Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

1:1 Complex of 4-nitrobenzoic acid and 4-nitropyridine *N*-oxide

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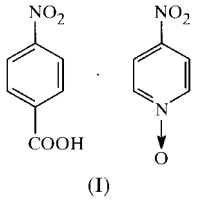
Received 10 September 1999
Accepted 25 October 1999

In the title co-crystal, $C_7H_5NO_4{\cdot}C_5H_4N_2O_3$, the two components are linked by an intermolecular hydrogen bond between the O—H and N—O groups [O···O 2.577 (3) Å]. The interplanar angle between the planes of the rings of the molecules is 5.3 (2)°. The rings are stacked in the crystal with a mean interplanar distance of 3.279 (3) Å.

Comment

Over several years, a systematic study of molecular complexes of 4-nitropyridine *N*-oxide (NPNO) with diverse hydrogen-bond donors (Moreno-Fuquen *et al.*, 1996) has been carried out. Some molecular complexes associated with NPNO show potential for application in non-linear optics; for example, the NPNO and 3-nitrophenol molecular complex has a satisfactory second harmonic generation (SHG) response (Moreno-Fuquen *et al.*, 1995). The synthesis and characterization of the title NPNO and 4-nitrobenzoic acid (PNBA) complex, (I), have a threefold purpose: (*a*) to add to the crystallographic information available on compounds based on NPNO, (*b*) to analyse the type of hydrogen bond in the title complex and (*c*) to explore its possible application in non-linear optics.



(I)

Fig. 1 shows the NPNO–PNBA adduct, (I), with the adopted atom-numbering scheme. The molecular complex is held together by an intermolecular hydrogen bond between O1 of the *N*-oxide group of NPNO and O—H of the carboxyl group of PNBA, with an O1···O5 distance of 2.577 (3) Å and an O1···HO5—O5 angle of 161 (3)°. The O5—HO5 and O1···HO5 distances are 0.95 (4) and 1.67 (4) Å, respectively. From the O···O bond length value, the strength of the hydrogen bond can be classified as strong (Emsley, 1984).

The dihedral angle formed by the planes which essentially contain the rings of the molecules is 5.3 (2)°. If one compares the values of bond lengths and angles in the title complex with the values in the free molecules , CCDC references (Allen *et al.*, 1991) NBZOAC06 (Tonogaki *et al.*, 1993) and NTPYRO1-1 (Wang *et al.*, 1976), the C6—C7 and C6—O5 bond lengths change from 1.488 (4) and 1.324 (4) Å in (I) to 1.500 (9) and 1.289 (9) Å in the free molecule, while the C1—N1, N1—C5 and O1—N1 bond lengths change from 1.353 (4), 1.348 (4) and 1.314 (3) Å in (I) to 1.369, 1.370 and 1.291 Å in the free molecule. There are no significant differences for the other parameters.

The molecules of (I) are stacked in the crystal with the NPNO ring at a mean interplanar distance of 3.279 (3) Å from the PNBA ring at $-x, 1-y, 1-z$. The presence of a centre of symmetry in the crystal inhibits an SHG response.

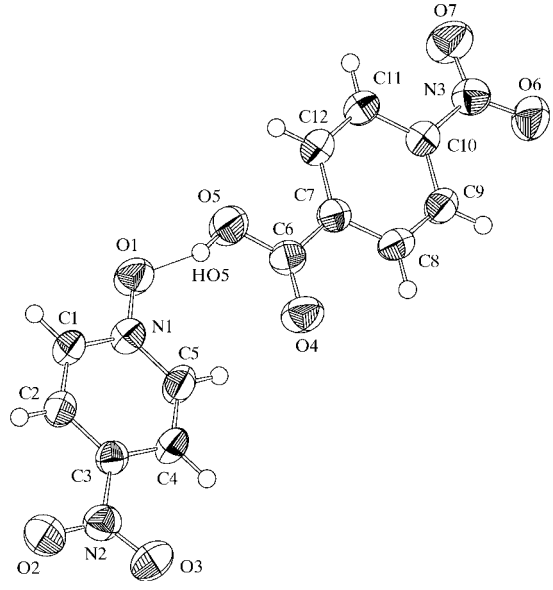


Figure 1
A *ZORTEP* (Zsolnai, 1995) plot of the asymmetric unit of (I) showing the atomic numbering scheme. Displacement ellipsoids are plotted at the 50% probability level and H atoms are shown as spheres of an arbitrary radius.

Experimental

Crystals of (I) used in the present work were obtained by slow evaporation from an equimolecular solution of NPNO and PNBA in absolute ethanol. The sublimation point is 414 (1) K.

Crystal data

$C_7H_5NO_4{\cdot}C_5H_4N_2O_3$
M_r = 307.22
Monoclinic, $P2_1/n$
a = 6.221 (1) Å
b = 22.263 (1) Å
c = 9.411 (1) Å
β = 97.30 (2)°
V = 1292.9 (3) Å^3
Z = 4
D_x = 1.578 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 9.25–18.32°
μ = 0.133 mm^{-1}
T = 293 K
Plate, yellow
0.18 × 0.15 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
2498 measured reflections
2280 independent reflections
1372 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 24.96^\circ$
$h = 0 \rightarrow 7$
$k = 0 \rightarrow 26$
$l = -11 \rightarrow 11$
2 standard reflections
frequency: 120 min
intensity decay: 1.52%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.132$
$S = 1.077$
2278 reflections
212 parameters
H atoms: see below
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 0.7798P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}
Extinction correction: *SHELXL*93 (Sheldrick, 1993)
Extinction coefficient: 0.178 (7)

The ring-H atoms were added at calculated positions and treated as riding using *SHELXL*93 (Sheldrick, 1993) defaults (C—H = 0.93Å) but were not refined. The HO5 atom was located from a difference Fourier map and its coordinates were refined.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *SDP* (Frenz, 1978); program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*93; molecular graphics: *ZORTEP* (Zsolnai, 1995); software used to prepare material for publication: *SHELXL*93.

The authors wish to acknowledge the Universidad del Valle and COLCIENCIAS (Colombia) and the Brazilian agencies FAPESP, FINEP and IQSC of the Universidade de São Paulo for partial financial support. RMF thanks Dr Martín Martinez-Ripoll of the Instituto Rocasolano and CSIC of Spain for free access to the Crystal Structure Database.

Table 1
Selected geometric parameters (Å, °).

O1—N1	1.314 (3)	O5—C6	1.324 (4)
N1—C5	1.348 (4)	C6—C7	1.488 (4)
N1—C1	1.353 (4)		
O2—N2—C3—C2	11.3 (4)	O7—N3—C10—C11	−11.6 (4)
O4—C6—C7—C12	−173.2 (3)		

Supplementary data for this paper are available from the IUCr electronic archives (Reference: NA1431). Services for accessing these data are described at the back of the journal.

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