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2-Amino-4-nitrophenol monohydrate

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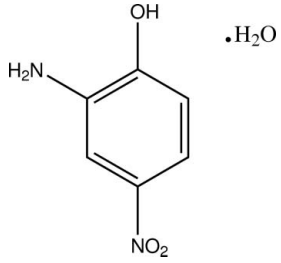
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.054; wR factor = 0.116; data-to-parameter ratio = 12.5.

The title compound, $C_6H_6N_2O_3\cdot H_2O$, crystallizes with two formula units in the asymmetric unit. The molecules are essentially planar with the nitro groups twisted slightly out of the ring planes [maximum deviations from the ring plane of 0.13 (2) and 0.22 (2) Å in the two molecules]. The respective O—N—C—C torsion angles are 6.0 (4) and 12.5 (4)°. In the crystal structure, molecules are linked by intermolecular N—H···O, C—H···O, O—H···O and O—H···N interactions into a three-dimensional network.

Related literature

For the use of nitroaromatics as intermediates in explosives, dyestuffs, pesticides and organic synthesis, see: Yan *et al.* (2006). For the occurrence of nitroaromatics in industrial wastes and as direct pollutants in the environment, see: Yan *et al.* (2006); Soojhawon *et al.* (2005). For related structures, see: Tanak *et al.* (2010); Bi *et al.* (2009); Garden *et al.* (2004).



Experimental

Crystal data

$C_6H_6N_2O_3\cdot H_2O$
M_r = 172.14
Monoclinic, $P2_1/n$
a = 7.539 (5) Å
b = 21.436 (5) Å
c = 9.714 (5) Å
β = 99.328 (5)°
V = 1549.1 (13) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.13 mm^{-1}
T = 296 K
0.62 × 0.30 × 0.05 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.578, T_{max} = 0.892
8719 measured reflections
3031 independent reflections
1598 reflections with $I > 2\sigma(I)$
R_{int} = 0.069

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.116
S = 0.98
3031 reflections
242 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H4···O2^{i}	0.89 (5)	2.51 (5)	3.382 (3)	165 (4)
N2—H5···O3^{ii}	0.89 (5)	2.47 (5)	3.317 (3)	159 (4)
N4—H10···O4^{iii}	0.92 (5)	2.18 (5)	3.062 (3)	159 (4)
N4—H11···O6^{iv}	0.88 (5)	2.28 (5)	3.064 (3)	147 (4)
O7—H13···N2^{ii}	0.89 (5)	2.00 (5)	2.877 (4)	172 (5)
O7—H14···O8^{v}	0.78 (5)	2.43 (5)	3.166 (4)	158 (5)
O8—H15···O2^{vi}	0.80 (5)	2.55 (5)	3.102 (3)	127 (4)
O8—H15···O5^{vi}	0.80 (5)	2.35 (5)	3.038 (3)	144 (5)
O8—H16···N4^{iv}	0.96 (5)	1.88 (5)	2.821 (4)	164 (4)
C6—H6···O1^{i}	0.93	2.47	3.304 (4)	150
C12—H12···O4^{iii}	0.93	2.54	3.254 (4)	133
O3—H1···O8	0.82	1.85	2.657 (3)	169
O6—H7···O7	0.82	1.81	2.619 (4)	168

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

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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: BT5342).

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supplementary materials

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2-Amino-4-nitrophenol monohydrate

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Comment

Nitroaromatics are widely used either as materials or as intermediates in explosives, dyestuffs, pesticides and organic synthesis (Yan *et al.*, 2006). Nitroaromatics occur as industrial wastes and direct pollutants in the environment, and are relatively soluble in water and detectable in rivers, ponds and soil (Yan *et al.*, 2006; Soojhawon *et al.*, 2005).

There is two independent molecules in the asymmetric unit of the title compound (I, Fig. 1). The bond lengths and angles in (I) have normal values, and are comparable with those in the related structures (Tanak *et al.*, 2010; Bi *et al.*, 2009; Garden *et al.*, 2004). The aromatic ring systems are almost planar with the maximum deviation, 0.13 (2) Å for atom O1 in the ring system C1—C6 and -0.22 (2) Å for atom O4 in the ring system C7—C12.

In the crystal structure, the molecules are linked by intermolecular N—H···O, C—H···O, O—H···O and O—H···N interactions (see Table I) into a three-dimensional network.

Experimental

The commercially available compound (Acros organics) was recrystallized from ethanol.

