materials

MDPI

Supplementary Materials

Quantum-Chemical Consideration of Al_2M_2 Tetranuclear Metal Clusters (M–3*d*-Element): Molecular/Electronic Structures and Thermodynamics

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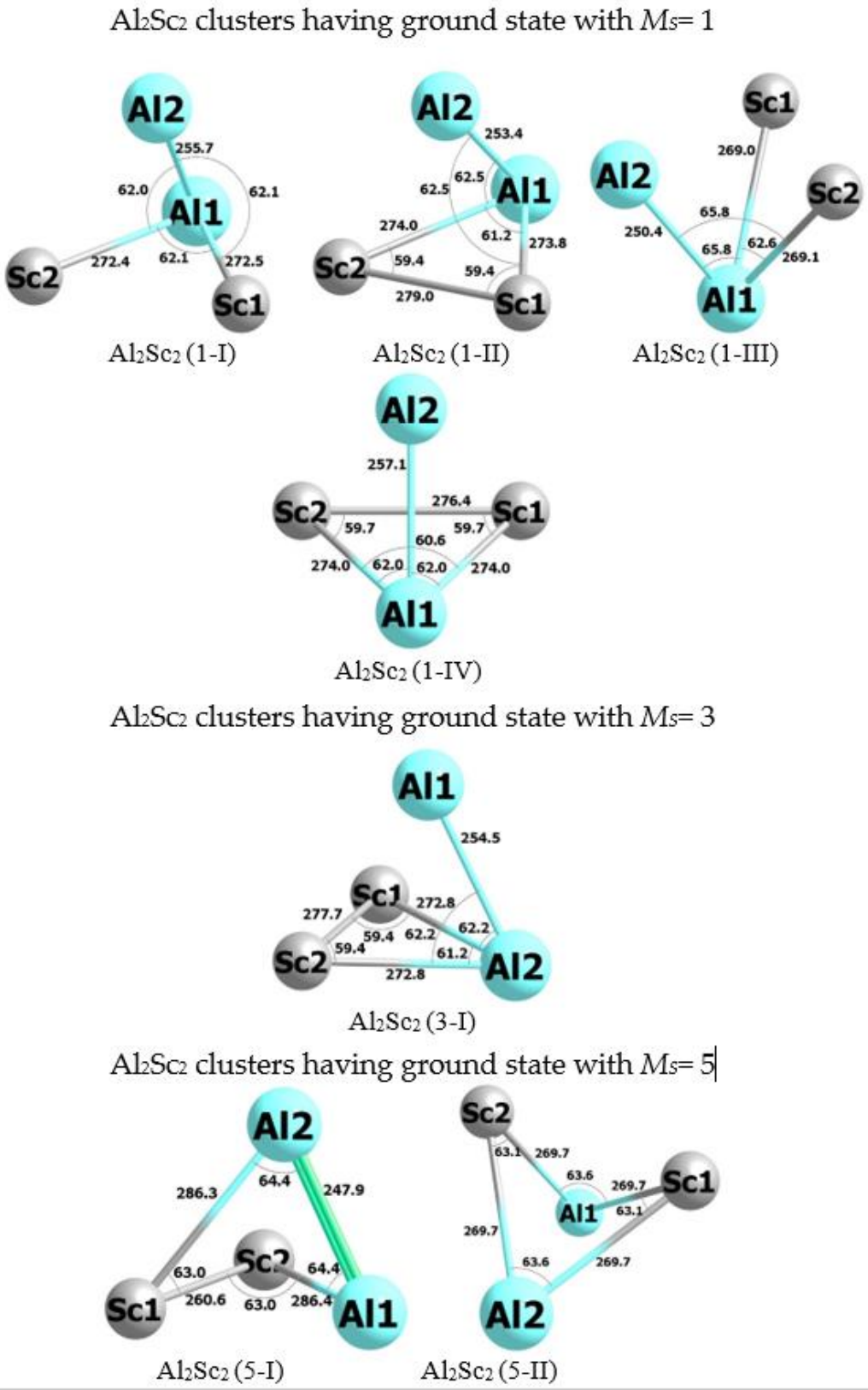


Figure S1. Molecular structures of Al_2Sc_2 metal clusters.

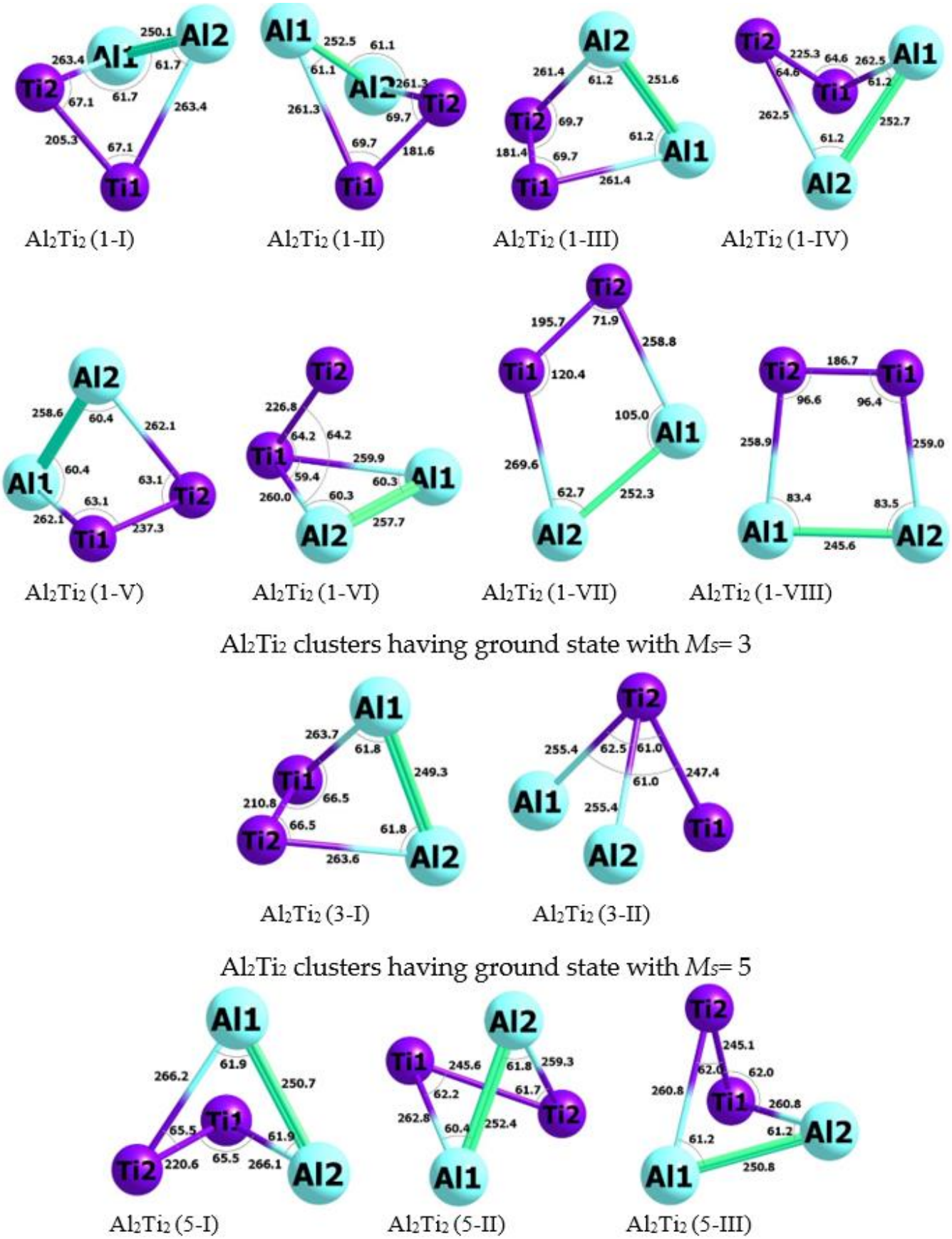


Figure S2. Molecular structures of Al_2Ti_2 metal clusters.

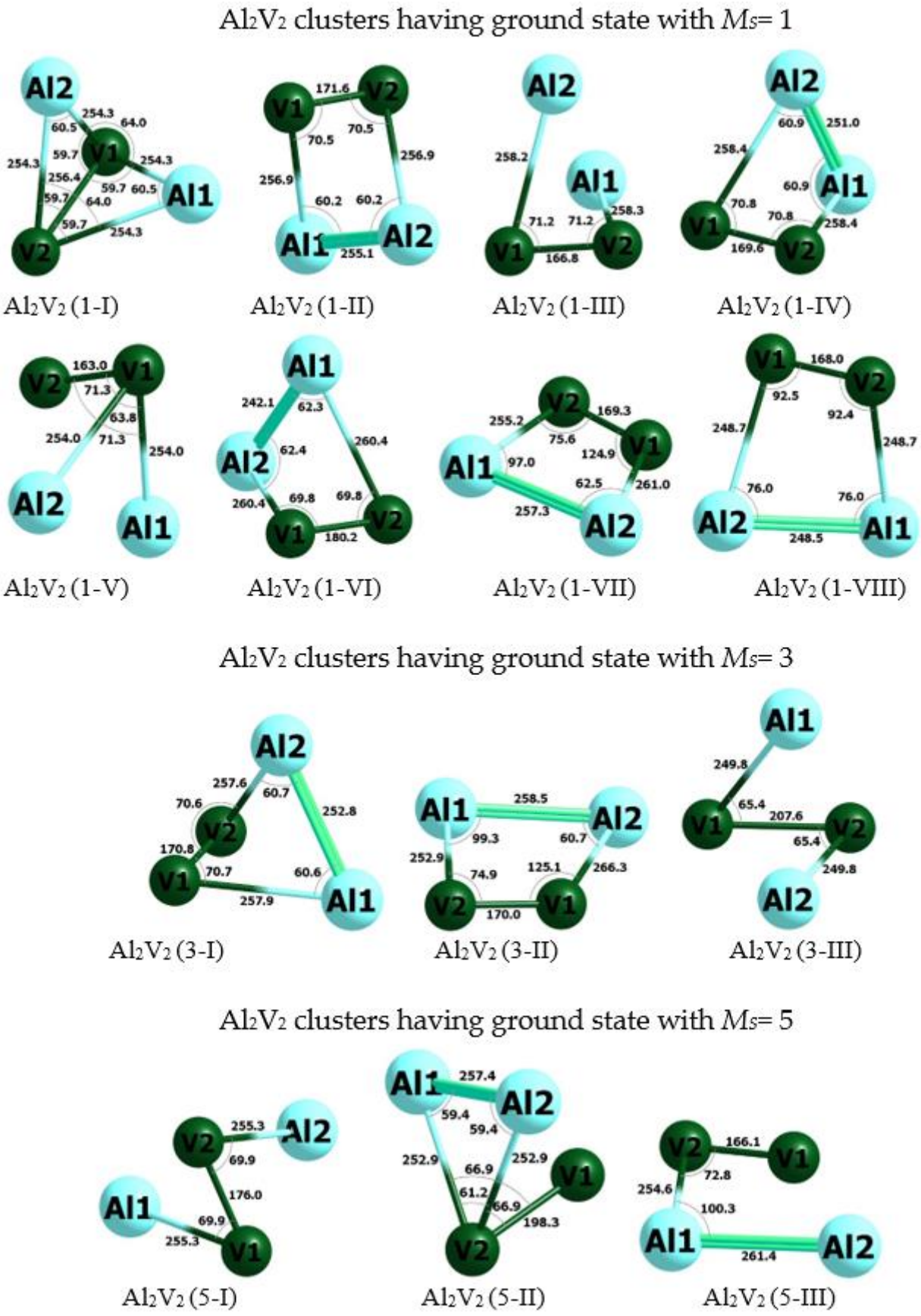


Figure S3. Molecular structures of Al_2V_2 metal clusters.

