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Phenazine–2,6-dihydroxybenzoic acid (1/1)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.112
Data-to-parameter ratio = 11.2

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

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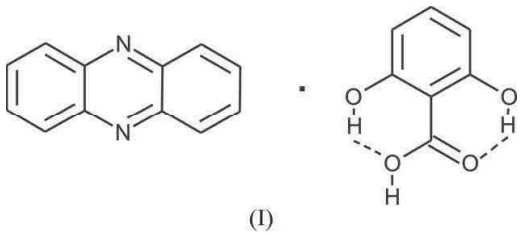
In the 1:1 cocrystal of phenazine with 2,6-dihydroxybenzoic acid, $C_{12}H_8N_2{\cdot}C_7H_6O_4$, the two symmetry-independent molecules of phenazine are located on inversion centres. The carboxyl group of the acid assumes the *syn* conformation. One of the phenazine molecules is connected to two acid molecules *via* strong O—H···N interactions, forming a discrete hydrogen-bonded assembly. The phenazine molecules are arranged into infinite columns by π–π stacking interactions, and the carboxylic acid molecules, which are strongly tilted relative to the heterocyclic molecules, occupy channels formed between these columns.

Comment

Phenazine (Phz) has been used extensively as a reagent in supramolecular synthesis (Batchelor *et al.*, 2000; Gdaniec *et al.*, 2005; Kutasi *et al.*, 2002; Munakata *et al.*, 1994; Pedireddi *et al.*, 1996; Thalladi, Smolka, Boese & Sustmann, 2000; Thalladi, Smolka, Gehrke *et al.*, 2000; Tomura & Yamashita, 2000). Thalladi, Smolka, Boese & Sustmann (2000) have shown that Phz forms cocrystals with some biphenols where the Phz molecules, arranged into stacks, form a robust host framework with one-dimensional channels filled by the phenolic molecules. The molecules in the channels and the Phz molecules are nearly perpendicular. In turn, carboxylic acids generally bind to Phz *via* O—H···N and C—H···N hydrogen bonds, generating an $R_2^2(8)$ motif (Bernstein *et al.*, 1995) which leads to a nearly coplanar arrangement of the heterocyclic ring and the carboxylic acid group.



(I)

In the course of our studies of the cocrystals of aza-aromatic compounds (Gdaniec *et al.*, 2005; Kadzewski & Gdaniec, 2006), we have prepared cocrystals, (I), of Phz with 2,6-dihydroxybenzoic acid (DHB), with the aim of checking whether the molecular organization in these cocrystals resembles that of Phz molecular complexes with phenols or that observed in complexes with carboxylic acids. Depending on the system of intramolecular hydrogen bonds within the molecule of DHB, which is related to the *syn* or *anti* form adopted by the carboxylic acid group, it can bind to hydrogen-