Electronic Suplementary Information for the article "*Structure, fragmentation patterns, and magnetic properties of small nickel oxide clusters*" by

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In the Figures 1-6 below are represented the putative ground state and first two low -energy isomers of $Ni_nO_m^{\pm,0}$ (n = 3-8; m = 1-9) clusters.

In the Figure 7 are shown the electronegativity, $(IP_v+EA_v)/2$, and the fundamental gap, IP_v-EA_v, of the Ni_4O_m neutral clusters for m = 1-7.

In the Tables 1-12 below we have collected the numerical values for several structural and electronic properties of neutral and charged $Ni_nO_m^{\pm,0}$ (n = 3-8; m = 1-9) clusters within the putative ground state and first two low -energy isomers.

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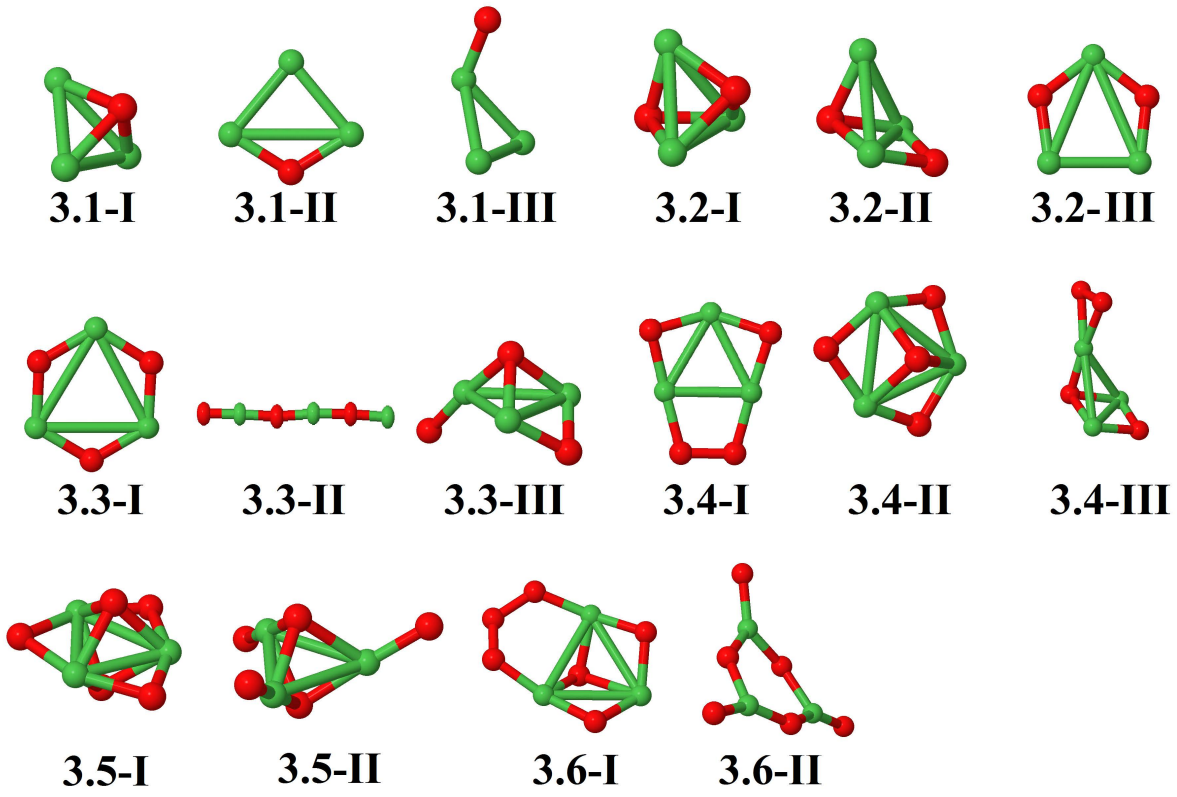

Fig. 1 Putative ground state and first two low-energy isomers of $[Ni_3O_m]^+$ with m = 1-6. The notation is 3.m-Label, with Label in roman letters in decreasing order of stability for each $(3, m)$.

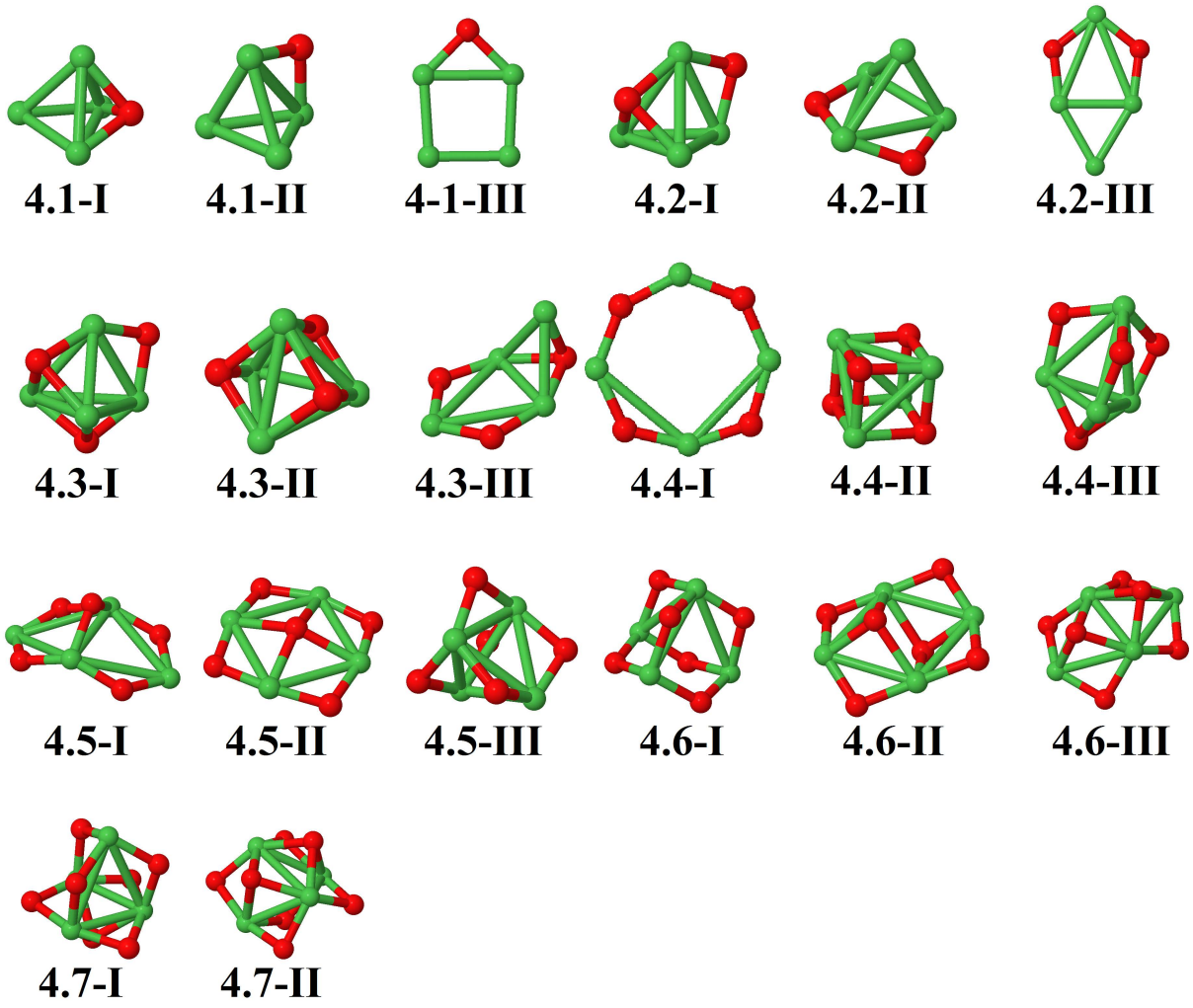

Fig. 2 Putative ground state and first two low-energy isomers of $[Ni_4O_m]^+$ with m = 1-7. The notation is 4.m-Label, with Label in roman letters in decreasing order of stability for each $(4,m)$.

