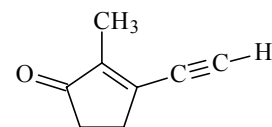


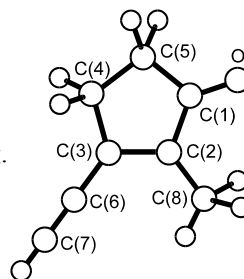
**836 C<sub>8</sub>H<sub>8</sub>O**ED, *ab initio*  
calculations**3-Ethynyl-2-methyl-2-cyclopenten-1-one****C<sub>s</sub>**

$r_a$	Å <sup>a)</sup>	$\theta_a$	deg <sup>a)</sup>
C(2)=C(3)	1.377(3)	C(5)-C(1)-C(2)	109.5(2)
C=O	1.227(1)	C(1)-C(2)=C(3)	108.5(2)
C(1)-C(2)	1.476(2)	C(2)=C(3)-C(4)	112.1(2)
C(3)-C(4)	1.526(1)	C(3)-C(4)-C(5)	105.3(2)
C(4)-C(5)	1.543(1)	C(4)-C(5)-C(1)	104.6(2)
C(1)-C(5)	1.536(1)	C(2)-C(1)=O	124.1(3)
C(2)-C(8)	1.487(2)	C(3)=C(2)-C(8)	130.2(3)
C(3)-C(6)	1.417(3)	C(2)=C(3)-C(6)	125.7(4)
C(6)≡C(7)	1.223(1)	C(3)-C(6)≡C(7)	180 <sup>b)</sup>
C(sp)-H	1.108(2)		
C(sp <sup>3</sup> )-H	1.113(2)		

Differences in the C-C bond lengths, between the C≡C and C=O bond lengths and in the valence and dihedral angles involving H atoms were all constrained to the values from MP2/6-31G\* calculations. The ethynyl group is coplanar with the ring. The temperature of the measurements was 76 °C.

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

<sup>b)</sup> Assumed at the value from MP2/6-31G\* calculations.



Trættemberg, M., Liebman, J.F., Hulce, M., Bohn, A.A., Rogers, D.W.: J. Chem. Soc., Perkin Trans. 2 (1997) 1925.