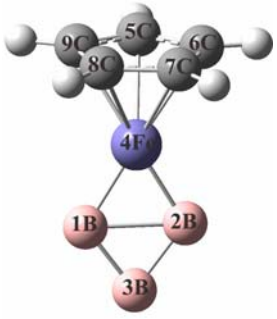
Supporting Information:

Scheme S1. Optimized geometries (B3LYP/6-311+G*) and some important geometrical parameters, (bond length (R, Å) and bond angle ((A, degree)) of different molecules

Molecules



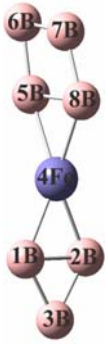
Cp-Fe-B_3

Bond Distances

R(1,2)=1.87; R(2,3)=R(1,3)=1.57
R(1,4)=R(2,4)=1.82
R(4,5)=R(4,6)=2.14
R(4,7)=R(4,8)=2.15, R(4,9)=2.18
R(5,6)=1.43,R(6,7)=R(7,8)=1.42
R(8,9)=R(9,5)=1.42

Bond Angles

A(1,2,3)=53.28; A(3,1,2)=53.34
A(2,3,1)=73.38
A(5,6,7)=107.88; A(6,7,8)=107.78
A(8,9,5)=107.72
A(7,8,9)=108.36; A(9,5,6)=108.18
A(1,4,2)=62.18
A(8,4,7)=38.61; A(7,4,6)=38.68
A(6,4,5)=39.02
A(5,4,9)=38.32; A(9,4,8)=38.23



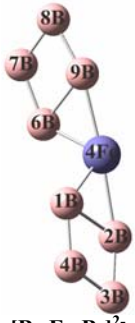
[B_4-Fe-B_3]$^-$

Bond Distances

R(1,2)=1.67; R(2,3)=R(1,3)=1.56
R(1,4)=R(2,4)=1.89
R(4,5)=1.91,R(4,8)=1.98
R(5,6)=R(7,8)=1.56
R(6,7)=1.52, R(5,8)=1.77

Bond Angles

A(1,2,3)=A(3,1,2)=57.57; A(2,3,1)=64.86
A(1,4,2)=52.64; A(4,1,2)= A(1,2,4)=63.68
A(5,6,7)=73.80
A(6,7,8)=116.08; A(7,8,5)=67.03
A(8,5,6)=103.09; A(5,4,8)=54.14
A(5,8,4)=64.95; A(4,5,8)=60.91
A(5,6,8)=41.42; A(5,7,8)=62.10
A(6,5,7)=52.22; A(6,8,7)=61.54



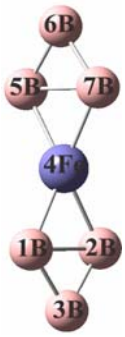
[B_4-Fe-B_4]$^{2-}$

Bond Distances

R(1,2)=R(6,9)=1.76
R(2,3)=R(8,9)=1.57
R(3,4)=R(7,8)=1.51
R(1,4)=R(6,7)=1.60
R(1,5)=R(6,5)=1.78
R(2,5)=R(9,5)=2.09

Bond Angles

A(1,2,3)=A(6,9,8)=104.84
A(2,3,4)=72.46; A(7,8,9)=72.53
A(3,4,1)=A(6,7,8)=117.81
A(4,1,2)= 64.85; A(9,6,7)=64.89
A(1,5,2)=A(6,5,9)=53.21
A(1,2,5)=54.10; A(5,9,6)=54.13
A(5,6,9)=70.75; A(2,1,5)=70.68
A(5,9,8)=52.56; A(4,2,3)=52.60



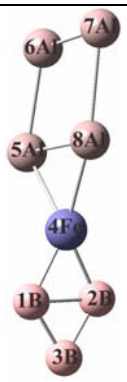
B_3-Fe-B_3

Bond Distances

R(1,2)=R(5,7)=1.89
R(2,3)=R(1,3)= 1.54
R(5,6)=R(6,7)=1.54
R(1,4)=R(2,4)=R(4,5)=R(4,7)=1.84

Bond Angles

A(1,2,3)=A(3,1,2)= 52.25
A(6,7,5)=A(7,5,6)=52.25
A(2,3,1)=A(5,6,7)=75.49
A(1,4,2)=A(5,4,7)=61.97
A(4,5,7)= A(4,7,5)= 59.01
A(1,2,5)= A(2,1,5)=59.01



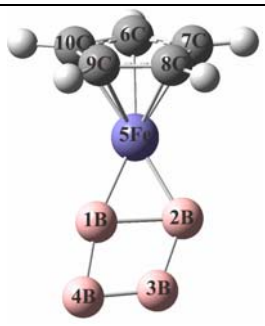
$[Al_4$-Fe-$B_3]^-$

Bond Distances

R(1,2)=1.72, R(1,3)= R(2,3)=1.58
R(1,4)= R(2,4)=1.84
R(5,6)=2.53; R(5,7)=2.55
R(7,8)=2.62; R(5,8)=2.76
R(4,5)=2.36; R(4,8)=2.34; R(6,8)=2.83

Bond Angles

A(1,2,3)= A(2,1,3)=56.84; A(1,3,2)=66.31
A(1,4,2)=55.98; A(1,2,4)= A(2,14)=62.01
A(5,4,8)=72.00; A(5,8,4)=54.26
A(4,5,8)=53.74; A(5,6,7)=119.97
A(6,7,8)=66.19; A(5,1,2)=109.45
A(6,5,8)=64.39; A(5,6,8)=61.84,
A(5,7,8)=32.33; A(6,5,7)=30.17
A(6,8,7)=55.68



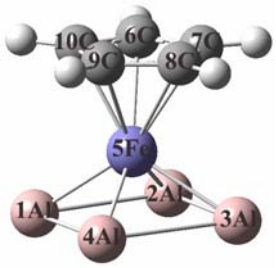
$[Cp$-Fe-$B_4]^-$

Bond Distances

R(1,2)=1.76; R(1,4)=1.56
R(2,3)=1.58; R(3,4)=1.52
R(1,5)=1.98; R(2,5)=1.88
R(3,5)=3.18; R(4,5)=3.51
R(6,7)= R(9,10)=1.42,
R(7,8)=R(8,9)= R(10,1)=1.43
R(6,5)= R(10.5)=2.15; R(7,5)=1.14
R(8,5)=2.07; R(9,5)=2.08

Bond Angles

A(1,2,3)=65.69; A(2,3,4)=116.80
A(2,1,4)=105.22; A(1,4,3)=72.29
A(1,4,2)=39.98; A(1,3,2)=61.86
A(4,1,3)=52.77; A(4,2,3)=30.90
A(1,5,2)=54.74; A(5,1,2)=60.11
A(1,2,5)=65.82
A(6,7,8)=107.41; A(7,8,9)=107.97
A(8,9,10)=108.28; A(9,10,1)=107.31
A(6,5,7)=38.59; A(7,5,8)=39.81
A(8,5,9)=40.26; A(9,5,10)=39.27
A(10,5,1)=38.87



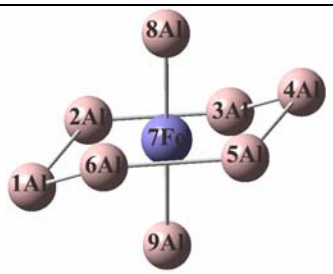
$[Cp$-Fe-$Al_4]^-$

Bond Distances

R(1,2)=R(1,4)=2.80
R(2,3)=R(3,4)=2.82
R(1,5)=2.31; R(3,7)=2.37
R(2,5)=R(4,5)=2.34
R(6,7)=R(7,8)=R(8,9)=1.42
R(9,10)= R(10,1)=1.42
R(6,5)= R(9,7)=2.25
R(7,5)= R(8,5)= 2.33
R(10,1)=2.21

Bond Angles

A(1,2,3)=89.49; A(2,3,4)=90.09
A(2,1,4)=90.90; A(1,4,3)=89.51
A(1,4,2)=44.55; A(1,3,2)=44.04
A(4,1,3)=45.44; A(4,2,3)=44.95
A(1,5,2)=74.05; A(2,5,3)=73.60
A(3,5,4)=73.61; A(1,2,4)=74.10
A(6,5,7)=36.07; A(7,5,8)=35.49
A(8,5,9)=36.16; A(9,5,10)=37.30
A(1,5,10)=37.23; A(6,7,8)=108.06
A(7,8,9)=108.07; A(8,9,10)=108.02
A(9,10,1)=107.80



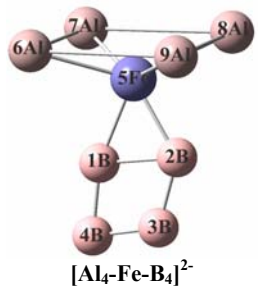
$[Al_4$-Fe-$Al_4]^{2-}$

Bond Distances

R(1,2)= R(4,5)=2.62
R(2,3)=2.64; R(1,4)=1.56
R(7,8)=R(7,9)=2.26;
R(3,7)=2.51; R(6,7)=2.49
R(3,4)=R(5,6)=R(1,6)=R(1,7)=2.65
R(4,7)=R(2,7)=R(5,7)=2.65