Refinement

C-bound H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The position of the H4, H5, H10, H11, H13, H14, H15 and H16 atoms were obtained from a difference map and these atoms were freely refined. The H atoms of the hydroxyl groups were refined using a riding model with O-H = 0.82Å and U_{iso}(H) = 1.5U_{eq}(O).

Figures

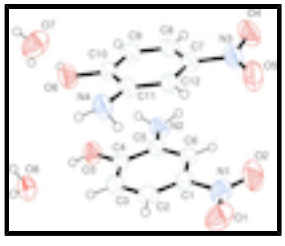

Fig. 1. The molecular structure of the title compound, showing the atom-numbering scheme and 50% probability diplacement ellipsoids.

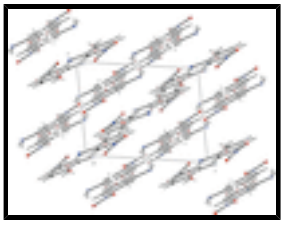

Fig. 2. The crystal packing of the title compound.

2-Amino-4-nitrophenol monohydrate

Crystal data

$C_6H_6N_2O_3·H_2O$	$F(000) = 720$
$M_r = 172.14$	$D_x = 1.476$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Hall symbol: -P 2yn	Cell parameters from 7016 reflections
$a = 7.539$ (5) Å	$\theta = 1.9$–$27.3°$
$b = 21.436$ (5) Å	$\mu = 0.13$ mm^{-1}
$c = 9.714$ (5) Å	$T = 296$ K
$\beta = 99.328$ (5)°	Prism, yellow
$V = 1549.1$ (13) Å^3	0.62 × 0.30 × 0.05 mm
$Z = 8$	

Data collection

Stoe IPDS II diffractometer	3031 independent reflections
Radiation source: fine-focus sealed tube	1598 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.069$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 26.0°$, $\theta_{min} = 1.9°$
rotation method scans	$h = -7 \rightarrow 9$
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)	$k = -26 \rightarrow 26$
$T_{min} = 0.578$, $T_{max} = 0.892$	$l = -11 \rightarrow 11$
8719 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0426P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{max} < 0.001$
3031 reflections	$\Delta\rho_{max} = 0.17$ e Å^{-3}
242 parameters	$\Delta\rho_{min} = -0.21$ e Å^{-3}

0 restraints

Primary atom site location: structure-invariant direct methods

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0063 (11)

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 $F^2 > \sigma(F^2)$ 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}
O3	0.6819 (3)	0.50238 (8)	0.1354 (2)	0.0700 (6)
H1	0.7078	0.4727	0.1882	0.105*
C11	0.4215 (3)	0.62410 (11)	0.4251 (3)	0.0524 (7)
O6	0.3203 (3)	0.52487 (8)	0.3513 (2)	0.0738 (6)
H7	0.2634	0.5061	0.2849	0.111*
C4	0.7466 (3)	0.55594 (11)	0.2003 (3)	0.0525 (7)
C5	0.7094 (3)	0.61040 (11)	0.1216 (3)	0.0521 (6)
C12	0.4337 (3)	0.68701 (11)	0.4013 (3)	0.0534 (7)
H12	0.4950	0.7129	0.4699	0.064*
O8	0.7879 (3)	0.39992 (9)	0.2795 (3)	0.0796 (7)
C2	0.9053 (4)	0.61399 (12)	0.3917 (3)	0.0581 (7)
H2	0.9702	0.6158	0.4816	0.070*
C10	0.3296 (3)	0.58634 (11)	0.3190 (3)	0.0540 (7)
N4	0.4880 (4)	0.59777 (11)	0.5561 (3)	0.0661 (7)
N2	0.6190 (4)	0.60576 (11)	−0.0165 (3)	0.0656 (7)
C1	0.8706 (4)	0.66709 (11)	0.3123 (3)	0.0543 (7)
C6	0.7737 (4)	0.66635 (11)	0.1799 (3)	0.0567 (7)
H6	0.7515	0.7033	0.1299	0.068*
O1	1.0411 (4)	0.72657 (11)	0.4830 (3)	0.0981 (8)
C3	0.8408 (4)	0.55795 (12)	0.3337 (3)	0.0580 (7)
H3	0.8612	0.5214	0.3853	0.070*
N3	0.3654 (4)	0.77812 (11)	0.2558 (3)	0.0690 (7)
N1	0.9413 (4)	0.72598 (12)	0.3708 (3)	0.0744 (8)
C9	0.2545 (4)	0.61152 (12)	0.1923 (3)	0.0612 (7)
H9	0.1966	0.5858	0.1219	0.073*
C8	0.2650 (4)	0.67473 (12)	0.1700 (3)	0.0614 (7)
H8	0.2126	0.6922	0.0856	0.074*
C7	0.3544 (4)	0.71151 (11)	0.2748 (3)	0.0540 (7)
O5	0.4692 (4)	0.80874 (9)	0.3407 (3)	0.0955 (8)

