12 **CBrCuO** **Bromo(carbonyl)copper** $C_{\infty v}$

MW Br–Cu–C=O

r_0	Å [a])
C=O	1.1277(6)
C–Cu	1.8022(9)
Cu–Br	2.182(4)

$r_{I\varepsilon}$	Å [a])
C=O	1.12821(8)
C–Cu	1.8027(1)
Cu–Br	2.1797(1)

$r_m^{(1)}$	Å [a])
C=O	1.12775(8)
C–Cu	1.8019(1)
Cu–Br	2.1788(1)

$r_m^{(2)}$	Å [a])
C=O	1.12721(2)
C–Cu	1.80238(2)
Cu–Br	2.17871(1)

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–Br distance is very similar to that observed in CuBr.

[a]) Estimated standard errors.

Walker, N.R., Gerry, M.C.L.: Inorg. Chem. **40** (2001) 6158.