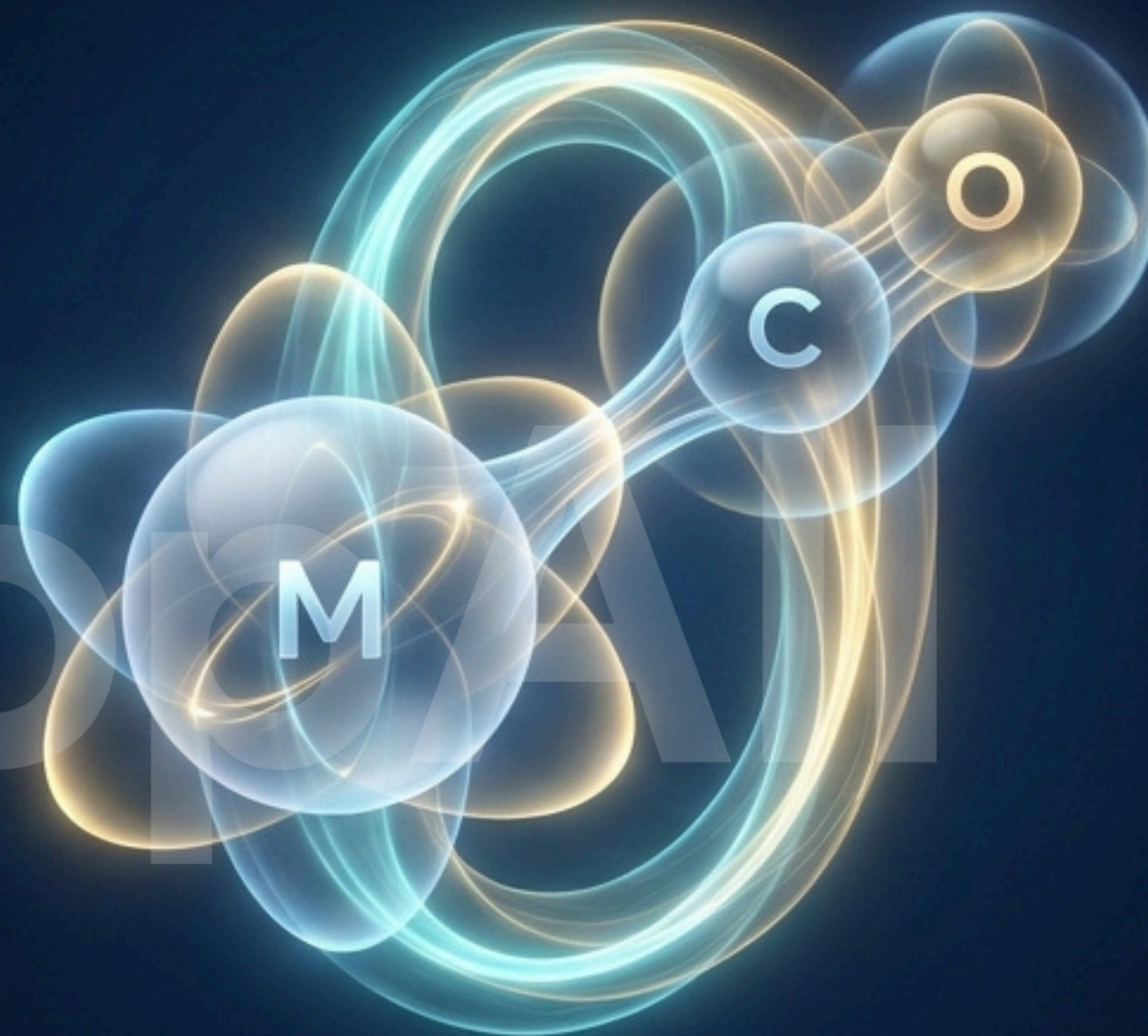


Bonding in Metal Carbonyls

A quantum blueprint of structures, electron flows, and the synergic effect.