O4	0.2702 (3)	0.80249 (9)	0.1563 (3)	0.0911 (8)
O2	0.9015 (4)	0.77391 (10)	0.3045 (3)	0.1136 (10)
O7	0.1271 (4)	0.45374 (12)	0.1652 (4)	0.1135 (11)
H11	0.513 (6)	0.558 (2)	0.552 (5)	0.170*
H5	0.544 (7)	0.574 (2)	−0.025 (5)	0.170*
H10	0.584 (7)	0.620 (2)	0.603 (5)	0.170*
H4	0.564 (7)	0.641 (2)	−0.048 (5)	0.170*
H15	0.808 (7)	0.368 (2)	0.243 (6)	0.170*
H16	0.686 (7)	0.394 (2)	0.327 (5)	0.170*
H13	0.201 (7)	0.432 (2)	0.122 (6)	0.170*
H14	0.055 (7)	0.431 (2)	0.188 (6)	0.170*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0838 (15)	0.0491 (10)	0.0692 (13)	−0.0074 (9)	−0.0118 (11)	0.0001 (10)
C11	0.0552 (17)	0.0446 (14)	0.0573 (18)	0.0031 (11)	0.0091 (13)	0.0025 (13)
O6	0.0843 (16)	0.0441 (10)	0.0885 (15)	−0.0017 (9)	0.0006 (11)	−0.0001 (10)
C4	0.0559 (17)	0.0441 (14)	0.0555 (18)	−0.0012 (12)	0.0031 (13)	−0.0018 (14)
C5	0.0512 (16)	0.0507 (14)	0.0534 (17)	0.0033 (12)	0.0056 (13)	−0.0005 (14)
C12	0.0575 (18)	0.0436 (14)	0.0573 (18)	0.0006 (11)	0.0038 (13)	0.0024 (13)
O8	0.0979 (19)	0.0521 (11)	0.0887 (18)	0.0038 (11)	0.0145 (13)	0.0065 (11)
C2	0.0568 (17)	0.0612 (17)	0.0530 (17)	0.0036 (13)	−0.0011 (13)	−0.0075 (15)
C10	0.0549 (18)	0.0402 (13)	0.068 (2)	0.0042 (11)	0.0126 (14)	0.0023 (14)
N4	0.0814 (19)	0.0477 (12)	0.0641 (17)	0.0015 (12)	−0.0041 (13)	0.0101 (13)
N2	0.0727 (18)	0.0609 (14)	0.0581 (16)	0.0057 (12)	−0.0050 (13)	0.0039 (13)
C1	0.0514 (16)	0.0478 (14)	0.064 (2)	−0.0011 (12)	0.0099 (14)	−0.0135 (14)
C6	0.0570 (17)	0.0458 (14)	0.068 (2)	0.0048 (12)	0.0128 (15)	0.0029 (15)
O1	0.0942 (18)	0.0970 (17)	0.0998 (19)	−0.0290 (13)	0.0057 (15)	−0.0430 (16)
C3	0.0661 (19)	0.0492 (14)	0.0557 (19)	0.0042 (12)	0.0007 (14)	0.0026 (13)
N3	0.0799 (19)	0.0529 (14)	0.0747 (19)	0.0083 (13)	0.0136 (15)	0.0146 (15)
N1	0.0694 (19)	0.0599 (17)	0.096 (2)	−0.0080 (13)	0.0205 (17)	−0.0282 (17)
C9	0.0613 (18)	0.0606 (16)	0.0597 (18)	0.0016 (13)	0.0039 (14)	−0.0047 (15)
C8	0.0599 (19)	0.0641 (17)	0.0594 (19)	0.0103 (14)	0.0075 (14)	0.0096 (15)
C7	0.0526 (17)	0.0459 (13)	0.0635 (19)	0.0067 (12)	0.0097 (14)	0.0088 (14)
O5	0.122 (2)	0.0524 (12)	0.104 (2)	−0.0134 (12)	−0.0068 (16)	0.0133 (13)
O4	0.1057 (19)	0.0673 (13)	0.0949 (18)	0.0214 (12)	−0.0002 (14)	0.0300 (13)
O2	0.137 (2)	0.0485 (13)	0.149 (3)	−0.0033 (13)	0.0030 (19)	−0.0150 (15)
O7	0.105 (2)	0.0883 (18)	0.156 (3)	−0.0325 (14)	0.0474 (18)	−0.0539 (18)

