Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Material

Theoretical Design of Stable Small Aluminum-Magnesium Binary Clusters

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Neutral Systems: Cartesians coordinates and relative energies

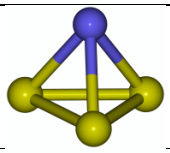
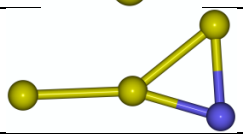
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{2v}		Al 0.000000000 0.000000000 1.616831000 Mg 0.000000000 1.789202000 -0.583856000 Mg 1.549495000 -0.894601000 -0.583856000 Mg -1.549495000 -0.894601000 -0.583856000			-840.909836	0.0
C_s		Al 1.886702000 -1.479443000 0.000000000 Mg -0.677724000 -2.555202000 0.000000000 Mg -1.366204000 3.593979000 0.000000000 Mg 0.000000000 0.563953000 0.000000000			-840.886530	14.6

Figure 1. Lowest energy isomers for $AlMg_3$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

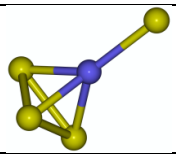
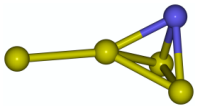
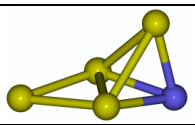
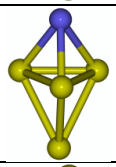
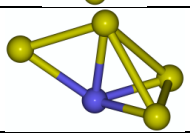
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{3v}		Al 0.000000000 0.000000000 0.695174000 Mg 0.000000000 1.761383000 -1.530805000 Mg -1.525402000 -0.880692000 -1.530805000 Mg 0.000000000 0.000000000 3.839311000 Mg 1.525402000 -0.880692000 -1.530805000			-1040.5576380	0.0
C_s		Al 1.695699000 -1.423428000 0.000000000 Mg -0.628634000 -1.744488000 1.544659000 Mg -0.628634000 4.148305000 0.000000000 Mg -0.628634000 -1.744488000 -1.544659000 Mg 0.048895000 0.882719000 0.000000000			-1040.5533193	2.7
C_s		Al 2.055569000 0.739319000 0.000000000 Mg -0.064068000 -0.448192000 1.598871000 Mg -0.064068000 2.424016000 0.000000000 Mg -0.064068000 -0.448192000 -1.598871000 Mg -2.034663000 -2.328560000 0.000000000			-1040.5530661	2.9
C_s		Al 2.385781000 0.156174000 0.000000000 Mg 0.056725000 1.765089000 0.000000000 Mg 0.056725000 -1.066184000 1.479797000 Mg -2.754769000 0.198092000 0.000000000 Mg 0.056725000 -1.066184000 -1.479797000			-1040.5514514	3.9
C_s		Al -1.115616000 -0.174305000 0.000000000 Mg -0.184033000 1.978239000 1.526124000 Mg 1.760682000 -0.668795000 0.000000000 Mg -0.184033000 -3.098853000 0.000000000 Mg -0.184033000 1.978239000 -1.526124000			-1040.5511481	4.1

Figure 2. Lowest energy isomers for $AlMg_4$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

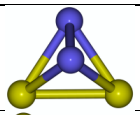
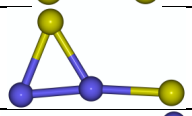
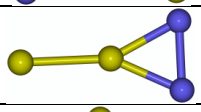
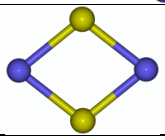
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{2v}		Al 0.000000000 1.334998000 -0.927331000 Al 0.000000000 -1.334998000 -0.927331000 Mg -1.547742000 0.000000000 1.004608000 Mg 1.547742000 0.000000000 1.004608000			-883.2480791	0.0
C_s		Al 0.000000000 0.561553000 0.000000000 Al -2.190935000 -0.598222000 0.000000000 Mg 2.301547000 2.216087000 0.000000000 Mg 0.071966000 -2.176363000 0.000000000			-883.2248378	14.6
C_{2v}		Al -1.225839130 0.000000000 1.910114525 Al 1.225839130 0.000000000 1.910114525 Mg 0.000000000 0.000000000 -3.740781454 Mg 0.000000000 0.000000000 -0.556715016			-883.2161035	20.1
D_{2h}		Al 0.000000000 0.000000000 2.297534000 Al 0.000000000 0.000000000 -2.297534000 Mg 0.000000000 1.842998000 0.000000000 Mg 0.000000000 -1.842998000 0.000000000			-883.2021853	28.8

Figure 3. Lowest energy isomers for Al_2Mg_2 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

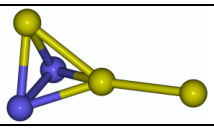
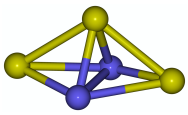
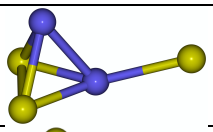
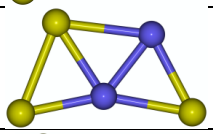
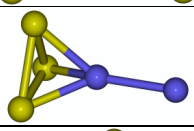
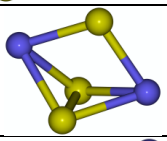
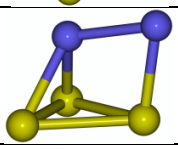
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al 0.539180000 -1.631006000 1.321245000 Al 0.539180000 -1.631006000 -1.321245000 Mg 0.539180000 4.134508000 0.000000000 Mg -1.915678000 -1.442216000 0.000000000 Mg 0.208274000 0.841554000 0.000000000			-1082.8932590	0.0
C_2		Al 0.000000000 1.422847000 -0.604767000 Al 0.000000000 -1.422847000 -0.604767000 Mg 2.700084000 0.536943000 -0.251825000 Mg 0.000000000 0.000000000 1.813978000 Mg -2.700084000 -0.536943000 -0.251825000			-1082.8927806	0.3
C_s		Al -1.777487000 -0.733480000 0.000000000 Al 0.677393000 0.565636000 0.000000000 Mg 0.397256000 3.707069000 0.000000000 Mg 0.397256000 -1.762620000 1.514312000 Mg 0.397256000 -1.762620000 -1.514312000			-1082.8915578	1.1
C_s		Al 0.000000000 0.678766000 0.000000000 Al 1.361733000 -1.465729000 0.000000000 Mg 2.913279000 0.923528000 0.000000000 Mg -1.758852000 -1.548091000 0.000000000 Mg -2.629637000 1.477106000 0.000000000			-1082.8871296	3.8
C_{3v}		Al 0.000000000 0.000000000 3.573304000 Al 0.000000000 0.000000000 0.724020000 Mg 0.000000000 1.717146000 -1.551812000 Mg -1.487092000 -0.858573000 -1.551812000 Mg 1.487092000 -0.858573000 -1.551812000			-1082.8859072	4.6
C_{2v}		Al 0.000000000 2.224155000 0.188701000 Al 0.000000000 -2.224155000 0.188701000 Mg -1.420427000 0.000000000 -1.190008000 Mg 1.420427000 0.000000000 -1.190008000 Mg 0.000000000 0.000000000 1.950709000			-1082.8853482	5.0
C_s		Al 2.564316000 -0.588085000 0.000000000 Al -0.109317000 -1.370611000 0.000000000 Mg -1.832148000 0.293501000 -1.468080000 Mg 0.901948000 1.626477000 0.000000000 Mg -1.832148000 0.293501000 1.468080000			-1082.8848651	5.3

