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Ornidazole hemihydrate

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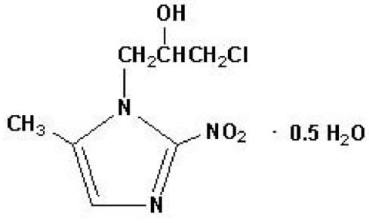
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.146; data-to-parameter ratio = 18.1.

The asymmetric unit of the racemic title compound, $C_7H_{10}ClN_3O_3\cdot0.5H_2O$, has two independent molecules of ornidazole. The crystal structure is formed *via* intermolecular hydrogen bonds involving the water molecules.

Related literature

For related literature, see: López Nigro *et al.* (2003).



Experimental

Crystal data

$C_7H_{10}ClN_3O_3\cdot0.5H_2O$
M_r = 228.64
Monoclinic, $C2/c$
a = 23.202 (8) Å
b = 8.289 (2) Å
c = 22.270 (7) Å
β = 103.996 (14)°
V = 4156 (2) Å^3
Z = 16
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 298 (1) K
0.31 × 0.28 × 0.25 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.890, T_{max} = 0.914
18814 measured reflections
4755 independent reflections
3287 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.026

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.146
S = 1.00
4755 reflections
263 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.62 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H701···O11^{i}	0.94	1.85	2.7854 (17)	169
O7—H702···N12	0.94	1.87	2.808 (2)	172
O11—H11···N22	0.93	1.80	2.726 (2)	174
O21—H21···O7^{ii}	0.97	1.71	2.6643 (18)	171

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

Data collection: *PROCESS-AUTO* (Rigaku/MSC & Rigaku, 2004); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC & Rigaku, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2037).

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  doi:10.1107/S1600536807045680

supplementary materials

Acta Cryst. (2007). E**63**, o4204 [**doi:10.1107/S1600536807045680**]

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Comment

5–Nitroimidazoles are a well–established group of antiprotozoan and antibacterial agents. 1–(2–Hydroxy–3–chloropropyl)–2–methyl–5–nitroimidazole (ornidazole) is a member of the nitroimidazole group so it is used for the treatment of susceptible protozoal infections and prophylaxis of anaerobic bacterial infections. Due to its antimicrobial activity it inhibits the growth of both anaerobic bacteria and certain anaerobic protozoa such as *Trichomonas vaginalis*, *Entamoeba histolytica* and *Giardia lamblia* (López Nigro *et al.*, 2003). The asymmetric unit have two independent molecules of ornidazole with the different chirality - C12 atom is *R* and C22 atom is *S* absolute configuration. The crystal structure of the title compound is formed by the system of intermolecular hydrogen bonds, which involve the water molecules.

Experimental

1–(2-Hydroxy–3–chloropropyl)–2-methyl–5–nitroimidazole was recrystallized from C_5H_5OH/H_2O (1:1) to give the ornidazole hemihydrate. Diffraction quality crystal was obtained by slow evaporation of at room temperature.

Refinement

The H atoms on the oxygen were located in a difference Fourier map and the other H atoms were placed in calculated posistion with C—H = 0.96–0.98 Å. All H atoms included in the final cycles of refinement as riding mode, with U_{iso}(H) = 1.2U_{eq} of the carrier atoms.

Figures

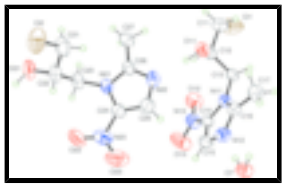

Fig. 1. The *ORTEP* view of the title complex with the numbering scheme. The displacement ellipsoids are drawn with the 50% probability level.

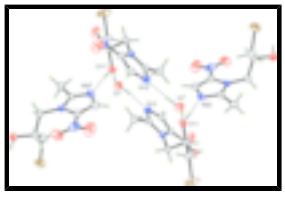

Fig. 2. View of the two crystallographically independent molecules linked by hydrogen bonds.

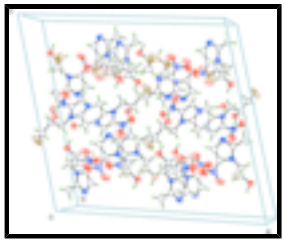

Fig. 3. Unit cell packing of the title compound.

