ساختار کریستالی N-بنزوئیل، N' و N'' -بیس (پیرولیدینیل) فسفریک تری آمید

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چکیده :
ساختار بلوری N-بنزوئیل، N' و N'' -بیس (پیرولیدینیل) فسفریک تری آمید توسط پرتو نگاری اشعه ایکس به دست آمد. فواصل پیوندی PN به میزان قابل ملاحظه ای کوتاهتر از پیوند ساده PN می باشد و تمام اتمهای نیتروژن در این مولکول تقریبا مسطح هستند. مولکول در شکل دیمرهای بوجود آمده از پیوندهای هیدروژنی یافت می شود و به علت شکلهای کنفورمری حلقه پیرولیدین مولکول به دو صورت در شبکه بلوری ظاهر می شود.

Introduction

Phosphoric triamides have found widespread use in organic and bio-chemistry.[1] The strong donor properties and lewis basicity make them excellent ligands for small and hard metal ions.[2] Some derivatives of these compounds are used in clinical practice as anticancer preparations.[3]

Results

We report here the results of the reaction of N-benzoyl phosphoramidic dichloride with pyrrolidine to form an organophosphorus compound, N-benzoyl, N′,N″-bis(pyrrolidinyl) phosphoric triamide. The investigated compound (Fig. 1) was synthesized according to a well-established method.[4] Single crystal of the product obtained from a solution of n-heptan and chloroform in the ratio (1:4) after slow evaporation at room temperature. Selected bond lengths and angles are shown in Table 1.

The P(1)-N(1), P(1)-N(2) and P(1)-N(3) bond lengths are 1.679(4), 1.618(4) and 1.615(4)Å, respectively. They are significantly shorter than the typical PN single bond length (1.77Å)[5] but much longer than the PN double bond length (1.57Å in ph_3P=N-). The share of partial multiple bond in P(1)-N(1) is less than P(1)-N(2) and P(1)-N(3) based on conjugation of nitrogen lone pair with carbonyl group. Similar data obtained for the P(2)-N(4), P(2)-N(5) and P(2)-N(6) bond lengths. (see Table1.)

The angles C(8)-N(2)-P(1), C(11)-N(2)-P(1), C(15)-N(3)-P(1), C(12)-N(3)-P(1) and C(16)-N(4)-P(2) are 128.5(3)°, 121.0(3)°, 120.6(3)°, 127.1(3)° and 125.1(3)° that confirm sp^2 hybridization for amino and amidic nitrogens in title compound.

Table 1. Selected Bond Lengths (Å) and Angles (deg) for title Compound.

P(1)-N(1)	1.679(4)	C(1)-N(1)	1.360(5)
P(1)-N(2)	1.618(4)	C(9)-C(10)	1.437(9)
P(1)-N(3)	1.615(4)	C(9')-C(10)	1.61(3)
O(2)-C(1)	1.217(5)	C(13)-C(14)	1.42(4)
P(1)-O(1)	1.487(3)	C(13)-C(14')	1.451(12)
O(1)-P(1)-N(1)	106.77(17)	C(11)-N(2)-P(1)	121.0(3)
O(1)-P(1)-N(2)	110.86(18)	C(12)-N(3)-P(1)	127.1(3)
O(1)-P(1)-N(3)	117.6(2)	C(15)-N(3)-P(1)	120.6(3)
N(3)-P(1)-N(2)	105.16(19)	C(16)-N(4)-P(2)	125.1(3)
N(2)-P(1)-N(1)	112.8(2)	C(23)-N(5)-P(2)	121.1(3)
N(3)-P(1)-N(1)	103.66(18)	C(26)-N(5)-P(2)	128.0(3)
O(3)-P(2)-N(5)	110.48(18)	C(27)-N(6)-P(2)	121.9(4)
O(3)-P(2)-N(6)	117.1(2)	C(30)-N(6)-P(2)	125.9(3)
N(5)-P(2)-N(6)	105.02(19)	C(13)-C(14)-C(15)	108.3(18)
O(3)-P(2)-N(4)	106.11(17)	C(13)-C(14')-C(15)	107.0(8)
N(5)-P(2)-N(4)	112.2(2)	C(10)-C(9)-C(8)	105.8(6)
N(6)-P(2)-N(4)	105.97(19)	C(8)-C(9')-C(10)	101.0(18)
C(1)-N(1)-P(1)	128.5(3)	C(9')-C(8)-C(9)	43.8(12)
C(8)-N(2)-P(1)	126.7(3)	N(2)-C(8)-C(9)	103.8(5)

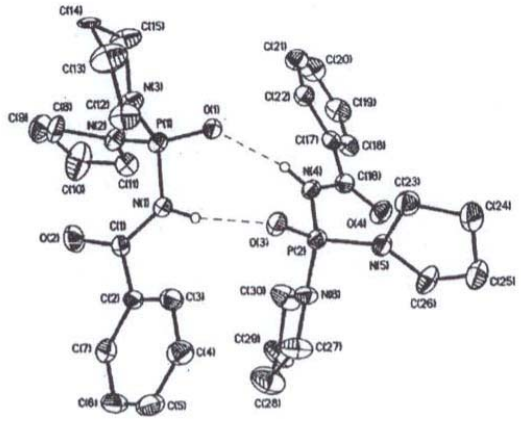

Fig. 1 The molecular structure of the title compound, showing the atom labeling scheme and 50% probability level displacement ellipsoids.

N-benzoyl, N′,N″-bis(pyrrolidinyl) phosphoric triamide appears as two crystallographically independent molecules based on the conformational forms of pyrrolidinyl groups. This ring in one conformer is planar but in another is deformed (C(9), C(9′) and C(14) and C(14′) in Figure 2).

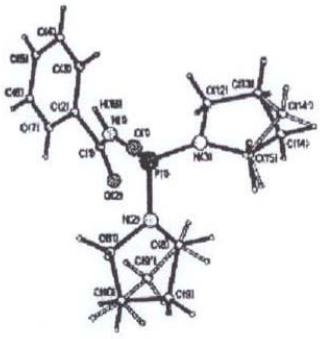

Fig. 2 A View of two conformers.

Also this compound obtained in the form of dimmers produced by hydrogen bonding. (See Figure 1).

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