

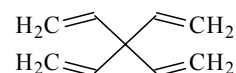
873  
ED

 $\text{C}_9\text{H}_{12}$ 
**3,3-Diethenyl-1,4-pentadiene**  
Tetravinylmethane

 $\text{C}_1$ 

$r_g$	$\text{\AA}^a$
C–H	1.101(2)
C=C	1.336(3)
C–C	1.522(3)

$\theta_a$	deg <sup>a)</sup>
C–C–C	109.5 <sup>b)</sup>
C–C=C	127.0(2)
C–C–H	117.0 <sup>b)</sup>
(C)C=C–H	123.7(7)
$\tau_1$ <sup>c)</sup> <sup>d)</sup>	24.8(15)
$\tau_2$ <sup>d)</sup> <sup>e)</sup>	–121.7(27)
$\tau_3$ <sup>d)</sup> <sup>f)</sup>	–8.6(18)
$\tau_4$ <sup>d)</sup> <sup>g)</sup>	–20.2(24)



The all-carbon frame of the molecule may be characterized by a carbon tetrahedron standing on three C=C legs out of one of the sides, C(2)C(4)C(6), of this tetrahedron, of approximately  $\text{C}_3$  symmetry.

The nozzle temperature was 23 °C.

<sup>a)</sup> Estimated total errors.

<sup>b)</sup> Assumed.

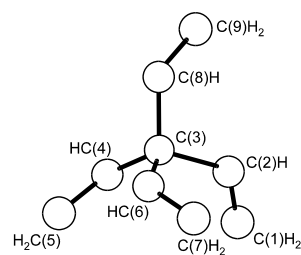
<sup>c)</sup> Torsional angle C(4)–C(3)–C(2)=C(1).

<sup>d)</sup> Zero degree for the eclipsed position, positive for clockwise rotation of the closer bond.

<sup>e)</sup> Torsional angle C(2)–C(3)–C(4)=C(5).

<sup>f)</sup> Torsional angle C(2)–C(3)–C(6)=C(7).

<sup>g)</sup> Torsional angle C(2)–C(3)–C(8)=C(9).



Schultz, G., Hargittai, I.: J. Mol. Struct. **445** (1998) 47.