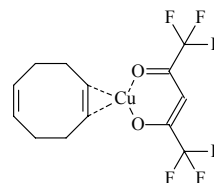


**919**      **C<sub>13</sub>H<sub>13</sub>CuF<sub>6</sub>O<sub>2</sub>**ED, *ab initio* and  
DFT calculations**[(1,2- $\eta$ )-1,5-cyclooctadiene](1,1,1,5,5,5-hexafluoro-  
2,4-pentanedionato- $\kappa$ O, $\kappa$ O')copper****C<sub>1</sub>**

$r_a$	$\text{\AA}^a$	$\theta_a$	deg $^a$
C(1)=C(2)	1.429(7)	C(2)=C(1)–C(8)	127.0(5)
C(5)=C(6)	1.353(19) <sup>b)</sup>	C(6)=C(5)–C(4)	129.9(16)
C(1)–C(8)	1.518(8)	C(1)=C(2)–C(3)	124.9(5)
C(4)–C(5)	1.518(8)	C(5)=C(6)–C(7)	121.8(17)
C(6)–C(7)	1.518(8)	C(1)–C(8)–C(7)	118.6(4)
C(2)–C(3)	1.534(5)	C(3)–C(4)–C(5)	118.6(4)
C(3)–C(4)	1.565(5)	C(2)–C(3)–C(4)	116.2(4)
C(7)–C(8)	1.565(5)	C(6)–C(7)–C(8)	116.2(4)
C(2')–C(3')	1.408(7)	Cu–O(1,2)–C(2',4')	119.5(7)
C(2')–C(1')	1.549(5)	C(1,2)–Cu–O(1,2)	109.2(5)
Cu–C(1)	1.940(13)	C(3)–C(2)=C(1)–C(8)	1.0 <sup>c)</sup>
Cu–C(2)	1.949(13)	C(4)–C(5)=C(6)–C(7)	2.0(15) <sup>b)</sup>
Cu–O(1)	1.944(9)	C(2)–C(3)–C(4)–C(5)	40.0(12)
C(2')=O(1)	1.280(10)	C(1)–C(8)–C(7)–C(6)	43.0(14)
C–F	1.332(3)	C(1)=C(2)–C(3)–C(4)	–85.1(9)
Cu...C(5)	2.672(23) <sup>b)</sup>	C(5)=C(6)–C(7)–C(8)	–90.2(12)
Cu...C(6)	2.769(25) <sup>b)</sup>	C(2)=C(1)–C(8)–C(7)	36.7(8)
C–H	1.124(8)	C(3)–C(4)–C(5)=C(6)	36.1(19)
		$\varphi^d$	27.8(16)



According to the results of BP86/AE1 and MP2/AE1 calculations, it was assumed in the ED analysis that the hexafluoropentanedionate fragment has local C<sub>2v</sub> symmetry and cyclooctadiene ligand has twist-boat conformation with very approximately C<sub>2</sub> local symmetry. The most stable structure is one in which one olefinic group of the cyclooctadiene ligand, C(1)=C(2), is coordinated to the square-planar Cu atom. The second bond, C(5)=C(6), is weakly associated with the Cu atom, and the cyclooctadiene ligand has a twist-boat conformation.

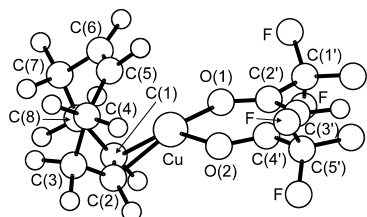
The nozzle temperature was *ca.* 413 K.

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

<sup>b)</sup> Flexibly restrained to the values from the calculations.

<sup>c)</sup> Assumed.

<sup>d)</sup> Folding angle of the CuC<sub>2</sub>O<sub>2</sub> core along the axis parallel to the C(1)=C(2) bond and passing through the Cu atom.



Hnyk, D., Bühl, M., Brain, P.T., Robertson, H.E., Rankin, D.W.H.: J. Am. Chem. Soc. **124** (2002) 8078.