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Unsaturated binuclear homoleptic nickel carbonyl anions $Ni_2(CO)_n^-$ (n = 4−6) featuring double three-center two-electron Ni−C−Ni bonds

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Table S1 The relative energies (in eV) of the low-lying isomers of $Ni_2(CO)_n^{-1/0}$ (n = 4−6) as well as their ADEs and VDEs (in eV) obtained by density functional calculations.

Species	Isomer	Relative Energy[a]	ADE		VDE	
			Calc.[a]	Exp.	Calc.[a]	Exp.
$Ni_2(CO)_4^-$	Ⅰ	0.00/0.00/0.00	1.84/2.20/1.81	1.77	1.97/2.28/1.95	1.88
$Ni_2(CO)_4$	Ⅱ	0.00/0.00/0.00				
$Ni_2(CO)_5^-$	Ⅲ	0.00/0.00/0.00	1.67/2.07/1.65	1.63	1.94/2.23/1.93	1.81
	Ⅳ	0.00/0.12/0.04	1.74/2.04/1.70		1.90/2.23/1.89	
$Ni_2(CO)_5$	Ⅴ	0.00/0.00/0.00				
	Ⅵ	0.29/0.07/0.25				
$Ni_2(CO)_6^-$	Ⅶ	0.00/0.00/0.00	1.98/2.33/1.96	2.10	2.16/2.46/2.17	2.17
	Ⅷ	0.09/0.26/0.06	2.18/2.59/2.21		2.33/2.71/2.36	
$Ni_2(CO)_6$	Ⅸ	0.00/0.00/0.00				
	Ⅹ	0.11/0.52/0.34				
	Ⅺ	0.04/0.18/0.03				

[a] Listed in the order of B3LYP, BP86, and MPW1PW91.

Table S2 DFT bond length, bond order, electron delocalization index, and IQA energetics profiles for the double carbonyl-bridged $Ni_2(CO)_4^-$ complex at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level. All data are in atomic units except distances in angstroms. The atomic labels are written as a superscript on the right of the element symbol.

interaction	distance	bond order				δ	E_{int}	V_{cl}	V_{xc}
		Wiberg	Mayer	G-J	N-M(3)				
Ni^1–Ni^8	2.305	0.106	0.367	0.151	0.155	0.390	-0.008	0.058	-0.066
Ni^1–C^4	1.829	0.501	0.906	0.533	0.544	0.960	-0.159	0.066	-0.225
Ni^1–O^7	2.960	0.096	0.091	0.134	0.151	0.161	-0.121	-0.106	-0.015
Ni^1–C^4O^7		0.597	0.997	0.667	0.695	1.121	-0.280	-0.040	-0.240
Ni^8–C^4	2.049	0.349	0.599	0.394	0.426	0.597	-0.080	0.049	-0.129
Ni^8–O^7	2.886	0.068	0.099	0.102	0.121	0.159	-0.103	-0.086	-0.017
Ni^8–C^4O^7		0.417	0.698	0.496	0.547	0.756	-0.183	-0.037	-0.146
Ni^1–C^2	1.737	0.762	1.128	0.858	0.863	1.313	-0.208	0.096	-0.304
Ni^1–O^5	2.895	0132	0.138	0.206	0.233	0.228	-0.133	-0.111	-0.022
Ni^1–C^2O^5		0.894	1.266	1.064	1.096	1.541	-0.341	-0.015	-0.326
Ni^8–C^9	1.728	0.898	1.327	0.967	1.026	1.391	-0.228	0.087	-0.315
Ni^8– O^{10}	2.887	0.148	0.154	0.220	0.261	0.251	-0.121	-0.097	-0.024
Ni^8–C^9O^{10}		1.046	1.481	1.187	1.287	1.642	-0.349	-0.010	-0.339
C^4–O^7	1.166	1.948	1.880	2.048	2.426	1.519	-1.324	-0.883	-0.441
C^2–O^5	1.159	1.974	1.979	2.106	2.475	1.531	-1.420	-0.979	-0.441
C^9–O^{10}	1.159	1.990	1.972	2.137	2.492	1.537	-1.413	-0.971	-0.442

Table S3 DFT bond length, bond order, electron delocalization index, and IQA energetics profiles for the double carbonyl-bridged $Ni_2(CO)_5^-$ complex at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level. All data are in atomic units except distances in angstroms. The atomic labels are written as a superscript on the right of the element symbol.

interaction	distance	bond order				δ	E_{int}	V_{cl}	V_{xc}
		Wiberg	Mayer	G-J	N-M(3)				
Ni^1–Ni^{10}	2.365	0.070	0.372	0.111	0.103	0.327	0.016	0.070	-0.054
Ni^1–C^3	2.309	0.307	0.612	0.362	0.668	0.622	-0.076	0.065	-0.141
Ni^1–O^9	2.983	0.064	0.075	0.103	0.111	0.131	-0.125	-0.111	-0.014
Ni^1–C^3O^9		0.371	0.687	0.465	0.779	0.743	-0.201	-0.046	-0.155
Ni^{10}–C^3	1.889	0.419	0.832	0.475	0.492	0.811	-0.123	0.068	-0.191
Ni^{10}–O^9	2.965	0.071	0.082	0.116	0.132	0.135	-0.128	-0.115	-0.013
Ni^{10}–C^3O^9		0.490	0.914	0.591	0.624	0.946	-0.251	-0.047	-0.204
Ni^1–C^2	1.774	0.611	1.178	0.697	0.668	1.142	-0.163	0.106	-0.269
Ni^1–O^6	2.928	0.107	0.114	0.172	0.185	0.191	-0.144	-0.126	-0.018
Ni^1–C^2O^6		0.718	1.292	0.869	0.853	1.333	-0.307	-0.020	-0.287
Ni^{10}–C^{11}	1.723	0.836	1.334	0.930	0.944	1.360	-0.208	0.107	-0.315
Ni^{10}–O^{12}	2.881	0.142	0.162	0.226	0.258	0.253	-0.143	-0.120	-0.023
Ni^{10}–$C^{11}O^{12}$		0.978	1.496	1.156	1.202	1.613	-0.351	-0.013	-0.338
C^3–O^9	1.168	1.974	1.921	2.068	2.455	1.540	-1.326	-0.881	-0.445
C^2–O^6	1.155	2.008	2.006	2.141	2.510	1.549	-1.449	-1.004	-0.445
C^{11}–O^{12}	1.157	1.999	1.983	2.131	2.487	1.531	-1.428	-0.986	-0.442

Table S4 DFT bond length, bond order, electron delocalization index, and IQA energetics profiles for the double carbonyl-bridged $Ni_2(CO)_6^-$ complex at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level. All data are in atomic units except distances in angstroms. The atomic labels are written as a superscript on the right of the element symbol.

interaction	distance	bond order				δ	E_{int}	V_{cl}	V_{xc}
		Wiberg	Mayer	G-J	N-M(3)				
Ni^1–Ni^{12}	2.505	0.045	0.287	0.078	0.066	0.224	0.041	0.075	-0.034
Ni^1–C^3	1.982	0.311	0.683	0.365	0.351	0.655	-0.074	0.078	-0.153
Ni^1–O^9	2.977	0.061	0.072	0.099	0.105	0.124	-0.136	-0.124	-0.013
Ni^1–C^3O^9		0.372	0.755	0.464	0.456	0.779	-0.210	-0.046	-0.166
Ni^1–C^2	1.779	0.617	1.188	0.709	0.675	1.138	-0.154	0.113	-0.267
Ni^1–O^6	2.930	0.112	0.122	0.181	0.193	0.197	-0.151	-0.132	-0.019
Ni^1–C^2O^6		0.729	1.310	0.890	0.869	1.335	-0.305	-0.019	-0.286
C^3–O^9	1.164	1.981	1.937	2.089	2.462	1.543	-1.359	-0.912	-0.447
C^2–O^6	1.152	2.026	2.023	2.163	2.526	1.553	-1.466	-1.020	-0.446

Table S5 Topological properties of the terminal and bridgd NiC BCPs in the $Ni_2(CO)_n^-$ (n = 4−6) complexes at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level. All data are in atomic units (a.u.). The atomic label are written as a superscript on the right of the element symbol.

