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4-*tert*-Butylpyridinium picrate

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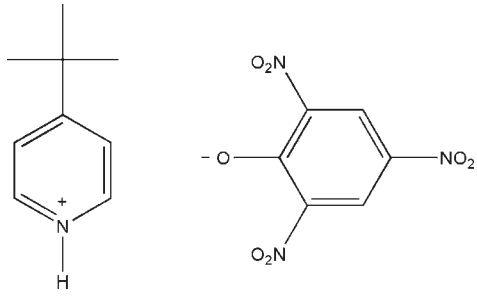
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.178; data-to-parameter ratio = 17.8.

In the title compound, $C_9H_{14}N^+\cdot C_6H_2N_3O_7^-$, the three nitro groups of the picrate anion are twisted out of the plane of the attached benzene ring; the dihedral angles are 32.8 (2), 10.5 (4) and 12.3 (4)°. The pyridinium cations and picrate anions are linked *via* bifurcated N—H···(O,O) hydrogen bonds. The ionic pairs are linked into a ribbon-like structure along [101] by C—H···O hydrogen bonds.

Related literature

For general background to picrate complexes, see: In *et al.* (1997); Zaderenko *et al.* (1997); Ashwell *et al.* (1995); Owen & White (1976); Shakir *et al.* (2009).



Experimental

Crystal data

$C_9H_{14}N^+\cdot C_6H_2N_3O_7^-$
M_r = 364.32
Monoclinic, $P2_1/n$
a = 5.7669 (12) Å
b = 26.798 (6) Å
c = 11.195 (3) Å
β = 97.335 (6)°
V = 1715.9 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 293 K
0.21 × 0.19 × 0.16 mm

Data collection

Bruker SMART APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.976, T_{max} = 0.982
16875 measured reflections
4318 independent reflections
2677 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.178
S = 1.05
4318 reflections
242 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.91 (3)	1.85 (3)	2.659 (2)	148 (2)
N1—H1···O7^{i}	0.91 (3)	2.38 (3)	3.085 (3)	135 (2)
C2—H2···O4^{ii}	0.93	2.45	3.131 (3)	130
C6—H6···O1^{iii}	0.93	2.42	3.137 (3)	133

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5056).

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supplementary materials

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4-*tert*-Butylpyridinium picrate

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Comment

It is well known that picric acid forms charge transfer molecular complexes with a number of aromatic compounds such as aromatic hydrocarbons and amines, through electrostatic or hydrogen bonding interactions (In *et al.*, 1997; Zaderenko *et al.*, 1997). The bonding of donor-acceptor picric acid complexes strongly depends on the nature of partners. Some of the picric acid complexes crystallize in centrosymmetric space group owing to non-linear optical properties (NLO) (Shakir *et al.*, 2009). This is due to the aggregation of the donor-acceptor molecules in a non-centrosymmetric manner which contributes to the bulk susceptibility from intermolecular charge transfer (Ashwell *et al.*,1995; Owen & White, 1976). We report here the crystal structure of the title salt.

The pyridinium ring of the cation (Fig.1) is planar (r.m.s. deviation 0.019 Å). In the picrate anion, the keto O atom deviates from the benzene plane by 0.139 (3) Å. The C11—O1 bond [1.245 (2) Å] assumes a partial double bond character. The C11—C12 [1.452 (3) Å] and C11—C16 [1.436 (3) Å] bond distances are longer than the other C—C bond lengths of the benzene ring. The three nitro groups are twisted out of the attached benzene ring by 32.8 (2)° [N17/O2/O3], 10.5 (4)° [N18/O4/O5] and 12.3 (4)° [N19/O6/O7].

In the crystal, the cations and anions are linked via N—H···O hydrogen bonds involving the phenolate O atom and one of the nitro O atoms. The ionic pairs are linked into a ribbon-like structure along the [101] by C—H···O hydrogen bonds (Fig.2).

Experimental

Equimolar solutions of 4-tertiarybutyl pyridine in methanol and picric acid in methanol were mixed together and the solution was stirred well for 1 h and the precipitated salt was filtered off. The salt was repeatedly recrystallised from methanol to get single crystals suitable for X-ray analysis.

Refinement

The N-bound H atom was located in a difference map and refined freely. C-bound H atoms were positioned geometrically (C–H = 0.93-0.96 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C) for methyl H and 1.2U_{eq}(C) for other H atoms. The displacement ellipsoids for the methyl carbons (C8-C10) of the tert-butyl group are elongated, suggesting possible disorder i.e free rotation of the tert-butyl group. Attempts to model the tert-butyl group as disordered over two sites did not give satisfactory results. Hence the original model was retained.