Structural & Quantum Mechanics

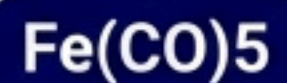
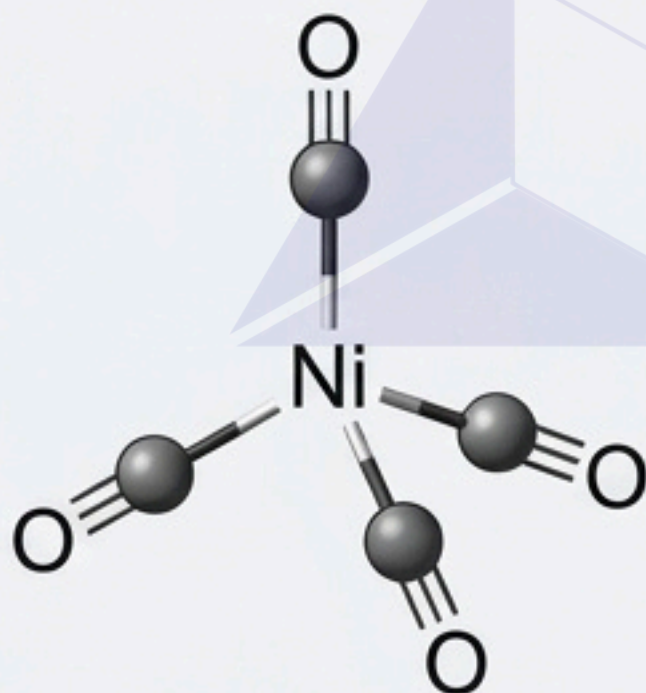


Mononuclear Carbonyl Architectures



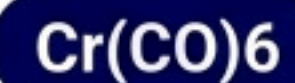
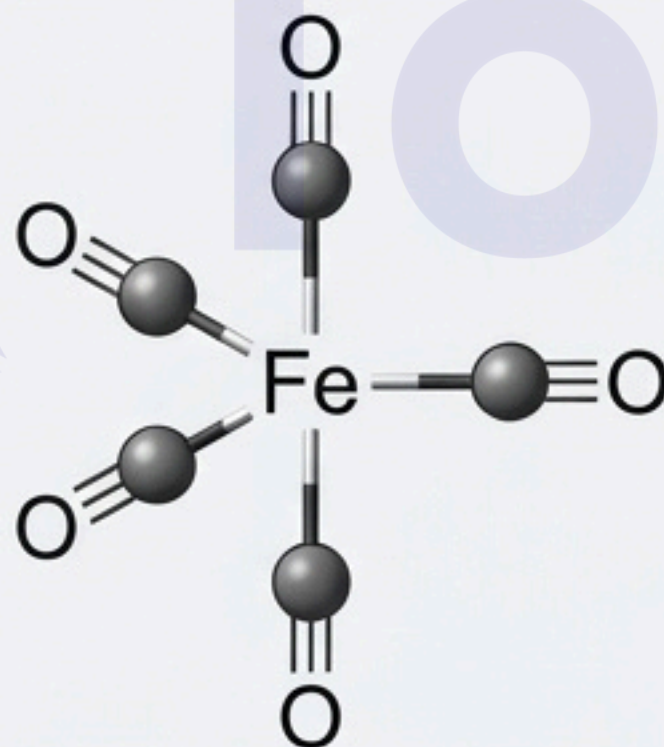
Tetracarbonylnickel(0)