Species	bond type	X–Y	ρ(r)	$\nabla^2\rho$(r)	G(r)	V(r)	E(r)
$Ni_2(CO)_4^-$	terminal	Ni^1–C^2	0.160	0.623	0.229	-0.303	-0.074
		Ni^8–C^9	0.165	0.619	0.234	-0.313	-0.079
	bridged	Ni^1–C^3	0.130	0.494	0.166	-0.209	-0.043
		Ni^8–C^3	0.081	0.256	0.079	-0.093	-0.015
$Ni_2(CO)_5^-$	terminal	Ni^1–C^2	0.147	0.587	0.206	-0.265	-0.059
		Ni^{10}–C^{11}	0.165	0.634	0.238	-0.318	-0.080
	bridged	Ni^1–C^3	0.085	0.276	0.084	-0.099	-0.015
		Ni^{10}–C^3	0.117	0.407	0.134	-0.166	-0.032
$Ni_2(CO)_6^-$	terminal	Ni^1–C^2	0.145	0.594	0.205	-0.262	-0.057
	bridged	Ni^1–C^3	0.095	0.318	0.098	-0.117	-0.019

Table S6 Molecular orbital atom-atom bonding character for the $Ni_2(CO)_n^-$ (n = 4−6) complexes at the B3LYP/Ni/Stuttgart+2*f*1*g*/C, O/aug–cc–pVTZ level. The numbers in parentheses are the contribution percentage of the metal center with the atomic label written as a superscript on the right of the element symbol.

Species	MO	bonding	nonbonding	antibonding
$Ni_2(CO)_4^-$	HOMO	0.056	0.913 (0.094 Ni^1/0.781 Ni^8)	0.031
	HOMO-1	0.002	0.994 (0.069 Ni^1/0.917 Ni^8)	0.004
	HOMO-2	0.026	0.778 (0.108 Ni^1/0..457 Ni^8)	0.196
	HOMO-3	0.019	0.850 (0.190 Ni^1/0.654 Ni^8)	0.130
	HOMO-4	0.059	0.892 (0.845 Ni^8)	0.049
	HOMO-5	0.024	0.887 (0.548 Ni^1/0.283 Ni^8)	0.089
	HOMO-6	0.048	0.937 (0.813 Ni^1/0.055 Ni^8)	0.015
	HOMO-7	0.015	0.948 (0.846 Ni^1)	0.037
	HOMO-8	0.158	0.664 (0.576 Ni^1)	0.178
	HOMO-9	0.027	0.908 (0.688 Ni^1/0.187 Ni^8)	0.064
$Ni_2(CO)_5^-$	HOMO	0.016	0.840 (0.434 Ni^1/0.244 Ni^{10})	0.144
	HOMO-1	0.020	0.796 (0.174 Ni^1/0.359 Ni^{10})	0.184
	HOMO-2	0.309	0.482 (0.270 Ni^1/0.051 Ni^{10})	0.209
	HOMO-3	0.026	0.955 (0.062 Ni^1/0.840 Ni^{10})	0.019
	HOMO-4	0.014	0.952 (0.094 Ni^{10})	0.034
	HOMO-5	0.016	0.934 (0.585 Ni^1/0.314 Ni^{10})	0.050
	HOMO-6	0.185	0.800 (0.517 Ni^1)	0.015
	HOMO-7	0.040	0.8863 (0.167 Ni^1/0.644 Ni^{10})	0.097
	HOMO-8	0.049	0.874 (0.837 Ni^1)	0.077
	HOMO-9	0.163	0.756 (0.720 Ni^1)	0.081
$Ni_2(CO)_6^-$	HOMO	0.125	0.792 (0.320 Ni^1/0.320 Ni^{12})	0.084
	HOMO-1	0.011	0.823 (0.274 Ni^1/0.274 Ni^{12})	0.166
	HOMO-2	0.071	0.806 (0.316 Ni^1/0.316 Ni^{12})	0.125
	HOMO-3	0.103	0.763 (0.348 Ni^1/0.348 Ni^{12})	0.133
	HOMO-4	0.062	0.854 (0.395 Ni^1/0.395 Ni^{12})	0.084
	HOMO-5	0.122	0.706 (0.301 Ni^1/0.301 Ni^{12})	0.172
	HOMO-6′	0.027	0.923 (0.461 Ni^1/0.461 Ni^{12})	0.049
	HOMO-7	0.027	0.927 (0.462 Ni^1/0.462 Ni^{12})	0.045
	HOMO-8	0.064	0.869 (0.432 Ni^1/0.432 Ni^{12})	0.067
	HOMO-9	0.022	0.943 (0.463 Ni^1/0.463 Ni^{12})	0.036

Table S7 Theoretical atomic net charges on the $Ni_2(CO)_n^-$ (n = 4−6). The atomic labels are written as a superscript on the right of the element symbol.

Species	fragment	NPA	Hirshfeld	Voronoi	MDC-q	AIM
$Ni_2CO_4^-$	Ni^1/Ni^8	0.249/0.132	0.045/0.033	0.105/0.063	0.277/0.169	0.392/0.320
	C^2O^5/C^9O^{10}	-0.273/-0.237	-0.268/-0.255	-0.293/-0.283	-0.235/-0.222	-0.384/-0.391
	C^4O^7	-0.435	-0.278	-0.297	-0.048	-0.469
$Ni_2CO_5^-$	Ni^1/Ni^{10}	0.317/0.271	0.110/0.091	0.152/0.142	0.315/0.138	0.481/0.448
	$C^2O^6/C^{11}O^{12}$	-0.259/-0.211	-0.259/-0.217	-0.238/-0.272	-0.282/-0.314	-0.339/-0.360
	C^5O^7	-0.430	-0.248	-0.273	-0.288	-0.445
$Ni_2CO_6^-$	Ni^1/Ni^{12}	0.216/0.216	0.125/0.125	0.168/0.168	0.195/0.195	0.521/0.521
	C^2O^6	-0.176	-0.198	-0.216	-0.250	-0.314
	C^3O^9	-0.364	-0.228	-0.235	-0.196	-0.393

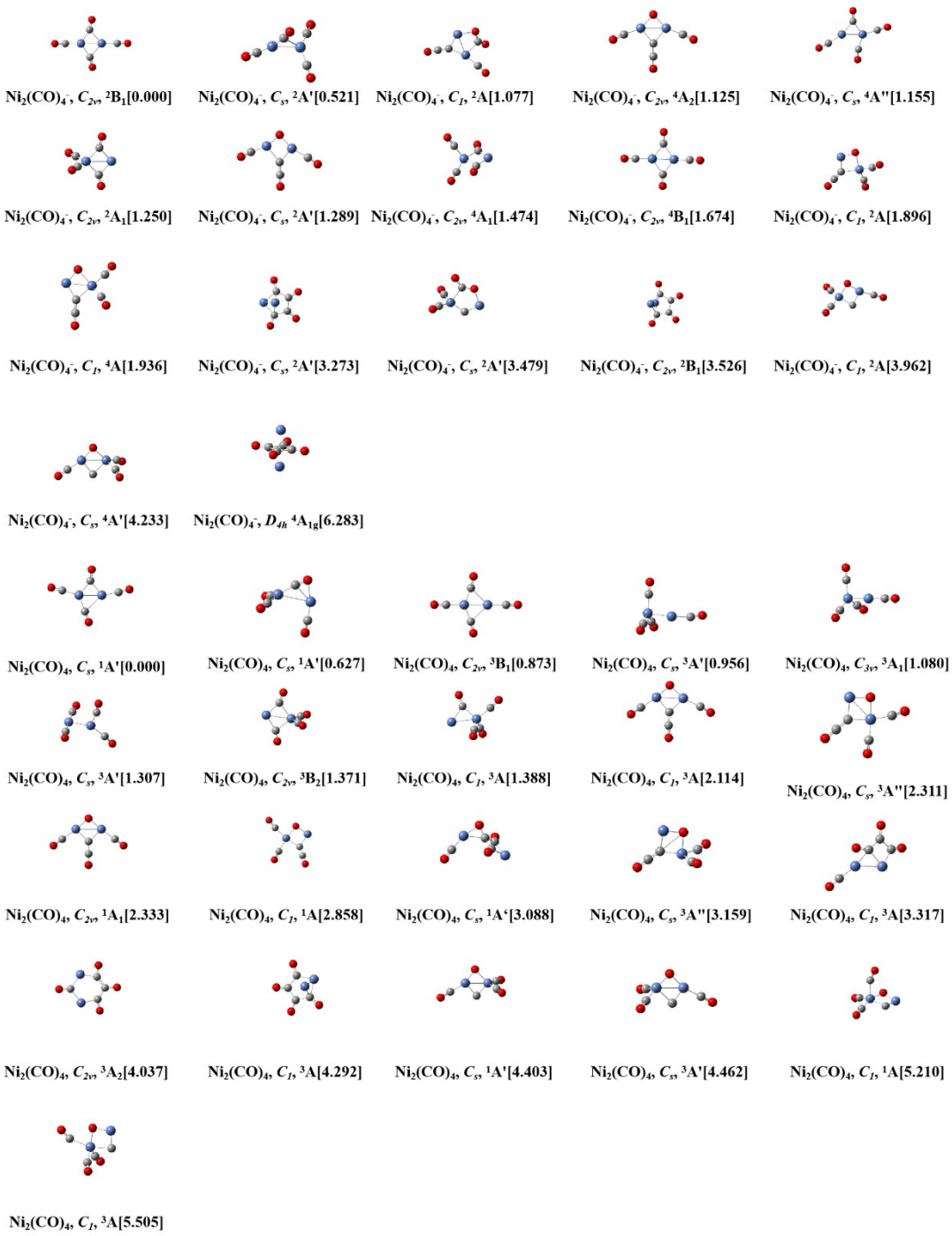

Fig. S1 Optimized ground-state and selected low-lying structures of $Ni_2(CO)_4^{-1/0}$ at the B3LYP/Ni /SDD/C, O/6−311+G* level of theory. The Ni, C and O are shown in blue, gray, and red, respectively. The relative energies to the neutral or anionic ground states are given in square brackets in eV.

