

1231  
ED, IR

**C<sub>3</sub>H<sub>6</sub>**

**Cyclopropane**

**D<sub>3h</sub>**

$r_z$	Å <sup>a)</sup>	$\theta_z$	deg <sup>a)</sup>
C–C	1.5127(12)	H–C–H	114.5(9)
C–H	1.0840(20)		
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$r_e$	Å <sup>a)</sup>	$\theta_e$	deg <sup>a)</sup>
C–C	1.501(44)	H–C–H	114.5(9)
C–H	1.083(5)		



The measurements were made at room temperature.

<sup>a)</sup> Estimated limits of error.

[1] Yamamoto, S., Nakata, M., Fukuyama, T., Kuchitsu, K.: J. Phys. Chem. **89** (1985) 3298.

See also: (ED) Bastiansen, O., Fritsch, F.N., Hedberg, K.: Acta Crystallogr. **17** (1964) 538.

MW

**Cyclopropane-1,1-*d*<sub>2</sub>**

**D<sub>3h</sub> (C<sub>2v</sub>)**

$r_0$	Å	$\theta_0$	deg
C–C	1.515321(75)	H–C–H	115.568(13)
C–H	1.07739(12)		
$\Delta[(C-H) - (C-D)]$	-0.001160(87)		
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$r_z$	Å	$\theta_z$	deg
C–C	1.5157(69)	H–C–H	115.5(10)
C–H	1.080(10)		
$\Delta[(C-H) - (C-D)]$	0.00029(48)		
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$r_e$	Å	$\theta_e$	deg
C–C	1.5101(21)	H–C–H	115.85(33)
C–H	1.0742(29)		

The authors of [3] state that, according to their correlations, the value  $r_e(C-H)$  given in [2] is too low and that the value 1.083 given in [1] is too high. They also think that the  $r_0(C-H)$  and  $r_z(C-H)$  values of [2] are too low and suggest to replace the latter by 1.0843(29) Å.

[2] Endo, Y., Chang, M.C., Hirota, E.: J. Mol. Spectrosc. **126** (1987) 63.

[3] Demaison, J., Włodarczak, G.: Struct. Chem. **5** (1994) 57.