GEOMETRY: Tetrahedral



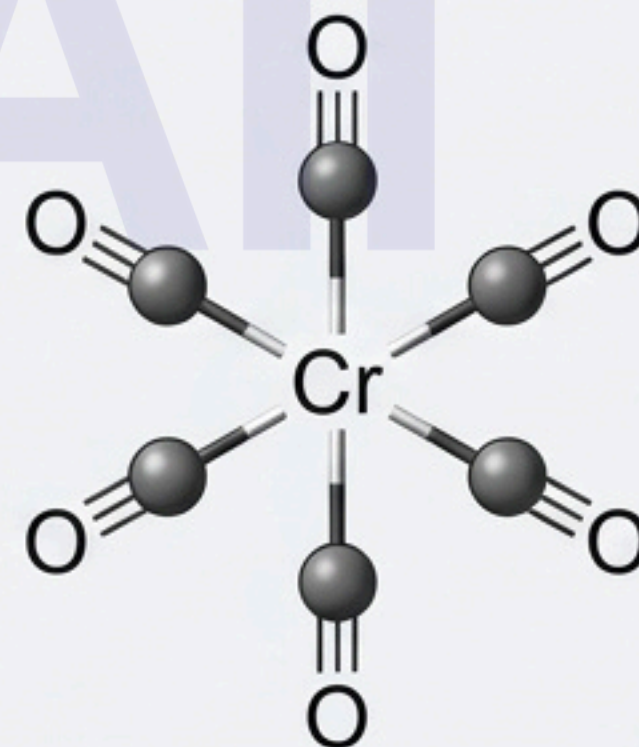
Pentacarbonyliron(0)

GEOMETRY: Trigonal Bipyramidal

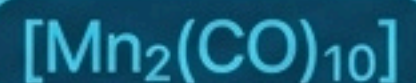


Hexacarbonylchromium(0)