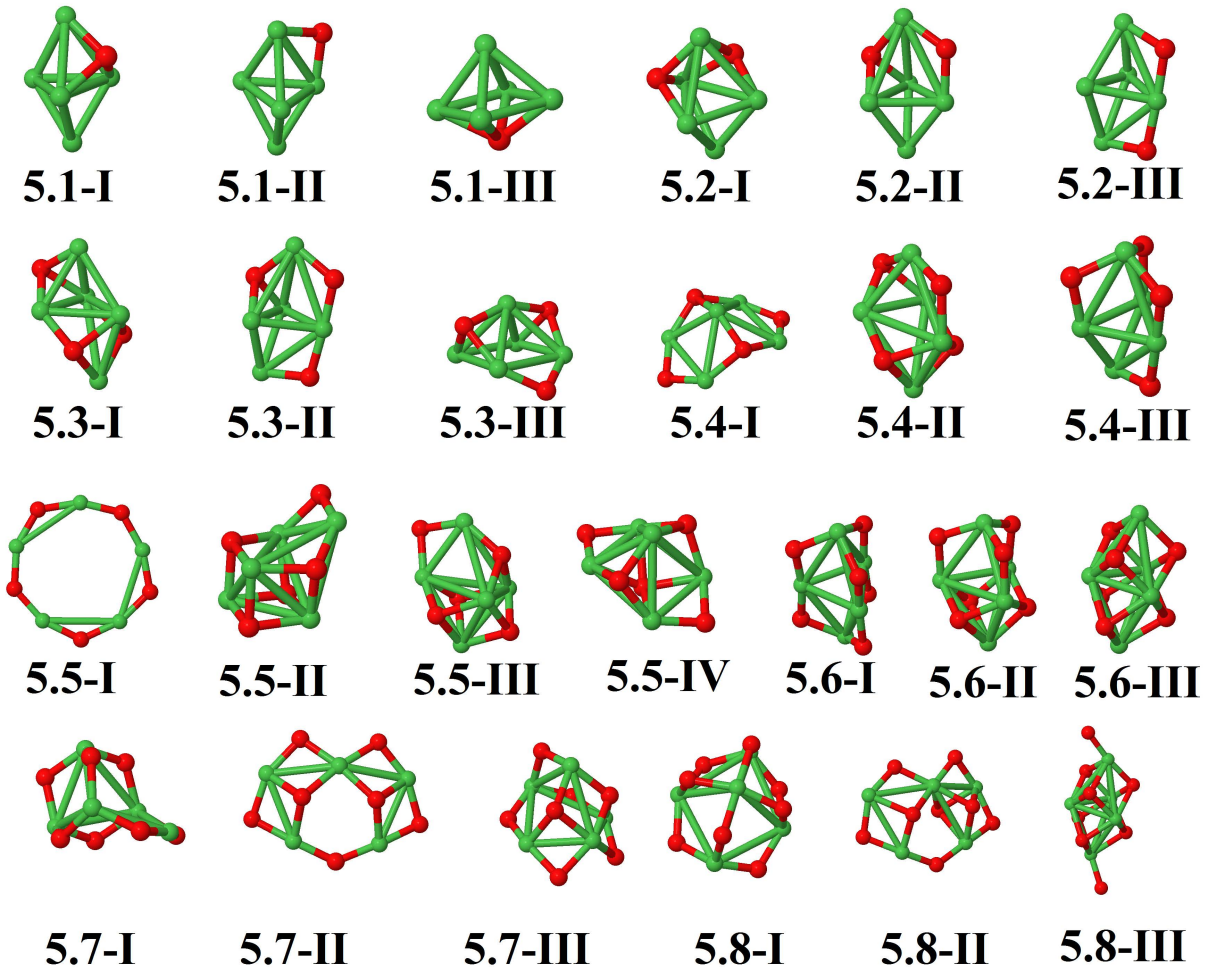

Fig. 3 Putative ground state and first two low-energy isomers of $[Ni_5O_m]^+$ with m = 1-8. The notation is 5.m-Label, with Label in roman letters in decreasing order of stability for each $(5, m)$.

