8 **CAuBrO** **Bromo(carbonyl)gold** **$C_{\infty v}$**

MW Br–Au–C=O

r_0	Å [a])
C=O	1.132(1)
C–Au	1.892(2)
Au–Br	2.3377(5)

r_s	Å [b])
C=O	1.1321(5)
C–Au	1.8917(5)
Au–Br	2.3363(5)

$r_{I\varepsilon}$	Å [a]) [c])
C=O	1.132160(5)
C–Au	1.891730(6)
Au–Br	2.336301(4)

$r_m^{(1)}$	Å [a]) [d])
C=O	1.13171(1)
C–Au	1.89095(2)
Au–Br	2.33535(1)

$r_m^{(2)}$	Å [a]) [e])
C=O	1.1341(5)
C–Au	1.8886(5)
Au–Br	2.3364(2)

The C=O bond is close to that of free CO, plus a relatively long Au–C bond.

[a]) Estimated standard errors.
[b]) Uncertainties were not estimated in the original paper.
[c]) $\varepsilon_0 = 0.4781(11)$ u Å^2 assumed.
[d]) $c = 0.03935(19)$ u^{½} Å assumed.
[e]) $c = 0.018(12)$ u^{½} Å and $d = 0.253$ u^{½} Å^2 assumed.

Evans, C.J., Reynard, L.M., Gerry, M.C.L.: Inorg. Chem. **40** (2001) 6123.