Figure 4. Lowest energy isomers for Al_2Mg_3 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

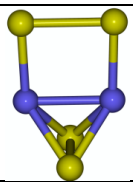
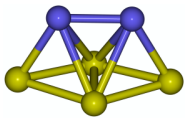
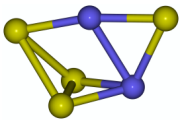
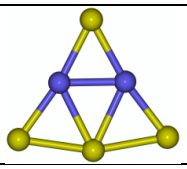
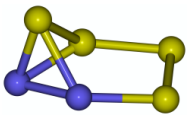
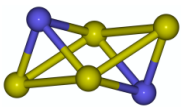
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{2v}		Al 0.000000000 1.459154000 -0.296288000 Al 0.000000000 -1.459154000 -0.296288000 Mg 1.462375000 0.000000000 -2.193220000 Mg -1.462375000 0.000000000 -2.193220000 Mg 0.000000000 -1.568979000 2.514198000 Mg 0.000000000 1.568979000 2.514198000			-1282.5648019	0.0
C_{2v}		Al 0.000000000 1.282809000 1.655708000 Al 0.000000000 -1.282809000 1.655708000 Mg 0.000000000 -2.672927000 -0.837552000 Mg -1.402903000 0.000000000 -0.956132000 Mg 0.000000000 2.672927000 -0.837552000 Mg 1.402903000 0.000000000 -0.956132000			-1282.5630678	1.1
C_s		Al -1.763437000 -0.616841000 0.000000000 Al 0.419757000 1.412067000 0.000000000 Mg 0.419757000 -1.599616000 1.419265000 Mg -2.198814000 2.260190000 0.000000000 Mg 0.419757000 -1.599616000 -1.419265000 Mg 2.814954000 0.077547000 0.000000000			-1282.5622203	1.6
C_{2v}		Al 0.000000000 1.298965000 0.756543000 Al 0.000000000 -1.298965000 0.756543000 Mg 0.000000000 0.000000000 3.222213000 Mg 0.000000000 2.937361000 -1.463671000 Mg 0.000000000 0.000000000 -1.934047000 Mg 0.000000000 -2.937361000 -1.463671000			-1282.5598666	3.1
C_1		Al 2.207632000 -0.373973000 -1.115227000 Al 0.635523000 1.531048000 -0.311474000 Mg -2.205563000 1.752591000 0.030412000 Mg -0.046438000 -1.686608000 -0.145780000 Mg -2.961804000 -1.264408000 0.118162000 Mg 2.133720000 -0.055072000 1.542799000			-1282.5589133	3.7
C_{2h}		Al 0.000000000 2.307250000 0.000000000 Al 0.000000000 -2.307250000 0.000000000 Mg 0.000000000 0.000000000 1.671181000 Mg -2.551689000 -1.372291000 0.000000000 Mg 0.000000000 0.000000000 -1.671181000 Mg 2.551689000 1.372291000 0.000000000			-1282.5573990	4.6

Figure 5. Lowest energy isomers for Al_2Mg_4 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

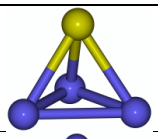
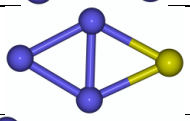
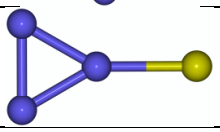
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al -0.774325768 -0.476461551 -1.579684076 Al 0.018304191 1.479691551 0.000000000 Al -0.774325768 -0.476461551 1.579684076 Mg 1.721536124 -0.592578487 0.000000000			-925.5731233	0.0
C_{2v}		Al 1.280754788 0.000000000 0.004375644 Al -1.280754788 0.000000000 0.004375644 Al 0.000000000 0.000000000 -2.302270767 Mg 0.000000000 0.000000000 2.580052593			-925.5663778	4.2
C_{2v}		Al 1.738520073 1.256765000 0.000000000 Al -0.455941927 0.000000000 0.000000000 Al 1.738520073 -1.256765000 0.000000000 Mg -3.398528927 0.000000000 0.000000000			-925.5613916	7.4

Figure 6. Lowest energy isomers for Al_3Mg and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

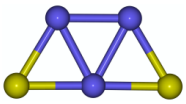
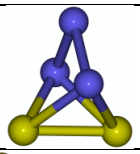
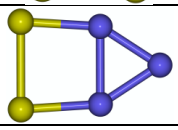
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{2v}		Al 1.283560000 0.000000000 1.402873000 Mg -2.728200000 0.000000000 -1.015253000 Mg 2.728200000 0.000000000 -1.015253000 Al -1.283560000 0.000000000 1.402873000 Al 0.000000000 0.000000000 -0.995838000			-1125.242573	0.0
C_{2v}		Al 2.045930383 0.000000000 -0.232699678 Al 0.000000000 0.000000000 -1.900310337 Al -2.045930383 0.000000000 -0.232699678 Mg 0.000000000 1.415243002 1.330630823 Mg 0.000000000 -1.415243002 1.330630823			-1125.236783	3.6
C_{2v}		Al 0.000000000 0.000000000 2.724387000 Al 0.000000000 1.359391000 0.629508000 Al 0.000000000 -1.359391000 0.629508000 Mg 0.000000000 -1.530843000 -2.157677000 Mg 0.000000000 1.530843000 -2.157677000			-1125.231371	7.0

Figure 7 Lowest energy isomers for Al_3Mg_2 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

