The structural properties of a noncentrosymmetric polymorph of 4-aminobenzoic acid

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Description

The crystal structure of a polymorph of 4-aminobenzoic acid (PABA), C7H7NO2, at 100 K is noncentrosymmetric, as opposed to centrosymmetric in the structures of the other known polymorphs. The two crystallographically independent PABA molecules form pseudocentrosymmetric O—H···O hydrogen-bonded dimers that are further linked by N—H···O hydrogen bonds into a three-dimensional network. The benzene rings stack in the b direction. The CO2 moieties are bent out slightly from the benzene ring plane.