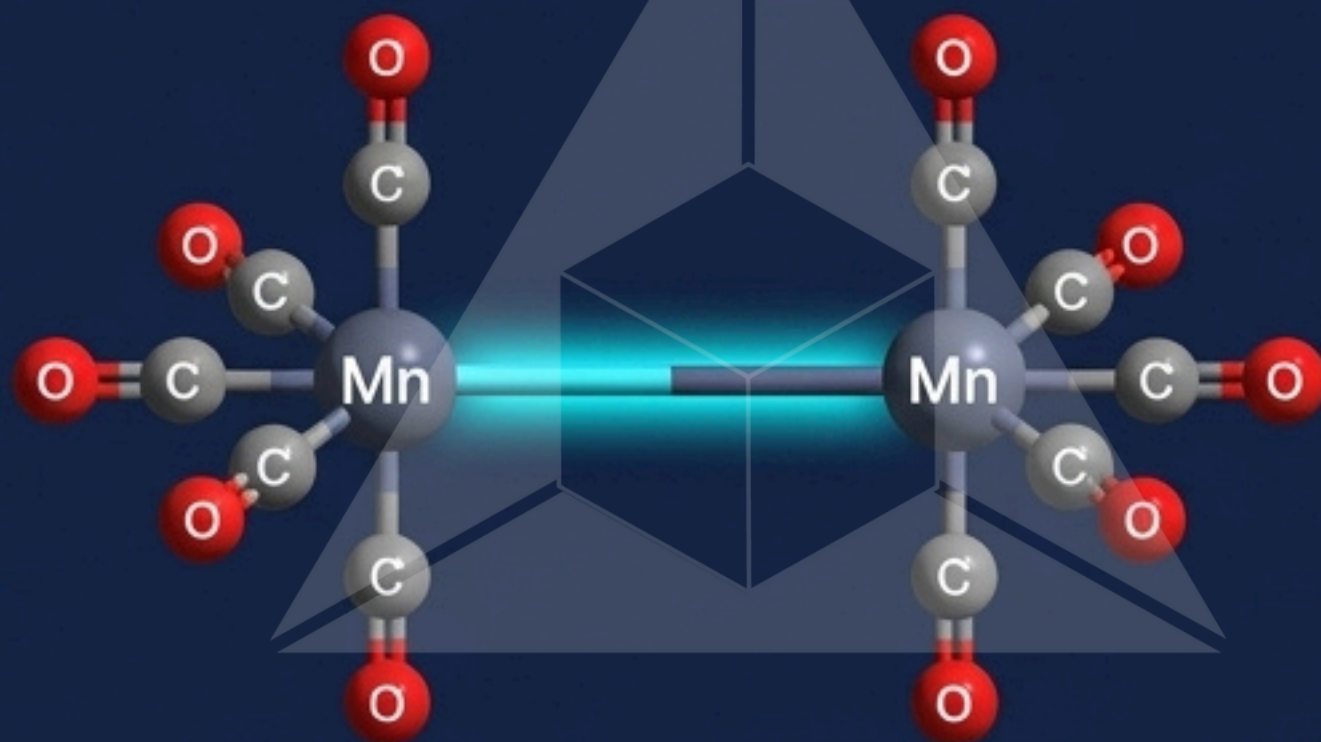
GEOMETRY: Octahedral



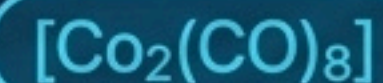
Dinuclear Carbonyl Architectures



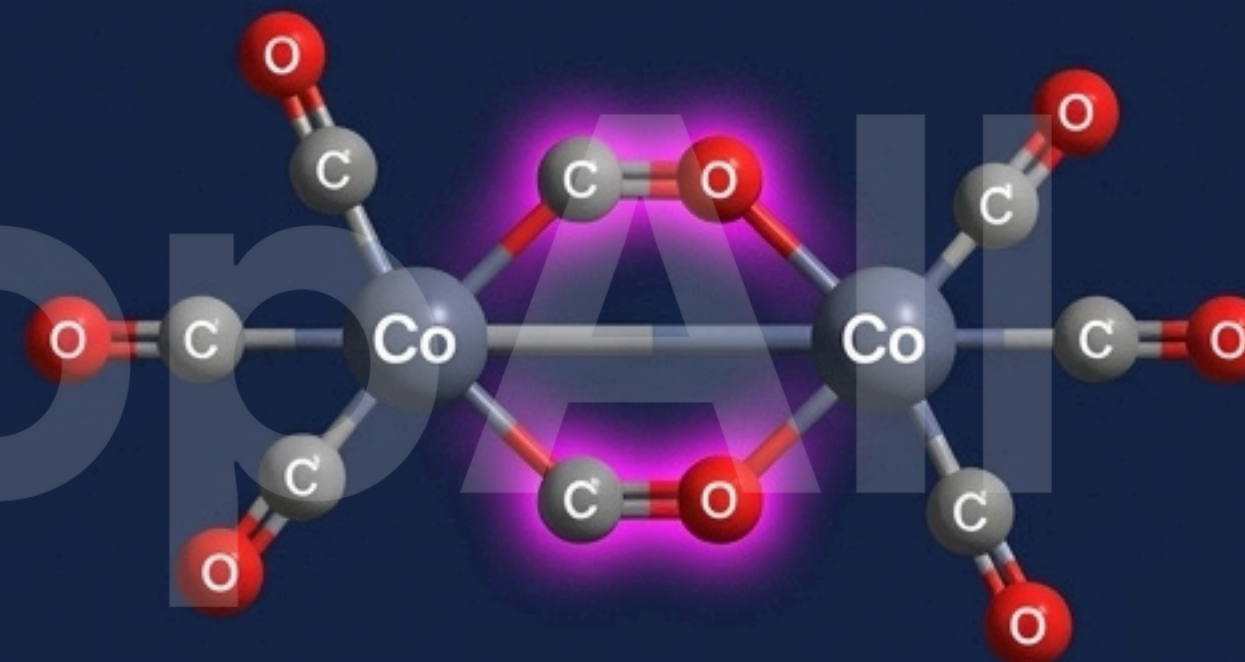
Decacarbonyldimanganese(0)



Composed of two distinct square pyramidal $\text{Mn}(\text{CO})_5$ units joined directly by a central metal-metal bond.



Octacarbonyldicobalt(0)



Features a direct Co-Co bond that is uniquely bridged by two coordinating CO groups, binding the complex together.



