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Crystal Structure of Diphenylphosphinic Acid

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The title compound diphenylphosphinic acid was structurally characterized by single crystal X-ray diffraction analysis. The crystals are monoclinic, space group P21/c with a = *11.474(2),* b = *6.0506(12),* c = *15.718(3) Å,* α = *90,* β = *99.93(3),* γ = *90°,* V = *1074.9(4) Å^3,* Z = *4,* F(000) = *452,* D_c = *1.342 g/cm^3,* μ = *0.230 mm^{-1}, the final* R = *0.0429 and* wR = *0.1192. A total of 10494 reflections were collected, of which 2545 were independent* (R_{int} = *0.0533). In the crystal packing diagram, intermolecular O—H… O hydrogen bonds stabilize the solid state of the title compound.*

Keywords Crystal structure; Phenyl; Phosphinic acid

Introduction

In recent year, phosphorus containing compounds have attracted much interest because of their widely applications in coordination chemistry as ligands [1–14]. As a continuation of our work on phosphorus chemistry [15–18], we obtained the single crystals of the title compound diphenylphosphinic acid and its structure was characterized by X-ray crystallography. In this paper, we describe the crystal structural characterization of diphenylphosphinic acid.

Experimental

Crystal structure determination

The crystal of the title compound with dimensions of 0.20 mm × 0.18 mm × 0.12 mm was mounted on a Rigaku Saturn CCD area detector diffractometer with a graphite-monochromated MoKα radiation (λ = 0.71073Å) by using a phi and scan modes at 293(2) K in the range of 2.92° ≤ θ ≤ 27.93°. The crystal belongs to monoclinic system with space group P21/c and crystal parameters of a = 11.474(2) Å, b = 6.0506(12) Å, c = 15.718(3) Å, α = 90°, β = 99.93(3)°, γ = 90°, V = 1074.9(4) A^3, D_c = 1.342 g/cm^3, The absorption coefficient μ = 0.230 mm^{-1}, and Z = 4. A summary of crystal data is presented in Table 1.

The structure was solved by direct methods with SHELXS-97 [19] and refined by the full-matrix least squares method on F^2 data using SHELXL-97 [20]. The empirical absorption corrections were applied to all intensity data. H atom of N-H was initially located in a difference Fourier map and were refined with the restraint Uiso(H) = 1.2Ueq(N). Other

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Table 1. Crystal data and structure refinement

Empirical formula	$C_{12}H_{10}O_2P$
Formula weight	217.17
Crystal system	Monoclinic
Unit cell dimensions	
a (Å)	11.474(2)
b (Å)	6.0506(12)
c (Å)	15.718(3)
Unit cell angles (°)	
α	90
β	99.93(3)
γ	90
Volume (Å^3)	1074.9(4)
Z	4
Temperature (K)	293(2)
space group	P21/c
Wavelength (Å)	0.71073
Calculated density (g/cm^3)	1.342
Absorption coefficient (mm^{-1})	0.230
F(000)	452
Crystal size (mm)	0.20 × 0.18 × 0.12
Theta range for data collection (^{o})	2.92 –27.93
Reflections collected	10494
Independent reflections	2545 [$R_{(int)} = 0.0533$]
Final R indices [$I>2\sigma(I)$]	$R_1 = 0.0429$, w$R_2 = 0.1192$

H atoms were positioned geometrically and refined using a riding model, with d(C—H) = 0.93–0.97 Å and Uiso(H) = 1.2Ueq(C) or 1.5Ueq(Cmethyl). The final full-matrix least squares refinement gave $R = 0.0429$ and $wR = 0.1192$.

Results and Discussion

The title compound diphenylphosphinic acid was confirmed by single-crystal X-ray diffraction analysis. The selected bond lengths and bond angles are listed in Table 2. The structure was solved by direct methods. Anisotropic displacement parameters were applied to all nonhydrogen atoms in full-matrix least-square refinements based on F^2. The hydrogen atoms were set in calculated positions with a common fixed isotropic thermal parameter.

The molecular structure and the packing view of the title compound are shown in Figs. 1 and 2, respectively. The title compound crystallizes in monoclinic space group P21/c with four molecules in the unit cell and one molecule in the asymmetric unit. As shown in Fig. 1, the molecular structure contains two phenyl groups attached to phosphorus atom. The P1-O1 bond length [1.4963(13) Å] is shorter than the P1-O2 bond length [1.5414(13) Å] indicating that P1-O1 is double bond and P1-O2 is single bond. The six-membered rings C1C2C3C4C5C6 and C7C8C9C10C11C12 are almost coplanar with the mean deviations of 0.0054 and 0.0022 Å, respectively. The dihedral angle between the two phenyl planes is 109.7°. The bond distances [P(1)-C(1) = 1.7908(19) Å, P(1)-C(7) = 1.7935(19) Å,

Table 2. Selected bond lengths (Å) and bond angles (°)

