Electronic supplementary material for:
What is the nature of bonding in $[Fe(CO)_3(NO)]^-$ and $[Fe(CO)_4]^{2-}$?

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Table S1 Energy Decomposition Analysis of $[Fe(CO)_3]^{2-}$-- CO at SR-ZORA-BP86-D4/TZP and SR-ZORA-BHandHLYP/TZP level of theory; energy components are given in kcal/mol relative to the chosen fragments; ΔQ is Hirshfeld charge, transferred between fragments; $E = E_{int} + E_{prep}$.

		E_{Pauli}	E_{elst}	E_{orb}	E_{disp}	E_{int}	E_{prep}	E	ΔQ
BP86-D4	$[Fe(CO)_3]^{2-}$ -- CO	135.45	-108.00	-114.70	-3.00	-90.25	20.77	-69.48	0.46 [a]
BHandHLYP	$[Fe(CO)_3]^{2-}$ -- CO	109.36	-97.48	-92.39	--	-80.50	11.12	-69.38	0.45 [a]

[a] charge is transferred from $[Fe(CO)_3]^{2-}$ fragment to CO fragment

Table S2 Energy Decomposition Analysis of $[Fe(CO)_3$--$NO]^{-}$ for different fragmentation patterns, i), ii) and iii) at SR-ZORA-BP86-D4/TZP level of theory; energy components are given in kcal/mol relative to the chosen fragments; $E_{rel}=E_{int}+E_{prep}$ relative to the relaxed $[Fe(CO)_3]^{-}$/NO pair; ΔQ is Hirshfeld charge, transferred between fragments.

		E_{Pauli}	E_{elst}	E_{orb}	E_{disp}	E_{int}	E_{prep}	E_{rel}	ΔQ
i)	$[Fe(CO)_3]^{2-}$--NO^+	126.23	-215.90	-356.01	-2.07	-447.74	57.14	-94.61	1.21[a]
ii)	$^2[Fe(CO)_3]^{-}$-- ^2NO	172.73	-91.94	-124.72	-2.67	-46.59	17.69	-28.92	0.46[b]
iii)	$^3[Fe(CO)_3]$-- $^3NO^{-}$	196.67	-177.83	-94.16	-3.13	-78.46	5.6	-28.92	0.29[c]

i) closed-shell singlet $[Fe(CO)_3NO]^{-}$ ii) and iii) open-shell singlet with "non-aufbau" occupation of KS-MOs $[Fe(CO)_3$-$NO]^{-}$

[a] charge is transferred from $[Fe(CO)_3]^{2-}$ fragment to NO^+ fragment

[b] charge is transferred from $[Fe(CO)_3]^{-}$ fragment to NO fragment

[c] charge is transferred from NO^{-} fragment to $[Fe(CO)_3]$

Table S3 Energy Decomposition Analysis of $[Fe(CO)_3$--$NO]^-$ for different fragmentation patterns, i), ii) and iii) at SR-ZORA-BHandHLYP/TZP level of theory; energy components are given in kcal/mol relative to the chosen fragments; $E_{rel}=E_{int}+E_{prep}$ relative to the relaxed $[Fe(CO)_3]^-$/NO pair; ΔQ is Hirshfeld charge, transferred between fragments.

		E_{Pauli}	E_{elst}	E_{orb}	E_{int}	E_{prep}	E_{rel}	ΔQ
i)	$[Fe(CO)_3]^{2-}$--NO^+	92.11	-204.08	-333.58	-445.45	61.54	-31.54	1.29[a]
ii)	$^2[Fe(CO)_3]^-$-- ^2NO	158.09	-86.58	-161.75	-90.24	40.65	-49.55	0.52[b]
iii)	$^3[Fe(CO)_3]$ -- $^3NO^-$	188.12	-172.09	-98.52	-82.50	9.1	-49.55	0.23[c]

i) closed-shell singlet $[Fe(CO)_3NO]^-$ ii) and iii) open-shell singlet $[Fe(CO)_3$-$NO]^-$

[a] charge is transferred from $[Fe(CO)_3]^{2-}$ fragment to NO^+ fragment

[b] charge is transferred from $[Fe(CO)_3]^-$ fragment to NO fragment

[c] charge is transferred from NO^- fragment to $[Fe(CO)_3]$