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$$E=mc^2$$



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Key Highlights

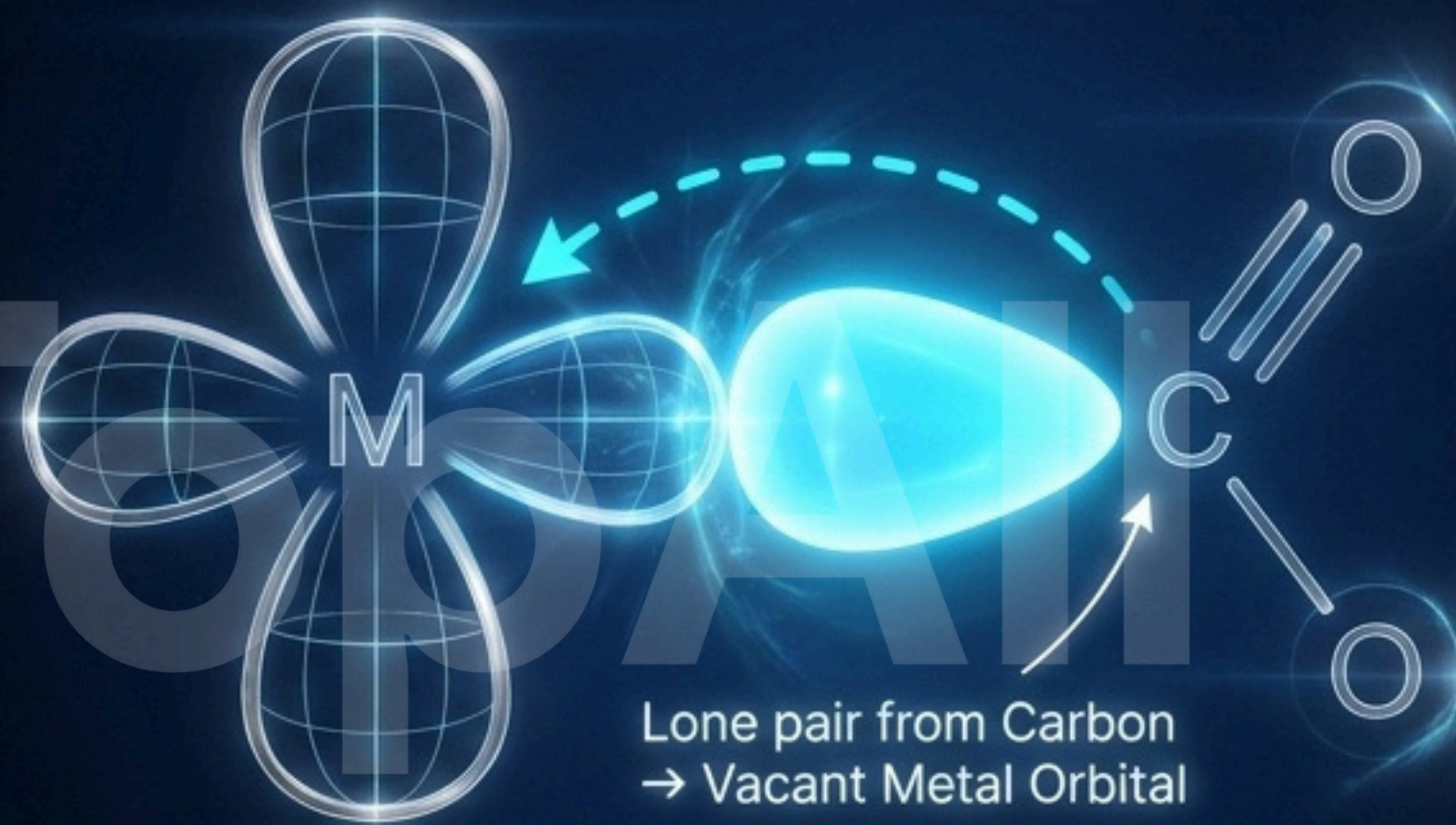
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Forward Donation: Building the Sigma Bond

