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5-Bromo-3-(methylaminocarbonyl)-pyridinium picrate

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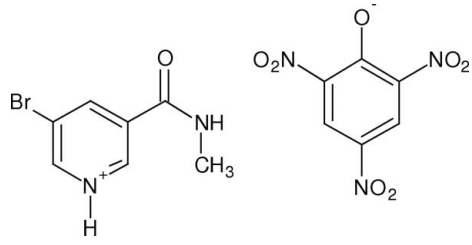
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.018 Å; R factor = 0.103; wR factor = 0.263; data-to-parameter ratio = 12.2.

In the title compound, $C_7H_8BrN_2O^+\cdot C_6H_2N_3O_7^-$, the cations and anions are connected by N—H···O hydrogen bonds. Whereas two nitro groups are almost coplanar with the aromatic ring of the picrate anion, the third one is significantly twisted [dihedral angle = 41 (2)°]. The ions crystallize in sheets parallel to the $(\overline{1}12)$ plane.

Related literature

For related structures, see: Anitha *et al.* (2005); Freeman & Bugg (1974); Jethmalani *et al.* (1996); Yathirajan *et al.* (2007). For related literature, see: Kagabu *et al.* (1998); Aranda & Morlock (2006).



Experimental

Crystal data

$C_7H_8BrN_2O^+\cdot C_6H_2N_3O_7^-$
M_r = 444.17
Triclinic, $P\overline{1}$
a = 4.6684 (7) Å
b = 7.0328 (11) Å
c = 12.842 (2) Å
α = 93.802 (13)°
β = 97.688 (13)°
γ = 98.280 (12)°
V = 411.90 (11) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.55 mm^{-1}
T = 173 (2) K
0.22 × 0.20 × 0.19 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.604, T_{max} = 0.643
6268 measured reflections
2966 independent reflections
2898 reflections with $I > 2\sigma(I)$
R_{int} = 0.122

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.103
$wR(F^2)$ = 0.263
S = 1.15
2966 reflections
244 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.15 e Å^{-3}
$\Delta\rho_{min}$ = −1.30 e Å^{-3}
Absolute structure: Flack (1983), with 1416 Friedel pairs
Flack parameter: 0.06 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88	2.23	2.865 (13)	129
N1—H1···O15^{ii}	0.88	2.28	2.964 (14)	135
N5—H5···O11	0.88	1.86	2.572 (15)	137
N5—H5···O12	0.88	2.15	2.885 (15)	140

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

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2557).

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supplementary materials

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5-Bromo-3-(methylaminocarbonyl)pyridinium picrate

B. K. Sarojini, B. Narayana, M. T. Swamy, H. S. Yathirajan and M. Bolte

Comment

Nicotinamide, also known as niacinamide, is the amide of niacin (vitamin B3) and used for the treatment of arthritis by aiding the body in its production of cartilage. A different use for this compound is an additive in energy drinks (Aranda & Morlock, 2006). The crystal structures of *N*-(4-bromophenyl)-5,6-dichloronicotinamide and 6-chloro-5-fluoro-*N*-(3-pyridyl)nicotinamide (Jethmalani *et al.*, 1996), the picrate salt of 1-methylnicotinamide (Freeman & Bugg, 1974) and nicotinium picrate (Anitha *et al.*, 2005) have been reported. In continuation of our work on picrate salts (Yathirajan *et al.*, 2007), the paper reports the crystal structure of the title compound, (I).

Compound (I), $[C_7H_8BrN_2O]^+[C_6H_2N_3O_7]^-$, consists of discrete 5-bromo-*N*-methylnicotinamidium cations and picrate anions connected by N—H···O and bifurcated N—H···(O,*O*) hydrogen bonds. Whereas two nitro groups are almost coplanar with the aromatic ring of the picrate anion [dihedral angles 4(2)° and 11 (2)°], the third one is significantly twisted [dihedral angle 41 (2)°]. The non-H atoms of the side chain of the cation are almost coplanar (r.m.s. deviation 0.015 Å) and this plane is inclined by 28.9 (8)° with respect to the heterocycle. The ion pairs crystallize in sheets parallel to the $(\bar{1}\bar{1}2)$ plane.