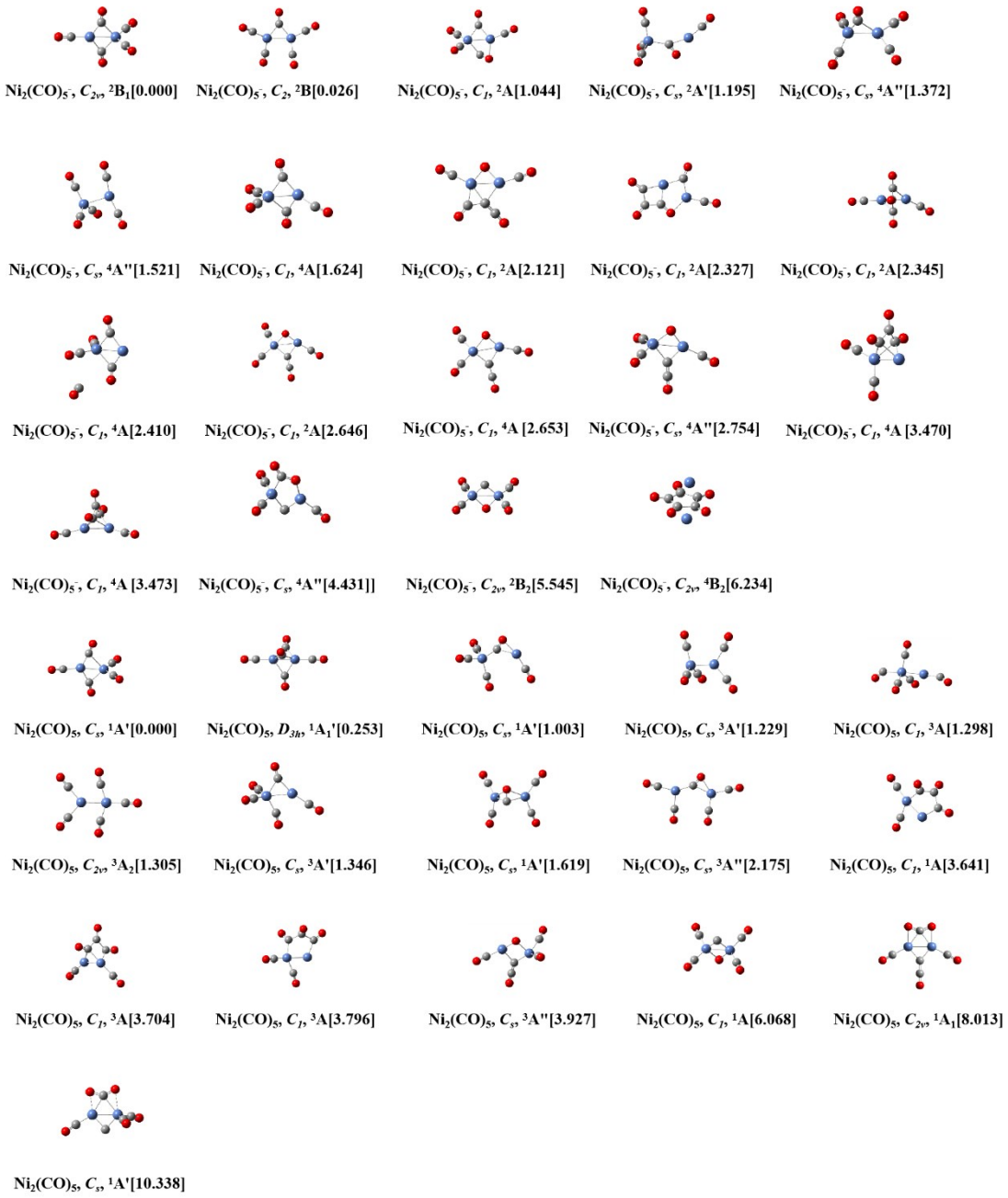

Fig. S2 Optimized ground-state and selected low-lying structures of $Ni_2(CO)_5^{-1/0}$ at the B3LYP/Ni /SDD/C, O/6−311+G* level of theory. The Ni, C and O are shown in blue, gray, and red, respectively. The relative energies to the neutral or anionic ground states are given in square brackets in eV.

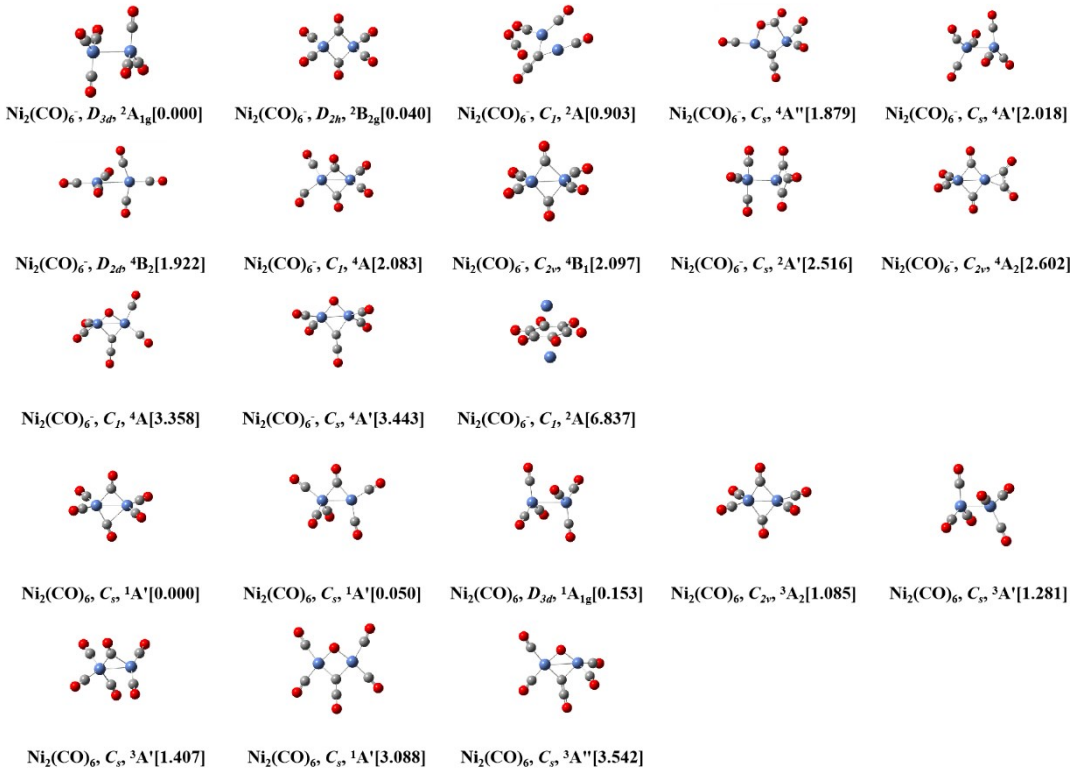

Fig. S3 Optimized ground-state and selected low-lying structures of $Ni_2(CO)_6^{-1/0}$ at the B3LYP/Ni /SDD/C, O/6−311+G* level of theory. The Ni, C and O are shown in blue, gray, and red, respectively. The relative energies to the neutral or anionic ground states are given in square brackets in eV.

