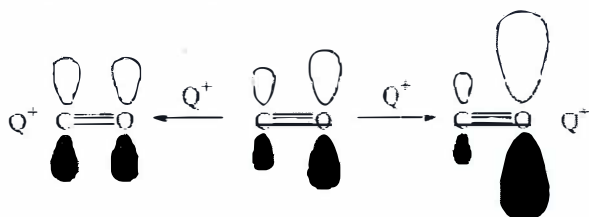


Carbonylkomplexe

5σ – bindend, antibindend, nichtbindend ??

Spezies	Konfiguration	d(C–O) pm	$\nu(\text{CO}) \text{ cm}^{-1}$	$f/\text{N cm}^{-1}$	Folgerung
CO	$(5\sigma)^2$	113	2143	18.56	
CO ⁺	$(5\sigma)^1$	111	2184	19.26	5σ schwach antibindend
CO*	$(5\sigma)^1(2\pi)^1$	S 124	1489		2π stark antibindend
		T 121	1715		
N ₂	$(5\sigma)^2$	110	2330	22.4	

(Johnson, Klemperer, 1977) S = Singulett-, T = Triplett-Zustand



„The 5σ HOMO of CO is not antibonding as it is often stated. The increase of the CO bond strength after CO binds through its carbon atom to a acceptor such as H⁺ is rather caused by the effect of the charge on the polarization of the bonding orbitals.“

(Durch Polarisation eher elektron. Struktur des N₂)

G. Frenking, J. Comp. Chem. 2007, 28, 117.

(Electronic structure of CO - an exercise in modern chemical bonding theory.)