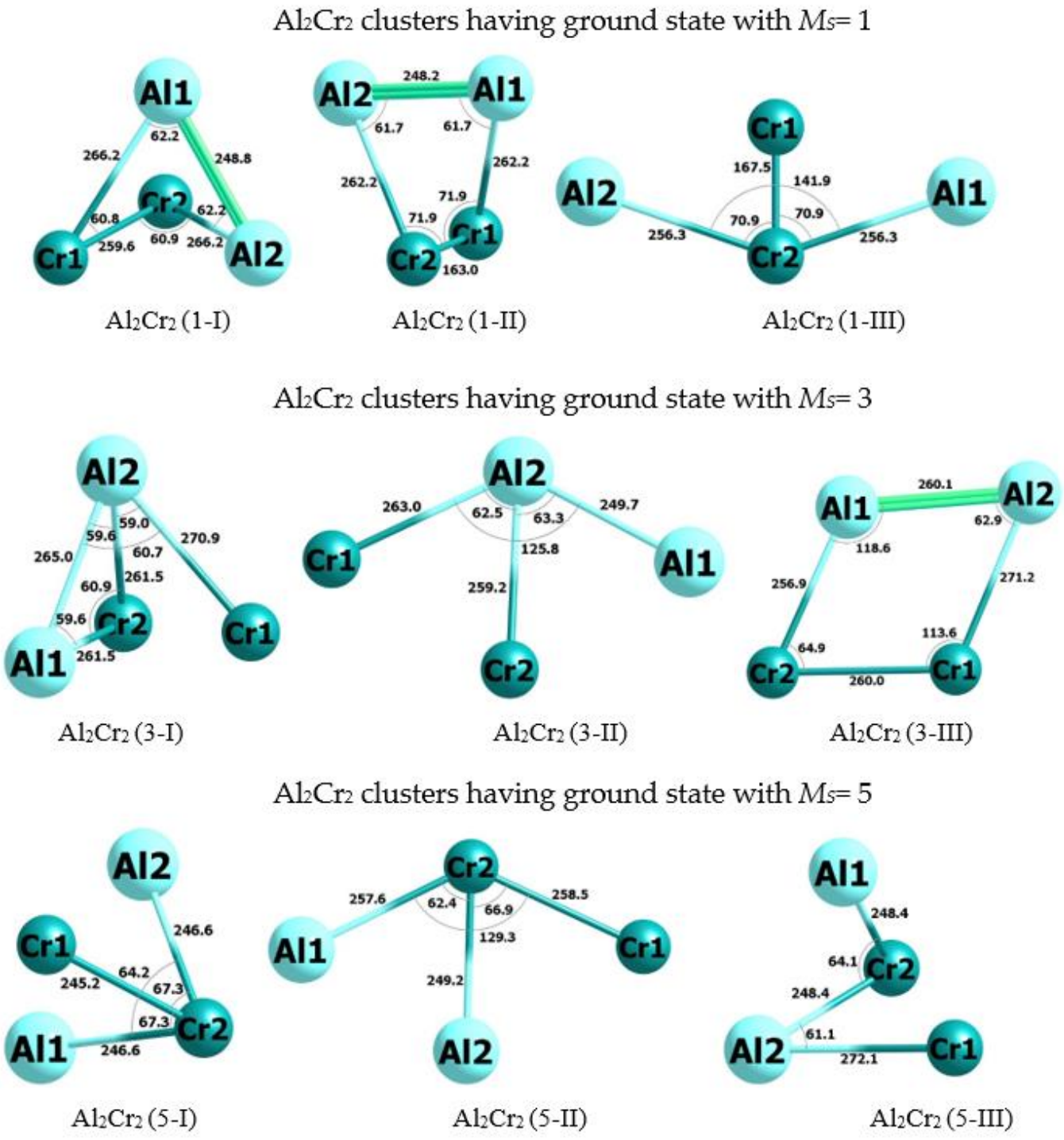
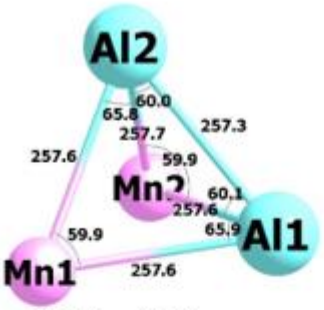
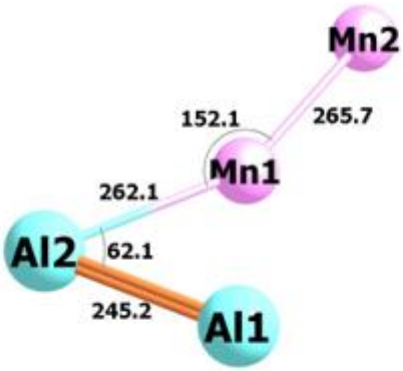


Figure S4. Molecular structures of Al_2Cr_2 metal clusters.

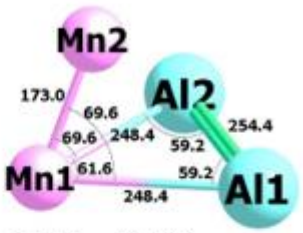
Al_2Mn_2 clusters having ground state with M_S= 1



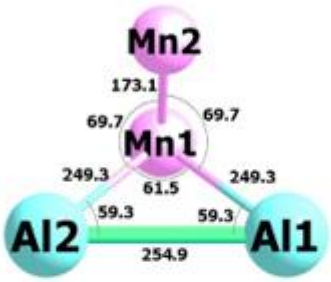
Al_2Mn_2 (1-I)



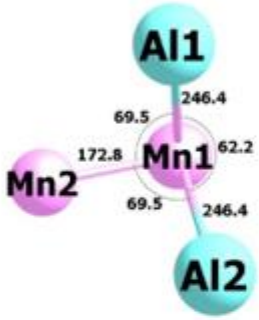
Al_2Mn_2 (1-II)



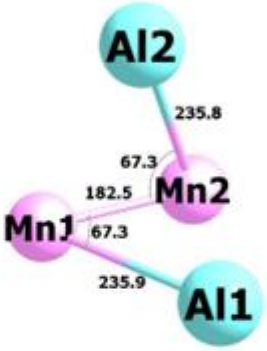
Al_2Mn_2 (1-III)



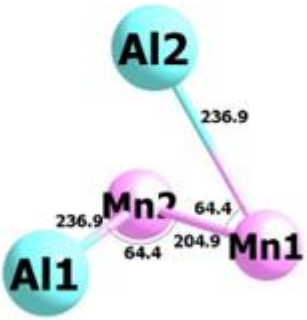
Al_2Mn_2 (1-IV)



Al_2Mn_2 (1-V)



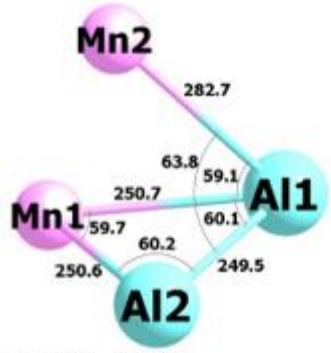
Al_2Mn_2 (1-VI)



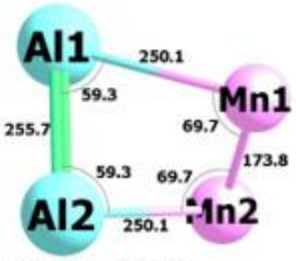
Al_2Mn_2 (1-VII)

Al_2Mn_2 (1-VIII)

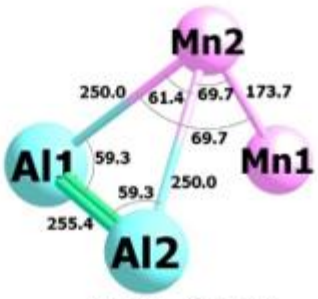
Al_2Mn_2 clusters having ground state with M_S= 3



Al_2Mn_2 (3-I)



Al_2Mn_2 (3-II)



Al_2Mn_2 (3-III)

