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4-Nitrophenol–urea (1/1)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.004 Å
R factor = 0.061
wR factor = 0.141
Data-to-parameter ratio = 12.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $C_6H_5NO_3{\cdot}CH_4N_2O$, 4-nitrophenol molecules are linked to urea molecules by O—H···O and N—H···O hydrogen bonds, forming a network structure.

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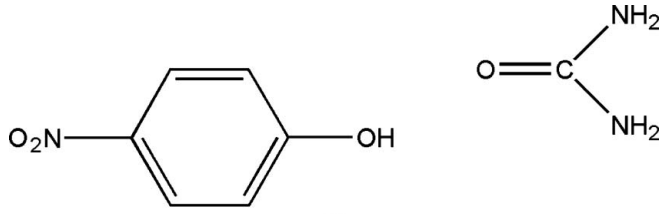
Comment

In the design of crystal structures, the assembly of molecular units in predefined arrangements is a key goal (Desiraju, 1995, 1997; Braga *et al.*, 1998). Directional intermolecular interactions are the primary tools in achieving this goal and hydrogen bonding is currently the best among them (Zaworotko, 1997; Braga & Grepioni, 2000).



(I)

The title compound, (I), forms a co-crystal (Fig. 1 and Table 1) in which 4-nitrophenol and urea molecules interact through multiple hydrogen bonds (Table 2) generating a three-dimensional network (Fig. 2).

Experimental

Urea (0.12 g, 2 mmol) and 4-nitrophenol (0.28 g, 2 mmol) were dissolved in dimethylformamide (10 ml). The reaction mixture was filtered. Colorless prism-shaped crystals separated from the filtrate after about a month.

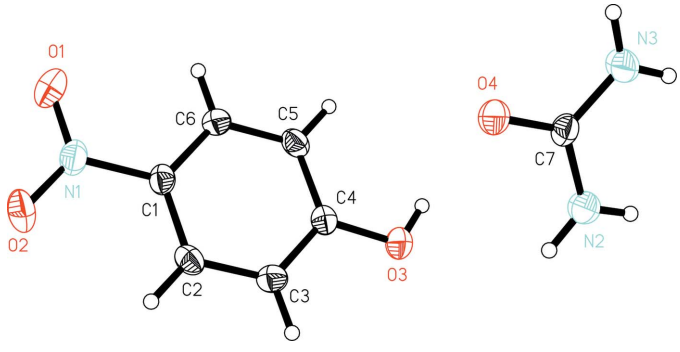


Figure 1
The structure of (I) with the atom numbering, showing displacement ellipsoids at the 50% probability level.

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Crystal data

$C_6H_5NO_3\cdot CH_4N_2O$
$M_r = 199.17$
Triclinic, $P\overline{1}$
$a = 3.7619\ (9)$ Å
$b = 10.230\ (2)$ Å
$c = 11.810\ (3)$ Å
$\alpha = 98.634\ (4)^\circ$
$\beta = 92.415\ (5)^\circ$
$\gamma = 99.326\ (4)^\circ$
$V = 442.38\ (18)$ Å^3
$Z = 2$
$D_x = 1.495$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1561 reflections
$\theta = 1.8$–25.1°
$\mu = 0.12$ mm^{-1}
$T = 298\ (2)$ K
Prism, colorless
0.23 × 0.13 × 0.05 mm

Data collection

Bruker SMART APEX area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.98$, $T_{max} = 0.99$
2362 measured reflections
1561 independent reflections
1234 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 25.1^\circ$
$h = -4 \rightarrow 4$
$k = -12 \rightarrow 12$
$l = -10 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.061$
$wR(F^2) = 0.141$
$S = 1.07$
1561 reflections
127 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2 + 0.2445P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.18$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—N1	1.225 (3)	C3—C4	1.386 (4)
O2—N1	1.230 (3)	C4—C5	1.390 (4)
O3—C4	1.341 (3)	C5—C6	1.365 (4)
N1—C1	1.444 (3)	O4—C7	1.243 (3)
C1—C6	1.385 (4)	N2—C7	1.339 (3)
C1—C2	1.386 (4)	N3—C7	1.323 (3)
C2—C3	1.368 (4)		
C4—O3—H3	109.4	O3—C4—C3	117.5 (2)
O1—N1—O2	122.0 (2)	O3—C4—C5	123.1 (2)
O1—N1—C1	119.0 (2)	C3—C4—C5	119.4 (2)
O2—N1—C1	119.0 (3)	C6—C5—C4	120.4 (2)
C6—C1—C2	121.1 (2)	C5—C6—C1	119.4 (2)
C6—C1—N1	119.7 (2)	O4—C7—N3	121.0 (2)
C2—C1—N1	119.2 (2)	O4—C7—N2	121.4 (3)
C3—C2—C1	118.9 (2)	N3—C7—N2	117.6 (2)
C2—C3—C4	120.8 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3C···O1^{i}	0.86	2.46	3.316 (3)	171
N3—H3B···O4^{ii}	0.86	2.14	3.000 (3)	174
N2—H2C···O2^{i}	0.86	2.32	3.118 (3)	155
O3—H3···O4^{iii}	0.82	1.79	2.613 (3)	177

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

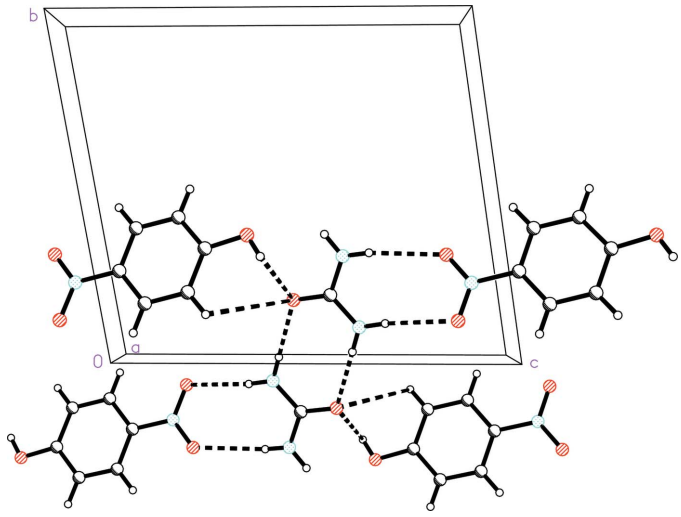

Figure 2
View parallel to the *a* axis of (I), showing hydrogen bonds as dashed lines.

The presence of two peaks in the difference Fourier map in two suitable locations showed atoms N2 and N3 to be protonated, and the H atoms attached to N2 and N3 were included in the refinement in calculated positions in the riding-model approximation (N—H = 0.86 Å), with U_{iso}(H) = 1.2U_{eq}(N). The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.82 (O—H) and 0.93 Å (C—H), and U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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