Experimental

5-Bromo-*N*-methylnicotinamide (2.15 g, 0.01 mol) was dissolved in 25 ml of 1:1 *v*/*v* alcohol-water mixture and few drops of dilute HCl were added and stirred well. To this, picric acid (2.29 g, 0.01 mol) in 30 ml of water was added dropwise and stirred for few minutes. The precipitated salt was filtered, dried and yellow blocks of (I) were obtained by slow evaporation of the ethanol solution. (m. p.: 401–403 K). Analysis for $C_{13}H_{10}BrN_5O_8$: Found (Calculated): C 35.04 (35.15); H 2.24 (2.27); N 15.71% (15.77%).

Refinement

The H atoms were geometrically placed (C—H = 0.95–0.98 Å, N—H = 0.88 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(methyl C).

Figures

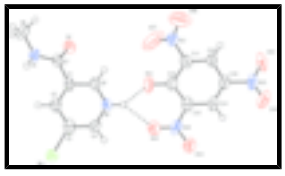

Fig. 1. Perspective view of (I) displacement ellipsoids for the non-hydrogen atoms are at the 50% probability level. Hydrogen bonds shown as dashed lines.

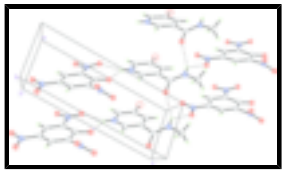

Fig. 2. Packing diagram of the title compound. Hydrogen bonds shown as dashed lines.

5-Bromo-3-(methylaminocarbonyl)pyridinium picrate

Crystal data

$C_7H_8BrN_2O^+·C_6H_2N_3O_7^-$	$Z = 1$
$M_r = 444.17$	$F_{000} = 222$
Triclinic, $P\overline{1}$	$D_x = 1.791$ Mg m^{-3}
Hall symbol: P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 4.6684$ (7) Å	Cell parameters from 5412 reflections
$b = 7.0328$ (11) Å	$\theta = 3.5$–25.7º
$c = 12.842$ (2) Å	$\mu = 2.55$ mm^{-1}
$\alpha = 93.802$ (13)º	$T = 173$ (2) K
$\beta = 97.688$ (13)º	Block, yellow
$\gamma = 98.280$ (12)º	0.22 × 0.20 × 0.19 mm
$V = 411.90$ (11) Å^3	

Data collection

Stoe IPDSII two-circle diffractometer	2966 independent reflections
Radiation source: fine-focus sealed tube	2898 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.122$
$T = 173$(2) K	$\theta_{max} = 25.6$º
ω scans	$\theta_{min} = 3.5$º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -5 \rightarrow 5$
$T_{min} = 0.604$, $T_{max} = 0.643$	$k = -8 \rightarrow 8$
6268 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.103$	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.263$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.15$	$\Delta\rho_{max} = 1.15$ e Å^{-3}
2966 reflections	$\Delta\rho_{min} = -1.30$ e Å^{-3}

244 parameters	Extinction correction: ., $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
3 restraints	Extinction coefficient:
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), 1416 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.06 (3)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1	0.80717 (7)	0.12358 (7)	0.79387 (6)	0.0446 (4)
O1	0.0789 (16)	0.8106 (13)	0.8851 (7)	0.0452 (18)
N1	0.547 (2)	0.8204 (15)	0.9724 (8)	0.040 (2)
H1	0.7077	0.7676	0.9783	0.048*
C1	0.379 (2)	0.5947 (18)	0.8161 (10)	0.041 (2)
C2	0.560 (3)	0.4597 (17)	0.8415 (10)	0.042 (2)
H2	0.6673	0.4644	0.9102	0.050*
C3	0.582 (3)	0.313 (2)	0.7614 (10)	0.050 (3)
C4	0.419 (2)	0.3107 (16)	0.6629 (9)	0.041 (2)
H4	0.4312	0.2147	0.6088	0.050*
N5	0.240 (3)	0.4456 (15)	0.6434 (8)	0.039 (2)
H5	0.1387	0.4418	0.5801	0.047*
C6	0.212 (3)	0.584 (2)	0.7170 (10)	0.040 (2)
H6	0.0800	0.6728	0.7018	0.048*
C7	0.323 (2)	0.7498 (19)	0.8939 (11)	0.038 (2)
C8	0.526 (3)	0.979 (2)	1.0457 (11)	0.056 (3)
H8A	0.3871	1.0576	1.0129	0.085*
H8B	0.7186	1.0586	1.0651	0.085*
H8C	0.4573	0.9299	1.1091	0.085*
C11	−0.484 (3)	0.7005 (19)	0.3974 (11)	0.047 (3)
C12	−0.299 (3)	0.5557 (19)	0.4251 (11)	0.046 (2)
C13	−0.292 (2)	0.4168 (19)	0.3371 (9)	0.045 (2)
C14	−0.469 (2)	0.4101 (18)	0.2417 (8)	0.042 (2)
H14	−0.4666	0.3117	0.1876	0.051*
C15	−0.649 (3)	0.5457 (19)	0.2252 (10)	0.046 (2)
C16	−0.654 (3)	0.6999 (18)	0.3012 (9)	0.042 (2)
H16	−0.7683	0.7986	0.2864	0.051*