Ornidazole hemihydrate

Crystal data

$C_7H_{10}ClN_3O_3 \cdot 0.5H_2O$	F_{000} = 1904.00
M_r = 228.64	D_x = 1.462 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71075 Å
Hall symbol: -C 2yc	Cell parameters from 14509 reflections
a = 23.202 (8) Å	θ = 3.1–27.5º
b = 8.289 (2) Å	μ = 0.36 mm^{-1}
c = 22.270 (7) Å	*T* = 298 (1) K
β = 103.996 (14)º	Block, colourless
V = 4156 (2) Å^3	0.31 × 0.28 × 0.25 mm
Z = 16	

Data collection

Rigaku R-AXIS RAPID diffractometer	3287 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	R_{int} = 0.026
ω scans	θ_{max} = 27.5º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −30→30
T_{min} = 0.890, T_{max} = 0.914	*k* = −10→9
18814 measured reflections	*l* = −28→28
4755 independent reflections	

Refinement

Refinement on F^2	$w = 1/[0.002F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$R[F^2 > 2\sigma(F^2)]$ = 0.045	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.146	$\Delta\rho_{max}$ = 0.59 e Å^{-3}
S = 1.01	$\Delta\rho_{min}$ = −0.62 e Å^{-3}
4755 reflections	Extinction correction: Larson, A. C. (1970). Crystallographic Computing, edited by F. R. Ahmed, pp. 291–294. Copenhagen: Munksgaard.
263 parameters	Extinction coefficient: 94 (36)
H-atom parameters constrained	

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 using all reflections. The weighted R–factor (*wR*) and goodness of fit (S) are based on F^2. R–factor (gt) are based on F. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating R–factor (gt).

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.51877 (3)	0.54256 (8)	0.64516 (4)	0.0940 (2)
Cl2	0.36375 (4)	1.26213 (8)	0.21447 (4)	0.0870 (2)
O7	0.12252 (6)	0.44528 (16)	0.43419 (6)	0.0487 (3)
O11	0.38555 (6)	0.74189 (13)	0.52290 (6)	0.0433 (3)
O12	0.43759 (6)	0.28657 (19)	0.48376 (8)	0.0615 (4)
O13	0.37775 (9)	0.1710 (2)	0.40646 (9)	0.0889 (6)
O21	0.43764 (6)	0.9665 (2)	0.18369 (6)	0.0604 (4)
O22	0.31344 (9)	0.6537 (2)	0.19209 (8)	0.0759 (5)
O23	0.25133 (9)	0.5497 (2)	0.23892 (10)	0.0952 (7)
N11	0.33913 (6)	0.42982 (16)	0.51646 (6)	0.0347 (3)
N12	0.24678 (6)	0.42340 (19)	0.45819 (8)	0.0454 (4)
N13	0.38789 (8)	0.2606 (2)	0.45115 (8)	0.0508 (4)
N21	0.38473 (6)	0.75918 (17)	0.30684 (6)	0.0384 (3)
N22	0.36136 (8)	0.7319 (2)	0.39693 (8)	0.0484 (4)
N23	0.29640 (8)	0.6258 (2)	0.23892 (9)	0.0590 (5)
C11	0.46743 (8)	0.6864 (2)	0.60469 (10)	0.0475 (5)
C12	0.42434 (8)	0.6139 (2)	0.54889 (8)	0.0374 (4)
C13	0.38913 (6)	0.4751 (2)	0.56720 (8)	0.0368 (4)
C14	0.33813 (8)	0.3374 (2)	0.46472 (8)	0.0388 (4)
C15	0.28143 (9)	0.3346 (2)	0.43015 (9)	0.0438 (4)
C16	0.28216 (8)	0.4799 (2)	0.51017 (8)	0.0378 (4)
C17	0.26214 (9)	0.5812 (2)	0.55585 (10)	0.0501 (5)
C21	0.39930 (12)	1.0974 (2)	0.26126 (11)	0.0650 (7)
C22	0.39831 (9)	0.9501 (2)	0.22289 (9)	0.0496 (5)
C23	0.41990 (8)	0.8002 (2)	0.26236 (9)	0.0459 (5)
C24	0.33042 (8)	0.6820 (2)	0.29689 (9)	0.0438 (4)
C25	0.31703 (9)	0.6678 (2)	0.35252 (10)	0.0506 (5)
C26	0.40150 (8)	0.7856 (2)	0.36831 (8)	0.0388 (4)
C27	0.45826 (9)	0.8620 (2)	0.40072 (9)	0.0519 (5)
H11	0.3781	0.7312	0.4804	0.052*
H21	0.4123	0.9602	0.1424	0.074*
H111	0.4450	0.7297	0.6326	0.057*
H112	0.4892	0.7728	0.5908	0.057*
H122	0.4460	0.5762	0.5189	0.045*
H131	0.3742	0.5078	0.6024	0.044*