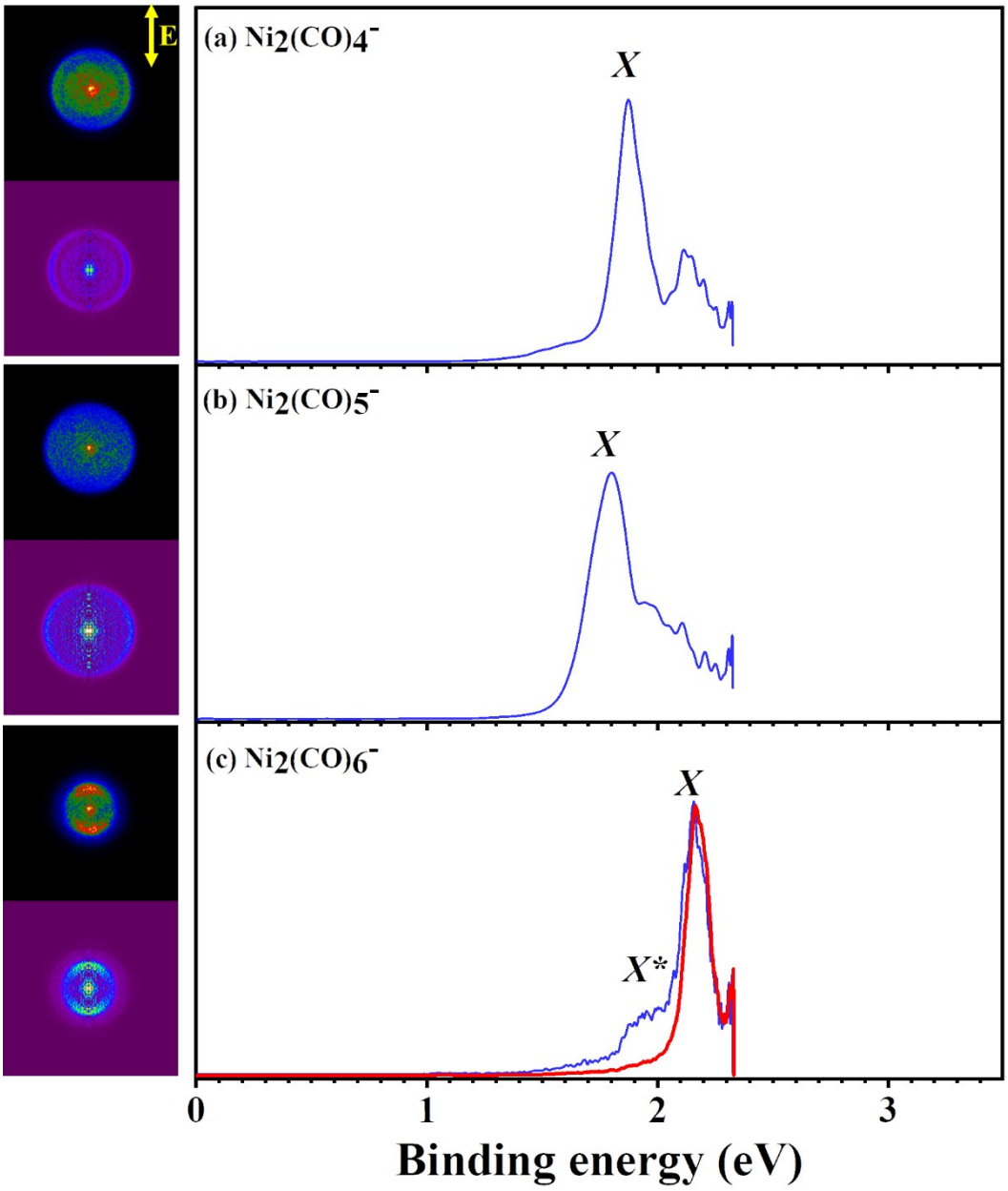

Fig. S4 The photoelectron spectra of $Ni_2(CO)_n^-$ (n = 4−6) recorded at 532 nm. Note that the blue and red curves in the spectra of $Ni_2(CO)_6^-$ were recorded at different mass-selected time.

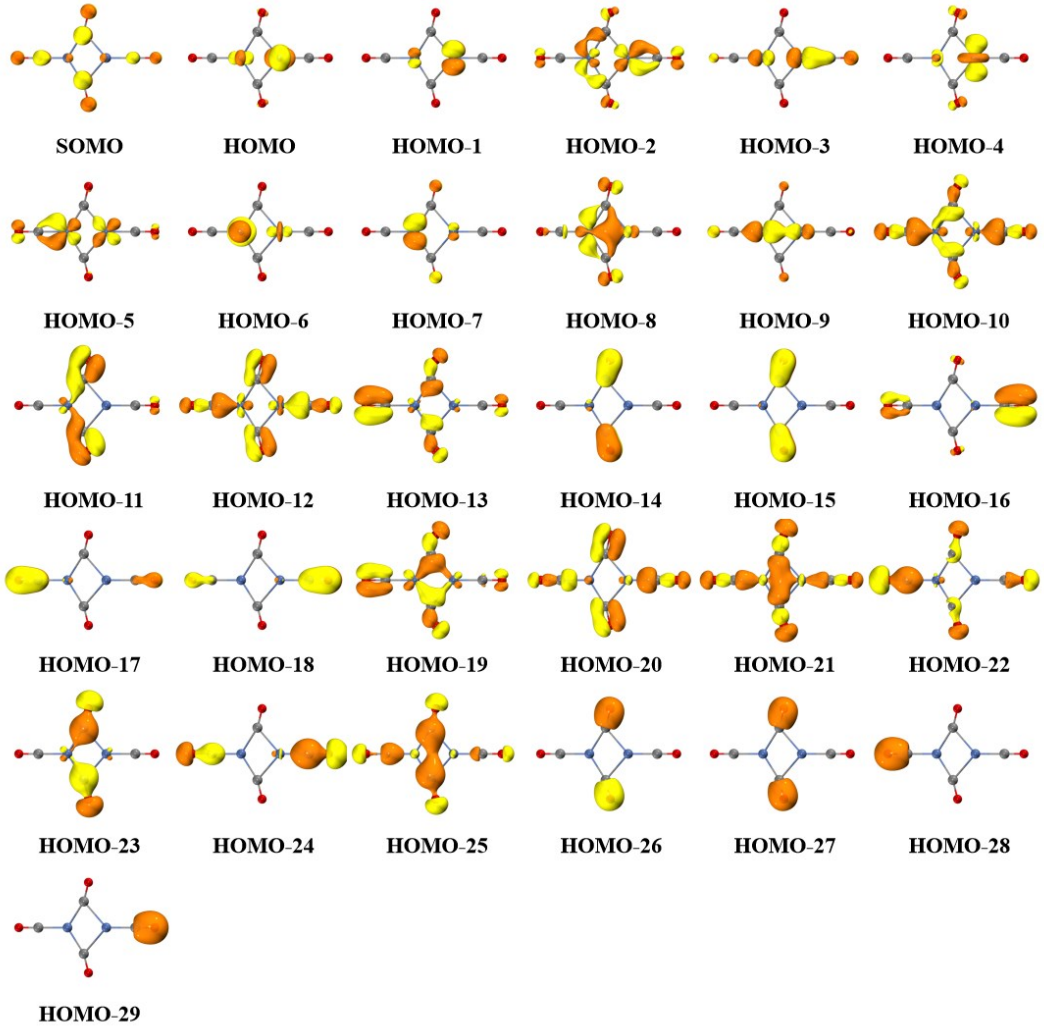

Fig. S5 Valence canonical molecular orbitals of the global minimum Ⅰ isomer of $Ni_2(CO)_4^-$ anion calculated at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level of theory. (isosurface = 0.06 a.u.)