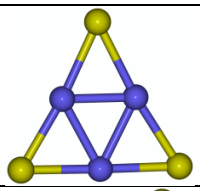
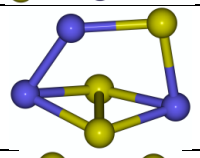
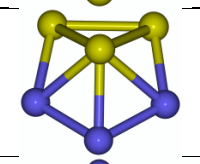
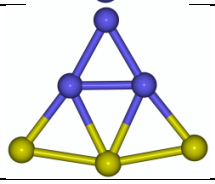
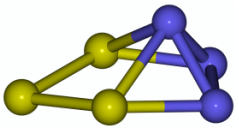
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{2v}		Al 1.259383772 0.000000000 0.770499443 Al 0.000000000 0.000000000 -1.653044051 Al -1.259383772 0.000000000 0.770499443 Mg 0.000000000 0.000000000 3.376187583 Mg 2.717626146 0.000000000 -1.625072217 Mg -2.717626146 0.000000000 -1.625072217			-1324.9053419	0.0
C_s		Al -2.440951000 0.227106000 0.000000000 Al 1.772405000 -1.523928000 0.000000000 Al -0.476877000 1.918768000 0.000000000 Mg -0.476877000 -0.974258000 1.523220000 Mg 2.194629000 1.274742000 0.000000000 Mg -0.476877000 -0.974258000 -1.523220000			-1324.9036416	1.1
C_s		Al 0.149908000 -2.310535000 0.000000000 Al -0.411182000 -0.709735000 1.958267000 Al -0.411182000 -0.709735000 -1.958267000 Mg 1.550860000 0.062720000 0.000000000 Mg -0.411182000 1.989060000 1.532006000 Mg -0.411182000 1.989060000 -1.532006000			-1324.9009437	2.8
C_{2v}		Al 0.000000000 0.000000000 3.007891000 Al 0.000000000 1.275556000 0.746566000 Al 0.000000000 -1.275556000 0.746566000 Mg 0.000000000 -2.984516000 -1.457485000 Mg 0.000000000 0.000000000 -1.961137000 Mg 0.000000000 2.984516000 -1.457485000			-1324.8971414	5.1
C_s		Al -0.180664000 -1.856547000 1.515456000 Al 1.435524000 -0.617794000 0.000000000 Al -0.180664000 -1.856547000 -1.515456000 Mg -0.180664000 0.867494000 2.069053000 Mg -0.802382000 2.956806000 0.000000000 Mg -0.180664000 0.867494000 -2.069053000			-1324.8930353	7.7

Figure 8. Lowest energy isomers for Al_3Mg_3 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

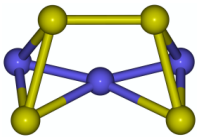
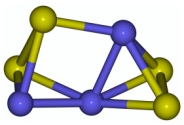
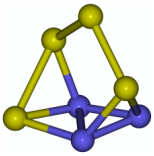
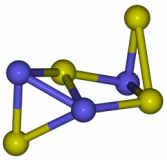
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al -0.686993000 1.087963000 2.543191000 Al -0.686993000 1.087963000 -2.543191000 Al -0.763397000 0.287949000 0.000000000 Mg 1.844741000 0.240502000 -1.585715000 Mg -0.686993000 -1.575101000 -2.413123000 Mg 1.844741000 0.240502000 1.585715000 Mg -0.686993000 -1.575101000 2.413123000			-1524.5720417	0.0
C_1		Al -2.206301000 -0.093059000 1.431355000 Al 0.200989000 -0.827964000 0.643508000 Al 1.022335000 1.323524000 -0.815997000 Mg -1.709116000 1.859346000 -0.706373000 Mg 2.434408000 -1.191069000 -1.120425000 Mg -2.339076000 -1.500176000 -0.889799000 Mg 2.678676000 0.395857000 1.352826000			-1524.5691309	1.8
C_1		Al 1.644610000 -0.068113000 1.202438000 Al 0.530362000 -1.547590000 -1.084569000 Al -0.322814000 -1.831668000 1.343625000 Mg 0.365572000 2.319410000 0.685297000 Mg -2.452683000 1.849779000 -0.214267000 Mg 2.288157000 0.689485000 -1.414763000 Mg -2.207550000 -1.124022000 -0.639551000			-1524.5657611	3.9
C_1		Al -2.502303000 -1.135481000 -0.882478000 Al 2.501198000 -0.005334000 1.437900000 Al -1.283428000 1.177846000 -0.897604000 Mg 1.459964000 1.771988000 -0.505439000 Mg -2.886473000 0.327639000 1.338586000 Mg 0.007657000 -1.051208000 0.583365000 Mg 2.810430000 -1.088537000 -1.045815000			-1524.5619774	6.3

Figure 9. Lowest energy isomers for Al_3Mg_4 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

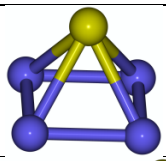
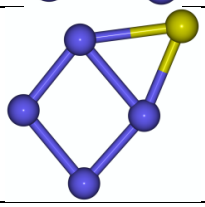
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{4v}		Al 1.334141989 1.334141989 -0.395590331 Al -1.334141989 1.334141989 -0.395590331 Al -1.334141989 -1.334141989 -0.395590331 Al 1.334141989 -1.334141989 -0.395590331 Mg 0.000000000 0.000000000 1.780048294			-1167.5998974	0.0
C_s		Al -1.236293000 -1.775208000 0.000000000 Al -2.364360000 0.560346000 0.000000000 Al 1.158660000 -1.173329000 0.000000000 Al 0.000000000 1.282733000 0.000000000 Mg 2.645493000 1.197579000 0.000000000			-1167.5894059	6.6

Figure 10. Lowest energy isomers for Al_4Mg and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

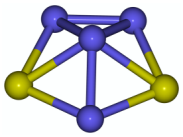
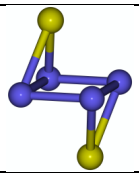
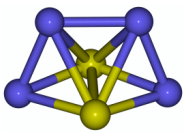
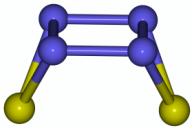
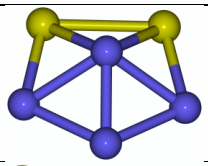
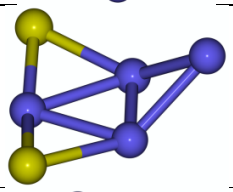
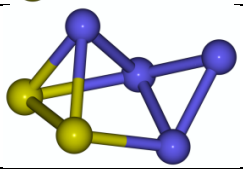
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al -0.308653000 1.853834000 1.252956000 Al 0.014771000 -2.272539000 0.000000000 Al -0.308653000 1.853834000 -1.252956000 Al 1.172356000 0.027215000 0.000000000 Mg -0.308653000 -0.792104000 -2.328295000 Mg -0.308653000 -0.792104000 2.328295000			-1367.2613402	0.0
C_s		Al -0.837291189 -1.002757462 1.377802000 Al 0.837291189 1.002757462 -1.377802000 Al -0.837291189 -1.002757462 -1.377802000 Al 0.837291189 1.002757462 1.377802000 Mg 2.255761944 -1.018074679 0.000000000 Mg -2.255761944 1.018074679 0.000000000			-1367.2610914	0.2
C_s		Al -0.000149000 -1.326030000 1.526489000 Al 0.000149000 -2.223305000 -0.853011000 Mg 1.623273000 0.000097000 -0.729600000 Al -0.000149000 2.223305000 -0.853011000 Al 0.000149000 1.326030000 1.526489000 Mg -1.623273000 -0.000097000 -0.729600000			-1367.2574835	2.4
C_s		Al 1.305515000 1.313283000 -0.733143000 Al -1.305515000 1.313283000 -0.733143000 Mg 0.000000000 -2.281577000 1.588478000 Al 1.305515000 -1.313283000 -0.733143000 Al -1.305515000 -1.313283000 -0.733143000 Mg 0.000000000 2.281577000 1.588478000			-1367.2567981	2.9
C_s		Al -0.000428000 0.072025000 1.043844000 Al -2.198064000 -0.716164000 -0.333411000 Al 0.001879000 -2.224368000 -0.043983000 Al 2.199211000 -0.712917000 -0.332124000 Mg -1.651340000 1.938975000 -0.180309000 Mg 1.648526000 1.940901000 -0.181877000			-1367.2541549	4.5
C_s		Al -0.239969000 0.909590000 1.234348000 Al -0.679419000 -1.532439000 0.000000000 Al 1.602376000 2.509007000 0.000000000 Al -0.239969000 0.909590000 -1.234348000 Mg -0.239969000 -1.514363000 2.674661000 Mg -0.239969000 -1.514363000 -2.674661000			-1367.2534852	4.9
C_1		Al 0.875417000 -0.845710000 1.422875000 Al -1.159116000 1.491773000 -0.662277000 Al -0.606477000 -1.271488000 -0.811339000 Al -2.518726000 -0.393519000 0.471929000 Mg 2.312597000 -0.812705000 -0.854454000 Mg 1.380381000 1.916561000 0.398167000			-1367.2484195	8.1