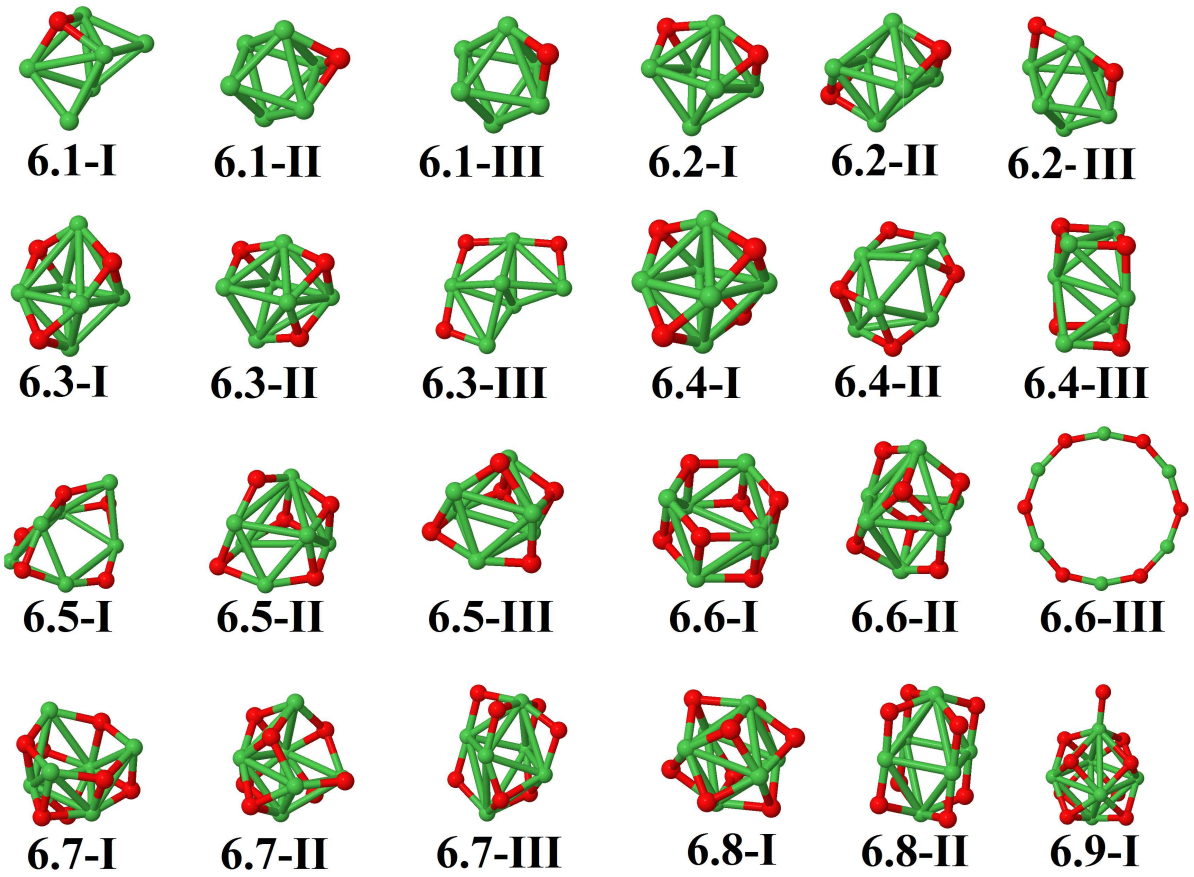

Fig. 4 Putative ground state and first two low-energy isomers of $[Ni_6O_m]^+$ with m = 1-9. The notation is 6.m-Label, with Label in roman letters in decreasing order of stability for each $(6, m)$.

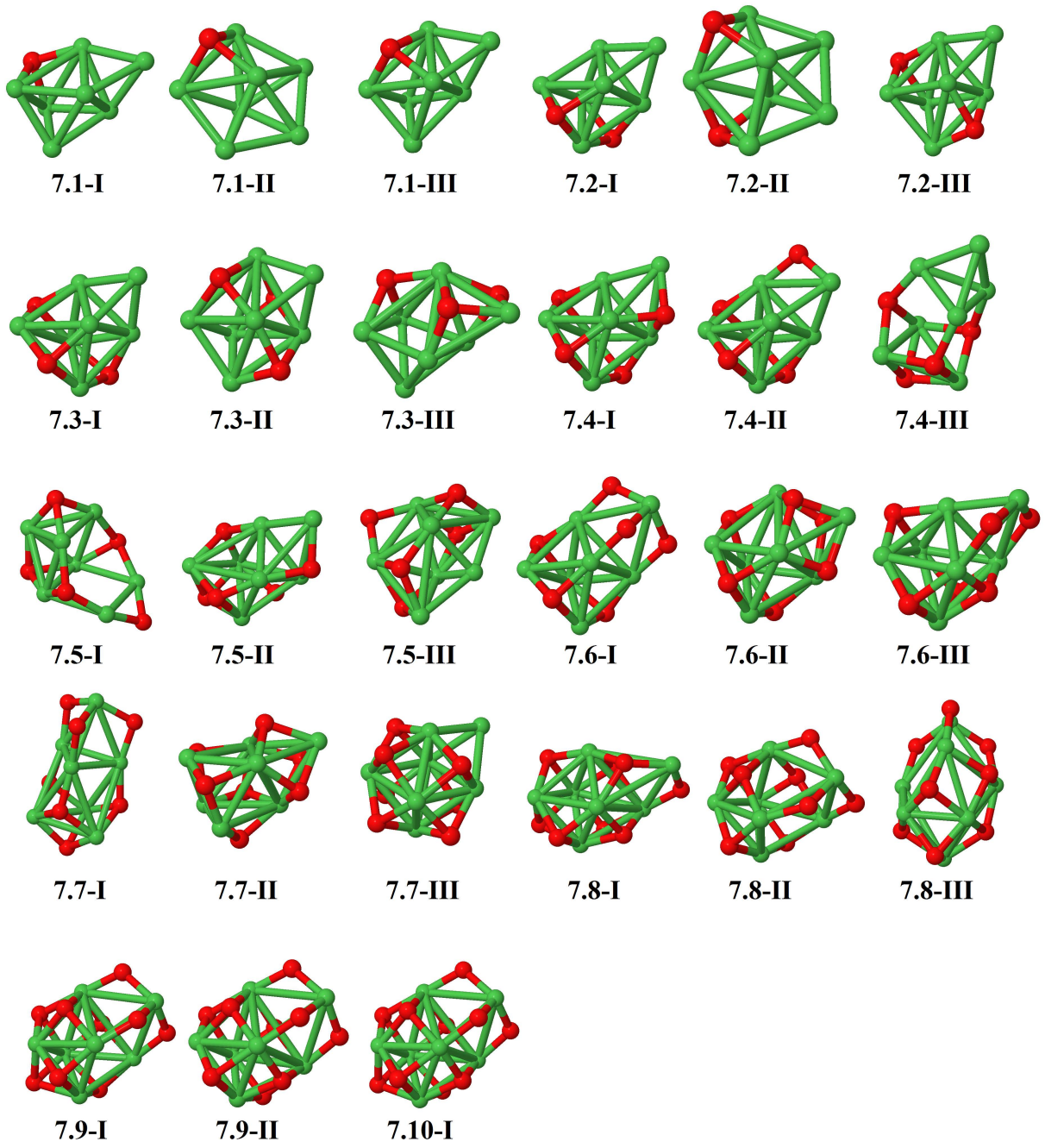

Fig. 5 Putative ground state and first two low-energy isomers of $[Ni_7O_m]^+$ with m = 1-10. The notation is 7.m-Label, with Label in roman letters in decreasing order of stability for each $(7, m)$.

