

1178  
IR

**C<sub>3</sub>H<sub>5</sub>**

**2-Propen-1-yl**  
Allyl radical

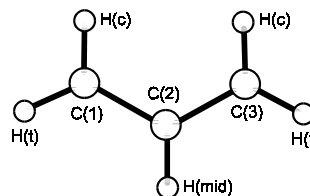
**C<sub>2v</sub>**

| $r_0$    | Å                   | $\theta_0$ | deg                 |
|----------|---------------------|------------|---------------------|
| C–C      | 1.3869(33)          | C–C–C      | 123.96(48)          |
| C–H(t)   | 1.082 <sup>a)</sup> | C–C–H(t)   | 121.2 <sup>b)</sup> |
| C–H(c)   | 1.085 <sup>a)</sup> | C–C–H(c)   | 121.5 <sup>b)</sup> |
| C–H(mid) | 1.087 <sup>a)</sup> |            |                     |

Structure derived from  $A_0$  and  $B_0$ .

<sup>a)</sup> Assumed value, uncertainty estimated 0.010 Å.

<sup>b)</sup> Assumed value, uncertainty estimated 1°.



Hirota, E., Yamada, C., Okunishi, M.: J. Chem. Phys. **97** (1992) 2963.

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| $r_g$     | Å <sup>a)</sup> | $\theta_a$ | deg <sup>a)</sup> |
|-----------|-----------------|------------|-------------------|
| C–C       | 1.428(13)       | C–C–C      | 124.6(34)         |
| C–H(mean) | 1.069(16)       | C(2)–C–H   | 120.9(34)         |

The free radicals, with 75% relative abundance, were produced by vacuum pyrolysis of 1,5-hexadiene at 960 °C.

The nozzle temperature was 960 °C.

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

Vajda, E., Tremmel, J., Rozsondai, B., Hargittai, I., Maltsev, A.K., Kagramanov, N.D., Nefedov, O.M.: J. Am. Chem. Soc. **108** (1986) 4352.