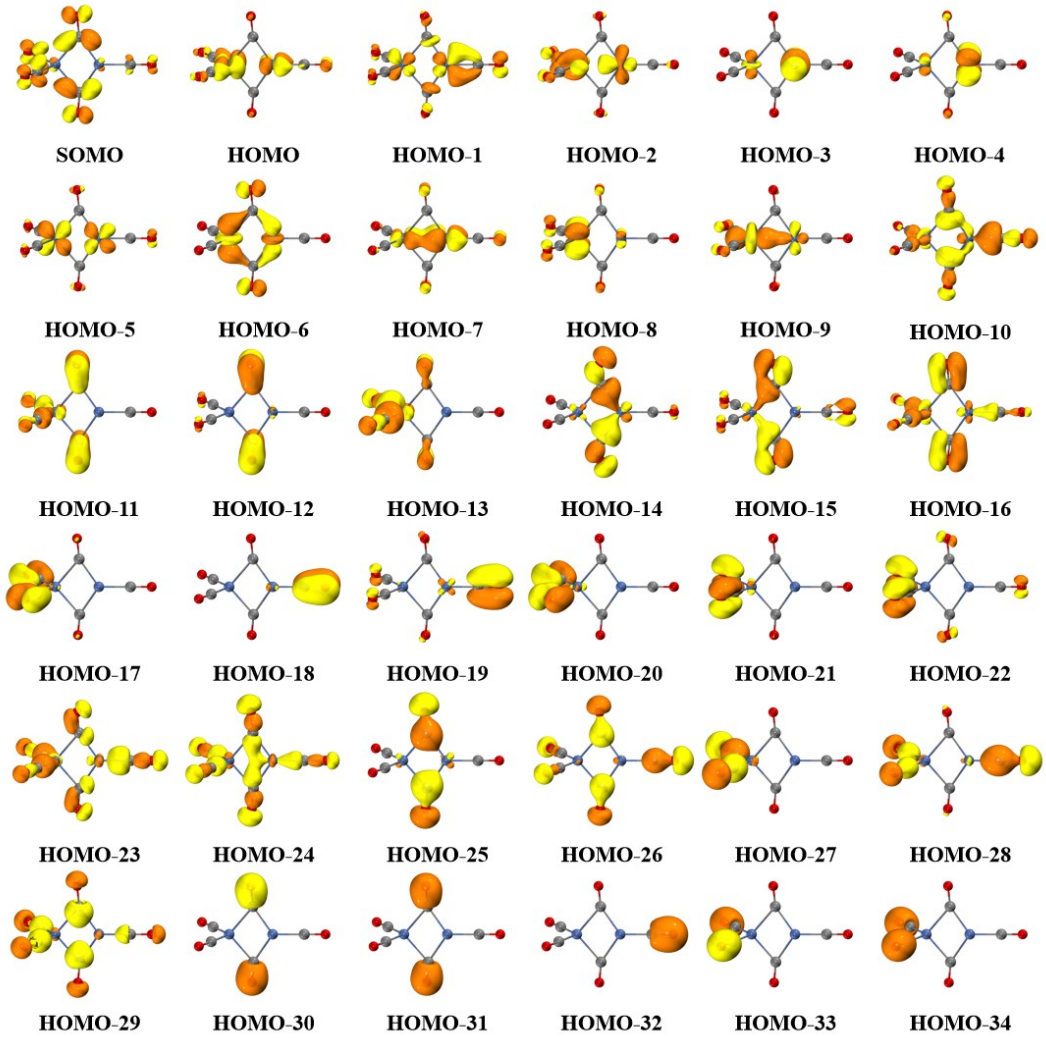

Fig. S6 Valence canonical molecular orbitals of the global minimum Ⅲ isomer of $Ni_2(CO)_5^-$ anion calculated at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level of theory. (isosurface = 0.06 a.u.)

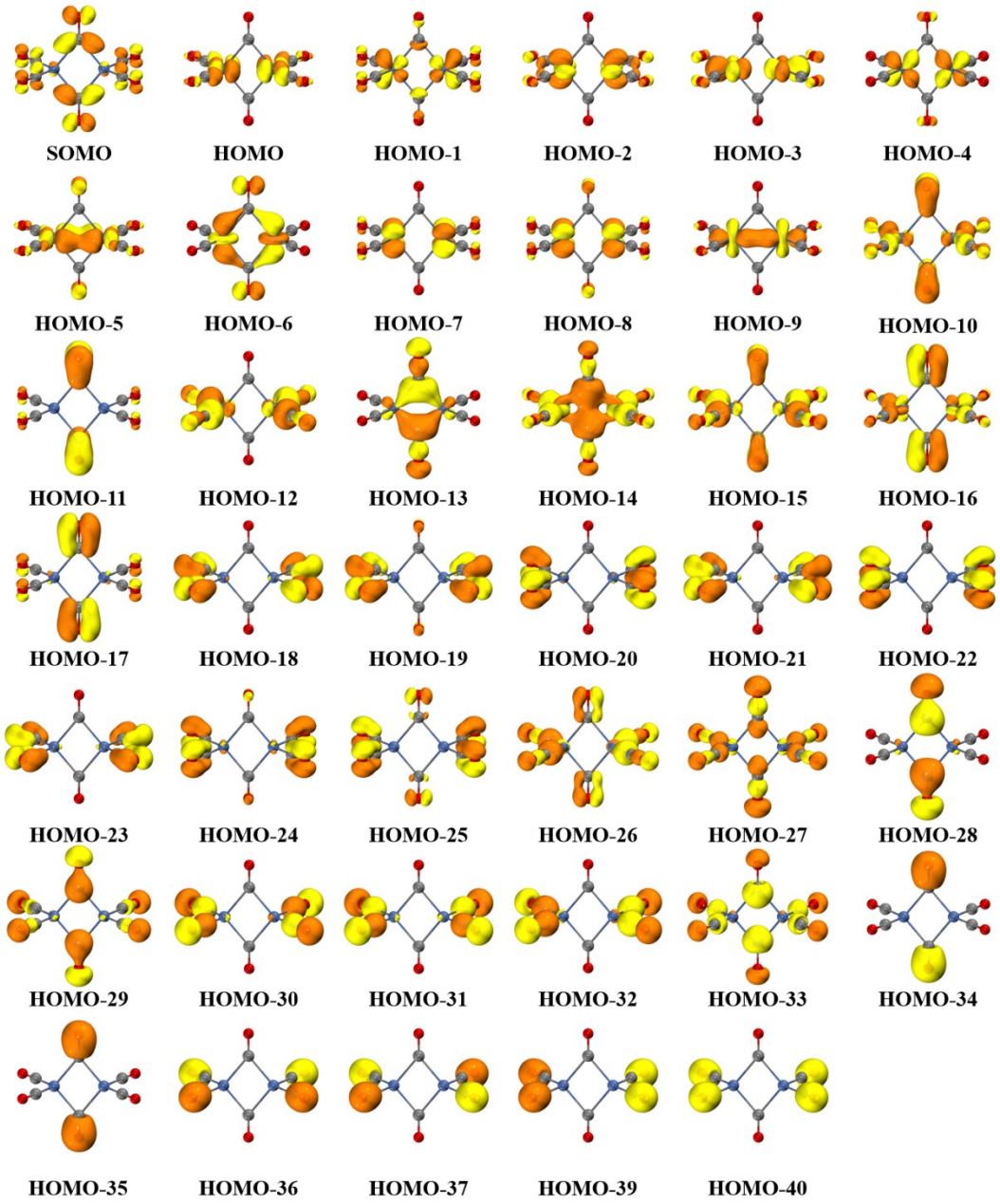

Fig. S7 Valence canonical molecular orbitals of the global minimum **VII** isomer of $Ni_2(CO)_6^-$ anion calculated at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level of theory. (isosurface = 0.06 a.u.)

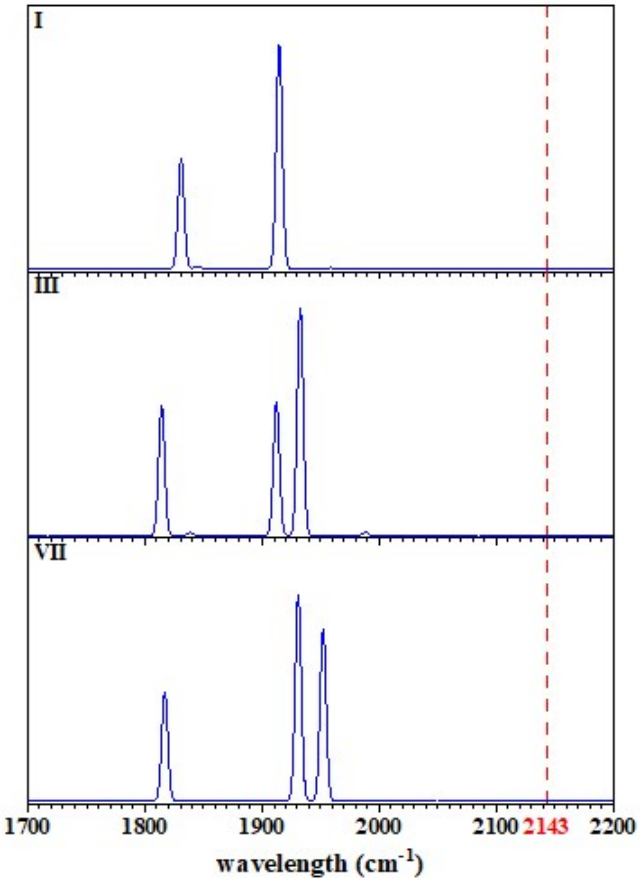

Fig. S8 Simulated infrared spectra of $Ni_2(CO)_n^{-1}$ (n = 4−6) ground-state complexes in the 1700−2200 cm^{-1} region at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug−cc−pVTZ level of theory (FWHM = 6 cm^{-1}).