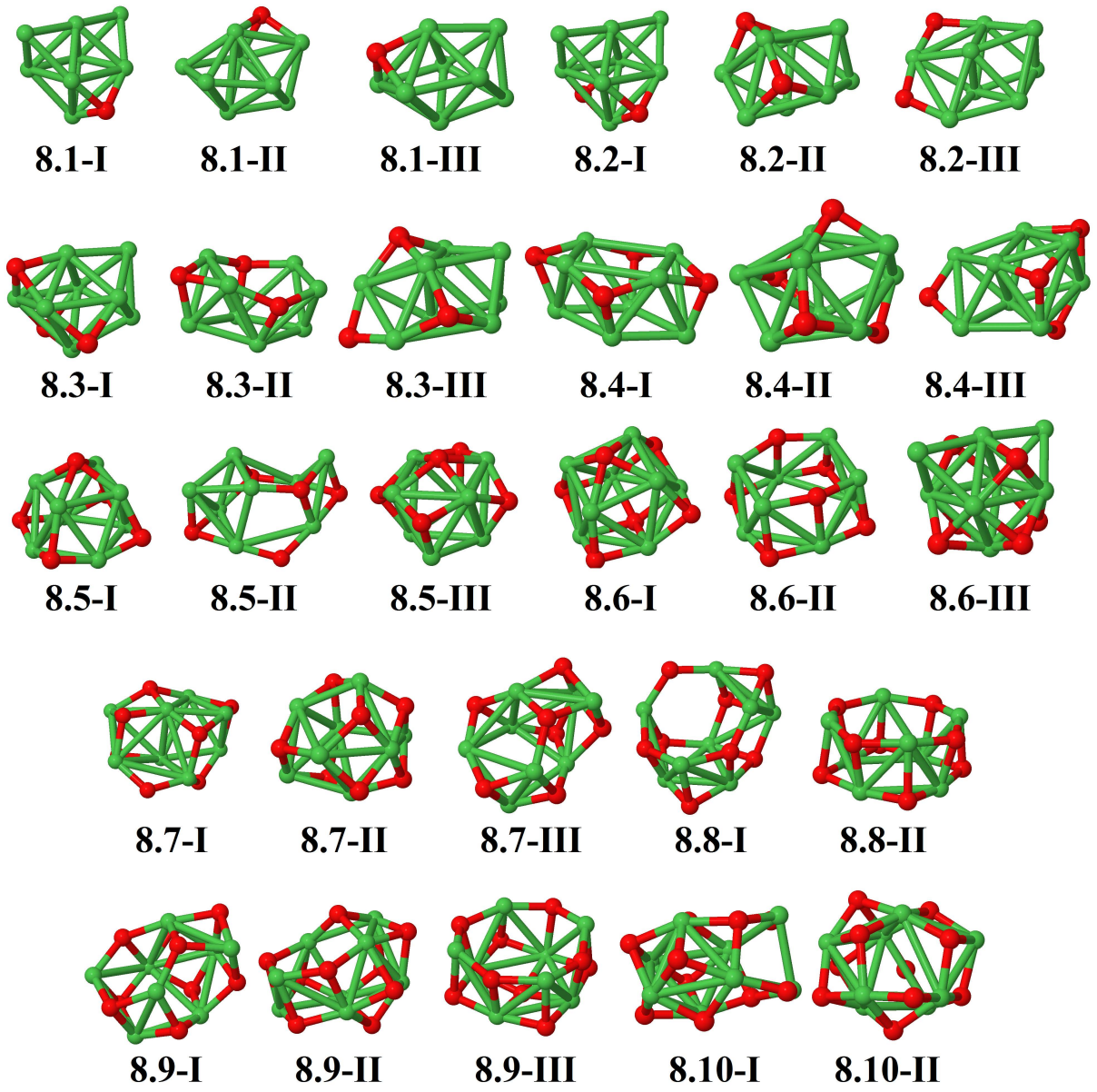

Fig. 6 Putative ground state and first two low-energy isomers of $[Ni_8O_m]^+$ with m = 1-10. The notation is 8.m-Label, with Label in roman letters in decreasing order of stability for each $(8, m)$.

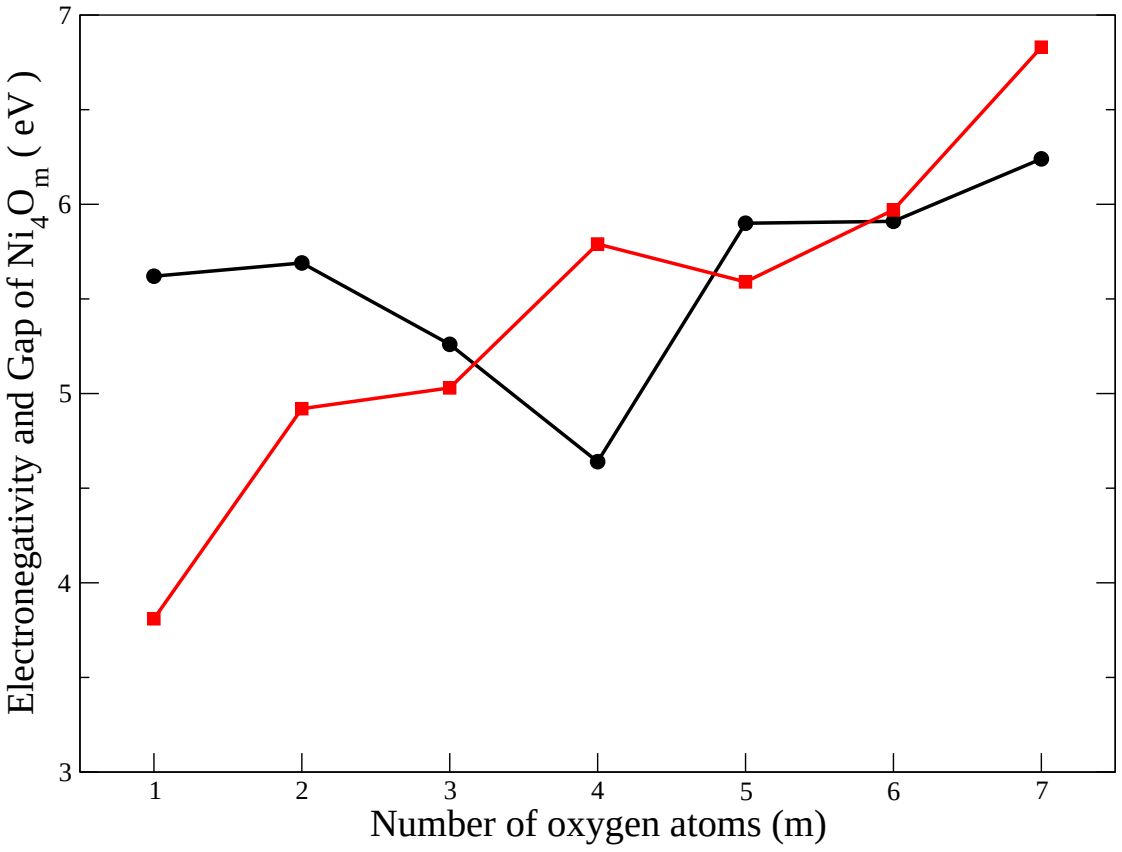

Fig. 7 Electronegativity, $(IP_v+EA_v)/2$, and fundamental gap, IP_v-EA_v, of Ni_4O_m neutral clusters.

Table 1 Several properties of low-energy isomers of neutral Ni_3O_m clusters with m = 1-6: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; I_p = ionization potential in eV; E_a = electron affinity in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature		neutral					
n.m-isomer	Sym	$E_b(n,m)$	I_p	E_a	μ	D(Ni-Ni)	D(Ni-O)
3.1-I	C_{3v}	2.69	6.56	0.72	4	2.38	1.94
3.1.II	C_s	2.66	7.01	1.10	4	2.34	1.84
3.1.III	C_{2v}	2.49	7.46	1.59	4	2.29	1.70
3.2-I	C_{2v}	3.01	6.99	1.20	2	2.50	1.97
3.2-II	C_s	3.11	7.15	1.47	4	2.43	1.92
3.2-III	C_s	3.16	7.54	2.13	4	2.46	1.82
3.3-I	D_{3h}	3.64	8.50	2.47	2	2.44	1.80
3.3-II	$C_{\infty v}$	3.27	7.57	2.59	2	-	1.74
3.3-III	C_s	3.33	7.98	2.56	4	2.55	1.85
3.4-I	C_s	3.52	8.66	2.95	4	2.52	1.81
3.4-II	C_{3v}	3.56	8.90	2.94	2	2.54	1.89
3.4-III	C_1	3.30	8.32	4.47	2	2.60	1.89
3.5-I	D_{3h}	3.42	8.98	3.23	4	2.53	1.94
3.5-II	C_1	3.36	9.45	4.17	6	2.67	1.88
3.6-I	C_s	3.43	8.74	3.49	4	2.83	1.87
3.6-II	C_s	3.44	9.69	4.49	4	3.23	1.76