Bond Angles

A(1,2,6)=33.31; A(1,6,2)=32.82
A(2,1,6)=113.86; A(3,4,5)=114.49
A(4,3,5)=A(5,3,4)=32.53; A(6,2,3)=86.35
A(2,3,5)=93.67; A(3,5,6)=86.12
A(2,6,5)=93.86; A(6,5,7)=38.59
A(7,5,8)=39.81; A(8,5,9)=40.26
A(9,5,10)=39.27



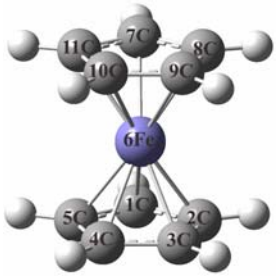
$[Al_4$-Fe-$B_4]^{2-}$

Bond Distances

R(1,2)=1.77; R(1,4)=1.59
R(2,3)=1.52; R(3,4)=1.57
R(1,5)=2.01; R(2,5)=1.87
R(4,5)=3.54; R(3,7)=3.17
R(6,7)=2.77; R(7,8)=3.27
R(8,9)=2.79; R(9,6)=3.28
R(6,5)= R(7,5)= 2.29
R(8,5)= R(9,5)=2.28

Bond Angles

A(1,2,3)=65.97; A(2,3,4)=116.76
A(2,1,4)=104.37; A(1,4,3)=72.90
A(1,4,2)=40.48; A(1,3,2)=61.84
A(4,1,3)=52.18; A(4,2,3)=30.82
A(6,7,8)=89.96; A(7,8,9)=90.06
A(8,9,6)=89.54; A(9,6,7)=90.42
A(6,7,9)=49.50; A(6,8,9)=49.79
A(7,6,8)=49.76; A(7,9,8)=49.48



Cp-Fe-Cp

Bond Distances

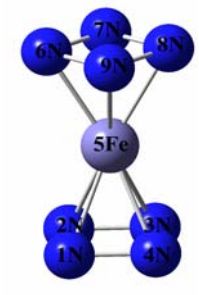
R(1,2)=R(2,3)=R(3,4)=R(4,5)=R(1,5)=1.42
R(7,8)=R(8,9)=R(9,10)=R(10,11)=R(7,11)=1.42
R(1,6)=R(2,6)=R(3,6)=R(4,6)=R(5,6)=2.08
R(6,7)=R(6,8)=R(6,9)=R(6,10)=R(6,11)=2.08

Bond Angles

A(1,2,3)=A(2,3,4)=A(3,4,5)=A(4,5,1)=A(5,1,2)=108
A(7,8,9)=A(8,9,10)=A(9,10,11)=A(10,11,7)=A(11,7,8)=108
A(4,6,3)=A(3,6,2)=A(2,6,1)=A(1,6,5)=A(5,6,4)=40.15
A(10,6,9)=A(9,6,8)=A(8,6,7)=A(7,6,11)=A(11,6,10)=40.15

Scheme S2. Optimized geometries (B3LYP/6-311+G*) and some important geometrical parameters, (bond length (R, Å) and bond angle ((A, degree)) of different molecules

Molecules



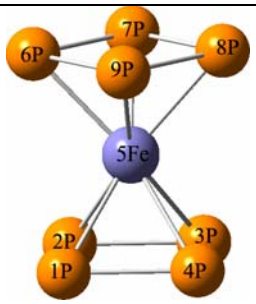
$[N_4\text{-Fe-}N_4]^{2-}$

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)=1.40
R(6,7)=R(7,8)=R(8,9)=R(9,6)=1.40
R(1,5)=R(2,5)=R(3,5)=R(4,5)=1.99
R(6,5)=R(7,5)=R(8,9)=R(9,5)=1.99

Bond Angles

A(1,2,3)=A(2,1,4)=A(6,7,8)=A(7,6,9)=90.02
A(2,3,4)=A(3,4,1)=A(7,8,9)=A(6,9,8)=89.97
A(1,5,2)=A(2,5,3)=A(3,5,4)=A(1,5,4)=41.07
A(6,5,7)=A(7,5,8)=A(8,5,9)=A(1,5,8)=41.07
A(1,2,4)=A(1,3,4)=A(2,1,3)=A(2,4,3)=45.00
A(6,7,9)=A(6,8,9)=A(7,6,8)=A(7,9,8)=45.00



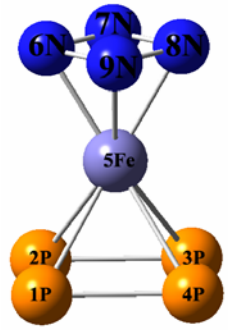
$[P_4\text{-Fe-}P_4]^{2-}$

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)=2.21
R(6,7)=R(7,8)=R(8,9)=R(9,6)=2.21
R(1,5)=R(2,5)=R(3,5)=R(4,5)=2.34
R(6,5)=R(7,5)=R(8,5)=R(9,5)=2.34

Bond Angles

A(1,5,2)=56.36; A(2,5 3)=56.30
A(3,5,4)=56.33; A(1,5,4)=56.41
A(6,5,9)=56.40; A(6,5,7)=56.34
A(7,5,8)=56.30; A(8,5,9)=56.34
A(1,2,3,)=90.04; A(23,4)=90.06
A(3,4,1)=89.96; A(2,1,4)=89.93
A(6,7,8)=90.05; A(7,8,9)=90.05
A(8,9,6)=90.05; A(7,6,9)=89.95



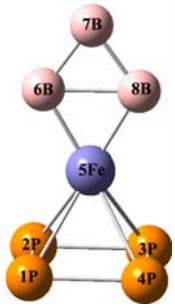
$[N_4\text{-Fe-}P_4]^{2-}$

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)=2.21
R(6,7)=R(7,8)=R(8,9)=R(9,6)=1.40
R(1,5)=R(2,5)=R(3,5)=R(4,5)=2.36
R(6,5)=R(7,5)=R(8,5)=R(9,5)=1.99

Bond Angles

A(1,5,2)=A(2,5,3)=A(3,5,4)=A(1,5,4)=55.95
A(6,5,7)=A(7,5,8)=A(8,5,9)=A(9,5,6)=40.99
A(1,2,3)=A(1,4,3)=90.00
A(2,3,4)=A(2,1,4)=89.99
A(6,7,8,)=A(6,9,8)=90.02
A(7,8,9)=A(7,6,9)= 89.99



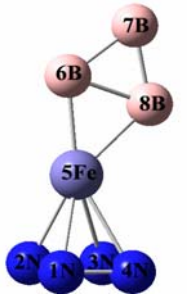
$[B_3\text{-Fe-}P_4]^{-}$

Bond Distances

R(6,7)=R(7,8)=1.58
R(6,8)=R(5,6)=R(5,8)=1.83
R(1,2)=R(2,3)=R(3,4)=R(4,1)=2.20
R(1,5)=R(2,5)=R(3,5)=R(4,5)=2.40

Bond Angles

A(7,8,6)=54.52; A(7,6,8)= 54.54
A(6,7,8)=70.93; A(6,5,8)=60.18
A(1,5,4)= A(2,5,3)=54.64
A(1,5,2)=54.35, A(3,5,4)=54.25
A(1,2,3)=A(2,1,4)=89.96
A(2,3,4)=A(1,4,3)=90.03



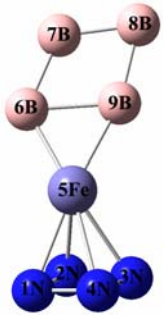
$[B_3\text{-Fe-}N_4]^{-}$

Bond Distances

R(6,7)=1.56; R(7,8)=1.54; R(6,8)= 1.68
R(5,6)=1.91; R(5,8)=1.89
R(2,3)=R(1,4)=1.39
R(3,4)=1.35,R(1,2)=1.42
R(2,5)= R(1,5)=1.98
R(3,5)=R(4,5)=2.09

Bond Angles

A(7,6,8)=56.62; A(7,8,6)=57.72
A(6,7,8)=66.66; A(6,5,8)= 52.57
A(2,5,3)=39.85; A(1,5,4)=39.88
A(1,5,2)=42.24; A(3,5,4)=37.80
A(2,3,4)=91.48; A(3,4,1)=91.44
A(2,1,4)=88.52; A(1,2,3)=88.57
A(2,4,3)=A(2,1,3)=44.99
A(1,3,4)=A(1,2,4)=45.03