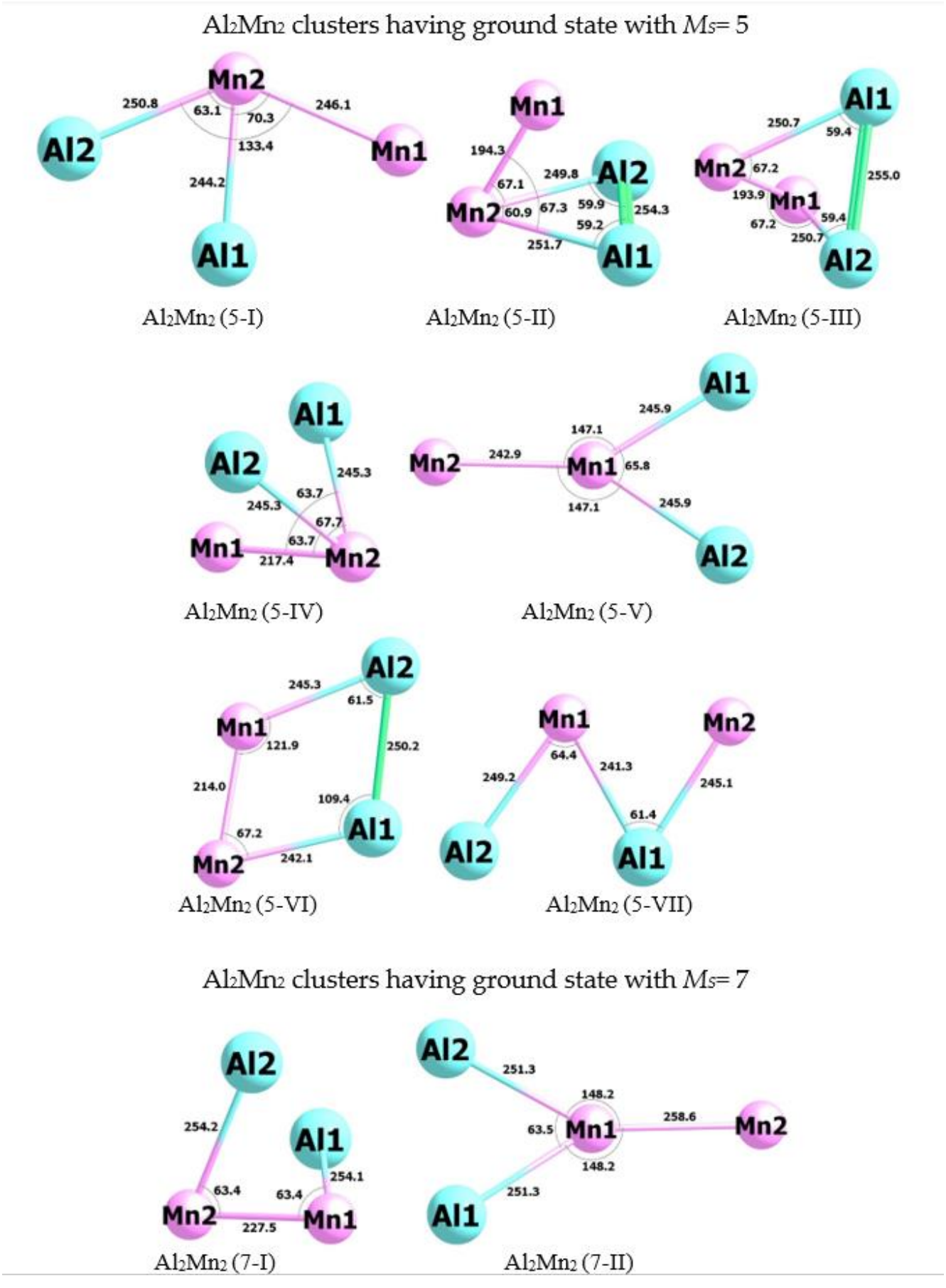
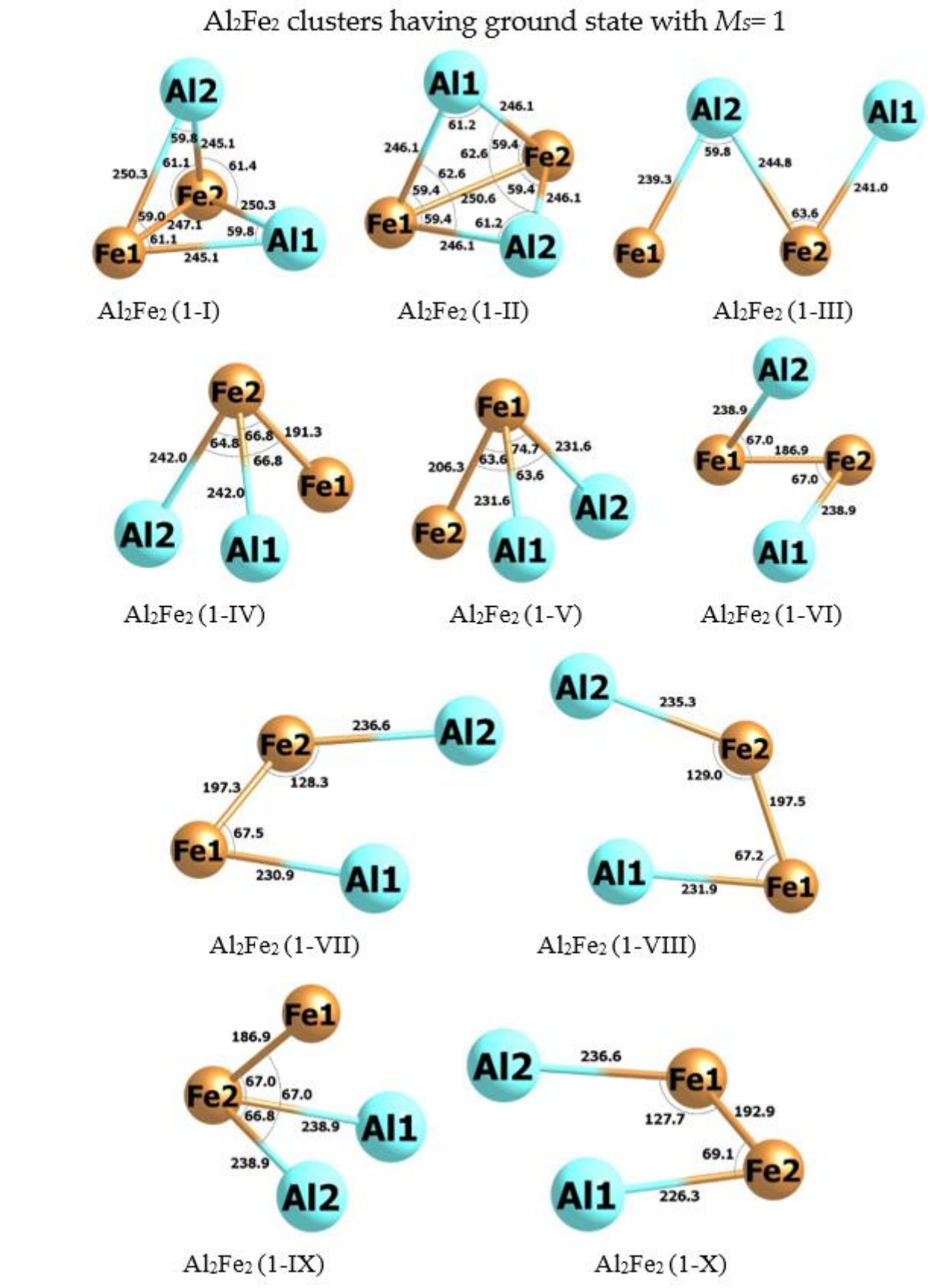


Figure S5. Molecular structures of Al_2Mn_2 metal clusters.


Al2Fe2 clusters having ground state with Ms= 1
Al2
Fe2
Fe1
Al1
59.8
245.1
61.1
61.4
250.3
250.3
59.0
247.1
59.8
61.1
245.1
Al2Fe2 (1-I)
Al1
246.1
61.2
246.1
62.6
59.4
Fe2
62.6
59.4
250.6
59.4
246.1
Fe1
59.4
61.2
Al2
246.1
Al2Fe2 (1-II)
Al2
Al1
59.8
244.8
239.3
241.0
63.6
Fe1
Fe2
Al2Fe2 (1-III)
Fe2
66.8
191.3
64.8
242.0
66.8
Fe1
242.0
Al2
Al1
Al2Fe2 (1-IV)
Fe1
74.7
231.6
206.3
63.6
63.6
231.6
Fe2
Al2
Al1
Al2Fe2 (1-V)
Al2
238.9
67.0
186.9
Fe1
Fe2
67.0
238.9
Al1
Al2Fe2 (1-VI)
Fe2
236.6
Al2
197.3
128.3
67.5
Fe1
230.9
Al1
Al2Fe2 (1-VII)
Al2
235.3
Fe2
129.0
197.5
67.2
Al1
231.9
Fe1
Al2Fe2 (1-VIII)
Fe1
186.9
67.0
Fe2
67.0
66.8
238.9
Al1
238.9
Al2
Al2Fe2 (1-IX)
Al2
236.6
Fe1
127.7
192.9
69.1
Fe2
Al1
226.3
Al2Fe2 (1-X)