N11	−0.491 (3)	0.8562 (17)	0.4781 (10)	0.049 (2)
N12	−0.103 (3)	0.2703 (18)	0.3510 (8)	0.051 (2)
N13	−0.839 (3)	0.5355 (19)	0.1231 (10)	0.055 (3)
O11	−0.172 (3)	0.553 (2)	0.5176 (8)	0.072 (3)
O12	0.081 (2)	0.2845 (16)	0.4273 (8)	0.060 (2)
O13	−0.115 (2)	0.143 (2)	0.2774 (9)	0.068 (3)
O14	−0.828 (3)	0.416 (2)	0.0549 (10)	0.073 (4)
O15	−1.009 (2)	0.660 (2)	0.1133 (10)	0.068 (3)
O16	−0.498 (6)	1.018 (3)	0.4500 (17)	0.124 (7)
O17	−0.488 (8)	0.822 (3)	0.5712 (18)	0.162 (14)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0394 (5)	0.0423 (5)	0.0511 (6)	0.0075 (3)	0.0010 (3)	0.0043 (3)
O1	0.030 (4)	0.049 (4)	0.054 (5)	0.008 (3)	−0.002 (3)	0.002 (4)
N1	0.031 (5)	0.049 (5)	0.038 (5)	0.008 (4)	−0.002 (4)	−0.006 (4)
C1	0.030 (5)	0.045 (6)	0.038 (6)	−0.008 (4)	−0.013 (4)	0.007 (5)
C2	0.040 (5)	0.043 (5)	0.038 (5)	−0.004 (4)	−0.001 (4)	0.006 (4)
C3	0.041 (6)	0.062 (7)	0.041 (6)	−0.011 (5)	−0.001 (5)	0.013 (5)
C4	0.039 (5)	0.041 (5)	0.040 (5)	0.004 (4)	0.001 (4)	−0.008 (4)
N5	0.041 (5)	0.038 (5)	0.034 (5)	0.007 (4)	−0.008 (4)	0.004 (4)
C6	0.040 (6)	0.051 (7)	0.031 (6)	0.015 (5)	−0.002 (5)	0.010 (5)
C7	0.025 (5)	0.041 (6)	0.044 (6)	0.000 (4)	−0.004 (5)	0.007 (5)
C8	0.050 (6)	0.066 (8)	0.049 (7)	0.006 (6)	0.004 (5)	−0.019 (6)
C11	0.045 (6)	0.052 (6)	0.044 (7)	0.011 (5)	−0.002 (5)	0.008 (5)
C12	0.047 (6)	0.051 (6)	0.036 (6)	0.006 (5)	−0.002 (5)	0.002 (5)
C13	0.036 (5)	0.057 (6)	0.038 (5)	0.000 (4)	−0.001 (4)	0.006 (5)
C14	0.040 (5)	0.056 (6)	0.026 (4)	−0.004 (5)	0.002 (4)	0.001 (4)
C15	0.048 (6)	0.048 (6)	0.034 (6)	−0.006 (5)	−0.003 (5)	0.002 (4)
C16	0.049 (6)	0.045 (5)	0.030 (5)	0.004 (4)	−0.003 (5)	0.008 (4)
N11	0.053 (6)	0.044 (6)	0.041 (6)	−0.005 (4)	−0.006 (4)	0.003 (5)
N12	0.053 (6)	0.064 (7)	0.032 (4)	0.008 (5)	0.001 (4)	−0.010 (4)
N13	0.051 (6)	0.066 (8)	0.038 (6)	−0.008 (5)	−0.016 (5)	0.006 (5)
O11	0.075 (7)	0.098 (9)	0.038 (5)	0.026 (6)	−0.019 (5)	−0.007 (5)
O12	0.063 (6)	0.065 (6)	0.050 (5)	0.020 (5)	−0.003 (4)	0.001 (4)
O13	0.063 (7)	0.079 (7)	0.058 (6)	0.028 (6)	−0.011 (5)	−0.015 (5)
O14	0.090 (9)	0.079 (8)	0.037 (6)	−0.016 (6)	0.000 (6)	−0.008 (6)
O15	0.047 (5)	0.098 (9)	0.055 (6)	0.009 (5)	−0.013 (5)	0.030 (6)
O16	0.20 (2)	0.078 (10)	0.115 (13)	0.060 (12)	0.048 (14)	0.026 (9)
O17	0.30 (4)	0.081 (12)	0.080 (13)	−0.013 (17)	0.014 (18)	−0.032 (11)