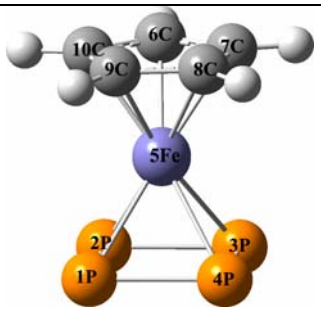
$[B_4\text{-Fe-}N_4]^{2-}$

Bond Distances

R(1,2)=1.39; R(2,3)=1.41
R(3,4)=1.38; R(1,4)=1.39
R(1,5)=2.04; R(2,5)=2.05
R(3,5)=2.07; R(4,5)=2.05
R(6,7)=1.60; R(7,8)=1.53
R(8,9)=1.58; R(6,9)= 1.77
R(5,6)=1.87; R(5,9)=1.99

Bond Angles

A(6,7,8)=119.79; A(7,8,9)=69.57
A(6,9,8)=107.17; A(7,6,9)=63.25;
A(6,8,7)=30.93; A(7,9,6)=53.68
A(8,6,9)=30.07; A(8,7,9)= 56.84
A(2,1,3)=45.55; A(2,3,1)=44.86
A(1,2,3)=89.49; A(2,3,4)=89.78;



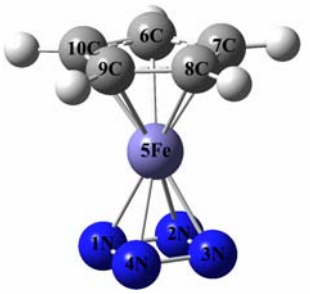
[Cp-Fe-P_4]$^-$

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)=2.20
R(1,5)=R(2,5)=R(3,5)=R(4,5)=2.36
R(6,5)=R(7,5)=2.07
R(5,8)=R(5,9)=2.09; R(5,10)=2.08
R(6,7)=R(7,8)=R(8,9)=R(9,10)=(10,1)=1.43

Bond Angles

A(1,2,3)= A(2,3,4)=89.99
A(3,4,1)=A(2,1,4)=90.00
A(1,5,2)=55.54; A(2,5,3)=55.62
A(3,5,4)=55.60; A(1,5,4)=55.52
A(2,1,3)= A(2,4,3)=45.00
A(1,2,4)= A(1,3,4)= 44.99
A(6,5,7)=40.44; A(7,5,8)=40.15
A(8,5,9)=39.85; A(9,5,10)=39.95
A(6,5,10)= 40.31; A(6,7,8)=107.95
A7,8,9)=108.03
A8,9,10)= 108.11 A(9,10,1)=108.00



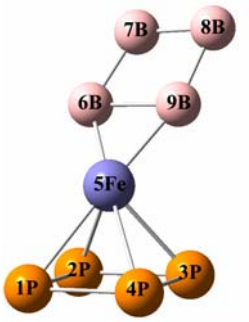
[Cp-Fe-N_4]$^-$

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)=1.40
R(1,5)=R(2,5)=R(3,5)=R(4,5)=1.98
R(6,5)=R(8,5)=2.07,
R(9,5)=R(10,5)=2.08; R(7,5)=2.06,
R(6,7)=R(7,8)=R(8,9)=R(9,10)=(10,1)=1.43

Bond Angles

A(1,2,3)= A(1,4,3)= A(2,1,4)=90.00
A(2,3,4)= 89.99
A(1,5,2)=41.26 A(2,5,3)=41.28
A(3,5,4)=41.27; A(1,5,4)=41.24,
A(2,1,3)= A(2,4,3)=45.00
A(1,2,4)= A(1,3,4)= 44.99
A(6,5,7)=40.42; A(7,5,8)=40.50
A(8,5,9)=40.30
A(9,5,10)=40.10 A(6,5,10)= 40.17
A(6,7,8)=107.92
A7,8,9)=107.95; A(8,9,10)= 108.05
A(9,10,1)=108.07



[B_4-Fe-P_4]$^{2-}$

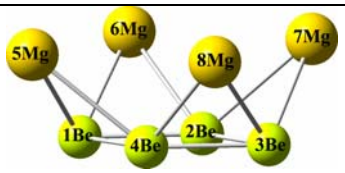
Bond Distances

R(1,5)=R(4,5)=2.43; R(1,2)=R(1,4)=2.22
R(2,3)=2.24; R(3,4)=2.21
R(2,5)=R(3,5)=2.29
R(6,7)=1.59; R(7,8)=1.52; R(8,9)=1.57
R(5,9)=1.98; R(5,6)=1.85; R(6,9)=1.75

Bond Angles

A(6,5,9)=54.16; A(5,9,6)=59.06
A(5,6,9)=66.77
A(6,7,9)=61.60; A(7,8,9)=71.48
A(7,6,9)=65.19; A(7,9,8)=52.81
A(1,5,2)=55.99; A(2,5,3)=58.50
A(3,5,4)=55.56
A(1,5,4)=54.33;
A(2,1,3)=45.35; A(2,4,3)=45.64
A(1,2,4)=45.09; A(1,3,4)=45.81
A(2,1,4)= A(1,2,3)=89.81
A(1,4,3)=90.74; A(2,3,4)=89.63

Scheme S3. Optimized geometries (B3LYP/6-311+G*) and some important geometrical parameters, (bond length(R,Å), and bond angle((A, degree)) of Mg_4Be_4 and different [Mg_4Be_4-M] metal clusters



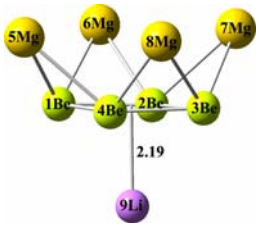
Mg_4Be_4

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.09,
R(5,6)=R(7,8)= 3.46; R (6,7)=R(8,5)= 3.55
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.51
R(1,5)=R(1,6)=R(3,8)=R(3,7)=2.37

Bond Angles

A(1,4,3)=A(1,2,3)= 123.00; A(4,1,2)=A(2,3,4)= 56.99
A(1,5,4)=A(4,8,3)=A(3,7,2)=A(2,6,1)= 50.54
A(6,5,8)=A(5,8,7)=A(8,7,6)=A(7,6,5)=90.00



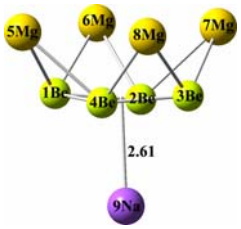
Mg_4Be_4-Li

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.07,
R(5,6)=R(7,8)= 3.68
R (6,7)=R(8,5)= 3.39
R(4,5)=R(4,8)= R(2,6)=R(2,7)=2.52
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.45

Bond Angles

A(1,4,3)=A(1,2,3)= 121.34
A(4,1,2)=A(2,3,4)= 58.57
A(1,5,4)=A(4,8,3)= 49.19
A(3,7,2)=A(2,6,1)= 49.19
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



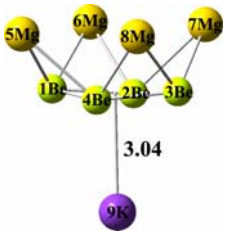
Mg_4Be_4-Na

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.08,
R(5,6)=3.78; R(7,8)= 3.70
R (6,7)= 3.41; R(8,5)= 3.28
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.55
R(1,5)=R(3,8)=2.46;R(1,6)=R(3,7)= 2.43

Bond Angles

A(1,4,3)= 122.16; A(1,2,3)= 120.64
A(4,1,2)=A(2,3,4)= 57.85
A(1,5,4)=A(4,8,3)= 48.56
A(3,7,2)= 49.20; A(2,6,1)= 49.27
A(6,5,8)= 90.14; A(5,8,7)= 91.65
A(8,7,6)= 89.63; A(7,6,5)= 88..31



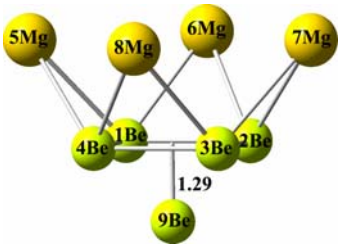
Mg_4Be_4-K

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.07
R(5,6)=R(7,8)= 3.72
R (6,7)=R(8,5)= 3.32
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.55
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.44

Bond Angles

A(1,4,3)=A(1,2,3)= 121.21
A(4,1,2)=A(2,3,4)= 57.91
A(1,5,4)=A(4,8,3)= 49.09
A(3,7,2)=A(2,6,1)= 49.09
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



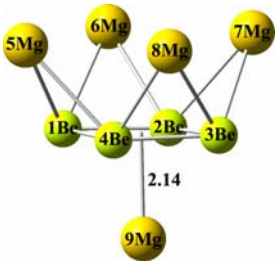
Mg_4Be_4-Be

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.16
R(5,6)=R(7,8)= R (6,7)=R(8,5)= 3.46
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.47
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.47

Bond Angles

A(1,4,3)=A(1,2,3)= 90.00
A(4,1,2)=A(2,3,4)= 90.00
A(1,5,4)=A(4,8,3)= 51.81
A(3,7,2)=A(2,6,1)= 51.81
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