Table 2 Several properties of low-energy isomers of $[Ni_3O_m]^{\pm}$ cationic and anionic clusters with m = 1-6: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature			cation/anion		
n.m-isomer	Sym	$E_b(n,m)$	μ	D(Ni-Ni)	D(Ni-O)
3.1-I	C_{3v}/C_1	2.98/2.84	3	2.44/2.42	1.89/1.92
3.1.II	C_{3v}/C_s	2.83/2.90	3	2.57/2.32	1.78/1.88
3.1.III	C_s/C_{2v}	2.55/2.85	5/3	2.34/2.28	1.74/1.72
3.2-I	D_{3h}/C_{2v}	3.24/3.31	5	2.58/2.57	1.96/1.99
3.2-II	C_s	3.22/3.38	5	2.62/2.42	1.91/1.95
3.2-III	C_{2v}/C_s	3.20/3.56	5	2.89/2.46	1.81/1.85
3.3-I	D_{3h}	3.51/4.03	1/3	3.12/2.51	1.79/1.82
3.3-II	$C_{\infty v}$	3.29/3.68	3/5	- / -	1.75/1.76
3.3-III	C_s	3.28/3.73	1/5	2.73/2.17	1.85/1.89
3.4-I	C_s	3.38/3.92	5	2.70/2.51	1.81/1.83
3.4-II	C_s/C_{3v}	3.35/3.95	5	2.79/2.51	1.89/1.94
3.4-III	C_1/ -	3.22/ -	5/-	2.74/ -	1.90/ -
3.5-I	D_{3h}	3.27/3.81	5/3	2.60/2.48	1.92/1.96
3.5-II	C_1/C_s	3.14/3.86	7	2.72/2.62	1.88/1.90
3.6-I	C_s	3.32/3.80	5/3	2.92/2.74	1.87/1.87
3.6-II	C_s/C_1	3.22/3.93	7/5	3.35/3.29	1.77/1.77

Table 3 Several properties of low-energy isomers of neutral Ni_4O_m clusters with m = 1-7: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; I_p = ionization potential in eV; E_a = electron affinity in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature			neutral				
n.m-isomer	Sym	$E_b(n,m)$	I_p	E_a	μ	D(Ni-Ni)	D(Ni-O)
4.1-I	C_{3v}	2.73	6.30	0.90	4	2.38	1.97
4.1-II	C_{2v}	2.76	6.55	1.06	4	2.41	1.83
4.1-III	C_{2v}	2.62	6.89	1.72	6	2.34	1.82
4.2-I	C_s	3.18	7.12	1.72	6	2.50	1.90
4.2-II	C_s	3.17	7.36	2.44	4	2.49	1.81
4.2-III	C_{2v}	3.19	7.55	2.33	6	2.48	1.82
4.3-I	C_s	3.47	7.13	2.52	0	2.50	1.83
4.3-II	C_{3v}	3.42	6.81	1.85	2	2.60	1.94
4.3-III	C_s	3.52	7.52	2.41	4	2.48	1.85
4.4-I	C_{2v}	3.80	8.09	3.53	2	2.68	1.79
4.4-II	T_d	3.74	7.73	1.61	0	2.71	1.98
4.4-III	C_{3v}	3.75	8.00	2.54	8	2.71	1.87
4.5-I	C_{2v}	3.69	7.89	3.30	2	2.76	1.81
4.5-II	C_{2v}	3.75	8.44	3.09	4	2.81	1.89
4.5-III	C_{2v}	3.66	7.64	3.56	4	2.55	1.82
4.6-I	C_2	3.72	8.72	3.61	2	2.92	1.83
4.6-II	D_{4h}	3.62	8.11	3.77	6	2.48	1.96
4.6-III	C_s	3.66	8.89	3.62	6	2.66	1.91
4.7-I	C_{3v}	3.59	9.09	4.17	4	2.63	1.89
4.7-II	C_{2v}	3.57	9.49	4.16	6	2.61	1.92

Table 4 Several properties of low-energy isomers of $[Ni_4O_m]^{\pm}$ cationic and anionic clusters with m = 1-7: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature				cation/anion	
n.m-isomer	Sym	$E_b(n,m)$	μ	D(Ni-Ni)	D(Ni-O)
4.1-I	C_s	3.01/2.88	5/3	2.52/2.39	1.91/1.97
4.1-II	C_{2v}/C_2	2.99/2.95	5	2.47/2.36	1.82/1.85
4.1-III	C_{2v}	2.78/2.94	5	2.36/2.38	1.81/1.82
4.2-I	C_s	3.28/3.45	5	2.58/2.48	1.86/1.90
4.2-II	C_s/ -	3.23/ -	7/-	2.64/ -	1.83/ -
4.2-III	C_{2v}/C_s	3.22/3.56	7/5	2.69/2.39	1.82/1.85
4.3-I	C_s/C_{3v}	3.55/3.81	7/5	2.74/2.46	1.90/1.85
4.3-II	C_{3v}	3.55/3.67	7/5	2.77/2.58	1.95/1.98
4.3-III	C_s	3.55/3.85	7/5	2.75/2.46	1.85/1.87
4.4-I	C_1/D_{4h}	3.67/4.15	5/7	3.23/2.46	1.78/1.82
4.4-II	T_d	3.66/3.85	1/7	2.78/2.69	1.96/2.00
4.4-III	C_{3v}/C_s	3.61/3.97	9/7	2.76/2.56	1.86/1.90
4.5-I	C_{2v}	3.67/4.05	1/3	3.08/2.68	1.78/1.84
4.5-II	C_{4v}/C_s	3.67/4.08	3/7	2.84/2.81	1.89/1.87
4.5-III	C_{2v}/C_s	3.67/4.04	5	3.08/2.64	1.79/1.84
4.6-I	C_{3v}/T_d	3.65/4.07	3/11	3.11/2.75	1.84/1.87
4.6-II	C_{2h}/D_{4h}	3.58/3.98	5	2.79/2.45	1.91/1.99
4.6-III	C_s	3.54/4.01	7/5	2.71/2.64	1.90/1.92
4.7-I	C_{3v}	3.46/3.96	9/3	2.81/2.55	1.89/1.89
4.7-II	C_{2v}/C_s	3.41/3.94	7/5	2.70/2.55	1.92/1.92