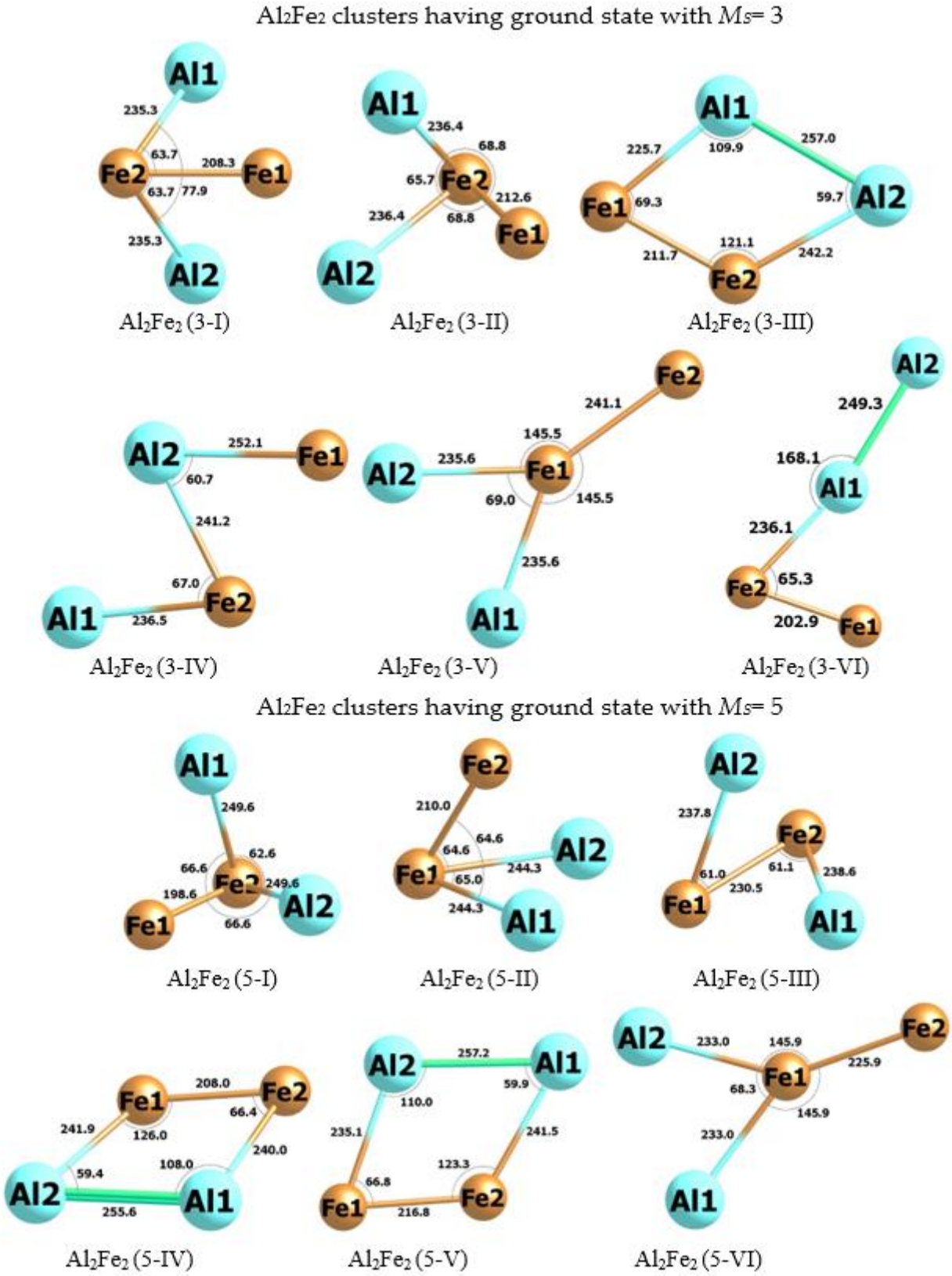
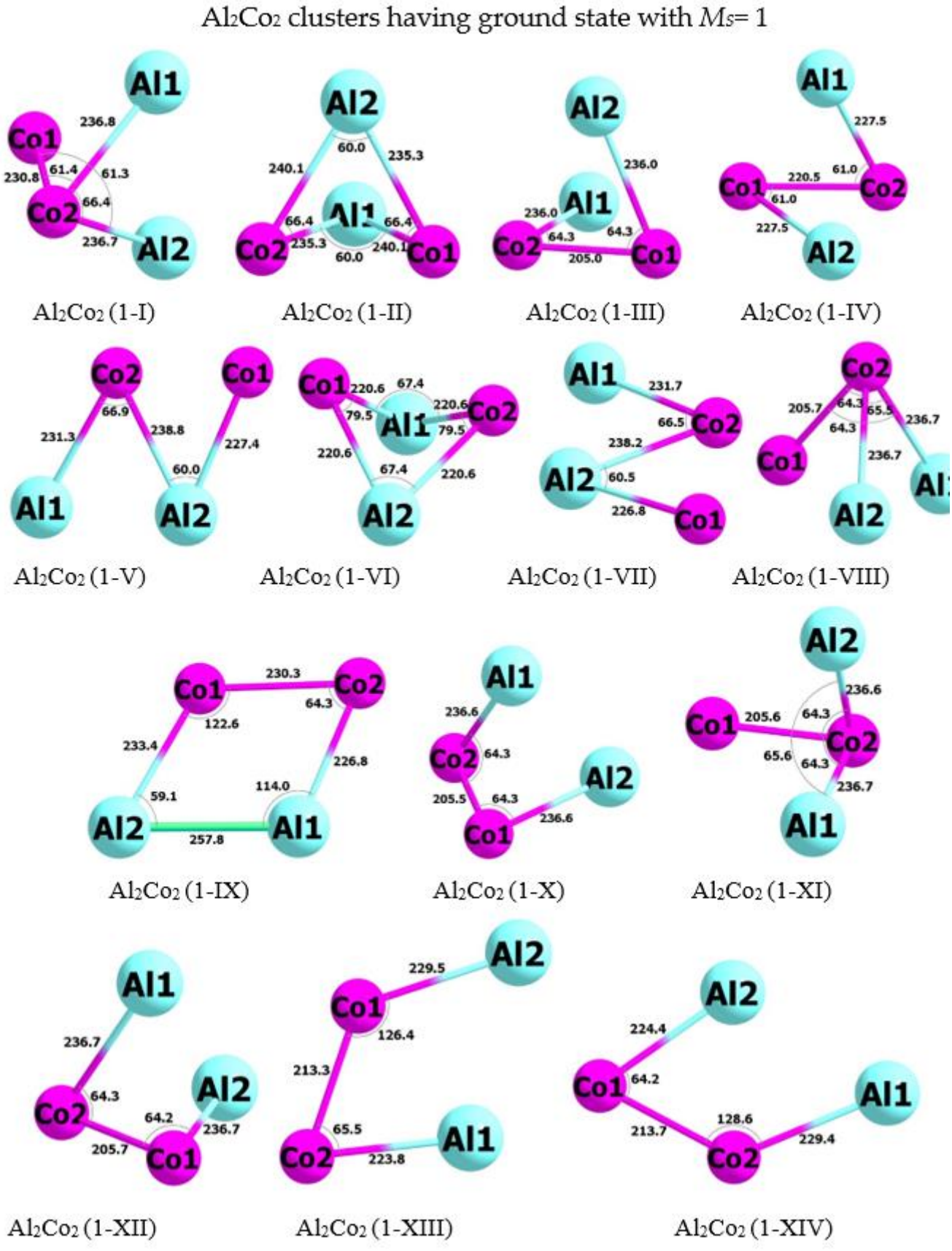


Figure S6. Molecular structures of Al_2Fe_2 metal clusters.


Al2Co2 clusters having ground state with Ms= 1
Al1
Co1
Co2
Al2
236.8
61.4
230.8
61.3
66.4
236.7
Al2Co2 (1-I)
Al2
60.0
235.3
240.1
66.4
66.4
235.3
60.0
240.1
Al2Co2 (1-II)
Al2
236.0
Al1
236.0
64.3
64.3
205.0
Al2Co2 (1-III)
Al1
227.5
220.5
61.0
Co1
Co2
61.0
227.5
Al2Co2 (1-IV)
Co2
Co1
66.9
231.3
238.8
227.4
60.0
Al1
Al2
Al2Co2 (1-V)
Co1
220.6
67.4
220.6
79.5
Al1
Co2
79.5
220.6
67.4
220.6
Al2
Al2Co2 (1-VI)
Al1
231.7
66.5
Co2
238.2
Al2
60.5
226.8
Co1
Al2Co2 (1-VII)
Co2
205.7
64.3
65.5
236.7
64.3
Co1
236.7
Al2
Al2Co2 (1-VIII)
Co1
230.3
Co2
64.3
122.6
233.4
226.8
59.1
114.0
Al2
257.8
Al1
Al2Co2 (1-IX)
Al1
236.6
Co2
64.3
Al2
205.5
64.3
Co1
236.6
Al2Co2 (1-X)
Al2
236.6
Co1
205.6
64.3
Co2
65.6
64.3
236.7
Al1
Al2Co2 (1-XI)
Al1
236.7
Co2
64.3
Al2
64.2
236.7
205.7
Co1
Al2Co2 (1-XII)
Al2
229.5
Co1
126.4
213.3
65.5
Co2
Al1
223.8
Al2Co2 (1-XIII)
Al2
224.4
Co1
64.2
Al1
128.6
213.7
229.4
Co2
Al2Co2 (1-XIV)

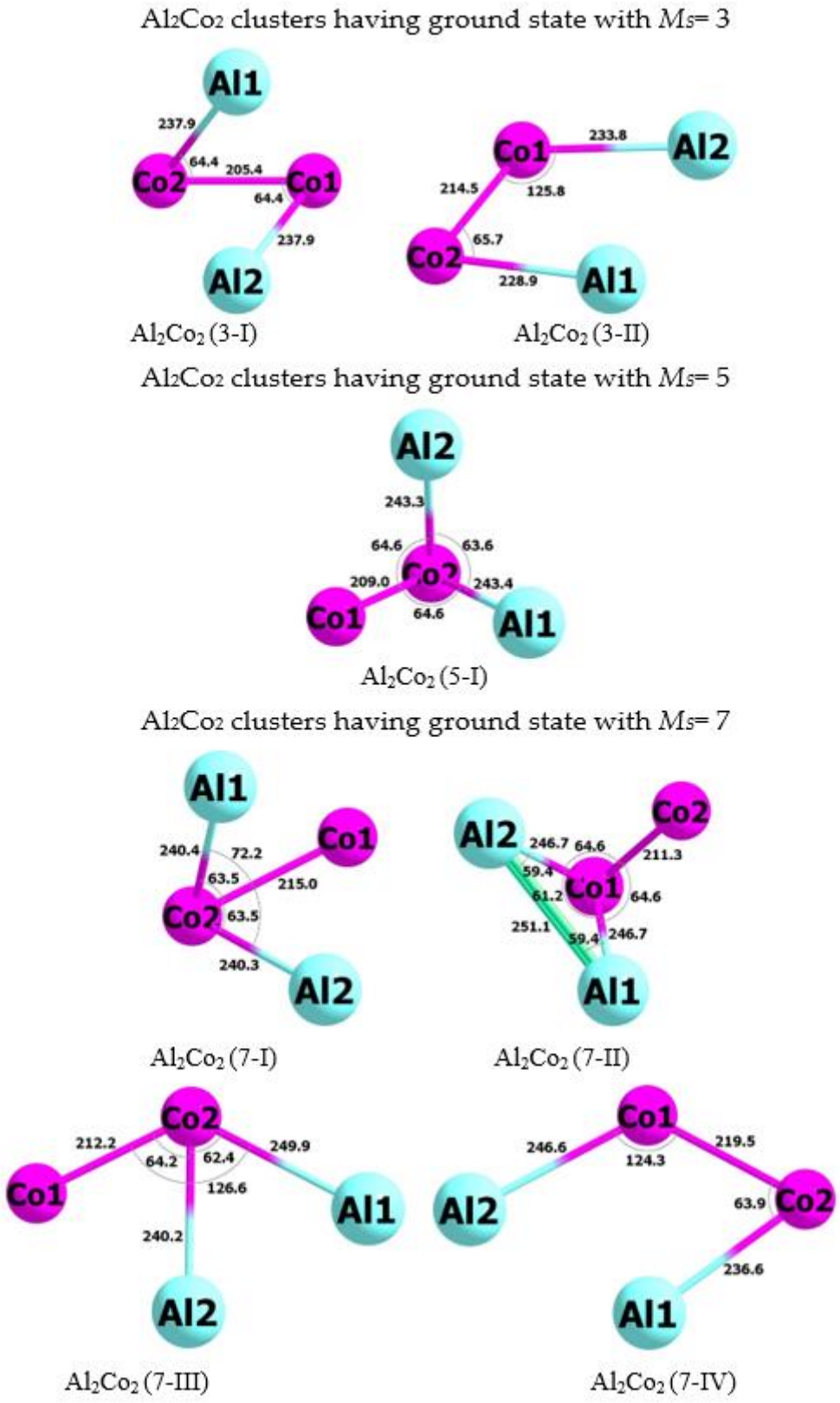


Figure S7. Molecular structures of Al_2Co_2 metal clusters.