Figure 11. Lowest energy isomers for Al_4Mg_2 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

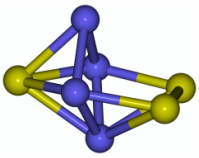
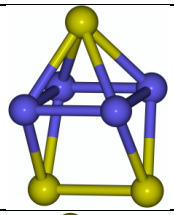
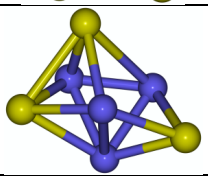
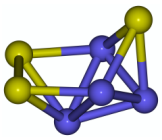
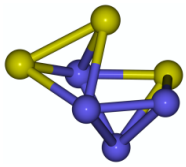
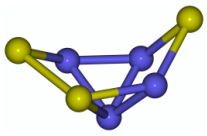
Symetry	Structure	Cartesians Coordinates				E (a.u)	ΔE
C_s		Al	-1.868980000	-0.868706000	0.000000000	-1566.9411262	0.0
		Al	-0.043005000	-0.526418000	1.923656000		
		Al	1.647957000	0.219759000	0.000000000		
		Al	-0.043005000	-0.526418000	-1.923656000		
		Mg	-0.043005000	2.202335000	1.545804000		
		Mg	-0.043005000	2.202335000	-1.545804000		
		Mg	0.418631000	-2.561073000	0.000000000		
C_{2v}		Al	-0.400484000	1.372675000	1.307540000	-1566.9402679	0.5
		Al	-0.421983000	-1.372689000	-1.300781000		
		Al	-0.395759000	-1.366971000	1.313300000		
		Al	-0.425413000	1.367003000	-1.306376000		
		Mg	2.190751000	1.543664000	-0.010684000		
		Mg	2.194624000	-1.539939000	-0.011197000		
		Mg	-2.604766000	-0.003744000	0.007057000		
C_1		Al	1.130381000	1.810877000	0.272818000	-1566.9373328	2.4
		Al	0.096819000	-1.817686000	0.590794000		
		Al	0.787903000	-0.260322000	-1.532211000		
		Al	-1.205912000	1.595480000	-0.579454000		
		Mg	2.666865000	-0.593666000	0.394295000		
		Mg	-1.489736000	0.224572000	1.897565000		
		Mg	-2.053752000	-1.069951000	-0.939802000		
C_s		Al	-0.888980000	-1.913706000	0.000000000	-1566.9366992	2.8
		Al	0.181392000	-0.536672000	1.943514000		
		Al	0.181392000	-0.536672000	-1.943514000		
		Al	-1.589400000	0.622920000	0.000000000		
		Mg	1.929110000	-1.783297000	0.000000000		
		Mg	0.181392000	2.172219000	1.575838000		
		Mg	0.181392000	2.172219000	-1.575838000		
C_1		Al	0.982386000	1.691336000	-0.452655000	-1566.9352143	3.7
		Al	-1.328348000	1.659224000	0.522545000		
		Al	0.228273000	-1.808804000	-0.389383000		
		Al	-1.094278000	0.099266000	-1.714370000		
		Mg	-2.225325000	-1.179822000	0.634894000		
		Mg	2.668538000	-0.529657000	-0.363388000		
		Mg	0.869751000	-0.068296000	1.931845000		
C_1		Al	-0.190256000	0.061711000	1.665665000	-1566.9284559	8.0
		Al	1.248949000	1.594190000	0.208134000		
		Al	1.433919000	-1.468152000	0.363078000		
		Al	-1.079504000	-1.822429000	0.092471000		
		Mg	-3.030575000	-0.246353000	-1.220804000		
		Mg	-1.506449000	1.951348000	0.039426000		
		Mg	3.006158000	0.065909000	-1.342083000		

Figure 12. Lowest energy isomers for Al_4Mg_3 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

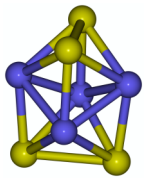
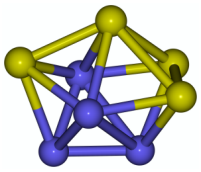
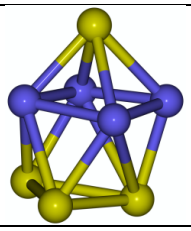
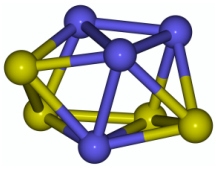
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
D_{2d}		Al 0.000000000 1.808380000 -0.575364000 Al 0.000000000 -1.808380000 -0.575364000 Mg -1.526055000 0.000000000 -2.146052000 Mg 1.526055000 0.000000000 -2.146052000 Al 1.808262000 0.000000000 0.575321000 Al -1.808262000 0.000000000 0.575321000 Mg 0.000000000 -1.526003000 2.146098000 Mg 0.000000000 1.526003000 2.146098000	-1766.6546251	0.0
C_s		Al 0.059104000 -0.605745000 1.838015000 Al 0.059104000 -0.605745000 -1.838015000 Al -1.877896000 0.751354000 0.000000000 Al -1.531085000 -1.714345000 0.000000000 Mg 1.300262000 -2.310149000 0.000000000 Mg 0.059104000 2.103629000 1.552243000 Mg 0.059104000 2.103629000 -1.552243000 Mg 2.146532000 0.458578000 0.000000000	-1766.6467647	4.9
C_s		Al 1.852559000 0.282353000 0.000000000 Al -1.454689000 -1.656805000 0.000000000 Al 0.103498000 -0.612000000 1.847707000 Al 0.103498000 -0.612000000 -1.847707000 Mg -2.202509000 0.949415000 0.000000000 Mg 1.340241000 -2.364657000 0.000000000 Mg 0.103498000 2.115116000 1.518113000 Mg 0.103498000 2.115116000 -1.518113000	-1766.6459491	5.5
C_1		Al -1.000168000 -0.003275000 1.691373000 Al 0.335462000 -1.960884000 0.013616000 Al 1.534504000 -0.164826000 1.603986000 Al -0.186882000 0.103378000 -1.770366000 Mg -1.882167000 1.809227000 -0.247728000 Mg 2.405058000 -0.333600000 -1.065133000 Mg 0.976179000 2.121528000 0.032900000 Mg -2.238896000 -1.402748000 -0.386866000	-1766.6447752	6.2