Table 5 Several properties of low-energy isomers of neutral Ni_5O_m clusters with m = 1-8: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; I_p = ionization potential in eV; E_a = electron affinity in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature			neutral				
$n.m$-isomer	Sym	$E_b(n,m)$	I_p	E_a	μ	D(Ni-Ni)	D(Ni-O)
5.1-I	C_{2v}	2.72	5.79	1.48	6	2.44	1.86
5.1-II	C_s	2.81	6.53	1.53	4	2.41	1.81
5.1-III	C_{4v}	2.68	6.06	0.95	4	2.42	1.98
5.2-I	C_s	3.20	6.68	1.98	4	2.55	1.93
5.2-II	C_s	3.19	6.77	2.01	6	2.52	1.89
5.2-III	C_{2v}	3.18	6.90	1.85	6	2.50	1.82
5.3-I	C_s	3.48	6.99	1.82	4	2.57	1.92
5.3-II	C_s	3.46	7.10	2.41	6	2.62	1.85
5.3-III	C_s	3.49	6.40	2.46	6	2.50	1.89
5.4-I	C_{2v}	3.75	7.79	2.87	8	2.56	1.87
5.4-II	C_1	3.68	7.35	2.55	8	2.65	1.92
5.4-III	C_s	3.61	7.99	2.83	4	2.59	1.81
5.5-I	C_{2v}	3.80	7.85	3.56	2	3.08	1.75
5.5-II	C_{2v}	3.74	7.52	2.57	2	2.81	1.95
5.5-III	C_1	3.73	7.61	2.54	2	2.80	1.93
5.5-IV	C_{2v}	3.72	7.44	2.89	2	2.61	1.81
5.6-I	C_{2v}	3.86	8.33	3.54	8	2.79	1.79
5.6-II	C_{3v}	3.80	8.03	3.15	8	2.78	1.91
5.6-III	D_{3h}	3.78	7.85	2.67	6	2.66	1.97
5.7-I	C_{2v}	3.80	7.40	3.79	6	2.98	1.80
5.7-II	C_s	3.83	8.55	3.52	0	2.13	1.85
5.7-III	C_s	3.82	8.54	3.55	4	2.83	1.86
5.8-I	C_s	3.77	8.81	4.06	6	2.98	1.81
5.8-II	C_1	3.73	8.63	3.87	8	2.90	1.91
5.8-III	C_2	3.67	8.93	4.02	6	2.72	1.94

Table 6 Several properties of low-energy isomers of $[Ni_5O_m]^{\pm}$ cationic and anionic clusters with m = 1-8: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature				cation/anion	
$n.m$-isomer	Sym	$E_b(n,m)$	μ	D(Ni-Ni)	D(Ni-O)
5.1-I	C_s/C_{2v}	3.05/2.95	5	2.51/2.44	1.89/1.88
5.1-II	C_s	3.01/3.04	5	2.45/2.41	1.81/1.85
5.1-III	C_{4v}	2.96/2.83	5/3	2.44/2.43	1.99/1.98
5.2-I	C_s/ -	3.35/ -	7/-	2.63/ -	1.93/ -
5.2-II	C_s	3.33/3.46	7/5	2.65/2.44	1.87/1.92
5.2-III	C_{2v}	3.30/3.43	5	2.51/2.49	1.80/1.83
5.3-I	C_s	3.57/3.69	7	2.71/2.58	1.92/1.95
5.3-II	C_s	3.53/3.74	5	2.69/2.53	1.83/1.87
5.3-III	C_s	3.53/3.78	7	2.61/2.51	1.87/1.91
5.4-I	C_s/C_{2v}	3.74/4.05	9/7	2.69/2.53	1.86/1.88
5.4-II	C_s	3.72/3.95	9/7	2.81/2.56	1.91/1.95
5.4-III	C_s	3.58/3.91	5/3	2.65/2.30	1.81/1.84
5.5-I	C_s/D_{5h}	3.78/4.14	1	3.17/2.88	1.75/1.77
5.5-II	C_{2v}	3.77/3.99	3/9	2.84/2.71	1.93/1.96
5.5-III	C_1/C_s	3.76/3.99	5/9	2.90/2.71	1.92/1.96
5.5-IV	C_1	3.75/3.99	11/7	2.90/2.63	1.94/1.92
5.6-I	D_{3h}	3.81/4.09	5/7	2.86/2.80	1.86/1.81
5.6-II	C_s	3.78/4.08	7	2.93/2.77	1.90/1.92
5.6-III	D_{3h}	3.77/4.01	7/5	2.73/2.66	1.96/1.98
5.7-I	C_2/C_{2v}	3.83/4.11	5	3.00/2.92	1.80/1.85
5.7-II	C_s	3.76/4.10	3	2.73/2.61	1.85/1.87
5.7-III	C_1/C_s	3.75/4.10	5	2.86/2.76	1.86/1.88
5.8-I	C_s	3.69/4.07	7/5	3.06/2.88	1.82/1.84
5.8-II	C_1	3.66/4.01	9/7	2.83/2.86	1.91/1.91
5.8-III	C_2/C_s	3.58/3.97	9/9	2.79/2.75	1.94/1.96

Table 7 Several properties of low-energy isomers of neutral Ni_6O_m clusters with m = 1-9: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; I_p = ionization potential in eV; E_a = electron affinity in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature			neutral				
n.m-isomer	Sym	$E_b(n,m)$	I_p	E_a	μ	D(Ni-Ni)	D(Ni-O)
6.1-I	C_s	2.88	6.33	1.39	6	2.45	1.95
6.1-II	C_{3v}	2.87	6.33	1.68	6	2.46	1.92
6.1-III	C_{2v}	2.86	6.60	1.85	6	2.43	1.84
6.2-I	C_{2v}	3.25	6.78	1.83	8	2.51	1.92
6.2-II	D_{3d}	3.18	6.64	1.72	4	2.48	1.90
6.2-III	C_{2v}	3.21	6.98	2.03	6	2.52	1.92
6.3-I	C_{3v}	3.56	7.15	3.15	8	2.52	1.92
6.3-II	C_s	3.44	6.83	2.05	6	2.53	1.93
6.3-III	C_{2v}	3.44	7.36	2.34	8	2.54	1.83
6.4-I	T_d	3.80	7.45	2.37	8	2.56	1.92
6.4-II	C_1	3.64	7.11	3.95	4	2.38	1.89
6.4-III	D_{2h}	3.63	7.07	2.35	6	2.62	1.92
6.5-I	C_1	3.80	7.40	3.90	10	2.83	1.88
6.5-II	C_1	3.78	7.24	2.74	10	1.73	1.92
6.5-III	C_{3v}	3.81	7.61	2.59	4	2.59	1.92
6.6-I	D_{3h}	3.87	7.21	2.89	2	2.58	1.93
6.6-II	C_s	3.86	7.19	2.92	2	2.79	1.92
6.6-III	C_1	3.82	7.80	3.90	2	3.09	1.75
6.7-I	C_{3v}	3.92	7.99	3.52	4	2.59	1.94
6.7-II	C_s	3.90	8.26	3.31	4	2.61	1.93
6.7-III	C_s	3.83	8.38	3.60	10	2.77	1.88
6.8-I	O_h	3.98	8.84	3.91	4	2.59	1.94
6.8-II	D_{4h}	3.82	8.76	4.25	6	2.64	1.83
6.9-I	C_{4v}	3.88	9.01	4.35	8	2.68	1.95