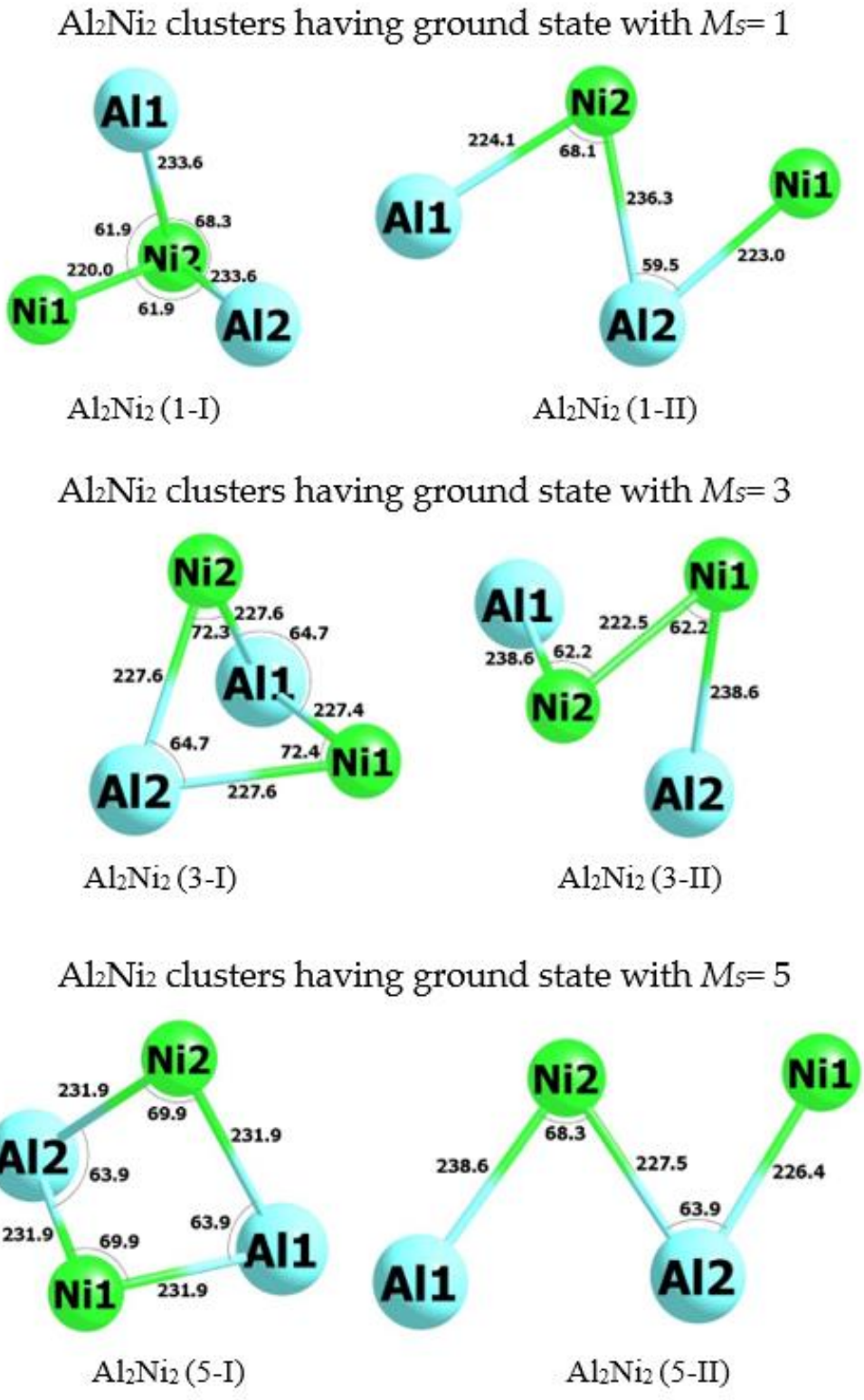
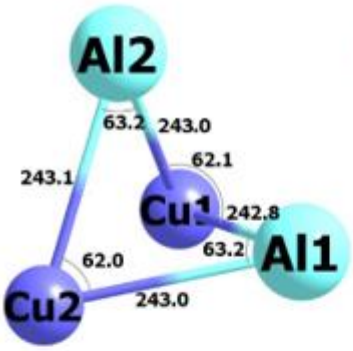
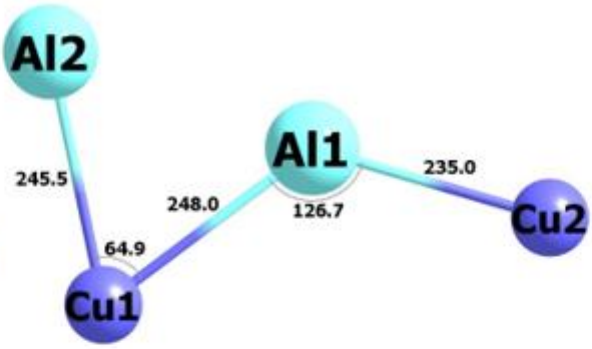


Figure S8. Molecular structures of Al_2Ni_2 metal clusters.

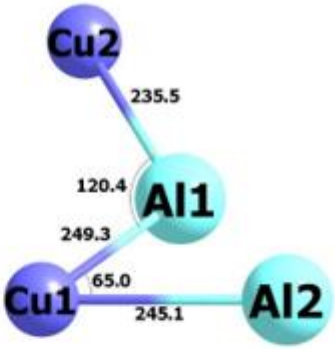
Al_2Cu_2 clusters having ground state with M_S= 1



Al_2Cu_2 (1-I)

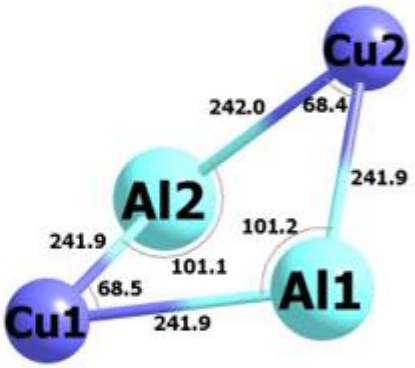


Al_2Cu_2 (1-II)

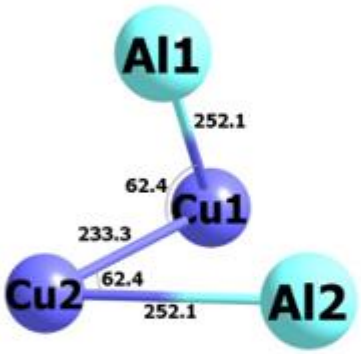


Al_2Cu_2 (1-III)

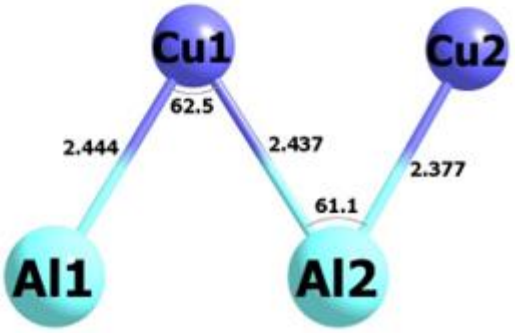
Al_2Cu_2 clusters having ground state with M_S= 3



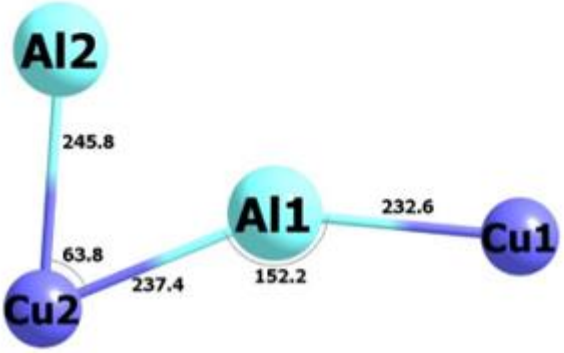
Al_2Cu_2 (3-I)



Al_2Cu_2 (3-II)



Al_2Cu_2 (3-III)



Al_2Cu_2 (3-IV)

