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4-Nitroaniline–2,4,6-trimethoxybenzaldehyde (1/1)

Abdullah M. Asiri,[a] Salman A. Khan,[a] Kong Wai Tan[b] and Seik Weng Ng[b]*

[a]Chemistry Department, Faculty of Science, King Abdul Aziz University, PO Box 80203, Jeddah 21589, Saudi Arabia, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: seikweng@um.edu.my

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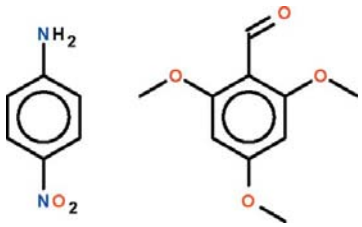
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.124; data-to-parameter ratio = 12.3.

In the title co-crystal, $C_6H_6N_2O_2.C_{10}H_{12}O_4$, the two components are held together by an N—H···$O_{aldehyde}$ hydrogen bond. Adjacent co-crystals are linked by weaker N—H···O_{nitro} hydrogen bonds, forming a linear chain. The two aromatic rings of the components are aligned at 75.2 (1)°. The crystal studied was a non-merohedral twin with a 24% minor component.

Related literature

For some examples of co-crystals of 4-nitroaniline, see: Bertolasi *et al.* (2001); Dederer & Gieren (1979); Huang *et al.* (1996); Koshima *et al.* (1996); Rashid & Deschamps (2006); Singh *et al.* (2003); Smith *et al.* (1997); Weber (1981); Zaitu *et al.* (1995). For the treatment of non-merohedral twins, see: Spek (2009).



Experimental

Crystal data

$C_6H_6N_2O_2\cdot C_{10}H_{12}O_4$ M_r = 334.32
Monoclinic, $P2_1/c$
a = 7.4409 (11) Å
b = 30.022 (5) Å
c = 6.9400 (11) Å
β = 93.237 (3)°
V = 1547.9 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100 K
0.15 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
8127 measured reflections
2722 independent reflections
1834 reflections with $I > 2\sigma(I)$
R_{int} = 0.059

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.124
S = 1.01
2722 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.41 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H12···O1	0.86	2.16	3.016 (3)	172
N1—H11···O5^{i}	0.86	2.50	3.288 (3)	152
N1—H11···O6^{i}	0.86	2.50	3.293 (3)	154

Symmetry code: (i) $x+1, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2271).

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