Figure 13. Lowest energy isomers for Al_4Mg_4 and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

Anionic Systems: Cartesians coordinates and relative energies

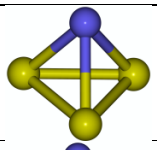
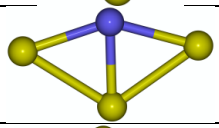
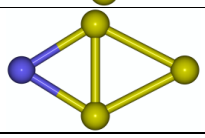
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{3v}		Al 0.000000000 0.000000000 1.609116000 Mg 0.000000000 1.767571000 -0.581069000 Mg -1.530762000 -0.883786000 -0.581069000 Mg 1.530762000 -0.883786000 -0.581069000			-840.9553120	0.0
C_{2v}		Al 0.000000000 0.000000000 1.039493097 Mg 2.695358946 0.000000000 0.215975003 Mg -2.695358946 0.000000000 0.215975003 Mg 0.000000000 0.000000000 -1.601308664			-840.9386925	10.4
C_s		Al 0.000000000 0.000000000 -2.395279246 Mg 0.000000000 0.000000000 2.795212301 Mg 1.457286289 0.000000000 -0.050343464 Mg -1.457286289 0.000000000 -0.050343464			-840.9296149	16.1

Figure 14. Lowest energy isomers for $AlMg_3^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

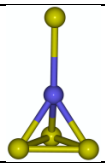
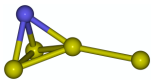
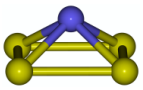
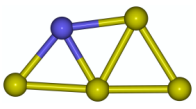
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{3v}		Al 0.000000000 0.000000000 0.635875000 Mg 0.000000000 1.751400000 -1.590304000 Mg 1.516757000 -0.875700000 -1.590304000 Mg -1.516757000 -0.875700000 -1.590304000 Mg 0.000000000 0.000000000 4.082047000			-1040.6058994	0.0
C_s		Al -1.691114000 -1.468990000 0.000000000 Mg 0.626744000 -1.767701000 1.529343000 Mg 0.626744000 4.291823000 0.000000000 Mg -0.048193000 0.834984000 0.000000000 Mg 0.626744000 -1.767701000 -1.529343000			-1040.6029724	1.8
C_{4v}		Al 0.000000000 0.000000000 1.065674314 Mg -1.751244113 1.751244113 -0.299702684 Mg 1.751244113 -1.751244113 -0.299702684 Mg -1.751244113 -1.751244113 -0.299702684 Mg 1.751244113 1.751244113 -0.299702684			-1040.6026812	2.0
C_{2v}		Al -1.354898000 -1.282304000 0.000000000 Mg -3.143702000 0.882914000 0.000000000 Mg 1.481720000 -1.643268000 0.000000000 Mg 0.000000000 1.080318000 0.000000000 Mg 3.129788000 1.069198000 0.000000000			-1040.5940815	7.4

Figure 15. Lowest energy isomers for $AlMg_4^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

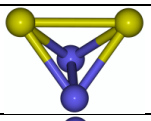
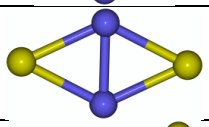
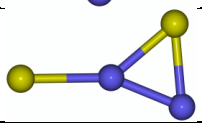
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{2v}		Al 0.000000000 1.278858000 -0.939643361 Al 0.000000000 -1.278858000 -0.939643361 Mg -1.682557137 0.000000000 1.057034532 Mg 1.682557137 0.000000000 1.057034532			-883.2915024	0.0
D_{2h}		Al 0.000000000 1.273295000 0.000000000 Al 0.000000000 -1.273295000 0.000000000 Mg 0.000000000 0.000000000 2.586977000 Mg 0.000000000 0.000000000 -2.586977000			-883.2877860	2.3
C_s		Al 0.000000000 0.430442000 0.000000000 Al 1.783301000 -1.358892000 0.000000000 Mg -1.118867000 3.191415000 0.000000000 Mg -0.813043000 -2.185594000 0.000000000			-883.2792282	7.7

Figure 16. Lowest energy isomers for $Al_2Mg_2^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

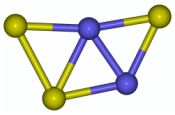
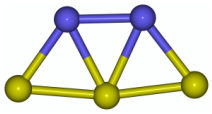
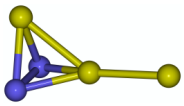
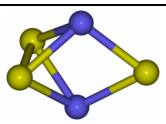
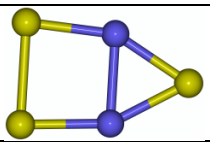
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al 0.000000000 0.856072000 0.000000000 Al -1.398026000 -1.309380000 0.000000000 Mg 1.426551000 -1.798315000 0.000000000 Mg -2.747120000 1.240469000 0.000000000 Mg 2.835097000 1.048929000 0.000000000			-1082.9482808	0.0
C_{2v}		Mg 0.000000000 2.951725000 0.903925000 Al 0.000000000 -1.267440000 -1.388634000 Mg 0.000000000 0.000000000 1.200857000 Mg 0.000000000 -2.951725000 0.903925000 Al 0.000000000 1.267440000 -1.388634000			-1082.9478688	0.3
C_s		Al -1.584709000 -0.783637000 1.268241000 Al -1.586534000 -0.794416000 -1.263053000 Mg -1.838050000 1.732466000 -0.005722000 Mg 0.988759000 -0.173481000 0.001380000 Mg 4.284805000 0.150571000 -0.001277000			-1082.9429413	3.3
C_{2v}		Al -1.676732000 -0.264398000 0.000000000 Al 1.677689000 -0.270183000 0.000000000 Mg -0.000346000 1.626954000 1.430737000 Mg -0.000346000 1.626954000 -1.430737000 Mg -0.000346000 -2.674779000 0.000000000			-1082.9418860	4.0
C_{2v}		Al 0.000000000 1.405893000 0.627977000 Al 0.000000000 -1.405893000 0.627977000 Mg 0.000000000 1.603054000 -2.189024000 Mg 0.000000000 0.000000000 3.017431000 Mg 0.000000000 -1.603054000 -2.189024000			-1082.9395303	5.5