Figures

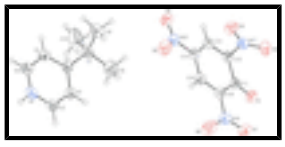

Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

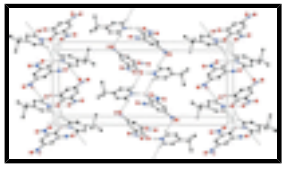

Fig. 2. The crystal packing of the title compound, viewed down the *a* axis. H atoms not involved in hydrogen bonding (dashed lines) have been omitted for clarity.

4-*tert*-Butylpyridinium picrate

Crystal data

$C_9H_{14}N^+·C_6H_2N_3O_7^-$	$F(000) = 760$
$M_r = 364.32$	$D_x = 1.410$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 2565 reflections
$a = 5.7669$ (12) Å	$\theta = 1.5$–$28.5°$
$b = 26.798$ (6) Å	$\mu = 0.11$ mm^{-1}
$c = 11.195$ (3) Å	$T = 293$ K
$\beta = 97.335$ (6)°	Block, colourless
$V = 1715.9$ (7) Å^3	0.21 × 0.19 × 0.16 mm
$Z = 4$	

Data collection

Bruker SMART APEXII area-detector diffractometer	4318 independent reflections
Radiation source: fine-focus sealed tube	2677 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.027$
ω and φ scans	$\theta_{max} = 28.5°$, $\theta_{min} = 1.5°$
Absorption correction: multi-scan (SADABS; Bruker, 2008)	$h = -7 \rightarrow 7$
$T_{min} = 0.976$, $T_{max} = 0.982$	$k = -34 \rightarrow 35$
16875 measured reflections	$l = -14 \rightarrow 15$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.055$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.178$	H atoms treated by a mixture of independent and constrained refinement

S = 1.05	$w = 1/[\sigma^2(F_o^2) + (0.0841P)^2 + 0.3243P]$ where $P = (F_o^2 + 2F_c^2)/3$
4318 reflections	$(\Delta/\sigma)_{max} = 0.001$
242 parameters	$\Delta\rho_{max} = 0.48$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.18$ e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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}
O1	0.2606 (3)	0.00115 (5)	0.17613 (13)	0.0663 (4)
O2	0.5627 (3)	−0.05436 (6)	0.32430 (15)	0.0744 (4)
O3	0.8672 (3)	−0.00990 (7)	0.37736 (16)	0.0800 (5)
O4	0.7078 (4)	0.14493 (6)	0.57283 (18)	0.0991 (7)
O5	0.3706 (4)	0.17951 (7)	0.5339 (2)	0.1081 (7)
O6	−0.1374 (4)	0.12612 (8)	0.1958 (3)	0.1319 (10)
O7	−0.1413 (3)	0.05113 (7)	0.13505 (15)	0.0829 (5)
N1	0.5892 (3)	0.43662 (7)	0.37124 (16)	0.0627 (4)
H1	0.516 (5)	0.4666 (11)	0.362 (3)	0.097 (9)*
C2	0.5004 (4)	0.39966 (9)	0.3030 (2)	0.0669 (6)
H2	0.3705	0.4053	0.2463	0.080*
C3	0.5967 (4)	0.35326 (8)	0.31436 (19)	0.0631 (5)
H3	0.5356	0.3277	0.2637	0.076*
C4	0.7843 (3)	0.34401 (7)	0.40070 (18)	0.0545 (5)
C5	0.8766 (4)	0.38456 (8)	0.46659 (19)	0.0667 (6)
H5	1.0077	0.3803	0.5233	0.080*
C6	0.7790 (4)	0.43054 (9)	0.45000 (19)	0.0715 (6)
H6	0.8451	0.4577	0.4937	0.086*
C7	0.8842 (4)	0.29206 (8)	0.4249 (2)	0.0732 (6)
C8	0.7573 (6)	0.25297 (11)	0.3428 (4)	0.1142 (11)
H8A	0.7858	0.2589	0.2613	0.171*
H8B	0.5925	0.2549	0.3475	0.171*
H8C	0.8134	0.2204	0.3677	0.171*
C9	0.8433 (7)	0.27804 (12)	0.5529 (3)	0.1227 (12)
H9A	0.8943	0.2444	0.5696	0.184*
H9B	0.6797	0.2807	0.5603	0.184*
H9C	0.9302	0.3002	0.6092	0.184*