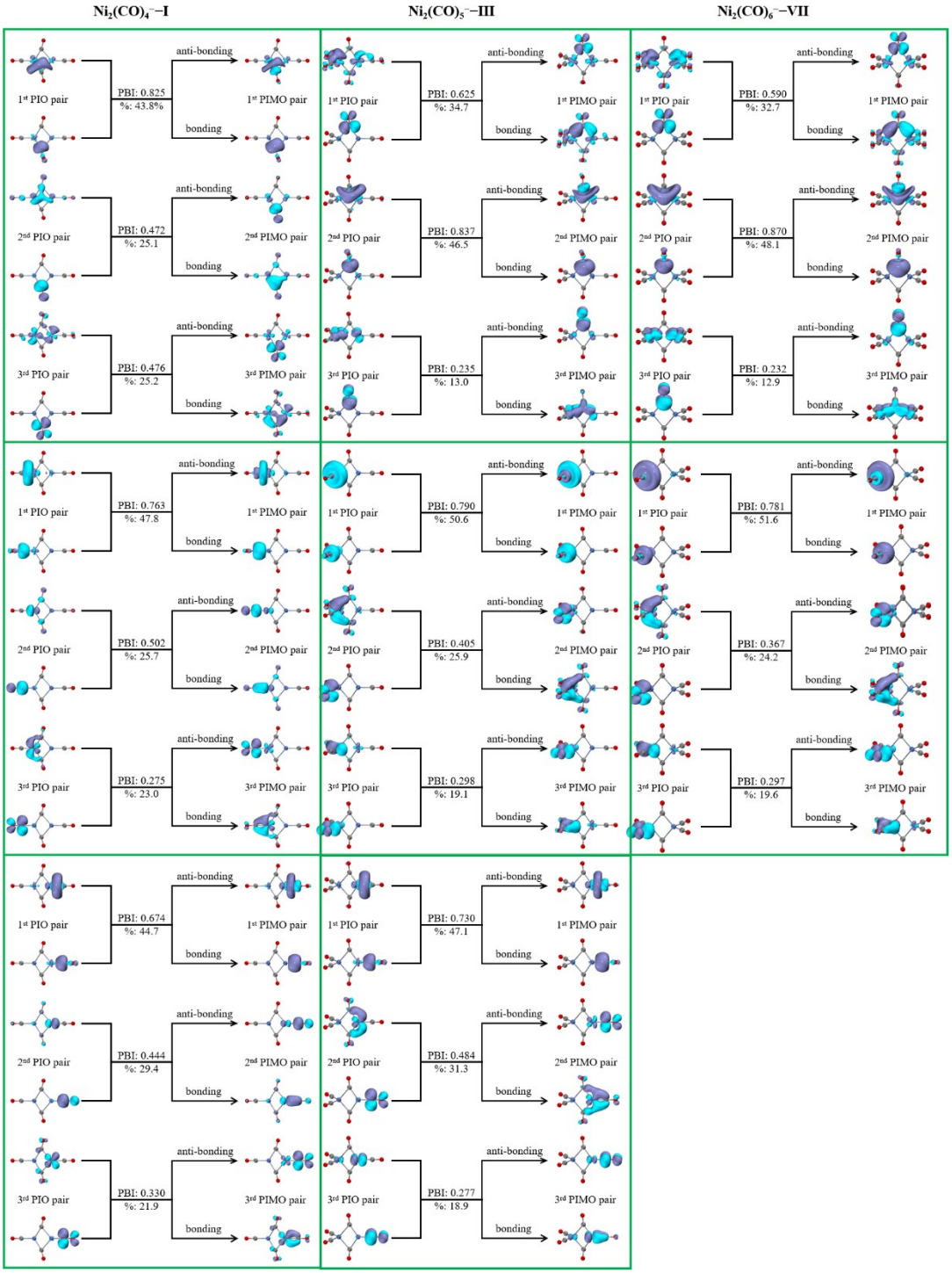

Fig. S9 Results of PIO analysis on the $Ni_2CO_n^-$ (n = 4–6) complex with a bridging or terminal carbonyl group as one fragment and the remaining moiety as the other fragment at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level of theory. The PIO-based bond index (PBI) and associated percentage contribution for each PIO pair are given. (isosurface = 0.06 a.u.)

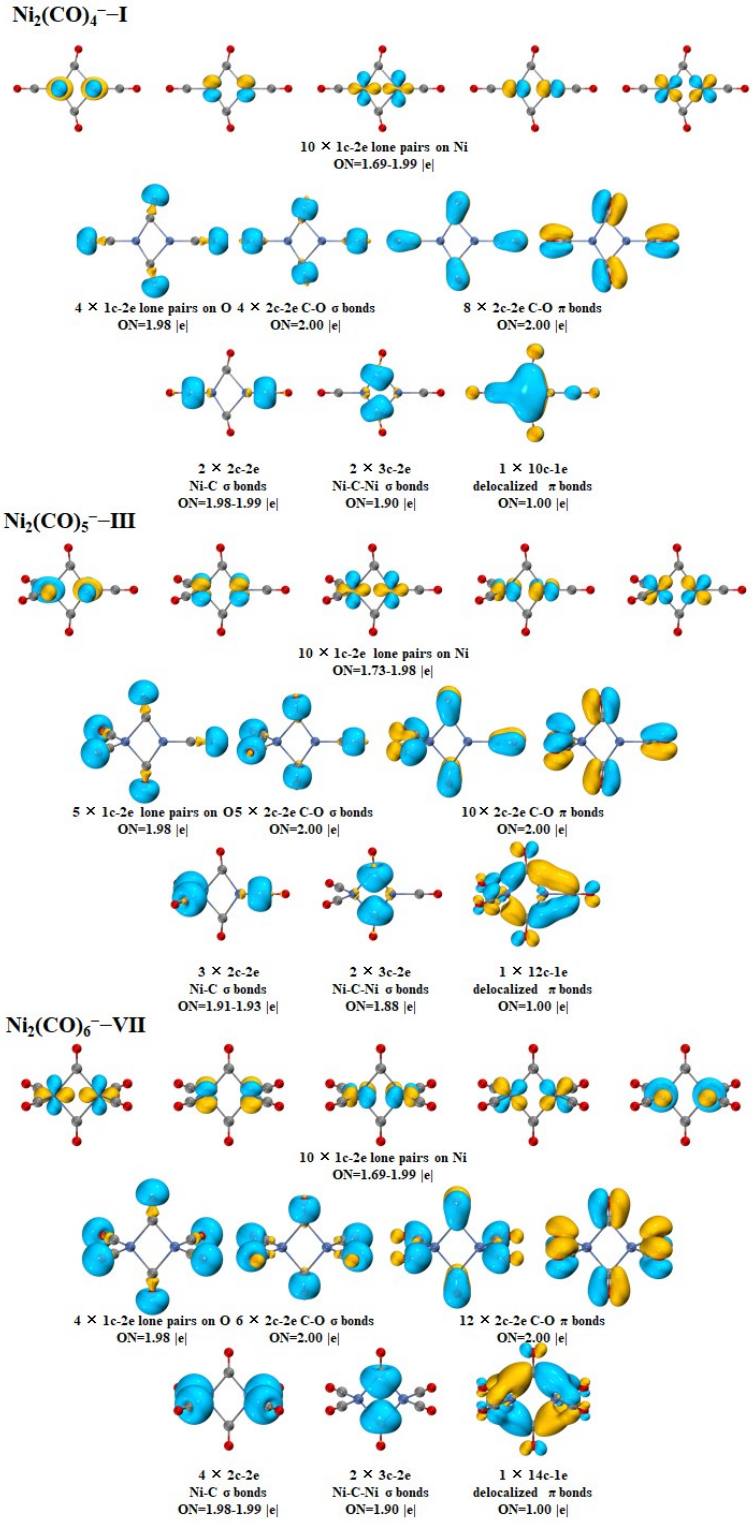

Fig. S10 The AdNDP analysis for the global minima of $Ni_2(CO)_n^-$ (n = 4−6) anions at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug−cc−pVTZ level. Occupation numbers (ONs) are shown. (isosurface = 0.08 a.u.)