Geometric parameters (Å, °)

O3—C4	1.361 (3)	N4—H11	0.88 (5)
O3—H1	0.8200	N4—H10	0.92 (5)
C11—C12	1.374 (3)	N2—H5	0.89 (5)
C11—C10	1.402 (4)	N2—H4	0.89 (5)
C11—N4	1.408 (4)	C1—C6	1.372 (4)
O6—C10	1.359 (3)	C1—N1	1.450 (3)
O6—H7	0.8200	C6—H6	0.9300

C4—C3	1.374 (4)	O1—N1	1.219 (4)
C4—C5	1.398 (3)	C3—H3	0.9300
C5—C6	1.380 (3)	N3—O4	1.223 (3)
C5—N2	1.406 (4)	N3—O5	1.230 (3)
C12—C7	1.380 (4)	N3—C7	1.444 (3)
C12—H12	0.9300	N1—O2	1.224 (3)
O8—H15	0.80 (5)	C9—C8	1.377 (4)
O8—H16	0.96 (5)	C9—H9	0.9300
C2—C1	1.376 (4)	C8—C7	1.374 (4)
C2—C3	1.382 (4)	C8—H8	0.9300
C2—H2	0.9300	O7—H13	0.89 (5)
C10—C9	1.378 (4)	O7—H14	0.78 (5)
C4—O3—H1	109.5	H5—N2—H4	112 (4)
C12—C11—C10	118.8 (2)	C6—C1—C2	122.7 (2)
C12—C11—N4	121.5 (3)	C6—C1—N1	118.9 (3)
C10—C11—N4	119.6 (2)	C2—C1—N1	118.4 (3)
C10—O6—H7	109.5	C1—C6—C5	119.5 (2)
O3—C4—C3	123.7 (2)	C1—C6—H6	120.2
O3—C4—C5	115.2 (2)	C5—C6—H6	120.2
C3—C4—C5	121.1 (2)	C4—C3—C2	120.4 (3)
C6—C5—C4	118.4 (2)	C4—C3—H3	119.8
C6—C5—N2	122.5 (2)	C2—C3—H3	119.8
C4—C5—N2	119.0 (2)	O4—N3—O5	122.0 (2)
C11—C12—C7	119.5 (3)	O4—N3—C7	119.0 (3)
C11—C12—H12	120.3	O5—N3—C7	119.1 (3)
C7—C12—H12	120.3	O1—N1—O2	121.6 (3)
H15—O8—H16	109 (4)	O1—N1—C1	119.6 (3)
C1—C2—C3	117.9 (2)	O2—N1—C1	118.7 (3)
C1—C2—H2	121.1	C8—C9—C10	120.0 (3)
C3—C2—H2	121.1	C8—C9—H9	120.0
O6—C10—C9	123.9 (3)	C10—C9—H9	120.0
O6—C10—C11	115.3 (2)	C7—C8—C9	118.8 (3)
C9—C10—C11	120.9 (2)	C7—C8—H8	120.6
C11—N4—H11	113 (3)	C9—C8—H8	120.6
C11—N4—H10	112 (3)	C8—C7—C12	122.0 (2)
H11—N4—H10	112 (4)	C8—C7—N3	120.3 (3)
C5—N2—H5	110 (3)	C12—C7—N3	117.7 (3)
C5—N2—H4	113 (3)	H13—O7—H14	109 (5)
O3—C4—C5—C6	−178.9 (2)	C5—C4—C3—C2	−1.8 (4)
C3—C4—C5—C6	1.6 (4)	C1—C2—C3—C4	0.6 (4)
O3—C4—C5—N2	−3.1 (4)	C6—C1—N1—O1	−173.4 (3)
C3—C4—C5—N2	177.4 (3)	C2—C1—N1—O1	6.0 (4)
C10—C11—C12—C7	0.6 (4)	C6—C1—N1—O2	5.2 (4)
N4—C11—C12—C7	−175.0 (2)	C2—C1—N1—O2	−175.4 (3)
C12—C11—C10—O6	−178.8 (2)	O6—C10—C9—C8	177.8 (2)
N4—C11—C10—O6	−3.2 (4)	C11—C10—C9—C8	−1.7 (4)
C12—C11—C10—C9	0.8 (4)	C10—C9—C8—C7	1.3 (4)
N4—C11—C10—C9	176.4 (3)	C9—C8—C7—C12	0.0 (4)

