

2,4,6-Trimethylbenzamide

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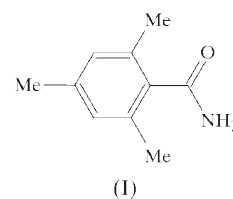
The crystal structure of the title compound, C₁₀H₁₃NO, displays an infinite one-dimensional network composed of primary amide molecules connected by N—H_a···O=C hydrogen bonds involving the *anti* NH amide H atoms, thus generating a C(4) motif. This network is additionally stabilized by a weak N—H_s··· π interaction between the *syn*-oriented amide H atom and the aromatic ring of a neighbouring molecule. The distance between the H atom and the ring centroid is 2.50 Å. The amide group and the aryl moiety are nearly perpendicular, forming an intramolecular dihedral angle of 84.69 (6)°.

Comment

Hydrogen-bonding interactions between amide H atoms and carbonyl O atoms give rise to a variety of assembly modes in crystals of primary amides (Leiserowitz & Hagler, 1983; Bernstein *et al.*, 1994). The most common modes are the centrosymmetric cyclic R₂²(8) hydrogen-bond motif, involving the *syn*-oriented H atoms, H_s (*syn* with respect to the adjacent C=O bond), and the C(4) hydrogen-bond motif, engaging the *anti*-oriented H atoms, H_a. Depending on the symmetry operation relating the centrosymmetric dimers along the C(4) chain, one- or two-dimensional hydrogen-bonded arrays can be generated in the solid state. For example, in the case of benzamide (Blake & Small, 1972), *o*-methylbenzamide (Kato *et al.*, 1979) and *m*-methylbenzamide (Orii *et al.*, 1963), formation of N—H_a···O hydrogen bonds between the translation-related centrosymmetric R₂²(8) dimers leads to one-dimensional networks. A similar assembly pattern was also observed in crystals of 4-methoxy-2,6-dimethylbenzamide (Mugnoli *et al.*, 1991), whereas neighbouring dimers along the C(4) chain in crystals of *p*-methylbenzamide are related by a glide plane that generates a two-dimensional array of the hydrogen-bonded molecules (Kato *et al.*, 1981).

Recently, it has been shown that introduction of a bulky triphenylmethyl group at the *p*-position of the benzamide molecule leads to crystal structures in which the centrosymmetric amide dimers are connected by weak N—H_a··· π

interactions (Reddy *et al.*, 2002). We report here the crystal structure of 2,4,6-trimethylbenzamide, (I), in which a new assembly mode was found for the aromatic primary amide. This mode is characterized by strong N—H_a···O hydrogen bonds accompanied by weak N—H_s··· π interactions (π denotes the aromatic ring centroid). A survey of the Cambridge Structural Database (Version 5.24, 296 427 entries; Allen, 2002) gave only three primary benzamide derivatives [HIXNIL (Pandurangi *et al.*, 1998), QELYUB (Zhang *et al.*, 1999) and TUVQIK (Kobayashi *et al.*, 2003)], in which the H··· π distance and the N—H··· π angle in the N—H··· π interactions fall in the ranges 2.0–3.0 Å and 120–180°, respectively.



The structure of (I), with its atom-numbering scheme, is shown in Fig. 1 and selected geometric parameters are given in Table 1. The carboxamide group and benzene moiety are

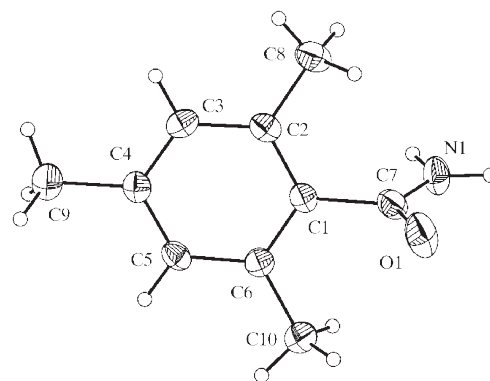


Figure 1

The molecule of (I), with displacement ellipsoids at the 50% probability level for non-H atoms.

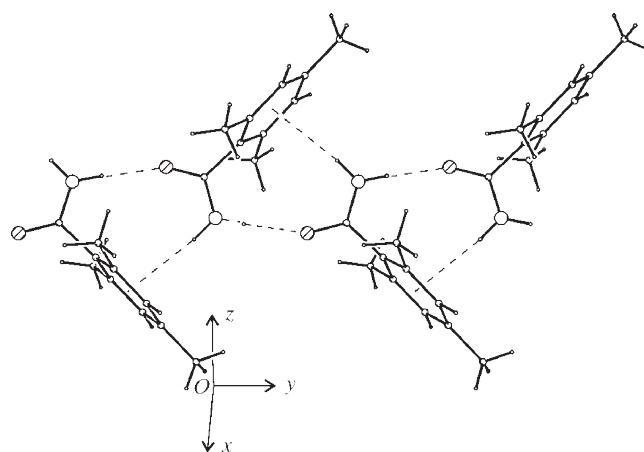


Figure 2

A hydrogen-bonded chain in (I), with N—H···O and N—H··· π interactions shown by dashed lines.