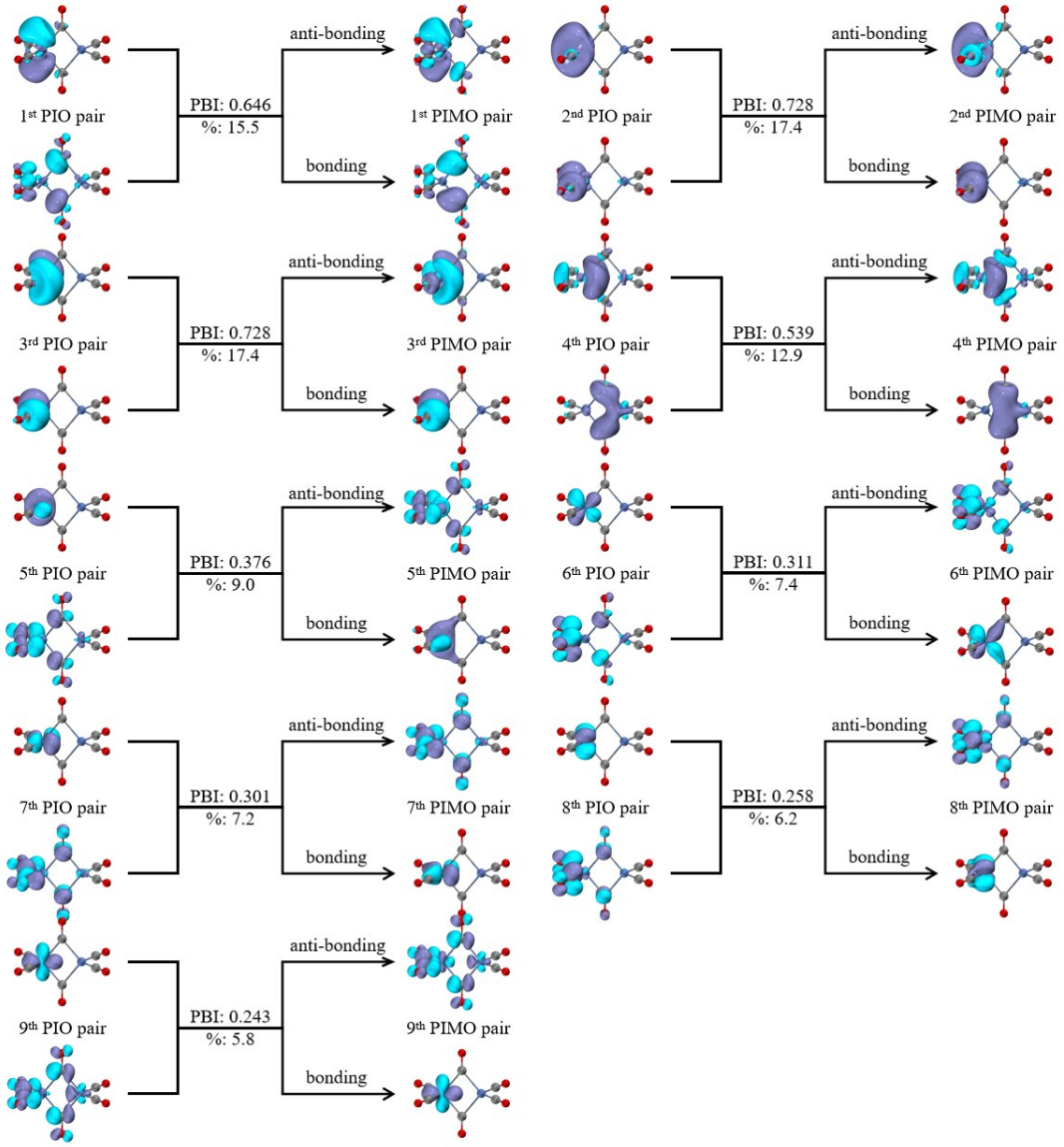

Fig. S11 Results of PIO analysis on the $Ni_2CO_6^-$ complex **Ⅶ** with Ni^1 atom as one fragment and the remaining moiety as the other fragment at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level of theory. (isosurface = 0.06 a.u.)

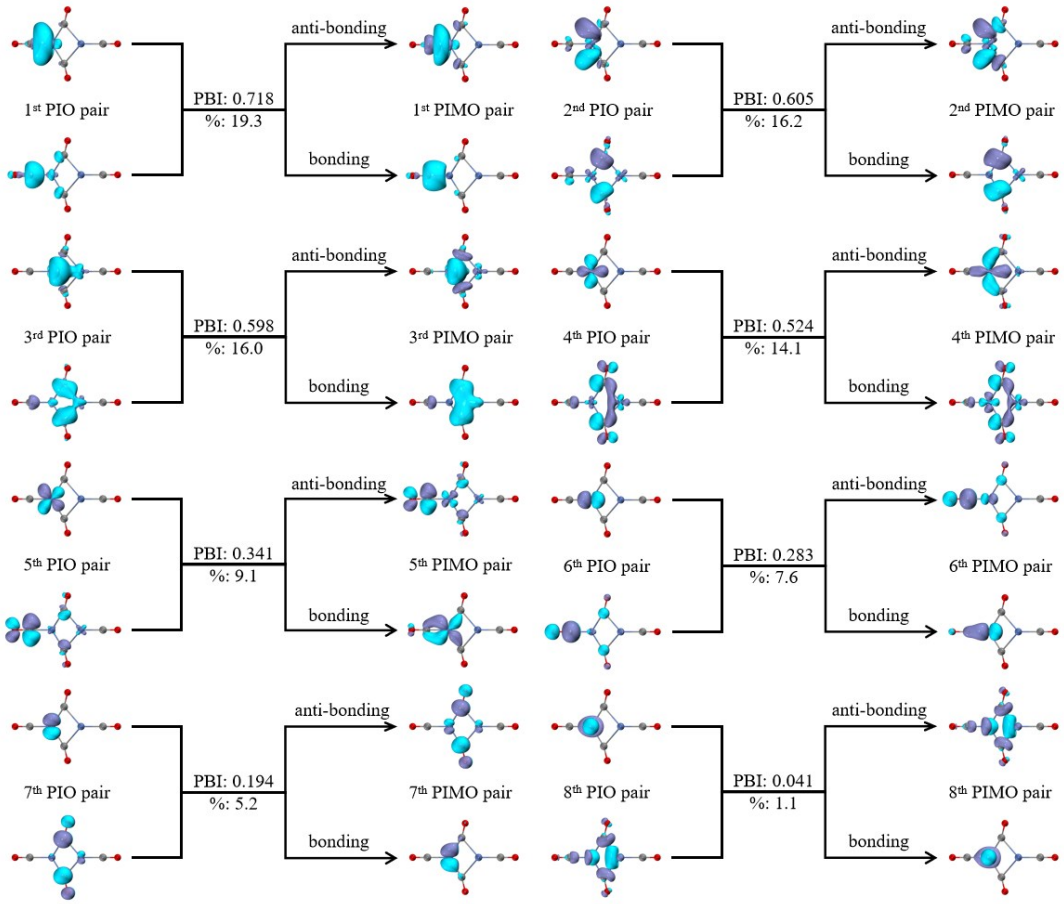

Fig. S12 Results of PIO analysis on the ground-state $Ni_2CO_4^-$ complex Ⅰ with Ni^1 atom as one fragment and the remaining moiety as the other fragment at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level of theory. (isosurface = 0.06 a.u.)

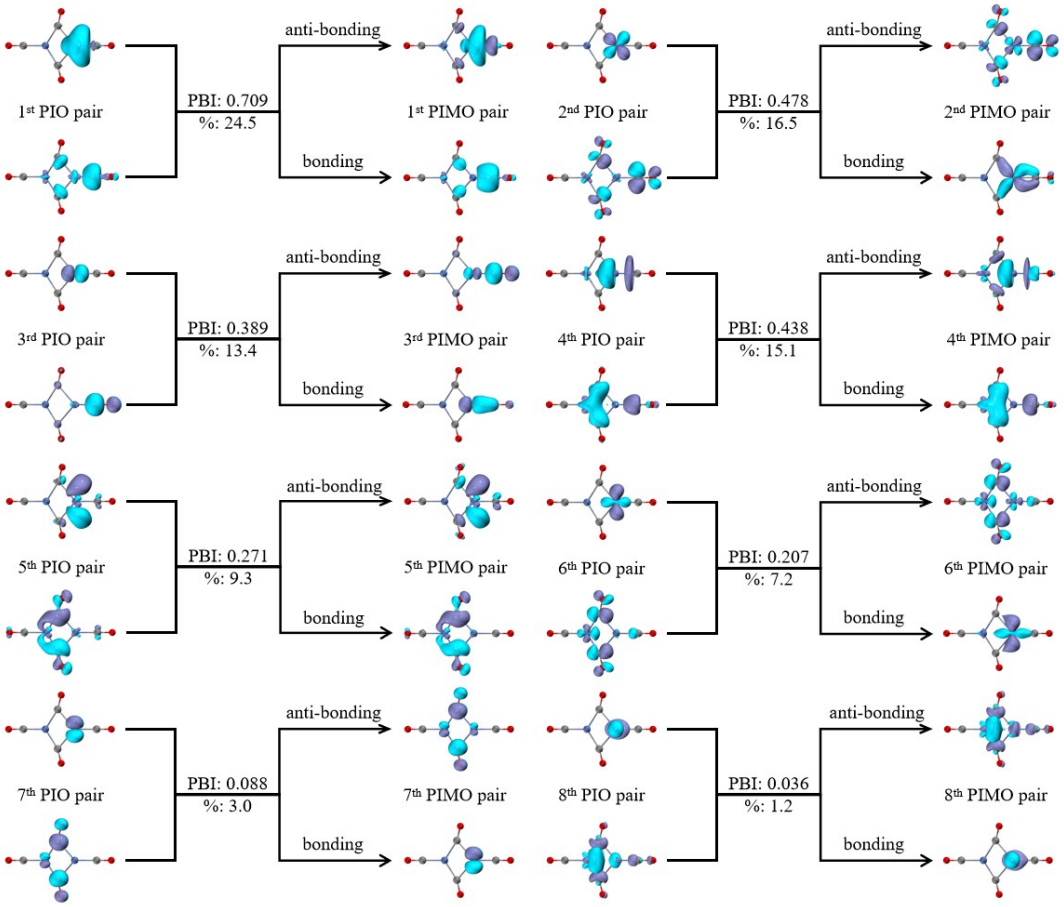

Fig. S13 Results of PIO analysis on the $Ni_2CO_4^-$ complex with Ni^8 atom as one fragment and the remaining moiety as the other fragment at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level of theory. (isosurface = 0.06 a.u.)

The cartesian coordinates of $Ni_2CO_n^{-/0}$ (n = 4–6) complexes at the B3LYP/Ni/Stuttgart+2f1g/C, O/aug–cc–pVTZ level of theory.