Geometric parameters (Å, °)

Br1—C3	1.848 (15)	C11—C16	1.373 (17)
O1—C7	1.268 (15)	C11—C12	1.461 (18)
N1—C7	1.363 (15)	C11—N11	1.464 (19)
N1—C8	1.436 (16)	C12—O11	1.257 (17)
N1—H1	0.8800	C12—C13	1.451 (18)

C1—C2	1.386 (18)	C13—C14	1.377 (15)
C1—C6	1.393 (17)	C13—N12	1.455 (18)
C1—C7	1.51 (2)	C14—C15	1.367 (19)
C2—C3	1.430 (19)	C14—H14	0.9500
C2—H2	0.9500	C15—C16	1.414 (19)
C3—C4	1.385 (16)	C15—N13	1.472 (15)
C4—N5	1.367 (16)	C16—H16	0.9500
C4—H4	0.9500	N11—O16	1.22 (2)
N5—C6	1.343 (18)	N11—O17	1.23 (3)
N5—H5	0.8800	N12—O12	1.202 (15)
C6—H6	0.9500	N12—O13	1.246 (16)
C8—H8A	0.9800	N13—O14	1.18 (2)
C8—H8B	0.9800	N13—O15	1.265 (19)
C8—H8C	0.9800		
C7—N1—C8	121.2 (11)	H8B—C8—H8C	109.5
C7—N1—H1	119.4	C16—C11—C12	124.6 (12)
C8—N1—H1	119.4	C16—C11—N11	117.9 (11)
C2—C1—C6	121.3 (14)	C12—C11—N11	117.5 (11)
C2—C1—C7	123.9 (10)	O11—C12—C13	125.6 (13)
C6—C1—C7	114.6 (11)	O11—C12—C11	121.6 (13)
C1—C2—C3	118.2 (11)	C13—C12—C11	112.8 (11)
C1—C2—H2	120.9	C14—C13—C12	123.0 (12)
C3—C2—H2	120.9	C14—C13—N12	117.8 (11)
C4—C3—C2	118.8 (12)	C12—C13—N12	119.1 (10)
C4—C3—Br1	121.6 (10)	C15—C14—C13	119.6 (11)
C2—C3—Br1	119.6 (9)	C15—C14—H14	120.2
N5—C4—C3	120.2 (11)	C13—C14—H14	120.2
N5—C4—H4	119.9	C14—C15—C16	122.6 (11)
C3—C4—H4	119.9	C14—C15—N13	118.9 (12)
C6—N5—C4	122.6 (10)	C16—C15—N13	118.4 (12)
C6—N5—H5	118.7	C11—C16—C15	117.0 (12)
C4—N5—H5	118.7	C11—C16—H16	121.5
N5—C6—C1	118.8 (12)	C15—C16—H16	121.5
N5—C6—H6	120.6	O16—N11—O17	122.2 (19)
C1—C6—H6	120.6	O16—N11—C11	117.8 (14)
O1—C7—N1	122.7 (13)	O17—N11—C11	120.0 (16)
O1—C7—C1	120.7 (11)	O12—N12—O13	120.9 (12)
N1—C7—C1	116.6 (10)	O12—N12—C13	120.0 (11)
N1—C8—H8A	109.5	O13—N12—C13	118.6 (10)
N1—C8—H8B	109.5	O14—N13—O15	122.9 (13)
H8A—C8—H8B	109.5	O14—N13—C15	120.6 (14)
N1—C8—H8C	109.5	O15—N13—C15	116.5 (13)
H8A—C8—H8C	109.5		
C6—C1—C2—C3	3.0 (16)	O11—C12—C13—N12	−7(2)
C7—C1—C2—C3	176.6 (9)	C11—C12—C13—N12	176.4 (11)
C1—C2—C3—C4	−1.0 (16)	C12—C13—C14—C15	3.9 (18)
C1—C2—C3—Br1	−177.0 (8)	N12—C13—C14—C15	−179.6 (11)
C2—C3—C4—N5	−0.2 (17)	C13—C14—C15—C16	2.7 (19)

