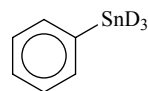


738 **C₆H₅Sn**ED, DFT
calculations**Phenylstannane-*d*₃**essentially C_s

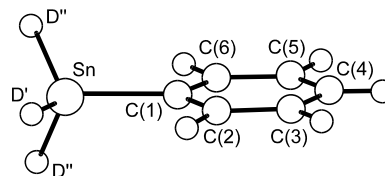
r_a	Å ^{a)}	θ_a	deg ^{a)}
Sn–C	2.131(7)	C–Sn–D'	113(4)
Sn–D'	1.686(14)	C–Sn–D''	115(4)
Sn–D''	1.687(14)	C(2)–C(1)–C(6)	119.6(8)
C(1)–C(2)	1.403(2)	C(1)–C(2)–C(3)	119.9(7)
C(3)–C(2,4)	1.395(2)	C(2)–C(3)–C(4)	120.5(2)
C(2)–H	1.099(9)	C(3)–C(4)–C(5)	119.6 ^{b)}
C(3)–H	1.098(9)	C(2)–C(1)–Sn–D'	0 ^{c)}
C(4)–H	1.088(9)	C(2)–C(1)–Sn–D''	±120.2 ^{c)}

According to the results of B3LYP/LANL2DZ calculations, the molecule has C₁ symmetry in the equilibrium position and a low barrier to internal rotation of the SnD₃ group, *ca.* 60 J mol^{−1}, at the C_s structure. The small differences in the bond distances and angles were assumed in the ED analysis at the values from quantum chemical calculations. The nozzle temperature was 22 °C.

^{a)} Twice the estimated standard errors including a systematic error.

^{b)} Assumed at the value from B3LYP/LANL2DZ calculations.

^{c)} Assumed.



Taraci, J., Zollner, S., McCartney, M.R., Menendez, J., Santana-Aranda, M.A., Smith, D.J., Haaland, A., Tutukin, A.V., Gundersen, G., Wolf, G., Kouvetakis, J.: J. Am. Chem. Soc. **123** (2001) 10980.