$Ni_2CO_4^-$---- Ⅰ

Ni	0.000000000000	0.000000000000	-1.145007000000
C	0.000000000000	0.000000000000	-2.881925000000
C	0.000000000000	1.552425000000	-0.176935000000
C	0.000000000000	-1.552425000000	-0.176935000000
O	0.000000000000	0.000000000000	-4.040497000000
O	0.000000000000	2.684898000000	0.101075000000
O	0.000000000000	-2.684898000000	0.101075000000
Ni	0.000000000000	0.000000000000	1.160053000000
C	0.000000000000	0.000000000000	2.887808000000
O	0.000000000000	0.000000000000	4.046677000000

Ni_2CO_4---- Ⅱ

Ni	0.000000000000	1.154458000000	0.000000000000
C	0.609340000000	2.833920000000	0.000000000000
C	-1.725501000000	0.682709000000	0.000000000000
C	1.377317000000	-0.170211000000	0.000000000000
O	0.981022000000	3.908338000000	0.000000000000
O	-2.831960000000	0.393400000000	0.000000000000
O	2.495897000000	-0.454658000000	0.000000000000
Ni	-0.224251000000	-1.178859000000	0.000000000000
C	-0.113093000000	-2.937758000000	0.000000000000

O	0.028872000000	-4.068171000000	0.000000000000

$Ni_2CO_5^-$----Ⅲ

Ni	0.000000000000	0.000000000000	-1.043187000000
C	0.000000000000	1.511718000000	-1.971703000000
C	-1.565139000000	0.000000000000	0.264342000000
C	0.000000000000	-1.511718000000	-1.971703000000
C	1.565139000000	0.000000000000	0.264342000000
O	0.000000000000	2.472849000000	-2.611656000000
O	2.728718000000	0.000000000000	0.161528000000
O	0.000000000000	-2.472849000000	-2.611656000000
O	-2.728718000000	0.000000000000	0.161528000000
Ni	0.000000000000	0.000000000000	1.321667000000
C	0.000000000000	0.000000000000	3.045373000000
O	0.000000000000	0.000000000000	4.202589000000

$Ni_2CO_5^-$----Ⅳ

Ni	0.000000000000	1.222040000000	0.028712000000
C	0.755261000000	1.362759000000	-1.579358000000
C	0.000000000000	0.000000000000	1.490653000000
C	-0.604312000000	2.704914000000	0.757489000000
O	-0.977314000000	3.697249000000	1.211563000000
O	0.000000000000	0.000000000000	2.668404000000
O	1.291844000000	1.515707000000	-2.588849000000
C	-0.755261000000	-1.362759000000	-1.579358000000

O	-1.291844000000	-1.515707000000	-2.588849000000
Ni	0.000000000000	-1.222040000000	0.028712000000
C	0.604312000000	-2.704914000000	0.757489000000
O	0.977314000000	-3.697249000000	1.211563000000

Ni_2CO_5----**V**

Ni	0.000000000000	0.000000000000	-1.077367000000
C	0.000000000000	1.577733000000	-1.969113000000
C	-1.605858000000	0.000000000000	0.412923000000
C	0.000000000000	-1.577733000000	-1.969113000000
C	1.605858000000	0.000000000000	0.412923000000
O	0.000000000000	2.552540000000	-2.554220000000
O	2.695097000000	0.000000000000	0.063135000000
O	0.000000000000	-2.552540000000	-2.554220000000
O	-2.695097000000	0.000000000000	0.063135000000
Ni	0.000000000000	0.000000000000	1.299281000000
C	0.000000000000	0.000000000000	3.087164000000
O	0.000000000000	0.000000000000	4.224385000000

Ni_2CO_5----**VI**

C	0.000000000000	1.702042000000	0.000000000000
O	0.000000000000	2.843653000000	0.000000000000
C	-1.474012000000	-0.851021000000	0.000000000000
O	-2.462675000000	-1.421826000000	0.000000000000

C	1.474012000000	-0.851021000000	0.000000000000
O	2.462675000000	-1.421826000000	0.000000000000
Ni	0.000000000000	0.000000000000	1.097695000000
C	0.000000000000	0.000000000000	2.875407000000
O	0.000000000000	0.000000000000	4.013645000000
Ni	0.000000000000	0.000000000000	-1.097695000000
C	0.000000000000	0.000000000000	-2.875407000000
O	0.000000000000	0.000000000000	-4.013645000000

$Ni_2CO_6^-$----**Ⅶ**

Ni	-1.252344000000	0.000000000000	0.000000000000
C	-2.174553000000	1.521511000000	0.000000000000
C	0.000000000000	0.000000000000	1.536389000000
C	-2.174553000000	-1.521511000000	0.000000000000
C	0.000000000000	0.000000000000	-1.536389000000
O	-2.834471000000	2.466089000000	0.000000000000
O	0.000000000000	0.000000000000	-2.700382000000
O	-2.834471000000	-2.466089000000	0.000000000000
O	0.000000000000	0.000000000000	2.700382000000
C	2.174553000000	1.521511000000	0.000000000000
O	2.834471000000	2.466089000000	0.000000000000
Ni	1.252344000000	0.000000000000	0.000000000000
C	2.174553000000	-1.521511000000	0.000000000000

O	2.834471000000	-2.466089000000	0.000000000000

$Ni_2CO_6^-$----Ⅷ

Ni	0.000000000000	0.000000000000	1.431028000000
C	0.000000000000	1.774743000000	1.591328000000
C	1.536972000000	-0.887371000000	1.591328000000
C	-1.536972000000	-0.887371000000	1.591328000000
C	-1.536972000000	0.887371000000	-1.591328000000
O	0.000000000000	2.919997000000	1.708456000000
O	-2.528791000000	1.459998000000	-1.708456000000
O	-2.528791000000	-1.459998000000	1.708456000000
O	2.528791000000	-1.459998000000	1.708456000000
C	1.536972000000	0.887371000000	-1.591328000000
O	2.528791000000	1.459998000000	-1.708456000000
Ni	0.000000000000	0.000000000000	-1.431028000000
C	0.000000000000	-1.774743000000	-1.591328000000
O	0.000000000000	-2.919997000000	-1.708456000000

Ni_2CO_6----Ⅸ

Ni	-0.049563000000	-1.336426000000	0.000000000000
C	0.012470000000	-2.184888000000	1.597998000000
C	1.699707000000	0.334125000000	0.000000000000
C	0.012470000000	-2.184888000000	-1.597998000000
C	-1.432669000000	0.029525000000	0.000000000000

O	0.012470000000	-2.763801000000	2.576648000000
O	-2.576415000000	-0.069898000000	0.000000000000
O	0.012470000000	-2.763801000000	-2.576648000000
O	2.753721000000	-0.101380000000	0.000000000000
C	-0.109130000000	2.223085000000	1.515526000000
O	-0.219649000000	2.878932000000	2.435881000000
Ni	0.101495000000	1.225279000000	0.000000000000
C	-0.109130000000	2.223085000000	-1.515526000000
O	-0.219649000000	2.878932000000	-2.435881000000

Ni_2CO_6----**X**

Ni	0.000000000000	0.000000000000	1.624003000000
C	0.000000000000	1.805034000000	1.687812000000
C	1.563206000000	-0.902517000000	1.687812000000
C	-1.563206000000	-0.902517000000	1.687812000000
C	-1.563206000000	0.902517000000	-1.687812000000
O	0.000000000000	2.940244000000	1.753648000000
O	-2.546326000000	1.470122000000	-1.753648000000
O	-2.546326000000	-1.470122000000	1.753648000000
O	2.546326000000	-1.470122000000	1.753648000000
C	1.563206000000	0.902517000000	-1.687812000000
O	2.546326000000	1.470122000000	-1.753648000000
Ni	0.000000000000	0.000000000000	-1.624003000000
C	0.000000000000	-1.805034000000	-1.687812000000

O	0.000000000000	-2.940244000000	-1.753648000000

Ni_2CO_6----**XI**

Ni	1.165417000000	0.131040000000	0.000000000000
C	1.122386000000	1.172323000000	1.509790000000
C	1.122386000000	1.172323000000	-1.509790000000
C	2.712142000000	-0.827340000000	0.000000000000
C	0.033120000000	-1.527161000000	0.000000000000
O	1.122386000000	1.805130000000	2.453821000000
O	3.705856000000	-1.376182000000	0.000000000000
O	1.122386000000	1.805130000000	-2.453821000000
O	0.221944000000	-2.667360000000	0.000000000000
C	-1.800217000000	1.526487000000	0.000000000000
O	-2.129795000000	2.613397000000	0.000000000000
Ni	-1.347517000000	-0.238022000000	0.000000000000
C	-2.779936000000	-1.311086000000	0.000000000000
O	-3.712838000000	-1.959838000000	0.000000000000