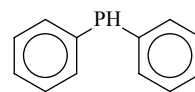


**907**      **C<sub>12</sub>H<sub>11</sub>P**ED, *ab initio* and  
DFT calculations**Diphenylphosphine****C<sub>1</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
P–C(1)	1.829(4)	P–C(1)–C(2)	120.4(16)
P–C(1')	1.833(4)	P–C(1')–C(2')	119.4(16)
C(1)–C(2)	1.407(1)	C(1)–C(2)–C(3)	122.4(16)
C(2)–C(3)	1.396(1)	C(2)–C(3)–C(4)	118.2(20)
C(3)–C(4)	1.400(1)	C(3)–C(4)–C(5)	119.3(12)
C(4)–C(5)	1.396(1)	C(4)–C(5)–C(6)	123.2(14) <sup>b)</sup>
C(5)–C(6)	1.400(1)	C(5)–C(6)–C(1)	117.4(15) <sup>b)</sup>
C(6)–C(1)	1.405(1)	C(6)–C(1)–C(2)	119.5(6) <sup>b)</sup>
C(1')–C(2')	1.402(1)	C(1')–P–C(1')	101.0(20)
C(2')–C(3')	1.402(1)	H–P–C(1)	98.0 <sup>c)</sup>
C(3')–C(4')	1.396(1)	H–P–C(1')	98.0 <sup>c)</sup>
C(4')–C(5')	1.402(1)	C(1)–P–C(1')–C(2')	154(7)
C(5')–C(6')	1.396(1)	C(1')–P–C(1)–C(2)	–65(7)
C(6')–C(1')	1.408(1)	H–P–C(1)–C(2)	–164(7) <sup>b)</sup>
C–C <sup>d)</sup>	1.401(1)	H–P–C(1')–C(2')	–107 <sup>b)</sup>
C–H <sup>d)</sup>	1.087(5)		
P–H	1.401 <sup>c)</sup>		

The experimental data reported in [1] were reanalyzed. The molecule was found to exist as a single asymmetric conformer with two different torsional angles around the P–C bonds. Differences in the C–C, P–C and P–C–C parameters were assumed at the values from HF/6-31G\* calculations. The C(*i*)–C(*j*)–C(*k*) and C(*i'*)–C(*j'*)–C(*k'*) angles were assumed to be equal to each other.

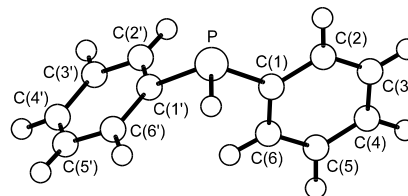
The temperature of the measurements was not stated.

<sup>a)</sup> Twice the estimated standard errors.

<sup>b)</sup> Dependent parameter.

<sup>c)</sup> Assumed according to the results of HF/6-31G\* calculations.

<sup>d)</sup> Mean value.



Naumov, V.A., Tafipol'skii, M.A., Naumov, A.V., Samdal, S.: Zh. Obshch. Khim. **72** No.12 (2002) 2002; Russ. J. Gen. Chem. (Engl. Transl.) **72** (2002) 1894.

[1] Naumov, V.A., Kataeva, O.N.: Zh. Strukt. Khim. **25** No.4 (1984) 140; J. Struct. Chem. (Engl. Transl.) **25** (1984) 642.

Replaces [II/25D \(3, 2809\)](#)