H132	0.4151	0.3827	0.5785	0.044*
H151	0.2684	0.2799	0.3929	0.053*
H171	0.2206	0.6048	0.5409	0.060*
H172	0.2684	0.5244	0.5945	0.060*
H173	0.2843	0.6800	0.5619	0.060*
H211	0.4402	1.1262	0.2802	0.078*
H212	0.3786	1.0757	0.2933	0.078*
H221	0.3579	0.9317	0.1978	0.060*
H231	0.4606	0.8191	0.2852	0.055*
H232	0.4187	0.7091	0.2347	0.055*
H251	0.2826	0.6213	0.3592	0.061*
H271	0.4599	0.8700	0.4441	0.062*
H272	0.4909	0.7975	0.3950	0.062*
H273	0.4608	0.9679	0.3841	0.062*
H701	0.1147	0.5476	0.4490	0.058*
H702	0.1637	0.4386	0.4380	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0725 (4)	0.0614 (3)	0.1148 (6)	0.0113 (3)	−0.0424 (4)	−0.0073 (3)
Cl2	0.1094 (5)	0.0701 (4)	0.0873 (5)	0.0288 (3)	0.0349 (4)	0.0337 (3)
O7	0.0426 (7)	0.0498 (7)	0.0506 (7)	0.0022 (5)	0.0053 (5)	−0.0054 (5)
O11	0.0546 (7)	0.0402 (6)	0.0349 (6)	0.0055 (5)	0.0103 (5)	0.0015 (5)
O12	0.0428 (7)	0.0742 (9)	0.0691 (10)	0.0090 (7)	0.0168 (7)	−0.0120 (8)
O13	0.0853 (12)	0.1008 (13)	0.0805 (12)	0.0155 (10)	0.0200 (10)	−0.0501 (11)
O21	0.0479 (7)	0.0967 (11)	0.0396 (7)	0.0034 (7)	0.0165 (6)	0.0138 (7)
O22	0.0980 (13)	0.0804 (11)	0.0395 (8)	−0.0058 (9)	−0.0024 (8)	−0.0063 (7)
O23	0.0642 (11)	0.1136 (15)	0.0996 (15)	−0.0259 (11)	0.0042 (10)	−0.0344 (12)
N11	0.0328 (7)	0.0361 (6)	0.0346 (7)	0.0018 (5)	0.0069 (5)	−0.0001 (5)
N12	0.0355 (7)	0.0486 (8)	0.0483 (9)	0.0001 (6)	0.0025 (6)	0.0026 (7)
N13	0.0540 (10)	0.0498 (9)	0.0506 (9)	0.0072 (7)	0.0167 (8)	−0.0085 (7)
N21	0.0413 (7)	0.0424 (7)	0.0313 (7)	0.0063 (6)	0.0083 (5)	0.0046 (5)
N22	0.0544 (9)	0.0546 (9)	0.0376 (8)	0.0031 (7)	0.0134 (7)	0.0078 (7)
N23	0.0562 (11)	0.0573 (10)	0.0544 (11)	0.0027 (9)	−0.0046 (8)	−0.0087 (8)
C11	0.0412 (9)	0.0422 (9)	0.0540 (11)	0.0029 (7)	0.0015 (8)	−0.0085 (8)
C12	0.0368 (8)	0.0372 (8)	0.0383 (9)	0.0032 (7)	0.0093 (7)	−0.0038 (7)
C13	0.0361 (8)	0.0416 (8)	0.0310 (8)	0.0013 (7)	0.0047 (6)	−0.0005 (6)
C14	0.0429 (9)	0.0363 (8)	0.0372 (9)	0.0008 (7)	0.0097 (7)	−0.0023 (6)
C15	0.0480 (10)	0.0429 (9)	0.0365 (9)	−0.0042 (8)	0.0024 (7)	−0.0026 (7)
C16	0.0342 (8)	0.0371 (8)	0.0416 (9)	0.0024 (7)	0.0084 (7)	0.0046 (7)
C17	0.0457 (10)	0.0535 (10)	0.0532 (11)	0.0095 (8)	0.0160 (9)	0.0003 (8)
C21	0.0857 (17)	0.0616 (12)	0.0488 (12)	0.0138 (12)	0.0181 (11)	0.0135 (10)
C22	0.0488 (10)	0.0629 (11)	0.0405 (10)	0.0081 (9)	0.0177 (8)	0.0127 (8)
C23	0.0440 (10)	0.0590 (11)	0.0365 (9)	0.0114 (8)	0.0135 (7)	0.0057 (8)
C24	0.0420 (9)	0.0460 (9)	0.0411 (10)	0.0029 (7)	0.0055 (7)	0.0017 (7)
C25	0.0481 (11)	0.0520 (10)	0.0519 (11)	−0.0038 (9)	0.0124 (9)	0.0058 (8)
C26	0.0431 (9)	0.0397 (8)	0.0328 (8)	0.0065 (7)	0.0077 (7)	0.0048 (6)