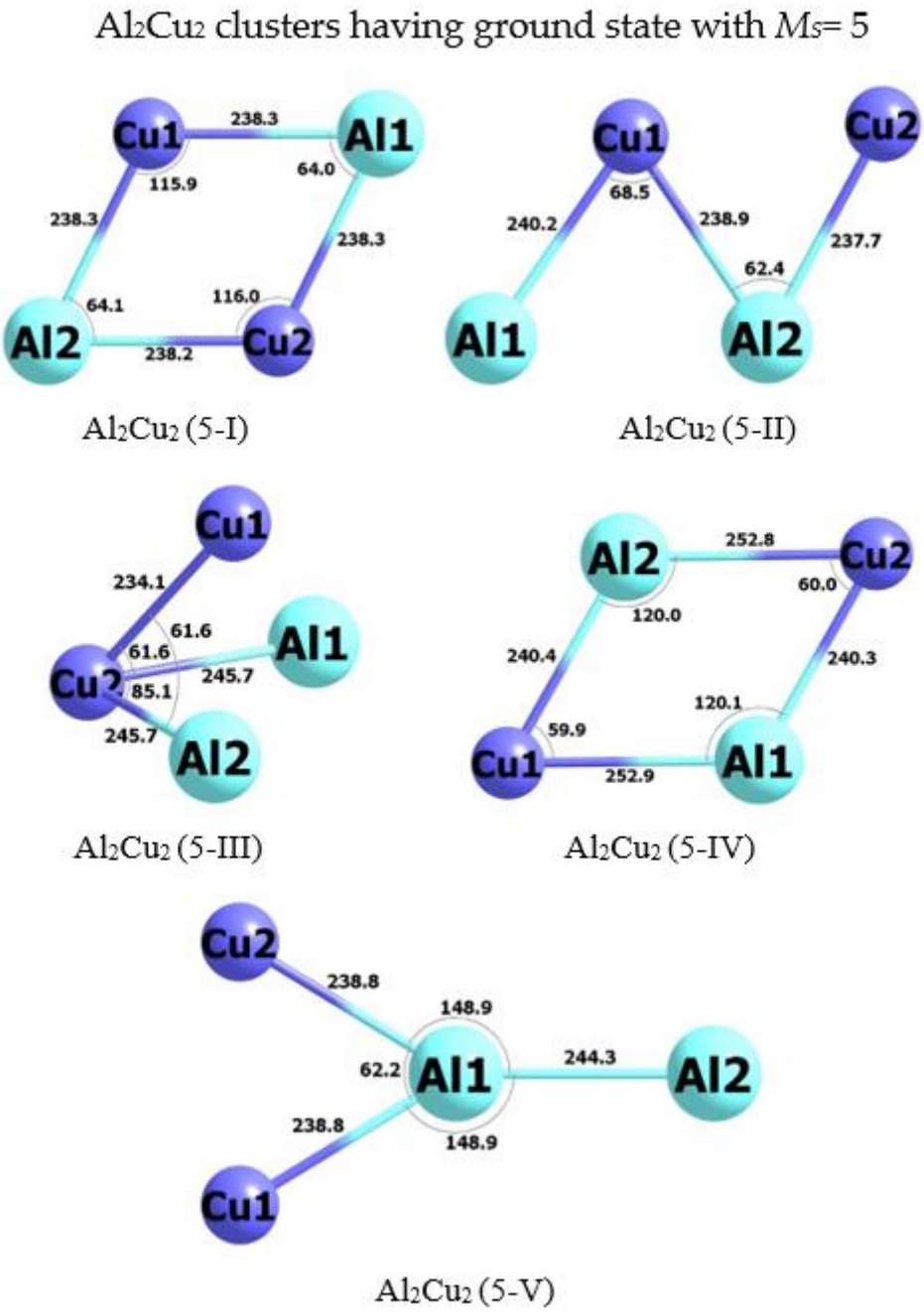


Figure S9. Molecular structures of Al_2Cu_2 metal clusters.

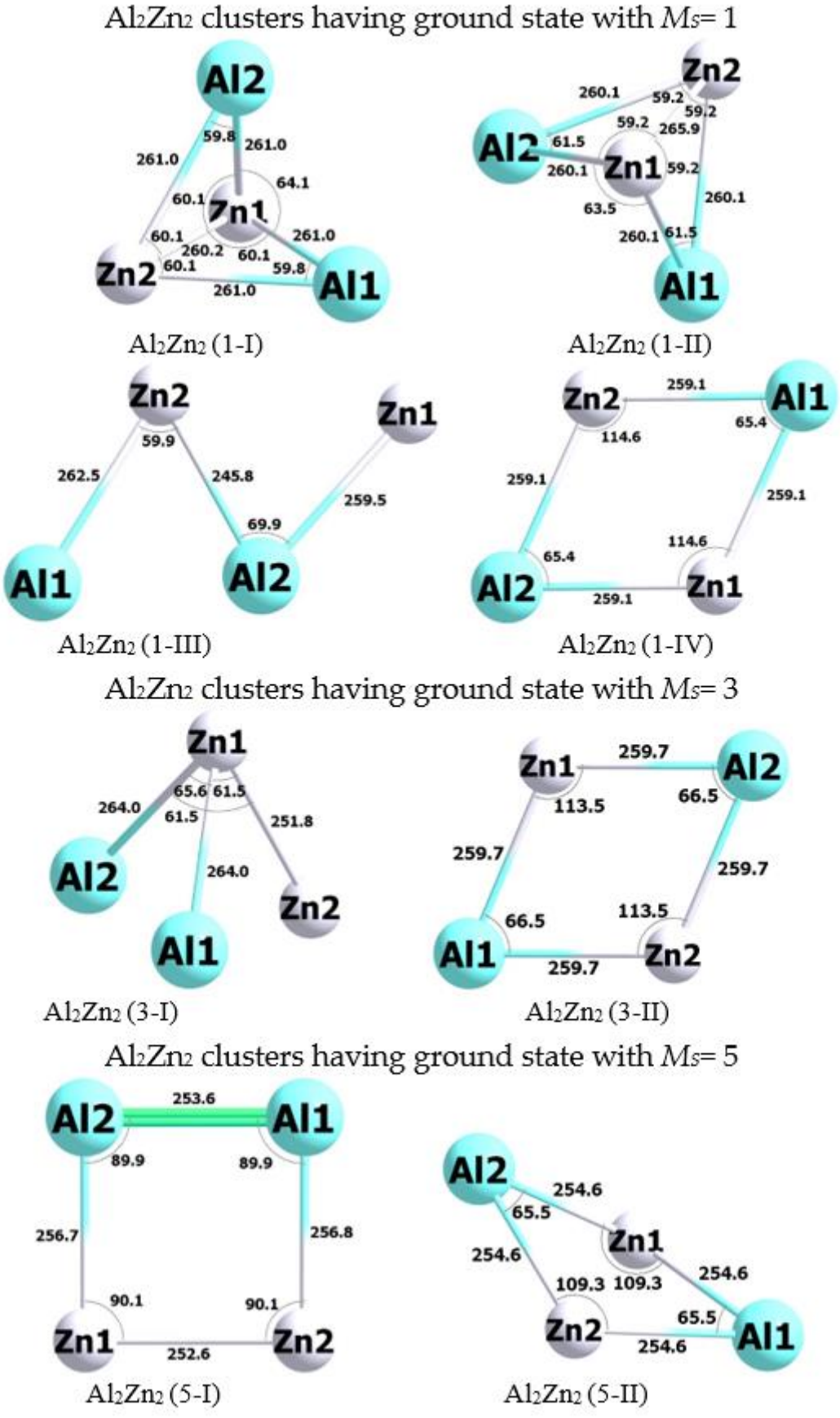


Figure S10. Molecular structures of Al_2Zn_2 metal clusters.

Table S1. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Sc_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Metal clusters with M_S= 3	
Al_2Sc_2 (1-I)*	15.0	**Al_2Sc_2 (3-I)**	**0.0**
Al_2Sc_2 (1-II)*	18.7	Metal clusters with M_S= 5	
Al_2Sc_2 (1-III)	46.5	Al2Sc2 (5-I)	18.6
Al_2Sc_2 (1-IV)	51.9	Al2Sc2 (5-II)	59.4

Table S2. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Ti_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Al_2Ti_2 (1-VIII)	105.0
Al_2Ti_2 (1-I)*	17.3	Metal clusters with M_S= 3	
Al_2Ti_2 (1-II)*	39.5	**Al_2Ti_2 (3-I)**	**0.0**
Al_2Ti_2 (1-III)	40.1	Al_2Ti_2 (3-II)	41.6
Al_2Ti_2 (1-IV)*	46.0	Metal clusters with M_S= 5	
Al_2Ti_2 (1-V)*	50.0	Al_2Ti_2 (5-I)	5.7
Al_2Ti_2 (1-VI)	55.2	Al_2Ti_2 (5-II)	12.7
Al_2Ti_2 (1-VII)*	90.9	Al_2Ti_2 (5-III)	14.4

Table S3. Relative energies and spin multiplicities of the ground states of various isomers of Al_2V_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Metal clusters with M_S= 3	
Al_2V_2 (1-I)*	2.7	**Al_2V_2 (3-I)**	**0.0**
Al_2V_2 (1-II)*	9.7	Al_2V_2 (3-II)	40.2
Al_2V_2 (1-III)*	13.9	Al_2V_2 (3-III)	112.5
Al_2V_2 (1-IV)*	17.0	Metal clusters with M_S= 5	
Al_2V_2 (1-V)	27.9	Al_2V_2 (5-I)	41.0
Al_2V_2 (1-VI)	33.9	Al_2V_2 (5-II)	61.5
Al_2V_2 (1-VII)*	38.1	Al_2V_2 (5-III)	100.8
Al_2V_2 (1-VIII)	42.6		

Table S4. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Cr_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Al_2Cr_2 (3-II)	63.7
Al_2Cr_2 (1-I)*	**0.0**	Al_2Cr_2 (3-III)	87.6
Al_2Cr_2 (1-II)	117.2	Metal clusters with M_S= 5	
Al_2Cr_2 (1-III)	213.7	Al_2Cr_2 (5-I)	172.1
Metal clusters with M_S= 3		Al_2Cr_2 (5-II)	180.1
Al_2Cr_2 (3-I)	32.7	Al_2Cr_2 (5-III)	192.6

Table S5. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Mn_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Al_2Mn_2 (3-III)	163.1
Al_2Mn_2 (1-I)*	**0.0**	Metal clusters with M_S= 5	
Al_2Mn_2 (1-II)*	152.5	Al_2Mn_2 (5-I)	140.6
Al_2Mn_2 (1-III)*	190.8	Al_2Mn_2 (5-II)	145.0
Al_2Mn_2 (1-IV)*	197.7	Al_2Mn_2 (5-III)	145.4
Al_2Mn_2 (1-V)	216.5	Al_2Mn_2 (5-IV)	151.8
Al_2Mn_2 (1-VI)*	250.3	Al_2Mn_2 (5-V)	161.9
Al_2Mn_2 (1-VII)*	307.4	Al_2Mn_2 (5-VI)	207.0
Al_2Mn_2 (1-VIII)	315.2	Al_2Mn_2 (5-VII)	214.3
Metal clusters with M_S= 3		Metal clusters with M_S= 7	
Al_2Mn_2 (3-I)	29.1	Al_2Mn_2 (7-I)	52.7
Al_2Mn_2 (3-II)	163.0	Al_2Mn_2 (7-II)	192.5

