عنوان مقاله:

A novel tubular hydrogen bond pattern in the crystal structure of a new diazaphosphole oxide: (4-Cl-C6H4NH)P(O)(1,2-NH)2C6H4

محل انتشار:

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خلاصه مقاله:

In this work, we report on the synthesis, spectroscopic characterization and X-ray crystal structure determination of a new diazaphosphole oxide, (4-Cl-C6H4NH)P(O)(1,2-NH)2C6H4 namely 2-[para-chloroanilino]-1,3,2λ4-diazaphosphol-2-one. This compound was synthesized in a two-step reaction, from POCl3 and 4-chloroaniline for the preparation of (4-Cl-C6H4NH)P(O)Cl2 phosphorus-chlorine reagent in the first step and then the reaction of 1,2-phenylenediamine with the phosphorus-chlorine compound. In the molecule, the P atom is bonded in a distorted tetrahedral P(O)[N]3 environment, with one of the O═P—N angle as the maximum angle at the P atom and the N—P—N angle within the ring as minimum angle. In the crystal packing, each molecule is surrounded with four neighbouring molecules through (N—H)2…O═P hydrogen bonds. These interactions form a tubular arrangement of fused hydrogen-bonded rings, of R33(12) and R34(14) graph-set motifs, along [001]. An N—H…π interaction exists in the tubular shape which does .not change the dimension of hydrogen bond pattern

کلمات کلیدی:

Diazaphosphole oxide, (N—H)2…O═P, N—H…π interaction, X-Ray crystallography

لینک ثابت مقاله در پایگاه سیویلیکا: