
Cl1···H8B^{ii}	2.8400	H1···H32^{ix}	2.5100
Cl1···H21^{i}	2.25 (4)	H2···O2^{viii}	2.7000
Cl1···H31	2.33 (3)	H2A···Cl1	2.2900
Cl1···H12^{iii}	2.8200	H2A···H8A	2.2100
S1···O1	3.3780 (17)	H2A···H10	2.6000
S1···C9^{iv}	3.568 (2)	H2A···C8	2.7500
S1···C10^{iv}	3.668 (2)	H2A···C10	3.0800
O1···C10^{iv}	3.332 (3)	H3···C10^{viii}	3.1000
O1···S1	3.3780 (17)	H3···C12^{viii}	3.0000
O1···C11^{iv}	3.267 (3)	H3···C11^{viii}	3.0300
O2···Cl1^{v}	3.178 (2)	H4···H12^{xii}	2.5900
O2···O3^{vi}	2.850 (3)	H4···C12^{xii}	2.9800
O2···O3	2.763 (3)	H8A···N2	2.7200
O3···O2^{vi}	2.850 (3)	H8A···Cl1	2.9300
O3···Cl1	3.145 (2)	H8A···H2A	2.2100
O3···N1^{vii}	2.738 (2)	H8B···H12^{i}	2.5700
O3···O2	2.763 (3)	H8B···Cl1^{iv}	2.8400
O2···H32	1.87 (5)	H10···Cl1	2.9400
O2···H2^{viii}	2.7000	H10···H2A	2.6000
O3···H22^{vi}	2.11 (4)	H11···Cl1^{v}	2.9300
O3···H1^{vii}	1.8800	H12···C8^{v}	3.0800
N1···O3^{ix}	2.738 (2)	H12···Cl1^{xiii}	2.8200
N1···N2	2.170 (2)	H12···H8B^{v}	2.5700
N2···N1	2.170 (2)	H12···H4^{xi}	2.5900
N2···Cl1	3.1032 (17)	H21···H32	2.51 (6)
N2···H8A	2.7200	H21···Cl1^{v}	2.25 (4)
C1···C1^{x}	3.550 (3)	H22···O3^{vi}	2.11 (4)
C1···C1^{viii}	3.544 (3)	H22···H32^{vi}	2.40 (6)
C3···C7^{x}	3.553 (3)	H22···H31^{vi}	2.53 (5)
C3···C7^{viii}	3.591 (3)	H22···H32	2.21 (6)
C7···C3^{viii}	3.591 (3)	H31···H22^{vi}	2.53 (5)
C7···C3^{x}	3.553 (3)	H31···Cl1	2.33 (3)
C9···S1^{ii}	3.568 (2)	H31···H1^{vii}	2.3700
C10···O1^{ii}	3.332 (3)	H32···H1^{vii}	2.5100

C10···S1^{ii}	3.668 (2)	H32···H21	2.51 (6)
C11···O1^{ii}	3.267 (3)	H32···H22	2.21 (6)
C8···H12^{i}	3.0800	H32···H22^{vi}	2.40 (6)
C8···H2A	2.7500	H32···O2	1.87 (5)
C7—S1—C8	102.18 (9)	O1—C9—C10	109.90 (19)
C9—O1—C12	106.11 (17)	O1—C9—C8	116.32 (16)
H21—O2—H22	108 (4)	C9—C10—C11	106.86 (18)
H31—O3—H32	106 (3)	C10—C11—C12	106.66 (19)
C1—N1—C7	109.38 (16)	O1—C12—C11	110.4 (2)
C6—N2—C7	109.01 (16)	C1—C2—H2	122.00
C7—N1—H1	125.00	C3—C2—H2	122.00
C1—N1—H1	125.00	C4—C3—H3	119.00
C7—N2—H2A	125.00	C2—C3—H3	119.00
C6—N2—H2A	126.00	C5—C4—H4	119.00
C2—C1—C6	121.30 (18)	C3—C4—H4	119.00
N1—C1—C2	132.42 (18)	C6—C5—H5	122.00
N1—C1—C6	106.27 (16)	C4—C5—H5	122.00
C1—C2—C3	116.37 (19)	S1—C8—H8A	109.00
C2—C3—C4	121.8 (2)	C9—C8—H8B	109.00
C3—C4—C5	122.05 (19)	S1—C8—H8B	109.00
C4—C5—C6	116.35 (18)	C9—C8—H8A	109.00
C1—C6—C5	122.17 (18)	H8A—C8—H8B	107.00
N2—C6—C5	131.46 (18)	C11—C10—H10	127.00
N2—C6—C1	106.38 (16)	C9—C10—H10	127.00
S1—C7—N1	122.31 (15)	C10—C11—H11	127.00
S1—C7—N2	128.73 (15)	C12—C11—H11	127.00
N1—C7—N2	108.96 (17)	C11—C12—H12	125.00
S1—C8—C9	114.64 (14)	O1—C12—H12	125.00
C8—C9—C10	133.77 (19)		
C8—S1—C7—N1	164.63 (17)	C2—C1—C6—N2	−179.44 (19)
C8—S1—C7—N2	−16.5 (2)	C2—C1—C6—C5	0.5 (3)
C7—S1—C8—C9	−74.29 (16)	N1—C1—C2—C3	−179.4 (2)
C12—O1—C9—C8	−179.37 (18)	N1—C1—C6—C5	179.77 (19)
C9—O1—C12—C11	−0.9 (3)	C1—C2—C3—C4	0.2 (3)
C12—O1—C9—C10	1.4 (2)	C2—C3—C4—C5	−0.2 (3)
C1—N1—C7—N2	−0.5 (2)	C3—C4—C5—C6	0.4 (3)
C7—N1—C1—C6	0.4 (2)	C4—C5—C6—C1	−0.5 (3)
C7—N1—C1—C2	179.6 (2)	C4—C5—C6—N2	179.4 (2)
C1—N1—C7—S1	178.54 (15)	S1—C8—C9—O1	−77.85 (19)
C6—N2—C7—S1	−178.54 (17)	S1—C8—C9—C10	101.1 (2)
C6—N2—C7—N1	0.4 (2)	O1—C9—C10—C11	−1.3 (2)
C7—N2—C6—C5	179.9 (2)	C8—C9—C10—C11	179.6 (2)
C7—N2—C6—C1	−0.2 (2)	C9—C10—C11—C12	0.7 (3)
N1—C1—C6—N2	−0.1 (2)	C10—C11—C12—O1	0.1 (3)
C6—C1—C2—C3	−0.3 (3)		

