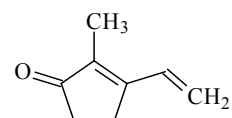


847 **C₈H₁₀O**ED, *ab initio*
calculations**3-Ethenyl-2-methyl-2-cyclopenten-1-one**

2-Methyl-3-vinyl-2-cyclopenten-1-one

C_s

r_a	\AA^a	θ_a	deg^a
C(2)=C(3)	1.363(2)	C(5)-C(1)-C(2)	108.8(3)
C=O	1.223(2)	C(1)-C(2)=C(3)	108.2(2)
C(1)-C(2)	1.482(1)	C(2)=C(3)-C(4)	113.2(3)
C(3)-C(4)	1.519(1)	C(3)-C(4)-C(5)	104.0(3)
C(4)-C(5)	1.536(1)	C(4)-C(5)-C(1)	105.7(3)
C(1)-C(5)	1.520(1)	C(2)-C(1)=O	126.7(10)
C(2)-C(8)	1.498(1)	C(3)=C(2)-C(8)	130.6(8)
C(3)-C(6)	1.467(1)	C(2)=C(3)-C(6)	127.1(5)
C(6)=C(7)	1.350(2)	C(3)-C(6)=C(7)	123.9(5)
C(sp ²)-H	1.020(6)	τ^b	180.0 ^c
C(sp ³)-H	1.116(3)		

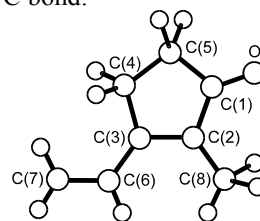
Differences in the C–C bond lengths, between the C(2)=C(3) and C(6)=C(7) bond lengths, and those in the valence and dihedral angles involving H atoms were all constrained to the values from MP2/6-31G* calculations. According to the results of HF/6-31G* calculations, the ethenyl group has *s-trans* orientation with respect to the C=C bond.

The temperature of the measurements was 36 °C.

^a) Estimated standard errors.

^b) C(2)=C(3)–C(6)=C(7) torsional angle.

^c) Assumed at the MP2/6-31G* value.



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