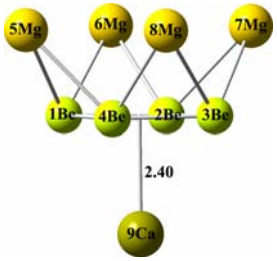
Mg_4Be_4-Mg

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.10
R(5,6)=R(7,8)= 3.39 ; R (6,7)=R(8,5)= 3.26
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.58
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.53

Bond Angles

A(1,4,3)=A(1,2,3)= 115.11
A(4,1,2)=A(2,3,4)= 64.82
A(1,5,4)=A(4,8,3)= 48.55
A(3,7,2)=A(2,6,1)= 48.55
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



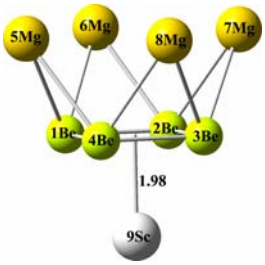
Mg_4Be_4-Ca

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.09
R(5,6)=R(7,8)= 3.55
R (6,7)=R(8,5)= 3.27
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.53
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.52

Bond Angles

A(1,4,3)=A(1,2,3)= 114.65
A(4,1,2)=A(2,3,4)= 65.32
A(1,5,4)=A(4,8,3)= 48.97
A(3,7,2)=A(2,6,1)= 48.97
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



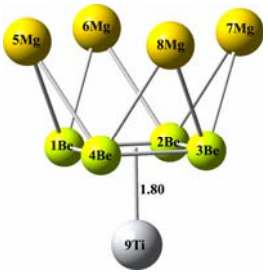
Mg_4Be_4-Sc

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.11
R(5,6)=R(7,8)= R (6,7)=R(8,5)= 3.10
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.51
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.51

Bond Angles

A(1,4,3)=A(1,2,3)= 90.00
A(4,1,2)=A(2,3,4)= 90.00
A(1,5,4)=A(4,8,3)= 49.71
A(3,7,2)=A(2,6,1)= 49.71
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



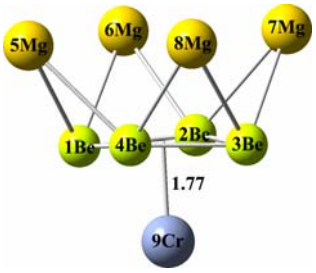
Mg_4Be_4-Ti

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)=2.07
R(5,6)=R(7,8)= R (6,7)=R(8,5)= 2.96
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.57
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.57

Bond Angles

A(1,4,3)=A(1,2,3)= 90.00
A(4,1,2)=A(2,3,4)= 90.00
A(1,5,4)=A(4,8,3)= 47.53
A(3,7,2)=A(2,6,1)= 47.53
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



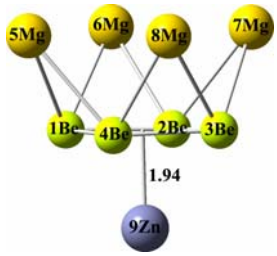
Mg_4Be_4-Cr

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.07
R(5,6)=R(7,8)= 3.19
R (6,7)=R(8,5)= 3.43
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.56
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.51

Bond Angles

A(1,4,3)=A(1,2,3)= 115.92
A(4,1,2)=A(2,3,4)= 63.82
A(1,5,4)=A(4,8,3)= 48.16
A(3,7,2)=A(2,6,1)= 48.16
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



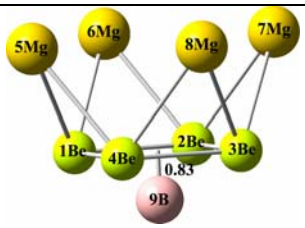
Mg_4Be_4-Zn

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.11
R(5,6)=R(7,8)= 2.22; R (6,7)=R(8,5)= 3.23
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.62
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.54

Bond Angles

A(1,4,3)=A(1,2,3)= 114.06
A(4,1,2)=A(2,3,4)= 65.88
A(1,5,4)=A(4,8,3)= 48.23
A(3,7,2)=A(2,6,1)= 48.23
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



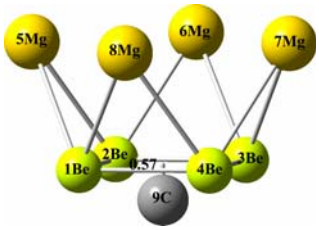
Mg_4Be_4-B

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.21
R(5,6)=R(7,8)=R (6,7)=R(8,5)= 3.19
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.48
R(1,5)=R(1,6)=R(3,8)=R(3,7)= 2.48

Bond Angles

A(1,4,3)=A(1,2,3)= 90.00
A(4,1,2)=A(2,3,4)= 90.00
A(1,5,4)=A(4,8,3)= 52.77
A(3,7,2)=A(2,6,1)= 52.77
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00



Mg_4Be_4-C

Bond Distances

R(1,2)=R(2,3)=R(3,4)=R(4,1)= 2.19
R(5,6)=R(7,8)= R (6,7)=R(8,5)= 3.05
R(4,5)=R(4,8)= R(2,6)=R(2,7)= 2.50
R(1,5)=R(1,6)=R(3,8)=R(3,7)=2.50

Bond Angles

A(1,4,3)=A(1,2,3)= 90.00
A(4,1,2)=A(2,3,4)= 90.00
A(1,5,4)=A(4,8,3)= 51.92
A(3,7,2)=A(2,6,1)= 51.92
A(6,5,8)=A(5,8,7)= 90.00
A(8,7,6)=A(7,6,5)= 90.00

Scheme S4. Optimized geometries (B3LYP/6-311+G*) and some important bond lengths(R, Å) of two different Be_6-Mg isomers and the transition state separating them.

<table>
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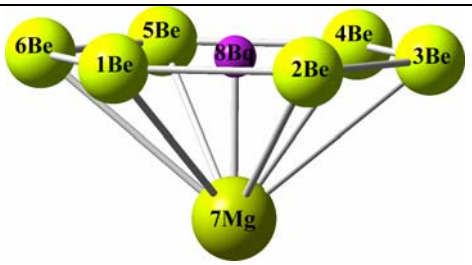
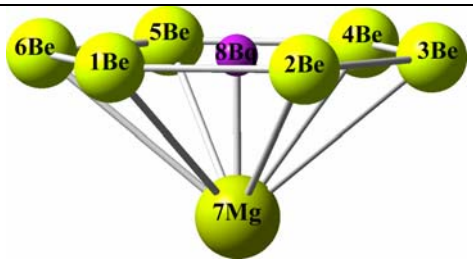
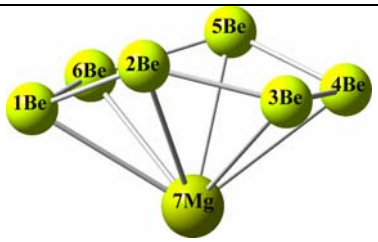
<td> 

Be_6–Mg I (C_{6v})
E = -288.370 (a.u.)
R17=2.70, R27=2.70, R37=2.70, R47=2.70, R57=2.70, R67=2.70, R87=1.71</td>
<td> 

Be_6–Mg II (C_{6v})
E = -288.370 (a.u.)
R17=2.71, R27=2.71, R37=2.71, R47=2.71, R57=2.70, R67=2.70, R87=1.72</td>
</tr>
<tr>
<td colspan="2">8(Bq)= Dummy atom at the center of the planar Be_6 ring.</td>
</tr>
<tr>
<td colspan="2"> 

Be_6-Mg (C_2) TS
E= -288.364 (a.u.)
R17=2.74, R27=2.71, R37=2.63, R47=2.74, R57=2.71, R67=2.63</td>
</tr>
</table>

Table S1. Total Energy (E, au), electronegativity (χ, eV), hardness (η, eV), electrophilicity (ω, eV) of different molecules involved in the substitution reactions

Molecules	E(au)	χ (eV)	η (eV)	ω (eV)
Al_4^{2-}	-969.741	-3.629	1.957	3.364
B_4^{2-}	-99.088	-5.135	1.711	7.705
B_3^-	-74.397	-0.678	3.368	0.068
Cp^-	-193.570	-1.512	3.423	0.334
Cp-Fe-Cp	-1650.883	3.400	3.695	1.564
$[Cp\text{-}Fe\text{-}Al_4]^-$	-2427.117	0.066	1.747	0.001
$[Al_4\text{-}Fe\text{-}Al_4]^{2-}$	-3203.326	-2.391	1.423	2.008
$[Cp\text{-}Fe\text{-}B_4]^-$	-1556.565	-0.301	2.128	0.021
$[B_4\text{-}Fe\text{-}B_4]^{2-}$	-1462.183	-3.183	1.512	3.351
$[Al_4\text{-}Fe\text{-}B_4]^{2-}$	-2332.783	-2.961	1.649	2.658
$B_3\text{-}Fe\text{-}B_3$	-1412.411	5.543	2.491	6.168
$[Al_4\text{-}Fe\text{-}B_3]^-$	-2307.909	0.797	1.273	0.250
$[B_4\text{-}Fe\text{-}B_3]^-$	-1437.380	0.803	1.724	0.187
$Cp\text{-}Fe\text{-}B_3$	-1531.634	4.610	2.349	4.523