Table S6. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Fe_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Al_2Fe_2 (3-II)	69.2
Al_2Fe_2 (1-I)*	48.7	Al_2Fe_2 (3-III)	143.8
Al_2Fe_2 (1-II)*	49.8	Al_2Fe_2 (3-IV)	147.3
Al_2Fe_2 (1-III)*	136.3	Al_2Fe_2 (3-V)	198.5
Al_2Fe_2 (1-IV)*	142.4	Al_2Fe_2 (3-VI)	236.3
Al_2Fe_2 (1-V)*	155.0	Metal clusters with M_S= 5	
Al_2Fe_2 (1-VI)	196.6	**Al_2Fe_2 (5-I)**	**0.0**
Al_2Fe_2 (1-VII)*	236.3	Al_2Fe_2 (5-II)	9.9
Al_2Fe_2 (1-VIII)*	245.5	Al_2Fe_2 (5-III)	53.5
Al_2Fe_2 (1-IX)	261.7	Al_2Fe_2 (5-IV)	55.2
Al_2Fe_2 (1-X)	307.0	Al_2Fe_2 (5-V)	70.6
Metal clusters with M_S= 3		Al_2Fe_2 (5-VI)	254.8
Al_2Fe_2 (3-I)	61.3		

Table S7. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Co_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Al_2Co_2 (1-XIII)*	173.1
Al_2Co_2 (1-I)*	72.7	Al_2Co_2 (1-XIV)	241.2
Al_2Co_2 (1-II)*	75.4	Metal clusters with M_S= 3	
Al_2Co_2 (1-III)*	81.4	Al_2Co_2 (3-I)	26.3
Al_2Co_2 (1-IV)*	85.8	Al_2Co_2 (3-II)	103.8
Al_2Co_2 (1-V)*	135.2	Metal clusters with M_S= 5	
Al_2Co_2 (1-VI)	139.2	**Al_2Co_2 (5-I)**	**0.0**
Al_2Co_2 (1-VII)*	141.0	Metal clusters with M_S= 7	
Al_2Co_2 (1-VIII)	146.7	Al_2Co_2 (7-I)	103.8
Al_2Co_2 (1-IX)*	148.4	Al_2Co_2 (7-II)	116.5
Al_2Co_2 (1-X)	167.1	Al_2Co_2 (7-III)	158.7
Al_2Co_2 (1-XI)	168.4	Al_2Co_2 (7-IV)	162.0
Al_2Co_2 (1-XII)	168.5		

Table S8. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Ni_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Al_2Ni_2 (3-II)	25.2
Al_2Ni_2 (1-I)	**0.0**	Metal clusters with M_S= 5	
Al_2Ni_2 (1-II)*	90.5	Al_2Ni_2 (5-I)	118.6
Metal clusters with M_S= 3		Al_2Ni_2 (5-II)	190.1
Al_2Ni_2 (3-I)	12.8		

Table S9. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Cu_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Al_2Cu_2 (3-IV)	127.5
Al_2Cu_2 (1-I)	**0.0**	Metal clusters with M_S= 5	
Al_2Cu_2 (1-II)*	114.6	Al_2Cu_2 (5-I)	215.3
Al_2Cu_2 (1-III)	115.7	Al_2Cu_2 (5-II)	229.0
Metal clusters with M_S= 3		Al_2Cu_2 (5-III)	245.4
Al_2Cu_2 (3-I)	79.3	Al_2Cu_2 (5-IV)	260.7
Al_2Cu_2 (3-II)	85.8	Al_2Cu_2 (5-V)	274.6
Al_2Cu_2 (3-III)	105.7		

Table S10. Relative energies and spin multiplicities of the ground states of various isomers of Al_2Zn_2 metal clusters.

Structure Designation	Relative Energy, kJ/mol	Structure Designation	Relative Energy, kJ/mol
Metal clusters with M_S= 1		Metal clusters with M_S= 3	
		Al_2Zn_2 (3-I)	16.3
Al_2Zn_2 (1-I)*	**0.0**	Al_2Zn_2 (3-II)	47.4
Al_2Zn_2 (1-II)	3.5	Metal clusters with M_S= 5	
Al_2Zn_2 (1-III)	45.4	Al_2Zn_2 (5-I)	82.0
Al_2Zn_2 (1-IV)*	60.9	Al_2Zn_2 (5-II)	151.3

Table S11. The values of energies (are given in eV) of highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals, and values of gap. The symbol "a" corresponds to electron with spin (+1/2), "b", to electron with spin (–l/2).

Cluster	HOMO (a)	LUMO (a)	Δ (a)	HOMO (b)	LUMO (b)	Δ (b)
			Al_2Sc_2			
Al_2Sc_2 (1-I)*	-3.443	-2.766	*0.677*	-3.384	-2.691	*0.693*
Al_2Sc_2 (1-II)*	-3.397	-2.773	*0.624*	-3.398	-2.773	*0.625*
Al_2Sc_2 (1-III)	-3.173	-3.098	*0.075*	-3.173	-3.098	*0.075*
Al_2Sc_2 (1-IV)	-3.159	-3.191	*-0.032*	-3.159	-3.191	*-0.032*
Al_2Sc_2 (3-I)	**-3.479**	**-2.842**	***0.637***	**-3.534**	**-2.617**	***0.917***
Al_2Sc_2 (5-1)	-3.321	-2.669	*0.652*	-3.839	-3.036	*0.802*
Al_2Sc_2 (5-2)	-3.303	-2.678	*0.625*	-3.386	-3.177	*0.209*
			Al_2Ti_2			
Al_2Ti_2 (1-I)*	-4.110	-3.369	*0.742*	-4.171	-3.248	*0.923*
Al_2Ti_2 (1-II)*	-3.830	-3.347	*0.482*	-3.830	-3.347	*0.482*
Al_2Ti_2 (1-III)	-3.830	-3.342	*0.488*	-3.830	-3.342	*0.488*
Al_2Ti_2 (1-IV)*	-3.793	-3.334	*0.459*	-3.793	-3.334	*0.459*
Al_2Ti_2 (1-V)*	-3.743	-3.240	*0.503*	-3.743	-3.240	*0.503*

Cluster	HOMO (a)	LUMO (a)	Δ (a)	HOMO (b)	LUMO (b)	Δ (b)
Al_2Ti_2 (1-VI)	-3.766	-3.495	*0.271*	-3.766	-3.495	*0.271*
Al_2Ti_2 (1-VII)*	-3.855	-3.045	*0.811*	-3.983	-3.278	*0.705*
Al_2Ti_2 (1-VIII)	-3.361	-3.071	*0.290*	-3.361	-3.071	*0.290*
Al_2Ti_2 (3-I)	**-4.212**	**-3.395**	***0.817***	**-3.998**	**-3.080**	***0.918***
Al_2Ti_2 (3-II)	-3.486	-3.238	*0.247*	-3.499	-2.582	*0.917*
Al_2Ti_2 (5-I)	-3.819	-3.433	*0.387*	-4.035	-3.318	*0.717*
Al_2Ti_2 (5-II)	-3.648	-3.364	*0.284*	-3.897	-3.049	*0.848*
Al_2Ti_2 (5-III)	-3.654	-3.482	*0.173*	-3.914	-3.116	*0.799*
			Al_2V_2			
Al_2V_2 (1-I)*	-3.854	-3.015	*0.839*	-3.854	-3.015	*0.839*
Al_2V_2 (1-II)*	-4.074	-3.557	*0.516*	-4.074	-3.557	*0.516*
Al_2V_2 (1-III)*	-3.897	-3.444	*0.453*	-3.897	-3.444	*0.453*
Al_2V_2 (1-IV)*	-4.050	-3.722	*0.328*	-4.114	-3.687	*0.427*
Al_2V_2 (1-V)	-3.857	-3.570	*0.287*	-3.857	-3.570	*0.287*
Al_2V_2 (1-VI)	-4.201	-3.984	*0.218*	-4.201	-3.984	*0.218*
Al_2V_2 (1-VII)*	-3.915	-3.287	*0.628*	-4.140	-2.957	*1.183*
Al_2V_2 (1-VIII)	-3.858	-3.250	*0.608*	-3.858	-3.250	*0.608*
Al_2V_2 (3-I)	**-4.157**	**-2.992**	***1.165***	**-4.010**	**-3.524**	***0.486***
Al_2V_2 (3-II)	-3.896	-3.033	*0.864*	-4.041	-3.285	*0.756*
Al_2V_2 (3-III)	-3.997	-3.814	*0.183*	-4.100	-3.661	*0.438*
Al_2V_2 (5-I)	-3.471	-2.585	*0.886*	-4.058	-3.241	*0.817*
Al_2V_2 (5-II)	-4.043	-3.151	*0.892*	-4.074	-3.654	*0.421*
Al_2V_2 (5-III)	-3.413	-2.834	*0.579*	-4.152	-3.689	*0.463*
			Al_2Cr_2			
Al_2Cr_2 (1-I)*	**-3.831**	**-3.143**	***0.688***	**-3.831**	**-3.143**	***0.688***
Al_2Cr_2 (1-II)	-4.336	-3.480	*0.856*	-4.336	-3.480	*0.856*
Al_2Cr_2 (1-III)	-4.107	-3.281	*0.826*	-4.107	-3.281	*0.826*
Al_2Cr_2 (3-I)	-3.459	-2.607	*0.852*	-4.622	-3.489	*1.133*
Al_2Cr_2 (3-II)	-3.817	-2.923	*0.894*	-4.453	-2.836	*1.618*
Al_2Cr_2 (3-III)	-3.614	-2.743	*0.870*	-4.379	-2.971	*1.408*
Al_2Cr_2 (5-I)	-3.593	-2.821	*0.772*	-4.316	-3.443	*0.873*
Al_2Cr_2 (5-II)	-3.409	-2.779	*0.630*	-4.747	-4.119	*0.628*
Al_2Cr_2 (5-III)	-3.576	-2.716	*0.860*	-4.536	-3.612	*0.925*
			Al_2Mn_2			
Al_2Mn_2 (1-I)*	**-3.708**	**-2.952**	***0.756***	**-3.708**	**-2.952**	***0.756***
Al_2Mn_2 (1-II)*	-3.929	-3.506	*0.423*	-3.598	-3.101	*0.498*
Al_2Mn_2 (1-III)*	-4.342	-3.389	*0.953*	-4.342	-3.389	*0.953*
Al_2Mn_2 (1-IV)*	-4.202	-3.665	*0.537*	-4.409	-3.161	*1.248*
Al_2Mn_2 (1-V)	-4.020	-3.815	*0.205*	-4.020	-3.815	*0.205*
Al_2Mn_2 (1-VI)*	-3.587	-2.601	*0.986*	-3.991	-3.849	*0.142*
Al_2Mn_2 (1-VII)*	-3.744	-3.588	*0.156*	-3.744	-3.587	*0.157*
Al_2Mn_2 (1-VIII)	-3.494	-3.338	*0.156*	-3.494	-3.338	*0.156*
Al_2Mn_2 (3-I)	-3.558	-3.136	*0.422*	-4.495	-3.441	*1.054*
Al_2Mn_2 (3-II)	-4.522	-3.620	*0.902*	-4.250	-3.344	*0.906*
Al_2Mn_2 (3-III)	-4.522	-3.619	*0.903*	-4.251	-3.344	*0.906*
Al_2Mn_2 (5-I)	-3.448	-3.273	*0.176*	-5.023	-3.710	*1.312*
Al_2Mn_2 (5-II)	-4.332	-4.143	*0.189*	-4.193	-3.307	*0.886*