Figure 17 Lowest energy isomers for $Al_2Mg_3^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

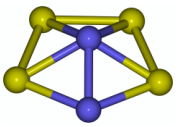
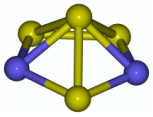
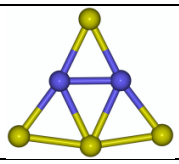
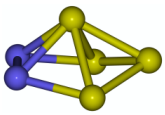
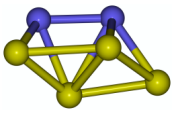
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al 0.177712000 -2.350873000 0.000000000 Al -0.924741000 0.020886000 0.000000000 Mg 0.202320000 2.153795000 1.529948000 Mg 0.202320000 -0.891719000 2.446261000 Mg 0.202320000 2.153795000 -1.529948000 Mg 0.202320000 -0.891719000 -2.446261000			-1282.6200927	0.0
C_s		Al -0.273935000 -0.657827000 2.070435000 Al -0.273935000 -0.657827000 -2.070435000 Mg -0.273935000 2.029680000 1.504735000 Mg -0.273935000 2.029680000 -1.504735000 Mg -0.400512000 -2.522229000 0.000000000 Mg 1.541907000 -0.111840000 0.000000000			-1282.6144068	3.6
C_s		Al -1.265763464 0.000000000 0.748915300 Al 1.265763464 0.000000000 0.748915300 Mg 0.000000000 0.000000000 -1.944521037 Mg -2.965021762 0.000000000 -1.523401958 Mg 2.965021762 0.000000000 -1.523401958 Mg 0.000000000 0.000000000 3.306367943			-1282.6133700	4.2
C_s		Al -1.924659000 -1.267083000 -0.173761000 Al -1.918597000 1.274071000 -0.173516000 Mg 0.737485000 2.152051000 -0.631499000 Mg 0.009283000 -0.002605000 1.570742000 Mg 2.687768000 -0.004304000 0.070775000 Mg 0.728992000 -2.152712000 -0.633801000			-1282.6129594	4.5
C_1		Al 1.522721000 1.587744000 0.058382000 Al -1.000485000 1.563373000 -0.590966000 Mg -0.476555000 -1.394563000 -1.258615000 Mg 0.147595000 -0.530559000 1.547731000 Mg 2.555377000 -1.059806000 -0.142373000 Mg -2.792173000 -0.428782000 0.430222000			-1282.6090442	6.9

Figure 18. Lowest energy isomers for $Al_2Mg_4^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

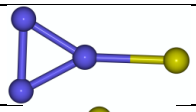
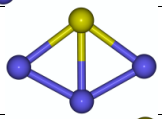
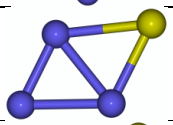
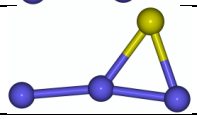
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{2v}		Al 0.000000000 1.257712000 -1.832472000 Al 0.000000000 0.000000000 0.363015000 Al 0.000000000 -1.257712000 -1.832472000 Mg 0.000000000 0.000000000 3.577089000			-925.6268320	0.0
C_{2v}		Al -2.248413000 0.000000000 0.063965570 Al 0.000000000 0.000000000 1.288745570 Al 2.248413000 0.000000000 0.063965570 Mg 0.000000000 0.000000000 -1.593664430			-925.6251751	1.0
C_s		Al 0.265164348 -1.387503391 0.000000000 Al -0.257927297 1.313187055 0.000000000 Al -2.226985809 -0.110297373 0.000000000 Mg 2.497065575 0.207677799 0.000000000			-925.6246362	1.4
C_{2v}		Al -3.055093214 -0.040419099 0.000000000 Al 2.000845081 1.141776988 0.000000000 Al -0.417167376 0.282275008 0.000000000 Mg 1.655241838 -1.556492402 0.000000000			-925.6136087	8.3

Figure 19. Lowest energy isomers for Al_3Mg^- and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

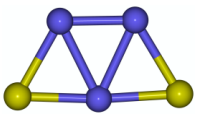
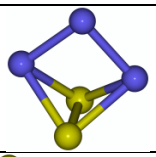
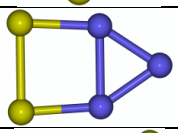
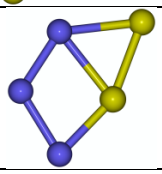
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_{2v}		Al 0.000000000 1.237780000 -1.461039000 Al 0.000000000 0.000000000 1.105044000 Al 0.000000000 -1.237780000 -1.461039000 Mg 0.000000000 2.663954000 0.984227000 Mg 0.000000000 -2.663954000 0.984227000			-1125.3093176	0.0
C_{2v}		Al 0.000000000 1.880099000 0.276873000 Al 0.000000000 0.000000000 2.115135000 Al 0.000000000 -1.880099000 0.276873000 Mg -1.387288000 0.000000000 -1.445643000 Mg 1.387288000 0.000000000 -1.445643000			-1125.3074975	1.1
C_{2v}		Al 0.000000000 1.386727000 0.621465000 Al 0.000000000 0.000000000 2.686883000 Al 0.000000000 -1.386727000 0.621465000 Mg 0.000000000 -1.528855000 -2.128648000 Mg 0.000000000 1.528855000 -2.128648000			-1125.3030407	3.9
C_s		Al -1.262460000 -1.561951000 0.000000000 Al -2.560385000 0.643409000 0.000000000 Al 1.201255000 -1.331306000 0.000000000 Mg 0.000000000 1.395491000 0.000000000 Mg 2.840055000 1.041845000 0.000000000			-1125.2970384	7.7

Figure 20. Lowest energy isomers for $Al_3Mg_2^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