Table 8 Several properties of low-energy isomers of $[Ni_6O_m]^{\pm}$ cationic and anionic clusters with m = 1-9: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature				cation/anion	
n.m-isomer	Sym	$E_b(n,m)$	μ	D(Ni-Ni)	D(Ni-O)
6.1-I	C_s	3.07/3.05	7/5	2.52/2.45	1.92/1.97
6.1-II	C_{2v}/C_{3v}	3.07/3.10	7	2.65/2.43	1.91/1.94
6.1-III	C_{2v}	3.02/3.06	7	2.45/2.42	1.82/1.86
6.2-I	C_{2v}	3.36/3.46	7	2.51/2.49	1.90/1.93
6.2-II	C_2/C_1	3.32/3.38	7/5	2.51/2.45	1.89/1.92
6.2-III	C_{2v}	3.30/3.45	5/7	2.47/2.45	1.83/1.84
6.3-I	C_s/C_{3v}	3.62/3.78	9/7	2.69/2.51	1.90/1.92
6.3-II	C	3.54/3.65	7	2.67/2.52	1.91/1.95
6.3-III	C_{2v}	3.48/3.69	7	2.56/2.52	1.80/1.83
6.4-I	T_d	3.83/4.02	5/7	2.59/2.54	1.89/1.92
6.4-II	C_1/ -	3.70/ -	9/-	2.71/ -	1.89/ -
6.4-III	D_{4h}/D_{2h}	3.70/3.86	7/5	2.71/2.55	1.89/1.93
6.5-I	C_1/D_{3h}	3.83/4.14	11/9	2.53/2.51	1.88/1.87
6.5-II	C_1	3.82/4.02	11/9	2.81/2.65	1.92/1.94
6.5-III	C_{3v}/C_1	3.82/4.03	5/7	2.68/2.58	1.92/2.01
6.6-I	C_s/C_{3v}	3.91/4.10	1/7	3.03/2.72	1.94/1.95
6.6-II	C_1/D_{2h}	3.91/4.10	3/11	2.77/2.60	1.91/2.01
6.6-III	D_{6h}/C_1	3.81/4.07	1/11	3.33/2.92	1.75/1.79
6.7-I	C_{3v}	3.90/4.18	7/3	2.67/2.58	1.94/1.94
6.7-II	C_s	3.86/4.15	5	2.67/2.67	1.92/1.94
6.7-III	C_s/C_1	3.78/4.10	11/9	2.83/2.74	1.87/1.89
6.8-I	O_h	3.90/4.25	5/3	2.62/2.58	1.94/1.95
6.8-II	D_{4h}	3.74/4.11	7/9	2.75/2.75	1.83/1.84
6.9-I	C_{4v}	3.79/4.16	9/7	2.76/2.66	1.95/1.95

Table 9 Several properties of low-energy isomers of neutral Ni_7O_m clusters with m = 1-10: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; I_p = ionization potential in eV; E_a = electron affinity in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature			neutral				
n.m-isomer	Sym	$E_b(n,m)$	I_p	E_a	μ	D(Ni-Ni)	D(Ni-O)
7.1-I	C_s	2.96	6.31	1.66	8	2.47	1.92
7.1-II	C_s	2.93	6.12	1.81	8	2.48	1.92
7.1-III	C_s	2.91	6.11	1.68	8	2.45	1.94
7.2-I	C_s	3.29	6.77	1.99	8	2.49	1.92
7.2-II	C_2	3.25	6.56	1.98	8	2.45	1.93
7.2-III	C_s	3.21	6.56	1.84	6	2.48	1.91
7.3-I	C_{3v}	3.58	7.95	2.13	8	2.50	1.92
7.3-II	C_{3v}	3.57	6.77	1.88	8	2.52	1.92
7.3-III	C_1	3.41	6.61	3.00	8	2.56	1.94
7.4-I	C_s	3.71	7.13	2.44	8	2.54	1.91
7.4-II	C_s	3.71	7.21	2.61	8	2.54	1.89
7.4-III	C_{3v}	3.58	6.53	2.53	4	2.53	1.93
7.5-I	C_s	3.87	7.52	3.06	10	2.54	1.90
7.5-II	C_s	3.72	6.86	2.60	8	2.66	1.80
7.5-III	C_{2v}	3.74	7.30	3.84	10	2.66	1.93
7.6-I	C_{3v}	3.89	7.43	3.40	12	2.65	1.88
7.6-II	C_{3v}	3.86	7.23	2.99	12	2.66	1.94
7.6-III	C_1	3.86	7.50	3.44	10	2.54	1.90
7.7-I	C_{3v}	3.93	7.55	2.99	2	2.82	1.88
7.7-II	C_s	3.89	7.60	3.00	6	2.72	1.94
7.7-III	C_{3v}	3.86	7.84	3.34	4	2.53	1.95
7.8-I	C_s	3.96	7.81	3.32	6	2.82	1.84
7.8-II	C_s	3.95	7.94	3.24	4	2.83	1.88
7.8-III	C_s	3.94	7.98	3.53	2	2.85	1.88
7.9-I	C_s	3.98	8.24	3.65	4	2.88	1.90
7.9-II	C_{3v}	3.96	8.26	3.63	4	2.85	1.90
7.10-I	C_{3v}	4.01	8.43	3.87	6	2.91	1.91

Table 10 Several properties of low-energy isomers of $[Ni_7O_m]^{\pm}$ cationic and anionic clusters with m = 1-10: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature				cation/anion	
n.m-isomer	Sym	$E_b(n,m)$	μ	D(Ni-Ni)	D(Ni-O)
7.1-I	C_s	3.14/3.15	7	2.50/2.44	1.90/1.93
7.1-II	C_s/C_1	3.13/3.14	7	2.49/2.47	1.91/1.95
7.1-III	C_1/C_s	3.11/3.10	7	2.58/2.45	1.90/1.93
7.2-I	C_1/C_s	3.40/3.50	9/7	2.52/2.47	1.91/1.92
7.2-II	C_2	3.38/3.45	7	2.51/2.48	1.91/1.95
7.2-III	C_s	3.34/3.40	7/5	2.52/2.47	1.90/1.93
7.3-I	C_s/C_{3v}	3.65/3.78	9/7	2.59/2.49	1.90/1.93
7.3-II	C_s/C_{3v}	3.57/3.65	9/7	2.66/2.52	1.90/1.93
7.3-III	C_1	3.52/3.70	9/7	2.62/2.69	1.93/1.94
7.4-I	C_s	3.76/3.92	9/7	2.61/2.53	1.90/1.93
7.4-II	C_1/C_s	3.75/3.93	9/7	2.67/2.55	1.88/1.90
7.4-III	C_{3v}	3.69/3.80	11/9	2.79/2.54	1.94/1.97
7.5-I	C_s/C_{2v}	3.89/4.12	11/9	2.62/2.53	1.88/1.91
7.5-II	C_s	3.79/3.93	9/7	2.73/2.66	1.92/1.94
7.5-III	C_s/C_{2v}	3.77/4.05	11/9	2.74/2.68	1.92/1.97
7.6-I	C_{3v}/C_s	3.91/4.14	5/11	2.79/2.63	1.84/1.89
7.6-II	C_1/C_{3v}	3.90/4.08	13/11	2.85/2.60	1.94/1.97
7.6-III	C_s/C_1	3.87/4.11	11/9	2.79/2.86	1.89/1.92
7.7-I	C_{3v}	3.94/4.14	1/5	2.84/2.78	1.88/1.92
7.7-II	C_s	3.91/4.10	11/7	2.79/2.68	1.93/1.95
7.7-III	C_{3v}	3.85/4.09	11/3	2.57/2.52	1.92/1.95
7.8-I	C_s	3.95/4.17	7/5	2.85/2.58	1.93/1.93
7.8-II	C_1/C_s	3.94/4.16	5/9	2.89/2.82	1.88/1.91
7.8-III	C_1/C_s	3.93/4.17	3	3.05/2.80	1.87/1.89
7.9-I	C_s	3.95/4.20	3/5	2.92/2.82	1.89/1.91
7.9-II	C_{3v}	3.93/4.18	11/5	2.95/2.82	1.91/1.91
7.10-I	C_{3v}	3.97/4.23	5	2.91/2.88	1.90/1.92

