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

Abdullah M. Asiri, a Salman A. Khan, a Kong Wai Tan b and Seik Weng Ng a,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 6 H 6 N 2 O 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).

Table 1

Hydrogen-bond geometry (Å, °).

<table>
<thead>
<tr>
<th>D—H⋯A</th>
<th>D—H</th>
<th>H⋯A</th>
<th>D⋯A</th>
<th>D—H⋯A</th>
</tr>
</thead>
<tbody>
<tr>
<td>N1—H12 ⋯O1</td>
<td>0.86</td>
<td>2.16</td>
<td>3.016 (3)</td>
<td>172</td>
</tr>
<tr>
<td>N1—H13 ⋯O5</td>
<td>0.86</td>
<td>2.50</td>
<td>3.288 (3)</td>
<td>152</td>
</tr>
<tr>
<td>N1—H14 ⋯O6</td>
<td>0.86</td>
<td>2.50</td>
<td>3.293 (3)</td>
<td>154</td>
</tr>
</tbody>
</table>

Symmetry code: (i) s + 1, −y + 1, z + 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).

References