Table S2. Total Energy (E, au), electronegativity (χ, eV), hardness (η, eV), electrophilicity (ω, eV) of different molecules involved in the substitution reactions

Molecules	E (au)	χ (eV)	η (eV)	ω (eV)
$[N_4\text{-}Fe\text{-}N_4]^{2-}$	-1701.573	-3.551	1.996	3.158
$[P_4\text{-}Fe\text{-}P_4]^{2-}$	-3994.880	-2.959	2.013	2.175
$[N_4\text{-}Fe\text{-}P_4]^{2-}$	-2848.227	-3.121	1.923	2.532
$[B_3\text{-}Fe\text{-}P_4]^-$	-2703.703	0.675	1.950	0.117
$[B_4\text{-}Fe\text{-}B_4]^{2-}$	-1462.183	-3.183	1.512	3.351
$[B_3\text{-}Fe\text{-}N_4]^-$	-1557.068	0.985	2.041	0.236
$B_3\text{-}Fe\text{-}B_3$	-1412.411	5.543	2.491	6.168
$[B_4\text{-}Fe\text{-}N_4]^{2-}$	-1581.862	-3.332	1.272	4.365
$[Cp\text{-}Fe\text{-}P_4]^-$	-2822.930	0.019	2.589	0.000
$[B_4\text{-}Fe\text{-}P_4]^{2-}$	-2728.518	-3.144	1.419	3.484
$[Cp\text{-}Fe\text{-}N_4]^-$	-1676.292	0.020	2.860	0.000
Cp-Fe-Cp	-1650.883	3.400	3.695	1.564
Cp^-	-193.570	-1.512	3.423	0.334
B_3^-	-74.397	-0.678	3.368	0.068
B_4^{2-}	-99.088	-5.135	1.711	7.705
N_4^{2-}	-218.781	-7.633	3.836	7.595
P_4^{2-}	-1365.475	-4.560	2.514	4.135

Table S3. Point group (PG), Nucleus independent chemical shift (NICS, ppm) values at different rings of molecules

Molecules	PG	NICS(0),ppm	
Al_4^{2-}	D_{4h}	-34.473	
B_4^{2-}	D_{4h}	-44.785	
B_3^-	D_{3h}	-73.599	
Cp^-	D_{5h}	-12.531	
Cp-Fe-Cp	D_{5h}	Cp (-45.871)	Cp (-45.871)
$[Al_4\text{-Fe-Cp}]^-$	C_s	Al_4 (-19.329)	Cp (-31.470)
$[Al_4\text{-Fe-}Al_4]^{2-}$	C_{2h}	Al_4 (2,3,5,6) (29583.330)	
$[Cp\text{-Fe-}B_4]^-$	C_1	B_4 (-16.178)	Cp (-56.558)
$[B_4\text{-Fe-}B_4]^{2-}$	C_2	B_4 (-25.549)	B_4 (-25.680)
$[Al_4\text{-Fe-}B_4]^{2-}$	C_s	Al_4 (158.627)	B_4 (-30.502)
$B_3\text{-Fe-}B_3$	D_{2d}	B_3 (-31.871)	B_3 (-31.867)
$[Al_4\text{-Fe-}B_3]^-$	C_s	B_3 (-2.813)	Al_4 (-10.268)
$[B_4\text{-Fe-}B_3]^-$	C_s	B_3 (9.598)	B_4 (9.530)
$Cp\text{-Fe-}B_3$	C_1	B_3(-6.740)	Cp(-12.926)

Table S4. Point group (PG), Nucleus independent chemical shift (NICS, ppm) values at different rings of molecules

Molecules	PG	NICS(0),ppm	
$[N_4\text{-Fe-}N_4]^{2-}$	S_8	N_4(-32.859)	N_4(-32.896)
$[P_4\text{-Fe-}P_4]^{2-}$	S_8	P_4(-8.988)	P_4(-9.005)
$[N_4\text{-Fe-}P_4]^{2-}$	C_{4v}	N_4(-20.631)	P_4(-19.478)
$[B_3\text{-Fe-}P_4]^-$	C_{2v}	P_4(24.924)	B_3(5.191)
$[B_4\text{-Fe-}B_4]^{2-}$	C_2	B_4(-24.490)	B_4(-8.252)
$[B_3\text{-Fe-}N_4]^-$	C_s	N_4(-59.576)	B_3(-61.762)
$B_3\text{-Fe-}B_3$	D_{2d}	B_3(-31.871)	B_3(-31.867)
$[B_4\text{-Fe-}N_4]^{2-}$	C_1	N_4(-7.598)	B_4(-4.076)
$[Cp\text{-Fe-}P_4]^-$	C_s	P_4(-15.059)	Cp(-39.158)
$[B_4\text{-Fe-}P_4]^{2-}$	C_1	B_4(-24.450)	P_4(-8.252)
$[Cp\text{-Fe-}N_4]^-$	C_1	Cp(-50.737)	N_4(-28.157)
Cp-Fe-Cp	D_{5h}	Cp (-45.871)	Cp (-45.871)
Cp^-	D_{5h}	-12.531	
B_3^-	D_{3h}	-73.599	
B_4^{2-}	D_{4h}	-44.785	
N_4^{2-}	D_{4h}	4.051	
P_4^{2-}	D_{4h}	9.692	

Table S5: Atomic charges ($Q_{k,}$(NPA)) and Fukui functions (f_k^+, f_k^- eV, (NPA)) values for different molecules involved in the substitution reactions

Molecules	Unit	Atomic charge (Q_k)	f_k^+(NPA)	f_k^-(NPA)
Cp-Fe-Cp (D_{5h})	Cp Cp Fe	-0.251,-0.251,-0.251,-0.251,-0.251 -0.251,-0.251,-0.251,-0.251,-0.251 0.218	-0.074,0.034,0.005,0.005,0.034 0.005,0.003,-0.074,0.034,0.005 0.899	0.037,0.038,0.036,0.036,0.038 0.036,0.038,0.037,0.038,0.036 0.286
$[Cp\text{-}Fe\text{-}Al_4]^-$ (C_s)	Cp Al_4 Fe	-0.339,-0.340,-0.343,-0.345,-0.347 0.261,0.253,0.250,0.254 -1.408	0.002,0.002,0.005,0.005,0.008 0.333,0.331,0.325,0.331 -0.371	0.021,0.036,0.009,0.004,0.020 0.186,0.077,0231,0.074 0.280
$[Al_4\text{-}Fe\text{-}Al_4]^{2-}$ (C_{2h})	Al_4 Al_4 Fe	-0.204,-0.196,-0.038,0.336 -0.042,0.336,-0.203,-0.194 -1.797	0.206,0.215,0.089,0.147 0.089,0.148,0.209,0.214 -0.316	0.236,0.194,0.050,0.076 0.052,0.074,0.237,0.191 -0.110
$[Cp\text{-}Fe\text{-}B_4]^-$ (C_1)	Cp B_4 Fe	-0.300,-0.281,-0.305,-0.256,-0.336 -0.320,-0.136,-0.234,-0.029 -0.029	0.003,0.027,0.025,0.019,0.010 0.042,0.068,0.027,0.028 0.576	0.012,0.055,0.025,-0.002,0.052 0.114,0.239,-0.048,0.043 0.547
$[B_4\text{-}Fe\text{-}B_4]^{2-}$ (C_2)	B_4 B_4 Fe	0.065,-0.298,-0.376,-0.286 -0.376,-0.286,0.065,-0.299 -0.209	0.010,0.001,0.018,0.031 0.018,0.030,0.010,0.001 0.881	0.006,-0.030,0.070,0.248 0.072,0.243,0.005,-0.042 0.427
$[Al_4\text{-}Fe\text{-}B_4]^{2-}$ (C_s)	Al_4 B_4 Fe	0.291,0.025,0.287,0.121 -0.364,-0.278,-0.178,-0.267 -1.638	0.263,0.121,0.283,0.111 0.023,-0.028,0.160,0.065 0.002	0.107,0.282,0.079,0.287 0.023,0.035,0.122,0.062 0.002
$B_3\text{-}Fe\text{-}B_3$ (D_{2d})	B_3 B_3 Fe	0.093,0.092,-0.047 0.093,-0.047,0.093 -0.278	0.115,0.110,0.284 0.112,0.287,0.118 -0.026	0.014,0.015,0.204 0.014,0.204,0.014 0.536
$[Al_4\text{-}Fe\text{-}B_3]^-$ (C_s)	Al_4 B_3 Fe	0.268,-0.025,-0.316,0.026 -0.124,-0.163,-0.125 -0.540	0.282,0.213,0.082,0.308 0.159,0.159,0.159 -0.363	-0.012,-0.070,0.244,0.252 -0.038,0.176,-0.041 0.489
$[B_4\text{-}Fe\text{-}B_3]^-$ (C_s)	B_4 B_3 Fe	-0.065,-0.258,-0.011,-0.189 -0.169,-0.166,-0.168 0.026	0.254,0.073,0.167,0.095 0.146,0.210,0.146 -0.091	0.187,0.146,0.002,-0.016 0.028,0.315,0.028 0.311
$Cp\text{-}Fe\text{-}B_3$ (C_1)	Cp B_3 Fe	-0.272,-0.248,-0.272,-0.256,-0.269 0.031,-0.016,0.026 0.102	0.037,0.044,0.032,0.041,0.038 0.208,0.294,0.206 -0.002	0.018,0.057,0.011,0.048,0.033 0.002,0.315,0.003 0.371