Table 11 Several properties of low-energy isomers of neutral Ni_8O_m clusters with m = 1-10: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; I_p = ionization potential in eV; E_a = electron affinity in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature			neutral				
$n.m$-isomer	Sym	$E_b(n,m)$	I_p	E_a	μ	D(Ni-Ni)	D(Ni-O)
8.1-I	C_s	3.03	6.32	1.76	8	2.45	1.92
8.1-II	C_1	3.00	6.30	1.70	8	2.51	1.93
8.1-III	C_s	2.99	6.35	1.88	8	2.53	1.90
8.2-I	C_{2v}	3.35	6.69	1.94	8	2.46	1.92
8.2-II	C_s	3.27	6.56	1.91	8	2.56	1.91
8.2-III	C_s	3.24	6.81	2.38	10	2.54	1.82
8.3-I	C_1	3.50	6.57	2.23	8	2.54	1.91
8.3-II	C_s	3.47	6.66	2.28	10	2.50	1.90
8.3-III	C_s	3.48	6.83	2.38	8	2.56	1.89
8.4-I	C_{2v}	3.67	7.15	2.62	10	2.53	1.91
8.4-II	S_2	3.64	6.88	2.32	8	2.58	1.90
8.4-III	C_1	3.64	7.06	2.69	10	2.51	1.90
8.5-I	C_{2v}	3.84	7.33	2.61	10	2.53	1.94
8.5-II	C_1	3.73	5.98	2.86	10	2.62	1.90
8.5-III	C_{2v}	3.70	7.09	2.78	12	2.60	2.09
8.6-I	C_{4v}	3.87	9.41	2.83	12	2.56	1.98
8.6-II	C_1	3.88	8.18	3.11	4	2.65	1.91
8.6-III	C_{2v}	3.72	7.39	2.92	4	2.52	1.94
8.7-I	C_1	3.94	7.33	3.26	10	2.70	1.91
8.7-II	C_s	3.92	7.27	2.96	12	2.77	1.93
8.7-III	C_1	3.92	7.46	2.93	8	2.80	1.94
8.8-I	C_1	3.97	7.40	3.20	4	2.71	1.83
8.8-II	C_s	3.96	7.30	3.40	8	2.75	1.92
8.9-I	C_1	3.97	7.06	3.72	8	2.78	1.92
8.9-II	C_1	4.00	7.82	3.35	8	2.93	1.93
8.9-III	C_1	3.97	7.39	3.66	12	2.78	1.94
8.10-I	C_1	4.02	7.92	3.99	2	2.80	1.85
8.10-II	C_1	4.00	8.07	3.93	4	2.60	1.91

Table 12 Several properties of low-energy isomers of $[Ni_8O_m]^{\pm}$ cationic and anionic clusters with m = 1-10: Sym = molecular symmetry; $E_b(n,m)$ = binding energy per atom in eV; μ = magnetic moment in Bohr magnetons (μ_B); D(Ni-Ni)= average distance between first neighbour nickel atoms in Å; D(Ni-O) = average distance between first neighbour nickel-oxygen atoms in Å

Signature				cation/anion	
$n.m$-isomer	Sym	$E_b(n,m)$	μ	D(Ni-Ni)	D(Ni-O)
8.1-I	C_s	3.18/3.21	9/7	2.48/2.46	1.91/1.93
8.1-II	C_1	3.15/3.17	9/7	2.54/2.51	1.92/1.94
8.1-III	C_s	3.15/3.19	9	2.52/2.53	1.90/1.94
8.2-I	C_{2v}	3.45/3.53	9/7	2.52/2.46	1.91/1.92
8.2-II	C_s	3.39/3.45	9/7	2.59/2.55	1.91/1.92
8.2-III	C_s	3.33/3.46	9	2.57/2.51	1.82/1.84
8.3-I	C_s/C_1	3.60/3.69	9/7	2.45/2.39	1.91/1.93
8.3-II	C_s	3.56/3.66	11/9	2.55/2.55	1.90/1.92
8.3-III	C_s	3.56/3.69	9/7	2.56/2.52	1.88/1.89
8.4-I	C_1/C_{2v}	3.72/3.88	11/9	2.61/2.51	1.90/1.92
8.4-II	C_1/s_4	3.70/3.82	9/7	2.63/2.57	1.89/1.91
8.4-III	C_s/C_1	3.69/3.85	11/9	2.62/2.60	1.89/1.91
8.5-I	C_{2v}	3.87/4.03	11/9	2.55/2.50	1.93/1.96
8.5-II	C_1	3.87/3.94	11/9	2.65/2.63	1.88/1.92
8.5-III	C_{2v}	3.75/3.91	13/11	2.63/2.64	1.96/1.98
8.6-I	C_{4v}	3.90/4.06	11	2.65/2.55	1.96/1.97
8.6-II	C_{2v}/C_1	3.85/4.10	7	2.68/2.80	1.90/1.89
8.6-III	C_{2v}	3.75/3.92	5/3	2.57/2.51	1.93/1.95
8.7-I	C_1	3.96/4.14	9	2.80/2.69	1.91/1.92
8.7-II	C_1/C_s	3.95/4.10	9/11	2.74/2.67	1.92/1.95
8.7-III	C_1	3.93/4.10	11/9	2.87/2.74	1.90/1.97
8.8-I	C_1	3.99/4.16	7	2.75/2.73	1.91/1.93
8.8-II	C_s/C_{4v}	3.98/4.15	5/7	2.76/2.78	1.92/1.93
8.9-I	C_1	4.00/4.18	7	2.80/2.66	1.86/1.93
8.9-II	C_1	3.99/4.20	9/7	2.75/2.89	1.93/1.94
8.9-III	C_s/C_1	3.98/4.18	11/7	2.81/2.77	1.87/1.87
8.10-I	C_2	4.01/4.24	9/7	2.81/2.78	1.91/1.92
8.10-II	C_1	3.98/4.21	9/7	2.65/2.54	1.93/1.93