C3—C2—C1—C6	0.8 (4)	C9—C8—C7—N3	−179.0 (2)
C3—C2—C1—N1	−178.6 (2)	C11—C12—C7—C8	−1.0 (4)
C2—C1—C6—C5	−0.9 (4)	C11—C12—C7—N3	178.0 (2)
N1—C1—C6—C5	178.4 (2)	O4—N3—C7—C8	12.1 (4)
C4—C5—C6—C1	−0.3 (4)	O5—N3—C7—C8	−168.4 (3)
N2—C5—C6—C1	−175.9 (3)	O4—N3—C7—C12	−166.9 (3)
O3—C4—C3—C2	178.7 (2)	O5—N3—C7—C12	12.5 (4)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H4···O2^{i}	0.89 (5)	2.51 (5)	3.382 (3)	165 (4)
N2—H5···O3^{ii}	0.89 (5)	2.47 (5)	3.317 (3)	159 (4)
N4—H10···O4^{iii}	0.92 (5)	2.18 (5)	3.062 (3)	159 (4)
N4—H11···O6^{iv}	0.88 (5)	2.28 (5)	3.064 (3)	147 (4)
O7—H13···N2^{ii}	0.89 (5)	2.00 (5)	2.877 (4)	172 (5)
O7—H14···O8^{v}	0.78 (5)	2.43 (5)	3.166 (4)	158 (5)
O8—H15···O2^{vi}	0.80 (5)	2.55 (5)	3.102 (3)	127 (4)
O8—H15···O5^{vi}	0.80 (5)	2.35 (5)	3.038 (3)	144 (5)
O8—H16···N4^{iv}	0.96 (5)	1.88 (5)	2.821 (4)	164 (4)
C6—H6···O1^{i}	0.93	2.47	3.304 (4)	150
C12—H12···O4^{iii}	0.93	2.54	3.254 (4)	133
O3—H1···O8	0.82	1.85	2.657 (3)	169
O6—H7···O7	0.82	1.81	2.619 (4)	168

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

Fig. 1

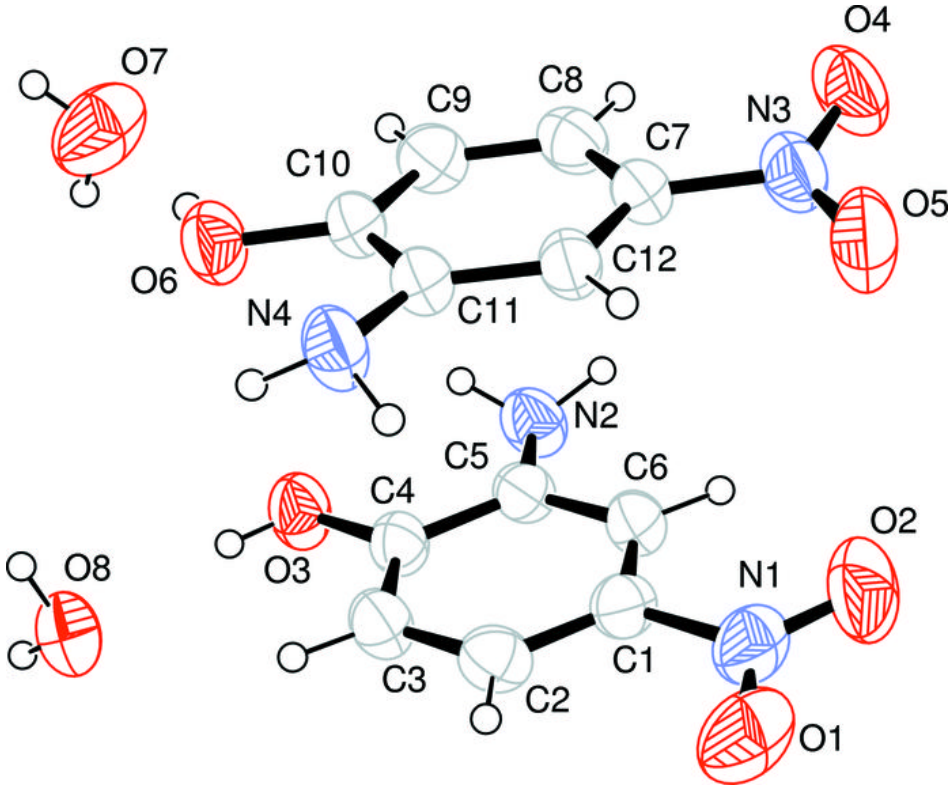
O7
O4
C9
C8
N3
C10
C7
O5
O6
C12
N4
C11
N2
C5
C6
C4
O2
O8
O3
N1
C3
C1
C2
O1

Fig. 2