Supporting Information

Structures and Energies of $[Co(CO)_n]^m$ (m = 0, 1+, 1–) and $HCo(CO)_n$: Density Functional Studies

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Table S1 B3LYP/6-311+G(d) total electronic energies (E_{tot}, au), zero-point energies (ZPE, kcal/mol), multiplicity, number of imaginary frequencies

Species	symmetry	multiplicity	ZPE	NImag	E_{tot} [a]
$[Co(CO)]^+$ (**1a**$^+$)	C_{∞_v}	3	4.5	0	−1495.81936
					(−1494.38703)
$[Co(CO)]^+$ (**1b**$^+$)	C_s	3	4.3	0	−1495.83313
					(−1494.39795)
$[Co(CO)_2]^+$ (**2**$^+$)	D_{∞_h}	3	9.8	0	−1609.24142
$[Co(CO)_3]^+$ (**3a**$^+$)	C_s	3	14.1	0	−1722.62314
$[Co(CO)_3]^+$ (**3b**$^+$)	D_{3h}	3	13.7	0	−1722.57100
$[Co(CO)_4]^+$ (**4a**$^+$)	C_{2v}	3	18.9	0	−1836.00433
$[Co(CO)_4]^+$ (**4b**$^+$)	D_{4h}	3	17.5	1	−1835.98261
$[Co(CO)_4]^+$ (**4c**$^+$)	D_{4h}	1	20.7	0	−1835.99201
$[Co(CO)_4]^+$ (**4d**$^+$)	C_{3v}	1	19.4	0	−1835.95523
$[Co(CO)_4]^+$ (**4e**$^+$)	T_d	3	17.4	2	−1835.99057
$[Co(CO)_5]^+$ (**5a**$^+$)	D_{3h}	1	25.8	0	−1949.37165
$[Co(CO)_5]^+$ (**5b**$^+$)	C_{4v}	1	25.7	1	−1949.36822
CoCO (**1a**)	C_{∞_v}	2	4.4	1	−1496.05623
					(−1494.59630)
CoCO (**1b**)	C_s	2	4.1	0	−1496.09017
					(−1494.62349)
$Co(CO)_2$ (**2a**)	D_{∞_h}	2	9.4	2	−1609.47126
$Co(CO)_2$ (**2b**)	C_s	2	9.4	0	−1609.50256
$Co(CO)_3$ (**3a**)	C_s	2	14.4	0	−1722.89305
$Co(CO)_3$ (**3b**)	D_{3h}	2	14.0	0	−1722.89224
$Co(CO)_4$ (**4**)	C_{3v}	2	19.4	0	−1836.27951
$[Co(CO)]^-$ (**1a**$^-$)	C_s	3	3.7	0	−1496.11910
$[Co(CO)]^-$ (**1b**$^-$)	C_{∞_v}	1	4.1	0	−1496.08222
$[Co(CO)_2]^-$ (**2**$^-$)	C_{2v}	1	9.5	0	−1609.53009

$[Co(CO)_3]^-$ (**3a**$^-$)	C_{3v}	1	14.3	0	–1722.95715
$[Co(CO)_3]^-$ (**3b**$^-$)	D_{3h}	1	14.2	1	–1722.95697
$[Co(CO)_4]^-$ (**4**$^-$)	T_d	1	20.1	0	–1836.37695
HCo(CO) (**1a-H**)	$C_{\infty v}$	3	7.7	0	–1496.68734
HCo(CO) (**1b-H**)	C_s	3	7.8	0	–1496.70305
HCo(CO) (**1c-H**)	$C_{\infty v}$	1	9.0	0	–1496.62788
HCo(CO) (**1d-H**)	C_s	1	8.7	0	–1496.65608
$HCo(CO)_2$ (**2a-H**)	C_{2v}	1	14.0	1	–1610.06889
$HCo(CO)_2$ (**2b-H**)	C_s	3	12.8	0	–1610.08156
$HCo(CO)_2$ (**2c-H**)	C_s	1	14.3	0	–1610.06997
$HCo(CO)_3$ (**3a-H**)	C_{2v}	1	19.7	0	–1723.48074
$HCo(CO)_3$ (**3b-H**)	C_{3v}	1	19.5	0	–1723.46387
$HCo(CO)_3$ (**3c-H**)	C_s	3	18.1	0	–1723.46388
$HCo(CO)_4$ (**4-H**)	C_{3v}	1	25.5	0	–1836.87546
$(HCO)Co(CO)_3$ (**6a**)	C_s	1	25.8	0	–1836.83079
$(HCO)Co(CO)_3$ (**6aT**)	C_s	3	24.7	0	–1836.81919
$(HCO)Co(CO)_3$ (**6b**)	C_s	1	26.7	0	–1836.84004
$(HCO)Co(CO)_3$ (**6bT**)	C_s	3	24.9	0	–1836.82140
$(HCO)Co(CO)_3$ (**6c**)	C_s	1	26.2	2	–1836.82113
$(HCO)Co(CO)_3$ (**6d**)	C_s	1	26.1	1	–1836.83178
H	K_h	2			–0.50216
CO	$C_{\infty v}$	1	3.2	0	–113.34905
Co^+	K_h	3			–1382.41974
Co	K_h	4			–1382.70337
Co^-	K_h	3			–1382.74131

a) The CCSD(T) values in parenthesis