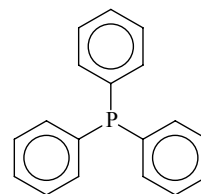
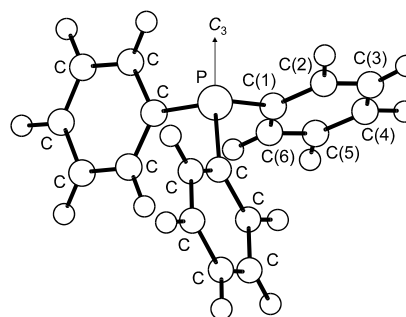


**937**      **C<sub>18</sub>H<sub>15</sub>P****Triphenylphosphine****C<sub>3</sub>**ED, *ab initio*  
calculations

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C–H (average)	1.098(3)	C(1)–C(2)–C(3)	121.3(11)
P–C	1.839(2)	C(2)–C(3)–C(4)	118.9(12)
C(1)–C(2)	1.404(1)	C(3)–C(4)–C(5)	120.2(7)
C(2)–C(3)	1.399 <sup>b)</sup>	C(4)–C(5)–C(6)	120.1(10) <sup>c)</sup>
C(3)–C(4)	1.400 <sup>b)</sup>	C(5)–C(6)–C(1)	119.2(10) <sup>c)</sup>
C(4)–C(5)	1.395 <sup>b)</sup>	C(6)–C(1)–C(2)	119.4(4) <sup>c)</sup>
C(5)–C(6)	1.396 <sup>b)</sup>	P–C–C	115.3(5)
C(1)–C(6)	1.408 <sup>b)</sup>	C–P–C	102.2(7)
C–C (average)	1.400 <sup>b)</sup>	$\tau^d$	32.2(35)



The temperature of the measurements was 170 °C.

<sup>a)</sup> Twice the estimated standard errors.<sup>b)</sup> Difference relative to the C(1)–C(2) bond length was assumed at the value from HF/6-31G\* calculations.<sup>c)</sup> Dependent parameter.<sup>d)</sup> Torsional angle C<sub>3</sub>...P–C(1)–C(2) from the *syn* position, where C<sub>3</sub> is the symmetry axis.

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