Symmetry codes: (i) *x*+1, *y*, *z*; (ii) *x*, −*y*+1/2, *z*+1/2; (iii) *x*+1, −*y*+1/2, *z*+1/2; (iv) *x*, −*y*+1/2, *z*−1/2; (v) *x*−1, *y*, *z*; (vi) −*x*, −*y*, −*z*+2; (vii) *x*, *y*, *z*+1; (viii) −*x*, −*y*, −*z*+1; (ix) *x*, *y*, *z*−1; (x) −*x*+1, −*y*, −*z*+1; (xi) −*x*, *y*+1/2, −*z*+3/2; (xii) −*x*, *y*−1/2, −*z*+3/2; (xiii) *x*−1, −*y*+1/2, *z*−1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{ix}	0.86	1.88	2.738 (2)	177
N2—H2A···Cl1	0.86	2.29	3.1032 (17)	159
O2—H21···Cl1^{v}	0.93 (4)	2.25 (4)	3.178 (2)	177 (4)
O2—H22···O3^{vi}	0.77 (4)	2.11 (4)	2.850 (3)	162 (4)
O3—H31···Cl1	0.83 (3)	2.33 (3)	3.145 (2)	170 (3)
O3—H32···O2	0.93 (4)	1.87 (5)	2.763 (3)	160 (4)
C12—H12···Cl1^{xiii}	0.93	2.82	3.673 (3)	152

Symmetry codes: (ix) *x*, *y*, *z*−1; (v) *x*−1, *y*, *z*; (vi) −*x*, −*y*, −*z*+2; (xiii) *x*−1, −*y*+1/2, *z*−1/2.

Fig. 1

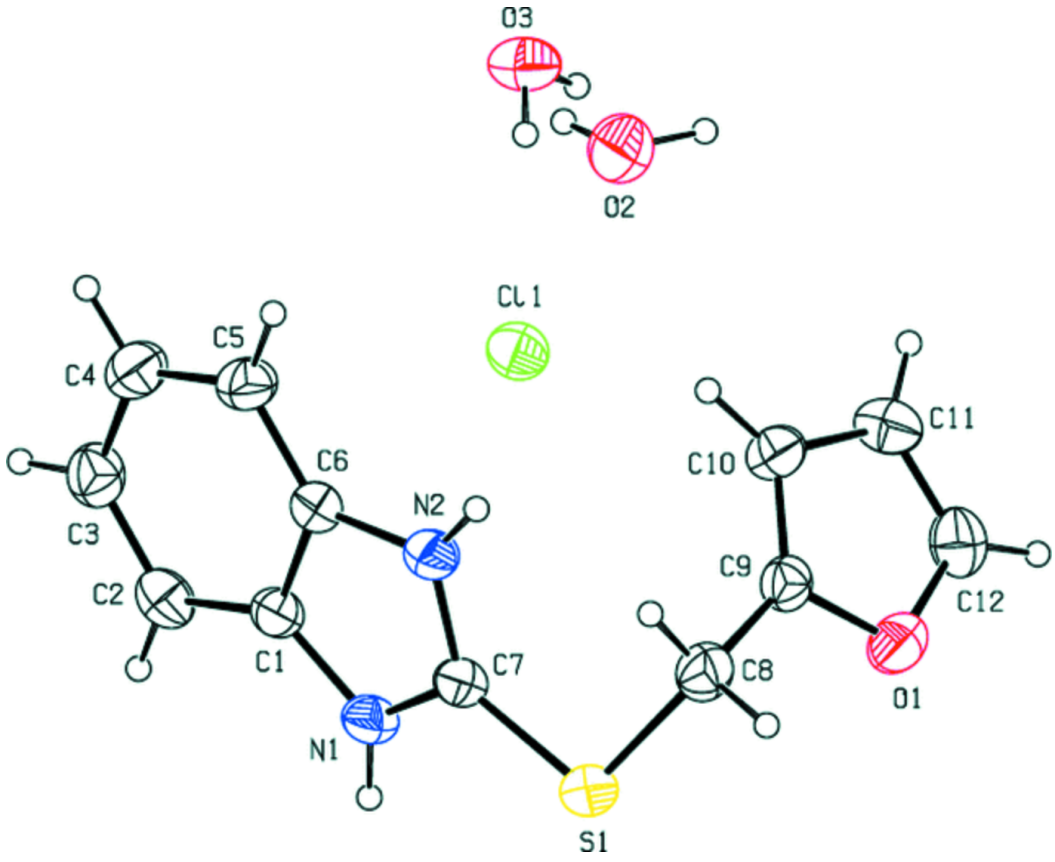

Fig. 2