σ Character

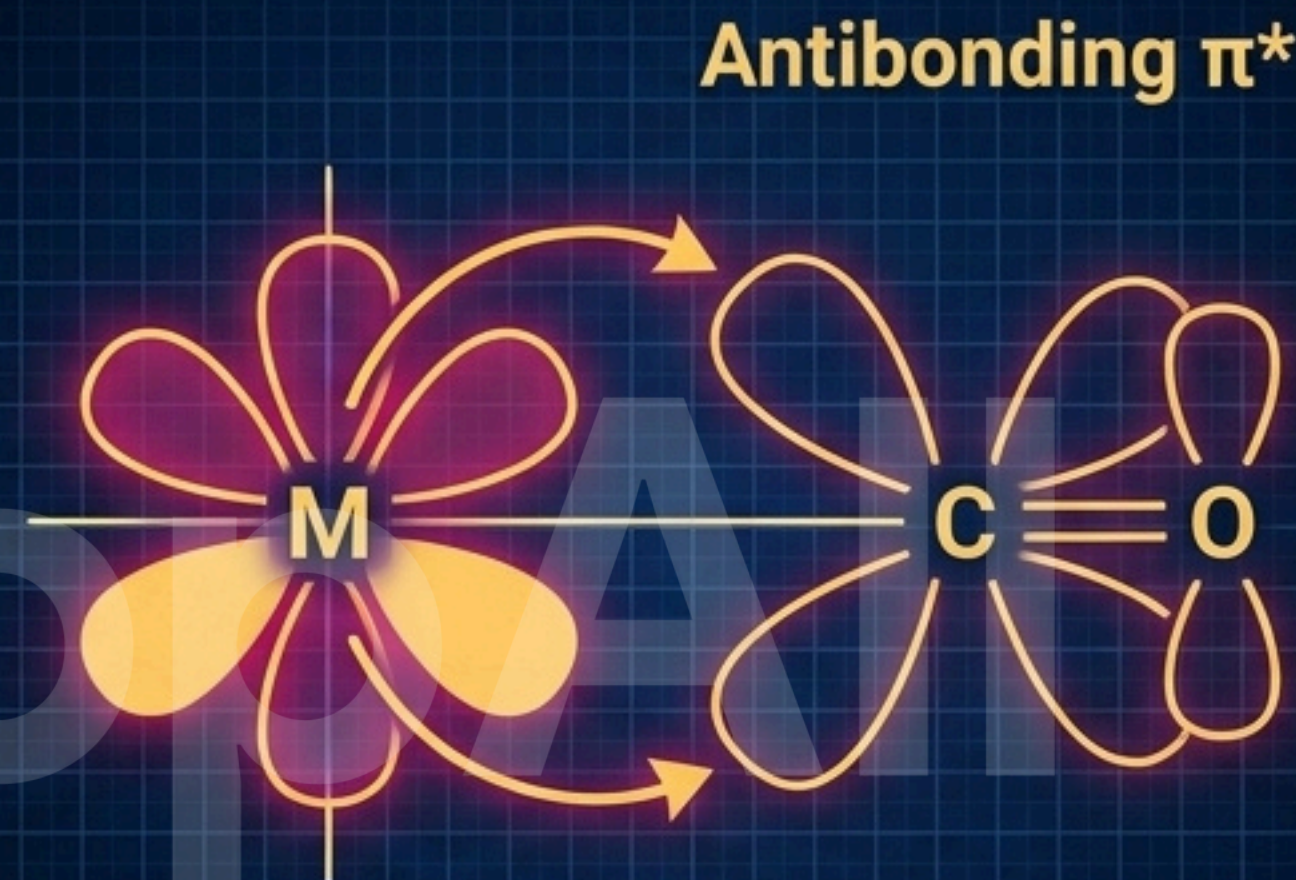
The foundational M–C bond is formed through a direct forward transfer of electron density. The carbonyl carbon acts as a Lewis base, donating a lone pair of electrons directly into a matching vacant orbital on the transition metal.