C10	1.1361 (5)	0.29230 (13)	0.4139 (6)	0.179 (3)
H10A	1.1620	0.3094	0.3415	0.268*
H10B	1.1913	0.2586	0.4110	0.268*
H10C	1.2193	0.3090	0.4822	0.268*
C11	0.3052 (3)	0.03289 (7)	0.25697 (16)	0.0529 (4)
C12	0.5135 (3)	0.03034 (7)	0.34450 (16)	0.0508 (4)
C13	0.5836 (3)	0.06717 (7)	0.42427 (17)	0.0545 (5)
H13	0.7245	0.0645	0.4745	0.065*
C14	0.4436 (4)	0.10853 (7)	0.42986 (18)	0.0594 (5)
C15	0.2372 (4)	0.11350 (7)	0.35493 (19)	0.0615 (5)
H15	0.1429	0.1413	0.3608	0.074*
C16	0.1713 (3)	0.07717 (7)	0.27149 (17)	0.0568 (5)
N17	0.6573 (3)	−0.01424 (6)	0.34792 (14)	0.0580 (4)
N18	0.5107 (4)	0.14682 (7)	0.51824 (18)	0.0770 (6)
N19	−0.0483 (3)	0.08495 (8)	0.19498 (17)	0.0707 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0751 (9)	0.0638 (9)	0.0581 (8)	−0.0153 (7)	0.0019 (7)	−0.0106 (7)
O2	0.0854 (10)	0.0527 (9)	0.0874 (11)	−0.0013 (7)	0.0194 (8)	−0.0060 (8)
O3	0.0656 (10)	0.0859 (12)	0.0845 (11)	0.0082 (8)	−0.0058 (8)	−0.0085 (9)
O4	0.1186 (14)	0.0598 (10)	0.1032 (13)	−0.0103 (9)	−0.0463 (12)	−0.0089 (9)
O5	0.1340 (17)	0.0605 (11)	0.1192 (16)	0.0156 (11)	−0.0245 (13)	−0.0300 (10)
O6	0.1079 (15)	0.0853 (15)	0.181 (2)	0.0249 (12)	−0.0669 (16)	−0.0217 (14)
O7	0.0782 (10)	0.0846 (11)	0.0774 (10)	−0.0123 (9)	−0.0226 (8)	−0.0048 (9)
N1	0.0751 (11)	0.0559 (10)	0.0575 (9)	0.0129 (9)	0.0101 (8)	0.0106 (8)
C2	0.0577 (11)	0.0668 (13)	0.0720 (13)	0.0010 (10)	−0.0075 (9)	0.0177 (11)
C3	0.0625 (12)	0.0542 (12)	0.0683 (12)	−0.0073 (9)	−0.0087 (9)	0.0063 (9)
C4	0.0507 (10)	0.0532 (10)	0.0587 (11)	0.0022 (8)	0.0038 (8)	0.0099 (8)
C5	0.0692 (13)	0.0670 (13)	0.0579 (11)	0.0038 (10)	−0.0148 (9)	0.0055 (10)
C6	0.0972 (16)	0.0614 (13)	0.0527 (11)	0.0015 (11)	−0.0024 (11)	−0.0025 (9)
C7	0.0648 (12)	0.0551 (12)	0.0963 (17)	0.0080 (10)	−0.0022 (11)	0.0165 (11)
C8	0.122 (3)	0.0661 (17)	0.150 (3)	0.0173 (16)	0.000 (2)	−0.0063 (18)
C9	0.161 (3)	0.084 (2)	0.114 (2)	0.001 (2)	−0.014 (2)	0.0452 (18)
C10	0.0698 (19)	0.087 (2)	0.386 (8)	0.0310 (16)	0.058 (3)	0.059 (3)
C11	0.0595 (11)	0.0507 (10)	0.0481 (9)	−0.0149 (8)	0.0051 (8)	0.0020 (8)
C12	0.0559 (10)	0.0482 (10)	0.0483 (9)	−0.0056 (8)	0.0069 (8)	0.0042 (8)
C13	0.0596 (10)	0.0497 (10)	0.0516 (10)	−0.0089 (8)	−0.0024 (8)	0.0057 (8)
C14	0.0733 (12)	0.0422 (10)	0.0590 (11)	−0.0101 (9)	−0.0054 (9)	0.0005 (8)
C15	0.0681 (12)	0.0457 (10)	0.0678 (12)	−0.0029 (9)	−0.0026 (9)	0.0033 (9)
C16	0.0572 (10)	0.0544 (11)	0.0560 (10)	−0.0081 (9)	−0.0042 (8)	0.0057 (9)
N17	0.0661 (11)	0.0581 (10)	0.0504 (9)	−0.0002 (8)	0.0096 (7)	−0.0010 (7)
N18	0.1021 (15)	0.0435 (10)	0.0770 (12)	−0.0075 (9)	−0.0203 (11)	−0.0017 (8)
N19	0.0655 (11)	0.0675 (12)	0.0741 (12)	−0.0054 (9)	−0.0102 (9)	0.0049 (9)