C27	0.0492 (11)	0.0606 (11)	0.0417 (10)	0.0022 (9)	0.0027 (8)	−0.0016 (8)

Geometric parameters (Å, °)

Cl1—C11	1.7702 (19)	C22—C23	1.534 (2)
Cl2—C21	1.793 (2)	C24—C25	1.353 (3)
O11—C12	1.421 (2)	C26—C27	1.482 (2)
O12—N13	1.224 (2)	O7—H701	0.944
O13—N13	1.218 (2)	O7—H702	0.940
O21—C22	1.414 (2)	O11—H11	0.925
O22—N23	1.223 (2)	O21—H21	0.965
O23—N23	1.221 (2)	C11—H111	0.970
N11—C13	1.4593 (19)	C11—H112	0.970
N11—C14	1.379 (2)	C12—H122	0.980
N11—C16	1.360 (2)	C13—H131	0.970
N12—C15	1.350 (2)	C13—H132	0.970
N12—C16	1.332 (2)	C15—H151	0.930
N13—C14	1.414 (2)	C17—H171	0.960
N21—C23	1.468 (2)	C17—H172	0.960
N21—C24	1.383 (2)	C17—H173	0.960
N21—C26	1.347 (2)	C21—H211	0.970
N22—C25	1.351 (2)	C21—H212	0.970
N22—C26	1.326 (2)	C22—H221	0.980
N23—C24	1.419 (2)	C23—H231	0.970
C11—C12	1.518 (2)	C23—H232	0.970
C12—C13	1.522 (2)	C25—H251	0.930
C14—C15	1.354 (2)	C27—H271	0.960
C16—C17	1.478 (2)	C27—H272	0.960
C21—C22	1.488 (3)	C27—H273	0.960
C13—N11—C14	129.75 (14)	Cl1—C11—H112	108.8
C13—N11—C16	124.89 (14)	C12—C11—H111	108.8
C14—N11—C16	105.31 (13)	C12—C11—H112	108.8
C15—N12—C16	106.46 (15)	H111—C11—H112	109.5
O12—N13—O13	124.1 (2)	O11—C12—H122	109.8
O12—N13—C14	119.65 (16)	C11—C12—H122	109.8
O13—N13—C14	116.28 (17)	C13—C12—H122	109.8
C23—N21—C24	129.28 (15)	N11—C13—H131	109.0
C23—N21—C26	125.24 (15)	N11—C13—H132	109.0
C24—N21—C26	105.43 (16)	C12—C13—H131	109.0
C25—N22—C26	106.19 (17)	C12—C13—H132	109.0
O22—N23—O23	123.43 (19)	H131—C13—H132	109.5
O22—N23—C24	119.36 (18)	N12—C15—H151	125.3
O23—N23—C24	117.2 (2)	C14—C15—H151	125.3
Cl1—C11—C12	112.27 (13)	C16—C17—H171	109.5
O11—C12—C11	105.34 (13)	C16—C17—H172	109.5
O11—C12—C13	110.20 (14)	C16—C17—H173	109.5
C11—C12—C13	111.70 (15)	H171—C17—H172	109.5
N11—C13—C12	111.38 (13)	H171—C17—H173	109.5
N11—C14—N13	125.40 (14)	H172—C17—H173	109.5