Table S6: Atomic charges(Q_k, NPA) and Fukui functions(f_k^+, f_k^-, eV, (NPA)) values for nucleophilic and electrophilic attacks respectively for different molecules involved in the substitution reactions

Molecules	**Unit**	**Atomic charges (Q_k)**	f_k^+ (NPA)	f_k^- (NPA)
$[N_4\text{-Fe-}N_4]^{2-}$ (S_8)	N_4	-0.321,-0.323,-0.321,-0.320	0.013,0.011,0.013,0.007	0.091,0.086,0.090,0.086
	N_4	-0.321,-0.320,-0.322,-0.323	0.013,0.007,0.013,0.011	0.088,0.089,0.088,0.089
	Fe	0.570	0.913	0.294
$[P_4\text{-Fe-}P_4]^{2-}$ (S_8)	P_4	-0.138,-0.138,-0.138,-0.138	0.029,0.029,0.029,0.029	0.093,0.094,0.095,0.094
	P_4	-0.138,-0.138,-0.138,-0.138	0.029,0.029,0.029,0.029	0.095,0.094,0.093,0.094
	Fe	-0.897	0.771	0.247
$[N_4\text{-Fe-}P_4]^{2-}$ (C_4v)	N_4	-0.259,-0.259,-0.259,-0.259	0.011,0.010,0.011,0.010	0.053,0.052,0.053,0.052
	P_4	-0.247,-0.247,-0.247,-0.247	0.029,0.029,0.028,0.030	0.148,0.146,0.148,0.146
	Fe	0.024	0.843	0.200
$[B_3\text{-Fe-}P_4]^{-}$ (C_2v)	P_4	-0.059,-0.152,-0.057	0.124.284,0.121	-0.029,0.298,-0.031
	B_3	-0.117,-0.117,-0.117,-0.117	0.163,0.163,0.151,0.154	0.110,0.115,0.112,0.114
	Fe	-0.262	-0.161	0.311
$[B_4\text{-Fe-}B_4]^{2-}$ (C_2)	B_4	0.065,-0.298,-0.376,-0.286	0.010,0.001,0.018,0.031	0.006,-0.030,0.070,0.248
	B_4	-0.376,-0.286,0.065,-0.267	0.018,0.030,0.010,0.001	0.072,0.243,0.005,-0.042
	Fe	-0.209	0.881	0.427
$[B_3\text{-Fe-}N_4]^{-}$ (C_s)	B_3	-0.357,-0.106,-0.146	0.091,0.374,0.170	0.201,0.274,0.056
	N_4	-0.180,-0.252,-0.257,-0.181	0.074,0.100,0.095,0.074	0.045,0.061,0.063,0.052
	Fe	0.478	0.024	0.249
$B_3\text{-Fe-}B_3$ (D_2d)	B_3	0.093,0.092,-0.047	0.115,0.110,.284	0.014,0.015,0.204
	B_3	0.093,-0.047,0.093	0.112,0.287,0.118	0.014,0.204,0.014
	Fe	-0.278	-0.026	0.536
$[B_4\text{-Fe-}N_4]^{2-}$ (C_1)	B_4	-0.266,-0.144,-0.402,-0.322	0.071,0.059,0.052,0.077	-0.049,0.078,0.104,0.298
	N_4	-0.279,-0.286,-0.325,-0.288	0.017,0.024,0.016,0.0191	0.029,0.070,0.042,0.098
	Fe	0.312	0.656	0.329
$[Cp\text{-Fe-}P_4]^{-}$ (C_s)	Cp	-0.265,-0.269,-0.269,-0.267,-0.263	0.045,0.012,0.012,0.045,-0.087	0.020,0.019,0.019,0.020,0.020
	P_4	-0.129,-0.127,-0.131,-0.132	0.032,0.030,0.033,0.032	0.144,0.145,0.144,0.144
	Fe	-.230	0.824	0.189
$[B_4\text{-Fe-}P_4]^{2-}$ (C_1)	B_4	-0.178,0.029,-0.391,-0.256	0.021,0.108,0.012,0.096	-0.070,-0.011,0.095,0.249
	P_4	-0.140,-0.324,-0.315,-0.114	0.045,-0.007,0.007,0.050	0.086,0.127,0.115,0.066
	Fe	-0.311	0.660	0.342
$[Cp\text{-Fe-}N_4]^{-}$ (C_1)	Cp	-0.299,-0.298,-0.297,-0.296,-0.295	0.032,0.033,-0.069,-0.069,0.058	0.038,0.038,0.039,0.040,0.041
	N_4	-0.248,-0.246,-0.248,-0.247	0.065,-0.064,-0.065,0.065	0.080,0.081,0.085,0.079
	Fe	0.432	0.928	0.302
[Cp-Fe-Cp] (D_{5h})	Cp	-0.251,-0.251,-0.251,-0.251,-0.251	-0.074,0.034,0.005,0.005,0.034	0.037,0.038,0.036,0.036,0.038
	Cp	-0.251,-0.251,-0.251,-0.251,-0.251	0.005,0.003,-0.074,0.034,0.005	0.036,0.038,0.037,0.038,0.036
	Fe	0.218	0.899	0.286

Table S7: Reaction enthalpy (ΔH, Kcal/mole) and reaction electrophilicity (Δω, eV) values of different molecules which are involved in the substitution reactions

No.	Reactions	ΔH (Kcal/mole)	Δω (eV)
1	$Cp\text{-}Fe\text{-}Cp + Al_4^{2-} = [Cp\text{-}Fe\text{-}Al_4]^- + Cp^-$	-99.305	-4.592
2	$[Cp\text{-}Fe\text{-}Al_4]^- + Al_4^{2-} = [Al_4\text{-}Fe\text{-}Al_4]^{2-} + Cp^-$	-81.875	-1.022
3	$Cp\text{-}Fe\text{-}Cp + B_4^{2-} = [Cp\text{-}Fe\text{-}B_4]^- + Cp^-$	-104.845	-8.913
4	$[Cp\text{-}Fe\text{-}B_4]^- + B_4^{2-} = [B_4\text{-}Fe\text{-}B_4]^{2-} + Cp^-$	-63.361	-4.041
5	$[Al_4\text{-}Fe\text{-}B_3]^- + Al_4^{2-} = [Al_4\text{-}Fe\text{-}Al_4]^{2-} + B_3^-$	-102.995	-1.537
6	$[B_4\text{-}Fe\text{-}B_3]^- + B_4^{2-} = [B_4\text{-}Fe\text{-}B_4]^{2-} + B_3^-$	-69.878	-4.473
7	$B_3\text{-}Fe\text{-}B_3 + Al_4^{2-} = [Al_4\text{-}Fe\text{-}B_3]^- + B_3^-$	-153.169	-9.213
8	$B_3\text{-}Fe\text{-}B_3 + B_4^{2-} = [B_4\text{-}Fe\text{-}B_3]^- + B_3^-$	-173.312	-13.618
9	$[Al_4\text{-}Fe\text{-}Cp]^- + B_4^{2-} = [Al_4\text{-}Fe\text{-}B_4]^{2-} + Cp^-$	-92.741	-4.715
10	$[Al_4\text{-}Fe\text{-}B_3]^- + B_4^{2-} = [B_4\text{-}Fe\text{-}Al_4]^{2-} + B_3^-$	-113.68	-5.229
11	$[Cp\text{-}Fe\text{-}B_4]^- + Al_4^{2-} = [Al_4\text{-}Fe\text{-}B_4]^{2-} + Cp^-$	-87.202	-0.393
12	$[B_4\text{-}Fe\text{-}B_4]^{2-} + Al_4^{2-} = [Al_4\text{-}Fe\text{-}B_4]^{2-} + B_4^{2-}$	-23.841	3.648
13	$[B_4\text{-}Fe\text{-}B_3]^- + Al_4^{2-} = [Al_4\text{-}Fe\text{-}B_4]^{2-} + B_3^-$	-93.72	-0.825
14	$[Al_4\text{-}Fe\text{-}Al_4]^{2-} + B_4^{2-} = [Al_4\text{-}Fe\text{-}B_4]^{2-} + Al_4^{2-}$	-10.866	-3.692
15	$B_3\text{-}Fe\text{-}B_3 + Cp^- = Cp\text{-}Fe\text{-}B_3 + B_3^-$	-29.251	-1.911
16	$Cp\text{-}Fe\text{-}B_3 + Cp^- = Cp\text{-}Fe\text{-}Cp + B_3^-$	-45.733	-3.225