Cluster	HOMO (a)	LUMO (a)	Δ (a)	HOMO (b)	LUMO (b)	Δ (b)
Al_2Mn_2 (5-III)	-4.317	-4.147	*0.171*	-4.237	-3.323	*0.913*
Al_2Mn_2 (5-IV)	-4.550	-3.927	*0.623*	-3.729	-2.854	*0.875*
Al_2Mn_2 (5-V)	-3.517	-2.615	*0.902*	-4.893	-3.594	*1.298*
Al_2Mn_2 (5-VI)	-4.244	-3.760	*0.484*	-3.713	-2.688	*1.025*
Al_2Mn_2 (5-VII)	-4.776	-3.948	*0.828*	-3.241	-2.677	*0.564*
Al_2Mn_2 (7-I)	-4.797	-3.776	*1.021*	-3.751	-3.013	*0.738*
Al_2Mn_2 (7-II)	-4.859	-3.609	*1.250*	-3.519	-3.030	*0.490*
			Al_2Fe_2			
Al_2Fe_2 (1-I)*	-3.897	-3.292	*0.604*	-3.897	-3.292	*0.604*
Al_2Fe_2 (1-II)*	-3.891	-3.256	*0.634*	-3.891	-3.256	*0.634*
Al_2Fe_2 (1-III)*	-3.488	-3.210	*0.277*	-3.940	-3.373	*0.567*
Al_2Fe_2 (1-IV)*	-4.532	-3.741	*0.792*	-4.532	-3.741	*0.792*
Al_2Fe_2 (1-V)*	-4.095	-2.981	*1.114*	-4.249	-3.629	*0.620*
Al_2Fe_2 (1-VI)	-4.011	-4.086	*-0.075*	-4.011	-4.086	*-0.075*
Al_2Fe_2 (1-VII)*	-4.073	-3.369	*0.704*	-4.074	-3.370	*0.703*
Al_2Fe_2 (1-VIII)*	-3.969	-3.408	*0.561*	-3.969	-3.408	*0.561*
Al_2Fe_2 (1-IX)	-3.631	-4.357	*-0.727*	-3.631	-4.357	*-0.727*
Al_2Fe_2 (1-X)	-3.516	-3.625	*-0.110*	-3.516	-3.625	*-0.110*
Al_2Fe_2 (3-I)	-4.651	-3.698	*0.953*	-3.761	-2.602	*1.159*
Al_2Fe_2 (3-II)	-4.385	-3.604	*0.781*	-3.972	-3.369	*0.604*
Al_2Fe_2 (3-III)	-3.946	-3.030	*0.916*	-4.067	-3.092	*0.975*
Al_2Fe_2 (3-IV)	-3.663	-3.356	*0.307*	-4.290	-3.546	*0.744*
Al_2Fe_2 (3-V)	-4.163	-3.342	*0.821*	-3.644	-3.191	*0.453*
Al_2Fe_2 (3-VI)	-4.410	-3.456	*0.954*	-3.122	-2.764	*0.358*
Al_2Fe_2 (5-I)	**-4.843**	**-3.723**	***1.120***	**-3.825**	**-3.555**	***0.270***
Al_2Fe_2 (5-II)	-4.737	-3.706	*1.031*	-3.720	-3.651	*0.070*
Al_2Fe_2 (5-III)	-4.198	-4.054	*0.144*	-3.961	-3.512	*0.449*
Al_2Fe_2 (5-IV)	-4.720	-3.141	*1.580*	-3.568	-2.874	*0.695*
Al_2Fe_2 (5-V)	-4.686	-3.056	*1.629*	-3.251	-2.937	*0.315*
Al_2Fe_2 (5-VI)	-3.597	-2.957	*0.640*	-4.313	-3.927	*0.386*
			Al_2Co_2			
Al_2Co_2 (1-I)*	-4.374	-3.825	*0.550*	-4.313	-3.707	*0.606*
Al_2Co_2 (1-II)*	-4.304	-3.782	*0.523*	-4.304	-3.782	*0.522*
Al_2Co_2 (1-III)*	-4.473	-3.853	*0.621*	-4.421	-3.950	*0.470*
Al_2Co_2 (1-IV)*	-4.217	-3.660	*0.557*	-3.882	-3.406	*0.476*
Al_2Co_2 (1-V)*	-3.902	-3.134	*0.768*	-3.990	-3.224	*0.767*
Al_2Co_2 (1-VI)	-3.599	-3.546	*0.053*	-3.599	-3.546	*0.053*
Al_2Co_2 (1-VII)*	-3.912	-3.327	*0.585*	-4.011	-3.212	*0.799*
Al_2Co_2 (1-VIII)	-4.207	-4.644	*-0.437*	-4.207	-4.644	*-0.437*
Al_2Co_2 (1-IX)*	-3.944	-3.155	*0.789*	-3.962	-3.444	*0.518*
Al_2Co_2 (1-X)	-4.050	-4.702	*-0.652*	-4.050	-4.702	*-0.652*
Al_2Co_2 (1-XI)	-4.159	-4.872	*-0.713*	-4.159	-4.872	*-0.713*
Al_2Co_2 (1-XII)	-4.159	-4.872	*-0.713*	-4.159	-4.872	*-0.713*
Al_2Co_2 (1-XIII)*	-3.910	-3.477	*0.432*	-3.909	-3.477	*0.432*
Al_2Co_2 (1-XIV)	-3.782	-4.208	*-0.426*	-3.782	-4.208	*-0.426*
Al_2Co_2 (3-I)	-4.586	-3.822	*0.764*	-3.872	-3.394	*0.478*
Al_2Co_2 (3-II)	-4.672	-3.079	*1.593*	-3.639	-3.151	*0.488*

Cluster	HOMO (a)	LUMO (a)	Δ (a)	HOMO (b)	LUMO (b)	Δ (b)
Al_2Co_2 (5-I)	**-4.544**	**-3.052**	***1.492***	**-4.691**	**-4.009**	***0.682***
Al_2Co_2 (7-I)	-3.659	-2.690	*0.969*	-4.715	-4.285	*0.430*
Al_2Co_2 (7-II)	-3.693	-2.551	*1.142*	-4.692	-4.439	*0.253*
Al_2Co_2 (7-III)	-4.039	-3.096	*0.943*	-4.796	-4.263	*0.533*
Al_2Co_2 (7-IV)	-4.041	-3.020	*1.021*	-4.734	-4.206	*0.528*
			Al_2Ni_2			
Al_2Ni_2 (1-I)	**-4.456**	**-3.767**	***0.689***	**-4.456**	**-3.767**	***0.689***
Al_2Ni_2 (1-II)*	-3.859	-3.244	*0.615*	-3.859	-3.244	*0.615*
Al_2Ni_2 (3-I)	-4.274	-3.045	*1.229*	-4.390	-3.819	*0.571*
Al_2Ni_2 (3-II)	-4.530	-3.097	*1.433*	-4.689	-4.438	*0.251*
Al_2Ni_2 (5-I)	-3.549	-2.426	*1.123*	-4.539	-4.236	*0.303*
Al_2Ni_2 (5-II)	-3.858	-3.013	*0.845*	-4.494	-4.259	*0.235*
			Al_2Cu_2			
Al_2Cu_2 (1-I)	**-4.586**	**-3.311**	***1.275***	**-4.586**	**-3.311**	***1.275***
Al_2Cu_2 (1-II)*	-4.182	-3.345	*0.838*	-4.182	-3.345	*0.838*
Al_2Cu_2 (1-III)	-4.165	-3.440	*0.725*	-4.165	-3.440	*0.725*
Al_2Cu_2 (3-I)	-3.603	-2.612	*0.992*	-5.222	-3.268	*1.954*
Al_2Cu_2 (3-II)	-3.650	-2.445	*1.205*	-5.105	-4.204	*0.901*
Al_2Cu_2 (3-III)	-4.001	-3.023	*0.978*	-4.954	-3.245	*1.709*
Al_2Cu_2 (3-IV)	-3.888	-2.720	*1.168*	-4.775	-3.449	*1.326*
Al_2Cu_2 (5-I)	-3.922	-2.831	*1.090*	-6.006	-3.816	*2.190*
Al_2Cu_2 (5-II)	-3.601	-2.558	*1.043*	-5.662	-4.192	*1.470*
Al_2Cu_2 (5-III)	-3.317	-3.000	*0.318*	-5.610	-4.080	*1.529*
Al_2Cu_2 (5-IV)	-3.673	-3.070	*0.602*	-5.751	-4.984	*0.767*
Al_2Cu_2 (5-V)	-3.377	-2.977	*0.400*	-5.930	-3.598	*2.333*
			Al_2Mn_2			
Al_2Zn_2 (1-I)*	**-3.718**	**-2.805**	***0.913***	**-3.718**	**-2.805**	***0.913***
Al_2Zn_2 (1-II)	-3.618	-2.939	*0.680*	-3.618	-2.939	*0.680*
Al_2Zn_2 (1-III)	-3.837	-3.410	*0.427*	-3.837	-3.410	*0.427*
Al_2Zn_2 (1-IV)*	-4.020	-3.319	*0.701*	-4.020	-3.319	*0.701*
Al_2Zn_2 (3-I)	-3.403	-2.876	*0.527*	-5.824	-3.012	*2.812*
Al_2Zn_2 (3-II)	-4.045	-2.950	*1.096*	-4.926	-3.192	*1.734*
Al_2Zn_2 (5-I)	-4.164	-2.333	*1.832*	-6.359	-3.380	*2.978*
Al_2Zn_2 (5-II)	-3.667	-2.847	*0.821*	-5.593	-3.914	*1.679*