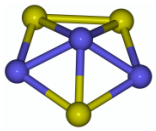
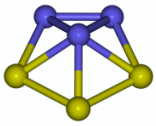
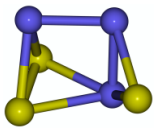
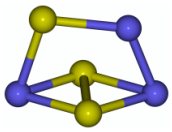
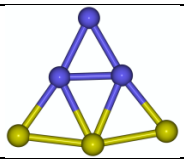
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al 0.191993000 -0.663073000 2.223698000 Al -1.051061000 -0.077989000 0.000000000 Al 0.191993000 -0.663073000 -2.223698000 Mg 0.338679000 -2.498504000 0.000000000 Mg 0.191993000 2.009825000 -1.575033000 Mg 0.191993000 2.009825000 1.575033000			-1324,9776067	0.0
C_s		Al -0.132045582 -1.095762601 0.000000000 Al 1.934377953 0.033139155 1.251123531 Al 1.934377953 0.033139155 -1.251123531 Mg -0.785064936 0.439654054 2.333400807 Mg -0.785064936 0.439654054 -2.333400807 Mg -2.633413743 0.278791328 0.000000000			-1324,9730090	2.9
C_1		Al 0.149908000 -2.310535000 0.000000000 Al -0.411182000 -0.709735000 1.958267000 Al -0.411182000 -0.709735000 -1.958267000 Mg 1.550860000 0.062720000 0.000000000 Mg -0.411182000 1.989060000 1.532006000 Mg -0.411182000 1.989060000 -1.532006000			-1324,9709316	4.2
C_s		Al 2.177960000 -1.016357000 -0.000075000 Al -1.227335000 1.623627000 -0.002495000 Al -2.344577000 -0.659085000 0.001817000 Mg -0.054638000 -0.829644000 1.591480000 Mg -0.056603000 -0.835130000 -1.589708000 Mg 1.621354000 1.720906000 -0.000957000			-1324,9697615	4.9
C_s		Al -0.180664000 -1.856547000 1.515456000 Mg -0.180664000 0.867494000 2.069053000 Al 1.435524000 -0.617794000 0.000000000 Al -0.180664000 -1.856547000 -1.515456000 Mg -0.802382000 2.956806000 0.000000000 Mg -0.180664000 0.867494000 -2.069053000			-1324,9657299	7.4

Figure 21. Lowest energy isomers for $Al_3Mg_3^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

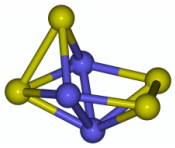
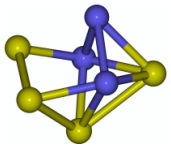
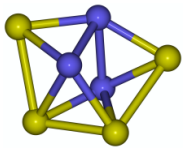
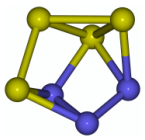
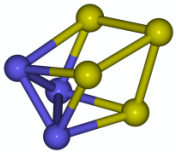
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al -0.081380000 -0.515605000 1.914446000 Al -0.081380000 -0.515605000 -1.914446000 Al 1.619828000 0.374367000 0.000000000 Mg -2.154565000 -1.319871000 0.000000000 Mg -0.081380000 2.216470000 -1.566921000 Mg 0.738835000 -2.401490000 0.000000000 Mg -0.081380000 2.216470000 1.566921000			-1524.653276	0.0
C_1		Al -0.078340000 -1.736183000 -0.798809000 Al -0.932526000 1.619147000 0.874763000 Al -0.878901000 0.758901000 -1.662456000 Mg 1.588165000 1.913382000 -0.147297000 Mg 2.551322000 -1.007646000 -0.301027000 Mg 0.357446000 -0.776290000 1.974802000 Mg -2.449685000 -0.824800000 0.192232000			-1524.64988	2.1
C_2		Al 0.000000000 1.818681000 -0.150165000 Al 0.000000000 0.000000000 1.937726000 Al 0.000000000 -1.818681000 -0.150165000 Mg 1.484514000 -0.064147000 -1.942655000 Mg -2.407640000 -0.998568000 1.055733000 Mg -1.484514000 0.064147000 -1.942655000 Mg 2.407640000 0.998568000 1.055733000			-1524.64730	3.7
C_1		Al 0.820088000 0.036035000 1.490597000 Al 1.494827000 -1.722662000 -0.445468000 Al -0.925440000 -1.847307000 0.120230000 Mg -1.914484000 0.041582000 -1.744312000 Mg -0.176938000 2.281307000 -0.359410000 Mg -1.948234000 0.541368000 1.342398000 Mg 2.534392000 0.964172000 -0.501149000			-1524.64652	4.2
C_1		Al -2.127520000 -0.545949000 0.000000000 Al -0.305499000 -1.587856000 1.560591000 Al -0.305499000 -1.587856000 -1.560591000 Mg -0.305499000 1.084983000 -1.963157000 Mg 1.993624000 -0.574866000 0.000000000 Mg 1.584100000 2.436700000 0.000000000 Mg -0.305499000 1.084983000 1.963157000			-1524.64305	6.4

Figure 22. Lowest energy isomers for $Al_3Mg_4^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

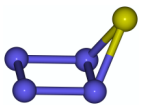
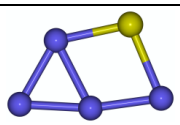
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al 0.432476000 -0.837730000 1.292302000 Al 0.432476000 1.727933000 1.294613000 Mg -1.874062000 -1.928772000 0.000000000 Al 0.432476000 -0.837730000 -1.292302000 Al 0.432476000 1.727933000 -1.294613000			-1167.6545357	0.0
C_s		Al -2.524396000 1.037814000 0.000000000 Al 0.000000000 1.138831000 0.000000000 Al -1.261223000 -1.240717000 0.000000000 Al 2.512589000 0.759261000 0.000000000 Mg 1.379116000 -1.836455000 0.000000000			-1167.6459799	5.4

Figure 23. Lowest energy isomers for Al_4Mg^- and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

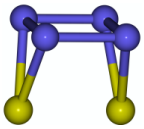
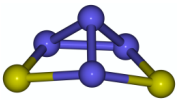
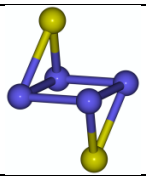
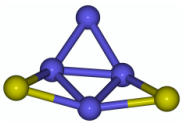
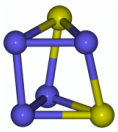
Symetry	Structure	Cartesians Coordinates				E (a.u)	ΔE
C_{2v}		Al	1.281572000	1.326485000	-0.830883790	-1367.3254496	0.0
		Al	-1.281572000	-1.326485000	-0.830883790		
		Al	1.281572000	-1.326485000	-0.830883790		
		Al	-1.281572000	1.326485000	-0.830883790		
		Mg	0.000000000	-1.678657000	1.800248210		
		Mg	0.000000000	1.678657000	1.800248210		
C_s		Al	1.791320550	-0.183491990	1.290240880	-1367.3239123	1.0
		Al	1.791320550	-0.183491990	-1.290240880		
		Al	0.064837150	1.297855870	0.000000000		
		Al	-2.170860240	0.124948090	0.000000000		
		Mg	-0.799834760	-0.571902480	2.345953750		
		Mg	-0.799834760	-0.571902480	-2.345953750		
C_s		Al	0.000913000	-1.303622000	1.377609000	-1367.3218006	2.3
		Al	0.000913000	1.309100000	-1.377995000		
		Al	0.000913000	-1.303622000	-1.377609000		
		Al	0.000913000	1.309100000	1.377995000		
		Mg	2.382054000	0.658390000	0.000000000		
		Mg	-2.386011000	-0.670259000	0.000000000		
C_s		Al	-1.355806000	2.646788000	0.000000000	-1367.3170149	5.3
		Al	0.773650000	-1.410851000	0.000000000		
		Al	0.151361000	0.854666000	1.271837000		
		Al	0.151361000	0.854666000	-1.271837000		
		Mg	0.151361000	-1.595354000	-2.720745000		
		Mg	0.151361000	-1.595354000	2.720745000		
C_s		Al	-1.343864000	-0.021732000	1.521993000	-1367.3160781	5.9
		Al	1.342100000	-0.025637000	1.523821000		
		Al	1.160007000	-1.579623000	-0.526103000		
		Mg	1.685393000	1.201870000	-1.087506000		
		Mg	-1.685104000	-1.167252000	-1.123792000		
		Al	-1.158511000	1.595037000	-0.478513000		

