

17 MW	CClCuO		Carbonylchlorocopper	$\text{C}_{\infty\text{v}}$ Cl–Cu–C=O
	r_0	\AA^{a}		
	C=O	1.128(1)		
	C–Cu	1.796(1)		
	Cu–Cl	2.0558(7)		
	r_{lg}	\AA^{a}		
	C=O	1.12872(7)		
	C–Cu	1.79493(9)		
	Cu–Cl	2.05480(5)		
	$r_{\text{m}}^{(1)}$	\AA^{a}		
	C=O	1.12818(7)		
	C–Cu	1.7940(1)		
	Cu–Cl	2.05379(7)		
	$r_{\text{m}}^{(2)}$	\AA^{a}		
	C=O	1.12755(1)		
	C–Cu	1.79447(1)		
	Cu–Cl	2.053419(8)		

The C=O distance is comparatively short and is close to that of free CO. The Cu–C distance is longer than that predicted by *ab initio* calculations, and the Cu–Cl distance is very similar to that observed in CuCl.

^a) Estimated standard errors.

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