Geometric parameters (Å, °)

O1—C11	1.245 (2)	C7—C9	1.529 (4)

O2—N17	1.219 (2)	C8—H8A	0.96
O3—N17	1.219 (2)	C8—H8B	0.96
O4—N18	1.221 (3)	C8—H8C	0.96
O5—N18	1.219 (3)	C9—H9A	0.96
O6—N19	1.218 (3)	C9—H9B	0.96
O7—N19	1.211 (2)	C9—H9C	0.96
N1—C2	1.314 (3)	C10—H10A	0.96
N1—C6	1.325 (3)	C10—H10B	0.96
N1—H1	0.91 (3)	C10—H10C	0.96
C2—C3	1.361 (3)	C11—C16	1.436 (3)
C2—H2	0.93	C11—C12	1.452 (3)
C3—C4	1.378 (3)	C12—C13	1.357 (3)
C3—H3	0.93	C12—N17	1.452 (3)
C4—C5	1.381 (3)	C13—C14	1.377 (3)
C4—C7	1.518 (3)	C13—H13	0.93
C5—C6	1.357 (3)	C14—C15	1.372 (3)
C5—H5	0.93	C14—N18	1.444 (3)
C6—H6	0.93	C15—C16	1.369 (3)
C7—C10	1.473 (4)	C15—H15	0.93
C7—C8	1.519 (4)	C16—N19	1.451 (3)
C2—N1—C6	121.45 (19)	H9B—C9—H9C	109.5
C2—N1—H1	117.2 (18)	C7—C10—H10A	109.5
C6—N1—H1	121.3 (18)	C7—C10—H10B	109.5
N1—C2—C3	120.67 (18)	H10A—C10—H10B	109.5
N1—C2—H2	119.7	C7—C10—H10C	109.5
C3—C2—H2	119.7	H10A—C10—H10C	109.5
C2—C3—C4	120.3 (2)	H10B—C10—H10C	109.5
C2—C3—H3	119.9	O1—C11—C16	125.64 (17)
C4—C3—H3	119.9	O1—C11—C12	122.35 (18)
C3—C4—C5	116.58 (18)	C16—C11—C12	111.90 (16)
C3—C4—C7	122.42 (19)	C13—C12—C11	124.14 (17)
C5—C4—C7	120.99 (18)	C13—C12—N17	117.36 (16)
C6—C5—C4	121.09 (18)	C11—C12—N17	118.50 (16)
C6—C5—H5	119.5	C12—C13—C14	119.20 (17)
C4—C5—H5	119.5	C12—C13—H13	120.4
N1—C6—C5	119.7 (2)	C14—C13—H13	120.4
N1—C6—H6	120.2	C15—C14—C13	121.19 (18)
C5—C6—H6	120.2	C15—C14—N18	119.05 (19)
C10—C7—C4	109.7 (2)	C13—C14—N18	119.73 (18)
C10—C7—C8	110.9 (3)	C16—C15—C14	119.45 (19)
C4—C7—C8	112.5 (2)	C16—C15—H15	120.3
C10—C7—C9	110.5 (3)	C14—C15—H15	120.3
C4—C7—C9	107.0 (2)	C15—C16—C11	123.94 (17)
C8—C7—C9	106.1 (2)	C15—C16—N19	116.49 (18)
C7—C8—H8A	109.5	C11—C16—N19	119.57 (17)
C7—C8—H8B	109.5	O3—N17—O2	122.98 (18)
H8A—C8—H8B	109.5	O3—N17—C12	118.23 (17)
C7—C8—H8C	109.5	O2—N17—C12	118.77 (17)
H8A—C8—H8C	109.5	O5—N18—O4	123.3 (2)