Br1—C3—C4—N5	175.7 (9)	C13—C14—C15—N13	−179.5 (11)
C3—C4—N5—C6	−0.4 (18)	C12—C11—C16—C15	1(2)
C4—N5—C6—C1	2.3 (18)	N11—C11—C16—C15	−178.5 (12)
C2—C1—C6—N5	−3.6 (17)	C14—C15—C16—C11	−5(2)
C7—C1—C6—N5	−177.8 (11)	N13—C15—C16—C11	177.1 (11)
C8—N1—C7—O1	−4.7 (19)	C16—C11—N11—O16	−39 (2)
C8—N1—C7—C1	174.8 (12)	C12—C11—N11—O16	140.9 (19)
C2—C1—C7—O1	−148.3 (11)	C16—C11—N11—O17	141 (2)
C6—C1—C7—O1	25.6 (15)	C12—C11—N11—O17	−39 (3)
C2—C1—C7—N1	32.1 (16)	C14—C13—N12—O12	170.6 (12)
C6—C1—C7—N1	−153.9 (11)	C12—C13—N12—O12	−12.7 (18)
C16—C11—C12—O11	−172.7 (15)	C14—C13—N12—O13	−1.7 (18)
N11—C11—C12—O11	7(2)	C12—C13—N12—O13	174.9 (12)
C16—C11—C12—C13	5(2)	C14—C15—N13—O14	−3(2)
N11—C11—C12—C13	−175.8 (11)	C16—C15—N13—O14	175.1 (14)
O11—C12—C13—C14	170.0 (14)	C14—C15—N13—O15	177.3 (12)
C11—C12—C13—C14	−7.1 (18)	C16—C15—N13—O15	−4.9 (19)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.23	2.865 (13)	129
N1—H1···O15^{ii}	0.88	2.28	2.964 (14)	135
N5—H5···O11	0.88	1.86	2.572 (15)	137
N5—H5···O12	0.88	2.15	2.885 (15)	140

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

Fig. 1

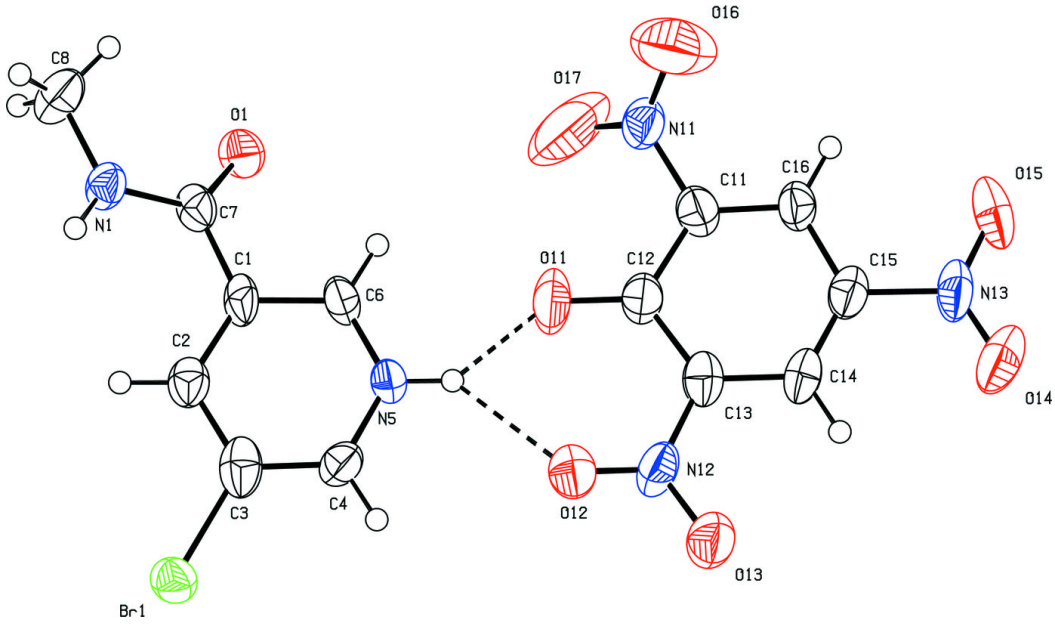
O16
O17
N11
C8
O1
C11
C16
O15
N1
C7
C12
C15
N13
C1
O11
C6
C2
C14
O14
N5
C13
N12
C3
C4
O12
O13
Br1

Fig. 2