Table S8: Reaction enthalpy (ΔH) and reaction electrophilicity (Δω) values of different molecules which are involved in the substitution reactions

Table 9: Energy (E, au), electronegativity (χ, eV), hardness (η, eV), and electrophilicity (ω, eV) for different atoms invole in the formation of different [Mg_4Be_4-M] clusters

No	Reactions	ΔH(Kcal/mole)	Δω(eV)
1	B_3-Fe-B_3 + N_4^{2-} = [B_3-Fe-N_4]$^-$ + B_3^-	-171.014	-13.458
2	[B_3-Fe-N_4]$^-$ + N_4^{2-} = [N_4-Fe-N_4]$^{2-}$ + B_3^-	-75.733	-4.605
3	[B_3-Fe-P_4]$^-$ + N_4^{2-} = [B_3-Fe-N_4]$^-$ + P_4^{2-}	-36.930	-3.339
4	B_3-Fe-B_3 + P_4^{2-} = [B_3-Fe-P_4]$^-$+ B_3^-	-134.084	-10.118
5	[B_3-Fe-P_4]$^-$ + P_4^{2-} = [P_4-Fe-P_4]$^{2-}$ + B^{3-}	-61.692	-2.010
6	[B_4-Fe-P_4]$^{2-}$ + N_4^{2-} = [B_4-Fe-N_4]$^{2-}$ + P_4^{2-}	-23.917	-2.578
7	[P_4-Fe-P_4]$^{2-}$ + N_4^{2-} = [N_4-Fe-P_4]$^{2-}$ + P_4^{2-}	-25.863	-3.102
8	[N_4-Fe-P_4]$^{2-}$ + N_4^{2-} = [N_4-Fe-N_4]$^{2-}$ + P_4^{2-}	-25.108	-2.833
9	[Cp-Fe-P_4]$^-$ + N_4^{2-} =[Cp-Fe-N_4]$^-$ + P_4^{2-}	-34.942	-3.459
10	[P_4-Fe-P_4]$^{2-}$ + B_4^{2-} = [B_4-Fe-P_4]$^{2-}$ + P_4^{2-}	-14.997	-2.260
11	[B_4-Fe-P_4]$^{2-}$ + B_4^{2-} = [B_4-Fe-B_4]$^{2-}$ + P_4^{2-}	-32.416	-3.703
12	Cp-Fe-B_3 + N_4^{2-} = [Cp-Fe-N_4]$^-$ + B_3^-	-171.850	-12.049
13	[B_4-Fe-N_4]$^{2-}$ + N_4^{2-} = [N_4-Fe-N_4]$^{2-}$ + B_4^{2-}	-12.056	-1.097
14	[B_4-Fe-N_4]$^{2-}$ + B_4^{2-} = [B_4-Fe-B_4]$^{2-}$ + N_4^{2-}	-8.498	-1.125
15	Cp-Fe-Cp + P_4^{2-} = [Cp-Fe-P_4]$^-$+ Cp^-	-91.175	-5.365
16	[Cp-Fe-P_4]$^-$ + P_4^{2-} = [P_4-Fe-P_4]$^{2-}$ + Cp^-	-29.618	-1.627
17	Cp-Fe-B_3 + P_4^{2-} = [Cp-Fe-P_4]$^-$ + B_3^-	-136.908	-8.590
18	Cp-Fe-Cp + N_4^{2-} =[Cp-Fe-N_4]$^-$ + Cp^-	-126.118	-8.824
19	[Cp-Fe-N_4]$^-$ + N_4^{2-} = [N_4-Fe-N_4]$^{2-}$ + Cp^-	-45.646	-4.102

Atoms	E (au)	χ (eV)	η (eV)	ω (eV)
Li	-7.491	3.087	2.529	1.884
Na	-162.287	3.003	2.418	1.864
K	-599.926	2.510	1.986	1.586
Be	-14.671	4.445	4.671	2.115
Mg	-200.093	3.752	3.976	1.770
Ca	-677.576	3.085	3.069	1.551
Sc	-760.621	3.506	4.607	1.334
Ti	-849.290	3.648	2.098	3.172
Cr	-1044.224	3.879	1.560	4.821
Zn	-1779.354	4.199	5.230	1.685
C	-37.792	5.706	4.064	4.006
B	-24.662	4.189	4.545	1.930

Table S10: Point group (PG), energy (E, au), electronegativity (χ, eV), hardness (η, eV), and electrophilicity (ω, eV) for different metal clusters

Molecules	PG	E (au)	χ (eV)	η (eV)	ω (eV)
Be_4	D_{4h}	-58.766	3.688	2.261	3.007
Mg_4	D_{4h}	-800.309	2.987	1.508	2.959
Mg_4Be_4	C_{2v}	-859.276	3.526	1.792	3.468
Mg_4Be_4-Li	C_{2v}	-866.838	3.423	1.821	3.217
Mg_4Be_4-Na	C_1	-1021.618	3.301	1.792	3.040
Mg_4Be_4-K	C_{2v}	-1459.259	3.118	1.770	2.747
Mg_4Be_4-Be	C_{4v}	-874.050	3.694	2.020	3.377
Mg_4Be_4-Mg	C_{2v}	-1059.404	3.545	1.874	3.353
Mg_4Be_4-Ca	C_{2v}	-1536.917	3.245	1.872	2.812
Mg_4Be_4-Sc	C_{4v}	-1620.007	3.319	1.805	3.051
Mg_4Be_4-Ti	C_{4v}	-1708.722	3.580	1.562	4.103
Mg_4Be_4-Cr	C_{2v}	-1903.673	2.906	1.131	3.734
Mg_4Be_4-Zn	C_{2v}	-2638.652	3.766	1.881	3.770
Mg_4Be_4-B	C_{4v}	-884.168	3.401	1.954	3.752
Mg_4Be_4-C	C_{4v}	-897.466	3.830	2.399	2.410

Table S11: Nucleus independent chemical shift (NICS(0), ppm) values at different rings of the molecules

Molecules	NICS(0) Ring(Mg_4)	NICS(0) Ring(Be_4)	Molecules	NICS(0) Ring(Mg_4)	NICS(0) Ring(Be_4)
Mg_4Be_4	-10.03	-15.13	Mg_4Be_4-Sc	-18.94	-66.30
Mg_4Be_4-Li	-10.87	-12.04	Mg_4Be_4-Ti	-2.92	-98.78
Mg_4Be_4-Na	-10.39	-11.67	Mg_4Be_4-Cr	-55.33	-471.90
Mg_4Be_4-K	-11.02	-10.39	Mg_4Be_4-Zn	15.80	-3.057
Mg_4Be_4-Be	-12.29	-31.16	Mg_4Be_4-B	-25.51	-56.80
Mg_4Be_4-Mg	8.18	-11.59	Mg_4Be_4-C	-32.33	-67.39
Mg_4Be_4-Ca	-4.62	-25.78			

Table S12: Formation reactions of different metal clusters and their reaction enthalpy (ΔH, Kcal/mole) and reaction electrophilicity (Δω, eV) values

Formation Reactions	ΔH (Kcal/mole)	Δω (eV)
$Mg_4 + Be_4 = Mg_4Be_4$	-123.979	-2.498
$Mg_4Be_4 + Li = Mg_4Be_4$-Li	-4.456	-0.780
$Mg_4Be_4 + Na = Mg_4Be_4$-Na	-34.067	-0.743
$Mg_4Be_4 + K = Mg_4Be_4$-K	-35.452	-0.556
$Mg_4Be_4 + Be = Mg_4Be_4$-Be	-23.163	-2.206
$Mg_4Be_4 + Mg = Mg_4Be_4$-Mg	-21.830	-1.885
$Mg_4Be_4 + Ca = Mg_4Be_4$-Ca	-40.587	-2.206
$Mg_4Be_4 + Sc = Mg_4Be_4$-Sc	-68.793	-1.751
$Mg_4Be_4 + Ti = Mg_4Be_4$-Ti	-97.014	-2.537
$Mg_4Be_4 + Cr = Mg_4Be_4$-Cr	-108.320	-4.555
$Mg_4Be_4 + Zn = Mg_4Be_4$-Zn	-14.264	-1.383
$Mg_4Be_4 + B = Mg_4Be_4$-B	-142.402	-1.646
$Mg_4Be_4 + C = Mg_4Be_4$-C	-247.214	-5.064