H8B—C8—H8C	109.5	O5—N18—C14	119.00 (19)
C7—C9—H9A	109.5	O4—N18—C14	117.7 (2)
C7—C9—H9B	109.5	O7—N19—O6	121.66 (19)
H9A—C9—H9B	109.5	O7—N19—C16	120.72 (19)
C7—C9—H9C	109.5	O6—N19—C16	117.60 (19)
H9A—C9—H9C	109.5		
C6—N1—C2—C3	2.4 (3)	C12—C13—C14—N18	177.02 (19)
N1—C2—C3—C4	2.2 (3)	C13—C14—C15—C16	−1.3 (3)
C2—C3—C4—C5	−4.7 (3)	N18—C14—C15—C16	−179.48 (19)
C2—C3—C4—C7	174.3 (2)	C14—C15—C16—C11	0.5 (3)
C3—C4—C5—C6	2.9 (3)	C14—C15—C16—N19	−179.75 (19)
C7—C4—C5—C6	−176.1 (2)	O1—C11—C16—C15	−173.87 (19)
C2—N1—C6—C5	−4.2 (3)	C12—C11—C16—C15	2.3 (3)
C4—C5—C6—N1	1.5 (4)	O1—C11—C16—N19	6.4 (3)
C3—C4—C7—C10	124.9 (3)	C12—C11—C16—N19	−177.37 (16)
C5—C4—C7—C10	−56.2 (4)	C13—C12—N17—O3	−31.6 (2)
C3—C4—C7—C8	0.9 (3)	C11—C12—N17—O3	148.47 (18)
C5—C4—C7—C8	179.9 (2)	C13—C12—N17—O2	146.61 (18)
C3—C4—C7—C9	−115.2 (3)	C11—C12—N17—O2	−33.3 (2)
C5—C4—C7—C9	63.7 (3)	C15—C14—N18—O5	8.6 (3)
O1—C11—C12—C13	171.42 (18)	C13—C14—N18—O5	−169.7 (2)
C16—C11—C12—C13	−4.9 (3)	C15—C14—N18—O4	−170.6 (2)
O1—C11—C12—N17	−8.6 (3)	C13—C14—N18—O4	11.1 (3)
C16—C11—C12—N17	175.02 (16)	C15—C16—N19—O7	−166.1 (2)
C11—C12—C13—C14	4.5 (3)	C11—C16—N19—O7	13.6 (3)
N17—C12—C13—C14	−175.42 (17)	C15—C16—N19—O6	12.1 (3)
C12—C13—C14—C15	−1.2 (3)	C11—C16—N19—O6	−168.2 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.91 (3)	1.85 (3)	2.659 (2)	148 (2)
N1—H1···O7^{i}	0.91 (3)	2.38 (3)	3.085 (3)	135 (2)
C2—H2···O4^{ii}	0.93	2.45	3.131 (3)	130
C6—H6···O1^{iii}	0.93	2.42	3.137 (3)	133

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

Fig. 1

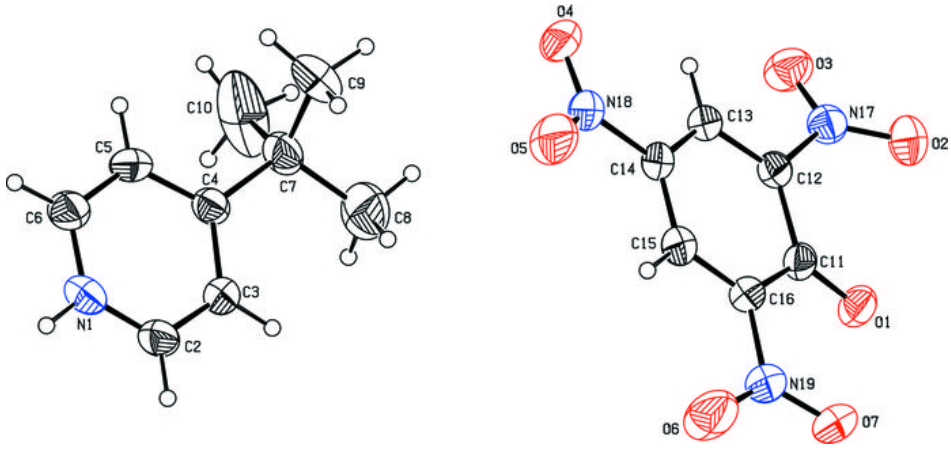
C9
C10
C5
C4
C7
C6
C8
C3
N1
C2
O4
O3
N18
C13
N17
O5
C14
C12
O2
C15
C11
C16
O1
N19
O6
O7

Fig. 2