Bond lengths			
P(1)-O(1)	1.4963(13)	C(4)-C(5)	1.365(3)
P(1)-O(2)	1.5414(13)	C(5)-C(6)	1.378(3)
P(1)-C(1)	1.7908(19)	C(7)-C(12)	1.383(3)
P(1)-C(7)	1.7935(19)	C(7)-C(8)	1.386(3)
C(1)-C(6)	1.381(3)	C(8)-C(9)	1.385(3)
C(1)-C(2)	1.384(3)	C(9)-C(10)	1.361(4)
C(2)-C(3)	1.383(3)	C(10)-C(11)	1.368(3)
C(3)-C(4)	1.375(3)	C(11)-C(12)	1.389(3)
Bond angles			
O(1)-P(1)-O(2)	116.42(8)	C(3)-C(2)-C(1)	120.2(2)
O(1)-P(1)-C(1)	110.87(9)	C(4)-C(3)-C(2)	120.3(2)
O(2)-P(1)-C(1)	107.36(8)	C(5)-C(4)-C(3)	119.8(2)
O(1)-P(1)-C(7)	110.12(8)	C(4)-C(5)-C(6)	120.1(2)
O(2)-P(1)-C(7)	103.66(8)	C(5)-C(6)-C(1)	121.0(2)
C(1)-P(1)-C(7)	107.91(8)	C(12)-C(7)-C(8)	119.44(19)
C(6)-C(1)-C(2)	118.6(2)	C(12)-C(7)-P(1)	120.03(15)
C(6)-C(1)-P(1)	119.80(16)	C(8)-C(7)-P(1)	120.52(15)
C(2)-C(1)-P(1)	121.62(15)	C(9)-C(8)-C(7)	119.7(2)

C(1)-C(6) = 1.381(3) Å, C(1)-C(2) = 1.384(3) Å, C(2)-C(3) = 1.383(3) Å, C(3)-C(4) = 1.375(3) Å and C(4)-C(5) = 1.365(3) Å] and bond angles [O(1)-P(1)-O(2) = 116.42(8)°, O(1)-P(1)-C(1) = 110.87(9)°, O(2)-P(1)-C(1) = 107.36(8)°, O(1)-P(1)-C(7) = 110.12(8)°, O(2)-P(1)-C(7) = 103.66(8)°, C(1)-P(1)-C(7) = 107.91(8)°, C(6)-C(1)-C(2) = 118.6(2)° and C(6)-C(1)-P(1) = 119.80(16)°] are comparable to other compounds [21–28].

As shown in Fig. 2, the crystal packing diagram of the title compound reveals that intermolecular O—H . . . O hydrogen bonds between amide groups stabilize the solid state.

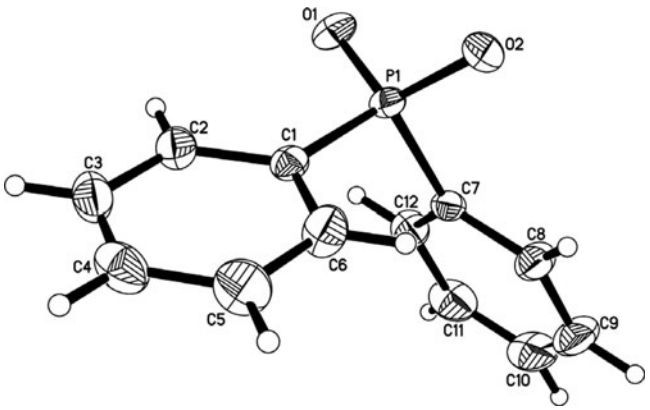

Figure 1. Molecular structure of the title compound.

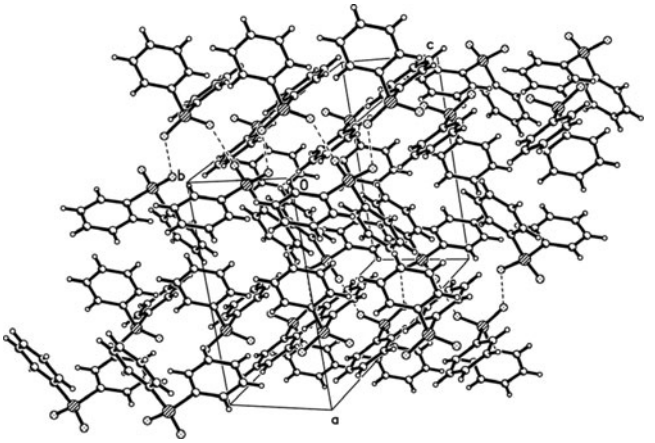

Figure 2. The crystal packing view of the title compound.

Conclusions

In summary, the title compound diphenylphosphinic acid has been characterized by X-ray diffraction analysis.

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Supplementary Information

Crystallographic data for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication number CCDC 1030675 for the title compound. Copies of the data can be obtained free of charge at http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; e-mail: deposit@ccdc.cam.ac.uk.

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