Back-Bonding: The Pi Interaction

π Character

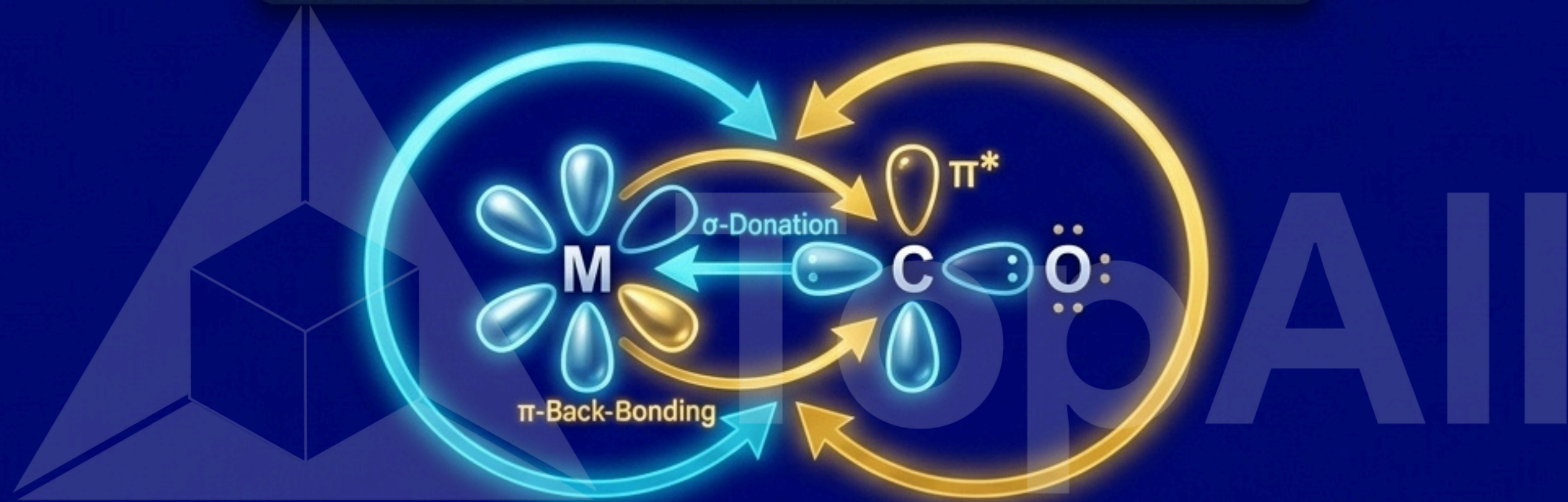
Simultaneously, the metal returns electron density back to the ligand. A pair of electrons from a filled metal d-orbital flows into the vacant, high-energy antibonding π^* orbital of the carbon monoxide.



**Filled Metal d-Orbital $\rightarrow$ Vacant
CO Antibonding π^* Orbital**

The Synergic Effect

σ -Donation pulls electron density toward the metal, making the metal electron-rich.



π -Back-Bonding relieves this density by pushing electrons back to the ligand, allowing further σ -donation.

This mutual, continuous reinforcement creates a synergic effect, dramatically strengthening the overall bond between the CO and the metal.

Key Takeaways: Metal Carbonyl Bonding



✓ Homoleptic Architectures

Structures range from simple tetrahedral Ni(CO)_4 and octahedral Cr(CO)_6 to complex dinuclear bridged forms like $[\text{Co}_2(\text{CO})_8]$.

✓ Forward σ -Donation

Ligand-to-metal bond formation occurs when the carbonyl carbon donates a lone electron pair into a vacant metal orbital.

✓ Reverse π -Back-Bonding

Metal-to-ligand bonding happens when filled metal d-orbitals push electron density into the vacant π^* antibonding orbital of CO.

✓ Synergic Strengthening

These dual electron flows create a mutually reinforcing feedback loop, profoundly stabilizing the resulting coordination compound.

Module Complete. You have mastered Section 5.6.



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