Figure 24. Lowest energy isomers for $Al_4Mg_2^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

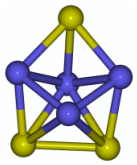
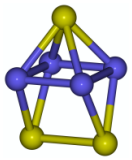
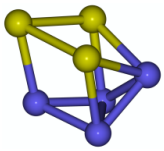
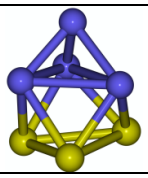
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
C_s		Al -1.977004000 0.012010000 0.000000000 Al -0.198023000 0.795335000 1.831695000 Al 1.720273000 -0.299231000 0.000000000 Al -0.198023000 0.795335000 -1.831695000 Mg 1.103220000 2.470241000 0.000000000 Mg -0.198023000 -1.941155000 1.500736000 Mg -0.198023000 -1.941155000 -1.500736000			-1567.0158484	0.0
C_{2v}		Al 1.334604078 1.359578859 -0.388395490 Al -1.334604078 -1.359578859 -0.388395490 Mg -1.511119967 0.000000000 2.128420699 Al -1.334604078 1.359578859 -0.388395490 Mg 0.000000000 0.000000000 -2.509167918 Mg 1.511119967 0.000000000 2.128420699 Al 1.334604078 -1.359578859 -0.388395490			-1567.0144214	0.9
C_s		Al 0.352629000 -1.532870000 1.513291000 Al 2.079041000 -0.241934000 0.000000000 Al 0.352629000 -1.532870000 -1.513291000 Al -1.682891000 -0.801309000 0.000000000 Mg 0.352629000 1.218681000 -1.869173000 Mg 0.352629000 1.218681000 1.869173000 Mg -1.898448000 2.014036000 0.000000000			-1567.0080348	4.9
C_s		Al -1.367065000 -1.938829000 0.000000000 Al -1.808018000 0.543269000 0.000000000 Al 0.265792000 -0.934999000 1.829107000 Al 0.265792000 -0.934999000 -1.829107000 Mg 0.265792000 1.828780000 1.581208000 Mg 0.265792000 1.828780000 -1.581208000 Mg 2.332207000 -0.119873000 0.000000000			-1567.0058174	6.3

Figure 25. Lowest energy isomers for $Al_4Mg_3^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.

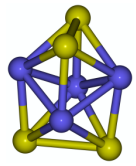
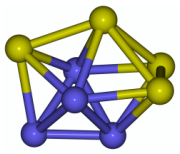
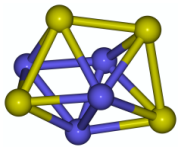
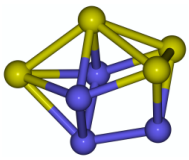
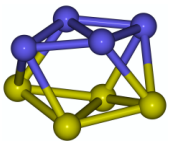
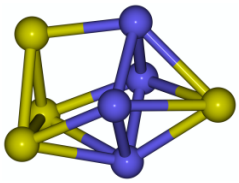
Symetry	Structure	Cartesians Coordinates			E (a.u)	ΔE
D_{2d}		Al 0.000000000 1.779961000 0.491124950 Mg -1.458806000 0.000000000 2.289426950 Al 1.779961000 0.000000000 -0.491124950 Mg 0.000000000 1.458806000 -2.289426950 Al 0.000000000 -1.779961000 0.491124950 Mg 1.458806000 0.000000000 2.289426950 Mg 0.000000000 -1.458806000 -2.289426950 Al -1.779961000 0.000000000 -0.491124950	-1766.7042412	0.0
C_s		Al 0.448630300 -1.801171940 0.000000000 Al -0.528021170 0.036059140 1.782191390 Al -0.528021170 0.036059140 -1.782191390 Al -2.078487140 -1.424209430 0.000000000 Mg 2.229208150 -0.086604130 1.485982170 Mg 0.642971240 2.103374410 0.000000000 Mg 2.229208150 -0.086604130 -1.485982170 Mg -2.191663430 1.485868860 0.000000000	-1766.7006244	2.3
C_1		Al 1.874311000 -0.198218000 1.465060000 Mg -1.836686000 1.872357000 -0.156811000 Mg -2.600735000 -1.213555000 -0.124311000 Al -0.344523000 -0.007062000 -1.737056000 Al 0.118149000 -1.890864000 0.103504000 Mg 1.091289000 2.045817000 -0.098300000 Mg 2.296200000 -0.538614000 -1.263538000 Al -0.678769000 0.096755000 1.685070000	-1766.6977950	4.0
C_s		Al -0.961859820 1.924284040 0.000000000 Mg 1.991333610 -0.688086940 -1.540417430 Mg -2.943336990 -0.461793820 0.000000000 Mg 1.991333610 -0.688086940 1.540417430 Al 1.560604160 1.650941860 0.000000000 Mg -0.307130110 -2.151548010 0.000000000 Al -0.637219510 0.053559420 1.790462290 Al -0.637219510 0.053559420 -1.790462290	-1766.6968382	4.7
C_2		Al 1.852559000 0.282353000 0.000000000 Al -1.454689000 -1.656805000 0.000000000 Al 0.103498000 -0.612000000 1.847707000 Al 0.103498000 -0.612000000 -1.847707000 Mg -2.202509000 0.949415000 0.000000000 Mg 1.340241000 -2.364657000 0.000000000 Mg 0.103498000 2.115116000 1.518113000 Mg 0.103498000 2.115116000 -1.518113000	-1766.6960452	5.1
C_1		Al -1.030077460 1.870305100 0.091612900 Al -0.368281560 -1.794836190 -0.069933640 Al -0.579276250 0.134509770 -1.804493170 Al -0.650904770 -0.042588800 1.831747350 Mg 2.027257370 -0.739413050 1.508551030 Mg -2.959386890 -0.474273860 -0.076218130 Mg 1.722717540 1.803038490 -0.015381240 Mg 2.056997020 -0.770690610 -1.469962880	-1766.6944601	6.1

Figure 26. Lowest energy isomers for $Al_4Mg_4^-$ and the relative energies in Kcal/mol at the CCSD(T)/Def2-TZVPP//B3lyp/Def2-TZVPP level. The Zero-point energy correction has been included.