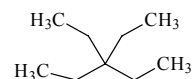


878 **C₉H₂₀**
ED, *ab initio*
calculations

3,3-Diethylpentane
Tetraethylmethane

D_{2d} (conformer I)
S₄ (conformer II)



r_a	$\text{\AA}^a)$	θ_a	$\text{deg}^a)$	
	D _{2d} , S ₄		D _{2d}	S ₄
C(1)–C(2)	1.532(2)	H–C(2)–H	107.2(16) ^{b)}	107.2(16) ^{b)}
C(2)–C(3)	1.554(2)	C(3)–C(2)–C(1)	115.5(5)	
C(1)–H	1.124(1)	C(2)–C(3)–C(4) ^{c)}	106.7(8)	108.6(18)
C(2)–H	1.124(1)	C(2)–C(3)–C(6) ^{c)}	110.9(4)	109.9(9)
		C(2)–C(1)–H ^{c)}	109.1(5)	
		C(3)–C(2)–H ^{c)} ^{d)}	106.9(5)	107.4(5)

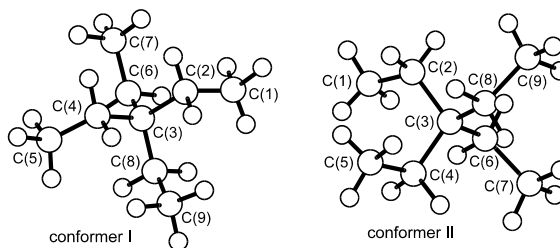
The molecule was found to exist as a mixture of conformer I of D_{2d} symmetry (66(2)%) and conformer II of S₄ symmetry (34(2)%). The distribution of conformers corresponds to the energy difference of 3.3(2) kJ mol^{−1}. Local C_{2v} symmetry was assumed for the CH₂ group and C_{3v} for C–CH₃. Differences between similar parameters were constrained to the values from MP2/6-31G* calculations, only the difference between the outer C–C–C bond angle and the central C–C–C bond angle for the D_{2d} conformer was refined. The nozzle temperature was 293 K.

^{a)} Estimated standard errors.

^{b)} Constrained to the value from MP2/6-31G* calculations.

^{c)} Dependent parameter.

^{d)} Difference between angles in the S₄ and D_{2d} conformers was assumed at 0.5° from MP2/6-31G* calculations.



Alder, R.W., Allen, P.R., Hnyk, D., Rankin, D.W.H., Robertson, H.E., Smart, B.A., Gillespie, R.J., Bytheway, I.: J. Org. Chem. **64** (1999) 4226.