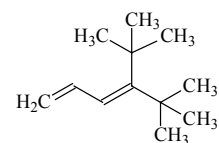


909  $C_{12}H_{22}$ ED, *ab initio*  
calculations

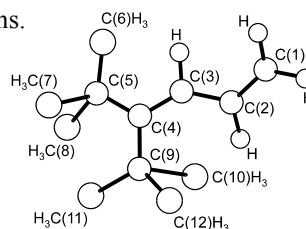
4-(1,1-Dimethylethyl)-5,5-dimethyl-1,3-hexadiene

1,1-Di-*t*-butyl-1,3-butadiene $C_1$ 

$r_a$	$\text{\AA}^a$	$\theta_a$	$\text{deg}^a$
C(3)=C(4)	1.380(6)	C(4)=C(3)-C(2)	128.2(16)
C(1)=C(2)	1.366 <sup>b)</sup>	C(3)-C(2)=C(1)	121.2(21)
C(2)-C(3)	1.533(22)	C(3)=C(4)-C(5)	116.1(6)
C(4)-C(5)	1.557(12)	C(3)=C(4)-C(9)	119.5 <sup>b)</sup>
C(4)-C(9)	1.563 <sup>b)</sup>	C(4)=C(3)-H	117.6 <sup>c)</sup>
C-C(methyl) <sup>d)</sup>	1.551(6)	C(2)-C(3)-H	109.7 <sup>c)</sup>
C(sp <sup>3</sup> )-H <sup>d)</sup>	1.122(14)	C(3)-C(2)-H	120.5 <sup>c)</sup>
C(sp <sup>2</sup> )-H <sup>d)</sup>	1.095 <sup>c)</sup>	C(1)=C(2)-H	117.6 <sup>c)</sup>
		C(4)-C(5)-C(6)	112.3 <sup>f)</sup>
		C(4)-C(5)-C(7)	109.5(10)
		C(4)-C(5)-C(8)	112.6 <sup>f)</sup>
		C(4)-C(9)-C(10)	110.2 <sup>f)</sup>
		C(4)-C(9)-C(11)	117.0 <sup>f)</sup>
		C(4)-C(9)-C(12)	109.2 <sup>f)</sup>
		C(3)=C(4)-C(5)-C(6)	-1.1(32)
		C(3)=C(4)-C(5)-C(7)	116.2 <sup>f)</sup>
		C(3)=C(4)-C(5)-C(8)	-120.0 <sup>f)</sup>
		C(3)=C(4)-C(9)-C(10)	44.2(21)
		C(3)=C(4)-C(9)-C(11)	162.0 <sup>f)</sup>
		C(3)=C(4)-C(9)-C(12)	-77.9 <sup>f)</sup>
		C(1)=C(2)-C(3)=C(4)	-192.5(151)



The nozzle was at 42.0 °C.

<sup>a)</sup> Uncertainties were unidentified, possibly estimated standard errors.<sup>b)</sup> Dependent parameter, tied to a similar parameter.<sup>c)</sup> Assumed at the value from HF/6-31G\* calculations.<sup>d)</sup> Mean value.<sup>e)</sup> Assumed.<sup>f)</sup> Differences in the C(4)-C-C(methyl) bond angles and in the C(3)=C(4)-C-C(methyl) torsional angles were assumed at the values from HF/6-31G\* calculations.

Hopf, H., Hänel, R., Trætteberg, M., Bakken, P.: Eur. J. Org. Chem. (1998) 467.