N11—C14—C15	107.59 (16)	Cl2—C21—H211	109.2
N13—C14—C15	127.01 (16)	Cl2—C21—H212	109.2
N12—C15—C14	109.45 (16)	C22—C21—H211	109.2
N11—C16—N12	111.18 (16)	C22—C21—H212	109.2
N11—C16—C17	124.20 (14)	H211—C21—H212	109.5
N12—C16—C17	124.61 (16)	O21—C22—H221	109.6
Cl2—C21—C22	110.50 (15)	C21—C22—H221	109.6
O21—C22—C21	110.69 (18)	C23—C22—H221	109.6
O21—C22—C23	105.16 (16)	N21—C23—H231	108.2
C21—C22—C23	112.22 (16)	N21—C23—H232	108.2
N21—C23—C22	114.63 (16)	C22—C23—H231	108.2
N21—C24—N23	125.63 (18)	C22—C23—H232	108.2
N21—C24—C25	107.19 (15)	H231—C23—H232	109.5
N23—C24—C25	127.17 (18)	N22—C25—H251	125.3
N22—C25—C24	109.48 (18)	C24—C25—H251	125.3
N21—C26—N22	111.71 (15)	C26—C27—H271	109.5
N21—C26—C27	124.64 (18)	C26—C27—H272	109.5
N22—C26—C27	123.64 (16)	C26—C27—H273	109.5
H701—O7—H702	107.3	H271—C27—H272	109.5
C12—O11—H11	106.7	H271—C27—H273	109.5
C22—O21—H21	104.3	H272—C27—H273	109.5
Cl1—C11—H111	108.8		
C13—N11—C14—N13	2.1 (2)	C24—N21—C26—N22	−0.6 (2)
C13—N11—C14—C15	−177.86 (16)	C24—N21—C26—C27	178.17 (17)
C14—N11—C13—C12	79.1 (2)	C26—N21—C24—N23	−178.00 (17)
C13—N11—C16—N12	177.80 (15)	C26—N21—C24—C25	0.8 (2)
C13—N11—C16—C17	−3.4 (2)	C25—N22—C26—N21	0.2 (2)
C16—N11—C13—C12	−97.8 (2)	C25—N22—C26—C27	−178.59 (17)
C14—N11—C16—N12	0.24 (19)	C26—N22—C25—C24	0.3 (2)
C14—N11—C16—C17	179.06 (17)	O22—N23—C24—N21	−4.4 (2)
C16—N11—C14—N13	179.52 (17)	O22—N23—C24—C25	177.1 (2)
C16—N11—C14—C15	−0.46 (19)	O23—N23—C24—N21	174.86 (19)
C15—N12—C16—N11	0.07 (19)	O23—N23—C24—C25	−3.6 (3)
C15—N12—C16—C17	−178.74 (18)	Cl1—C11—C12—O11	178.33 (13)
C16—N12—C15—C14	−0.4 (2)	Cl1—C11—C12—C13	58.69 (19)
O12—N13—C14—N11	−7.1 (2)	O11—C12—C13—N11	50.51 (19)
O12—N13—C14—C15	172.92 (19)	C11—C12—C13—N11	167.24 (14)
O13—N13—C14—N11	173.08 (18)	N11—C14—C15—N12	0.5 (2)
O13—N13—C14—C15	−6.9 (2)	N13—C14—C15—N12	−179.46 (17)
C23—N21—C24—N23	−0.5 (3)	Cl2—C21—C22—O21	71.3 (2)
C23—N21—C24—C25	178.28 (17)	Cl2—C21—C22—C23	−171.55 (15)
C24—N21—C23—C22	78.6 (2)	O21—C22—C23—N21	−179.62 (14)
C23—N21—C26—N22	−178.24 (16)	C21—C22—C23—N21	60.0 (2)
C23—N21—C26—C27	0.5 (2)	N21—C24—C25—N22	−0.7 (2)
C26—N21—C23—C22	−104.36 (19)	N23—C24—C25—N22	178.05 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

O7—H701···O11^{i}	0.94	1.85	2.7854 (17)	169
O7—H702···N12	0.94	1.87	2.808 (2)	172
O11—H11···N22	0.93	1.80	2.726 (2)	174
O21—H21···O7^{ii}	0.97	1.71	2.6643 (18)	171

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

Fig. 1

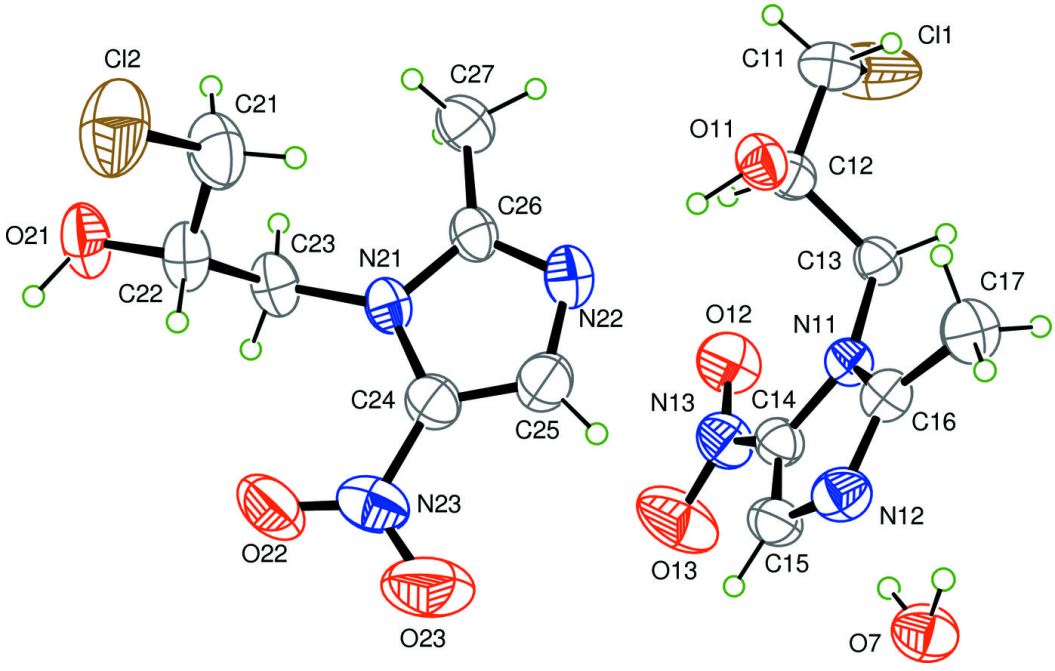
Cl2
C21
C27
O21
C23
N21
C26
C22
N22
C24
C25
N23
O22
O23
Cl1
C11
O11
C12
C13
C17
O12
N11
N13
C14
C16
N12
O13
C15
O7

Fig. 2

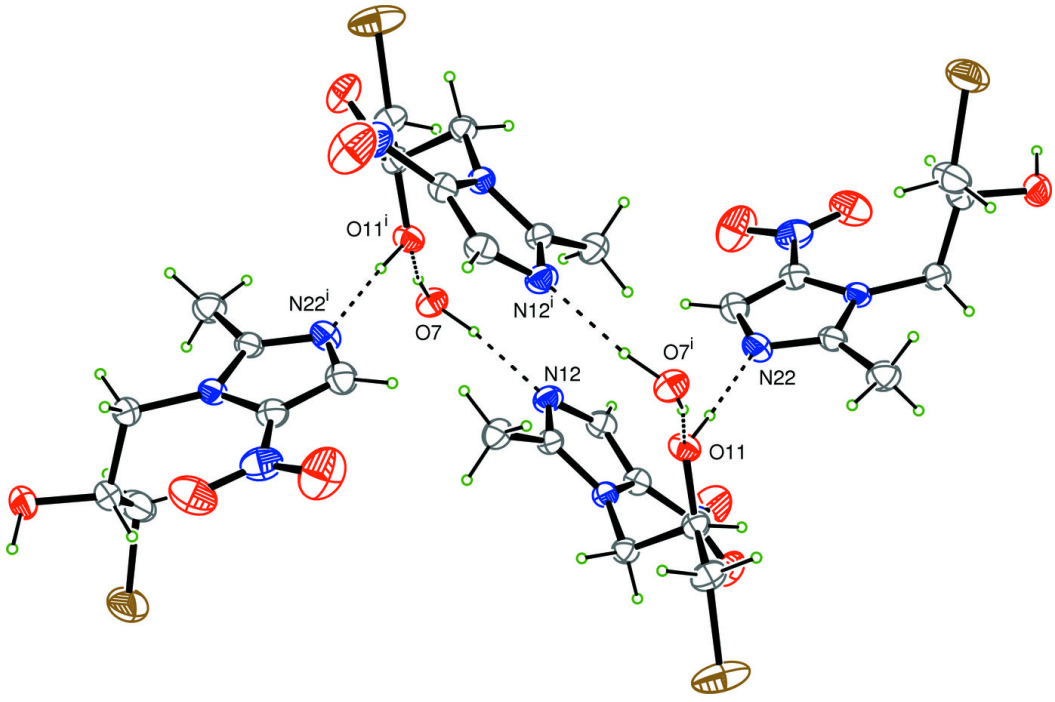

Fig. 3