Table S13: Atomic charges (Q_k(NPA)) and Fukui functions (f_k^+, f_k^-, eV, (NPA)) and philicity (ω_k^+, ω_k^-, eV, (NPA)) values for nucleophilic and electrophilic attacks respectively for different metal cluster

Molecules	Unit	Atomic Charge (Q_k) (NPA)	f_k^+ (NPA)	f_k^- (NPA)	ω_k^+ (NPA)	ω_k^- (NPA)
Mg_4 Be_4 (C_{2v})	Mg_4	0.346, 0.347	0.136, 0.137	0.099, 0.099	0.472, 0.474	0.343, 0.342
		0.346, 0.346	0.136, 0.137	0.099, 0.099	0.473, 0.474	0.343, 0.342
	Be_4	-0.211, -0.482	0.096, 0.130	0.156, 0.148	0.333, 0.451	0.541, 0.513
		-0.483, -0.210	0.130, 0.098	0.148, 0.153	0.452, 0.339	0.514, 0.530
Mg_4 Be_4-Li (C_{2v})	Mg_4	0.333, 0.334	0.148, 0.148	0.154, 0.155	0.476, 0.476	0.497, 0.498
		0.336, 0.336	0.148, 0.148	0.155, 0.154	0.477, 0.477	0.497, 0.498
	Be_4	-0.259, -0.564	0.049, 0.091	0.046, 0.100	0.158, 0.292	0.148, 0.321
		-0.575, -0.263	0.078, 0.047	0.091, 0.047	0.250, 0.153	0.294, 0.150
	Li	0.322	0.143	0.097	0.459	0.314
Mg_4 Be_4-Na (C_1)	Mg_4	0.339, 0.328	0.147, 0.145	0.145, 0.143	0.446, 0.440	0.441, 0.435
		0.326, 0.315	0.138, 0.135	0.143, 0.140	0.419, 0.410	0.434, 0.425
	Be_4	-0.287, -0.569	0.039, 0.045	0.048, 0.067	0.117, 0.136	0.146, 0.203
		-0.491, -0.252	0.106, 0.044	0.112, 0.052	0.323, 0.133	0.341, 0.157
	Na	0.291	0.203	0.151	0.616	0.458
Mg_4 Be_4-K (C_{2v})	Mg_4	0.313, 0.314	0.136, 0.136	0.137, 0.137	0.374, 0.374	0.377, 0.375
		0.313, 0.314	0.136, 0.136	0.137, 0.137	0.375, 0.374	0.378, 0.375
	Be_4	-0.302, -0.567	0.036, 0.063	0.058, 0.096	0.099, 0.173	0.159, 0.264
		-0.568, -0.298	0.063, 0.037	0.095, 0.052	0.173, 0.102	0.262, 0.143
	K	0.482	0.256	0.150	0.704	0.413
Mg_4 Be_4-Be (C_{4v})	Mg_4	0.343, 0.344	0.106, 0.106	0.088, 0.088	0.358, 0.358	0.298, 0.298
		0.344, 0.344	0.106, 0.106	0.088, 0.088	0.358, 0.359	0.298, 0.298
	Be_4	-0.400, -0.401	0.081, 0.081	0.139, 0.137	0.275, 0.274	0.470, 0.463
		-0.401, -0.401	0.081, 0.081	0.137, 0.139	0.274, 0.273	0.463, 0.468
	Be	0.230	0.250	0.095	0.846	0.322
Mg_4 Be_4-Mg (C_{2v})	Mg_4	0.266, 0.266	0.105, 0.105	0.163, 0.163	0.352, 0.352	0.547, 0.548
		0.264, 0.264	0.104, 0.104	0.164, 0.164	0.348, 0.348	0.550, 0.551
	Be_4	-0.269, -0.489	-0.020, 0.232	0.050, 0.078	-0.050, 0.779	0.166, 0.261
		-0.491, -0.270	0.229, -0.020	0.080, 0.050	0.767, -0.050	0.267, 0.167
	Mg	0.459	0.153	0.088	0.512	0.297
Mg_4 Be_4-Ca (C_{2v})	Mg_4	0.270, 0.270	0.090, 0.090	0.297, 0.297	0.254, 0.257	0.236, 0.234
		0.270, 0.270	0.090, 0.091	0.297, 0.297	0.252, 0.254	0.235, 0.234
	Be_4	-0.311, -0.594	-0.000, 0.172	0.205, -0.010	-0.000, 0.483	0.576, -0.035
		-0.594, -0.310	0.170, 0.002	-0.010, 0.202	0.477, 0.007	-0.039, 0.569
	Ca	0.729	0.295	0.286	0.830	0.803
Mg_4 Be_4-Sc (C_{4v})	Mg_4	0.320, 0.319	0.082, 0.081	0.083, 0.083	0.249, 0.247	0.252, 0.253
		0.320, 0.320	0.079, 0.079	0.082, 0.082	0.243, 0.240	0.251, 0.251
	Be_4	-0.093, -0.090	0.082, 0.081	0.081, 0.083	0.289, 0.289	0.247, 0.253
		-0.090, -0.093	0.079, 0.079	0.080, 0.082	0.271, 0.284	0.245, 0.251
	Sc	-0.913	0.082	0.344	0.940	1.048
Mg_4 Be_4-Ti (C_{4v})	Mg_4	0.357, 0.357	0.128, 0.128	0.059, 0.059	0.527, 0.527	0.241, 0.241
		0.357, 0.357	0.128, 0.128	0.059, 0.059	0.527, 0.527	0.241, 0.241
	Be_4	0.068, 0.069	0.131, 0.132	0.107, 0.106	0.540, 0.541	0.440, 0.437
		0.069, 0.068	0.131, 0.132	0.106, 0.107	0.541, 0.540	0.437, 0.440
	Ti	-1.703	-0.040	0.337	-0.160	1.384
Mg_4 Be_4-Cr (C_{2v})	Mg_4	0.323, 0.323	0.122, 0.123	0.143, 0.143	0.455, 0.458	0.535, 0.534
		0.323, 0.324	0.122, 0.123	0.143, 0.143	0.456, 0.459	0.535, 0.533
	Be_4	0.036, -0.115	0.008, 0.019	0.021, 0.003	0.030, 0.071	0.079, 0.012
		-0.114, 0.038	0.019, 0.010	0.002, 0.091	0.072, 0.037	0.009, 0.071

	Cr	-1.139	0.454	0.382	1.696	1.426
Mg_4 Be_4-Zn (C_{2v})	Mg_4	0.254, 0.254	0.102, 0.099	0.162, 0.162	0.385, 0.375	0.609, 0.611
		0.256, 0.255	0.104, 0.101	0.161, 0.161	0.393, 0.382	0.607, 0.609
	Be_4	-0.233, -0.395	-0.011, 0.272	0.022, 0.134	-0.040, 1.025	0.082, 0.505
		-0.391, -0.234	0.277, -0.020	0.128, 0.023	1.043, -0.080	0.483, 0.089
	Zn	0.233	0.075	0.046	0.285	0.174
Mg_4 Be_4-B (C_{4v})	Mg_4	0.356, 0.355	0.956, 0.955	0.113, 0.115	0.359, 0.355	0.425, 0.433
		0.355, 0.356	0.956, 0.955	0.113, 0.115	0.359, 0.356	0.425, 0.432
	Be_4	0.489, 0.482	0.177,0.109	0.089, 0.094	0.438, 0.408	0.333, 0.353
		0.482, 0.481	0.109, 0.109	0.094, 0.097	0.410, 0.409	0.351, 0.365
	B	-3.356	0.175	0.169	0.658	0.635
Mg_4 Be_4-C (C_{4v})	Mg_4	0.351, 0.353	0.104, 0.092	0.094, 0.094	0.251, 0.221	0.226, 0.226
		0.351, 0.352	0.090, 0.106	0.094, 0.094	0.218, 0.255	0.227, 0.226
	Be_4	0.487, 0.489	0.034, 0.251	0.130, 0.116	0.082, 0.605	0.314, 0.279
		0.487, 0.484	0.248, 0.033	0.122, 0.128	0.598, 0.079	0.294, 0.308
	C	-3.353	0.042	0.129	0.100	0.311

Table S14: Energy (E, au), Point Group (PG), Electronegativity (χ, eV), Chemical Hardness (η, eV) and Electrophilicity (ω, eV) values of two different Be_6-Mg isomers.

Isomers	E (a.u.)	PG	χ (eV)	η (eV)	ω (eV)
Be_6-Mg (I)	-288.370	C_{6v}	3.715	1.949	3.541
Be_6-Mg (TS)	-288.364	C_2	3.848	1.952	3.792
Be_6-Mg (II)	-288.370	C_{6v}	3.713	1.949	3.537

Table S15: Nucleus independent chemical shift (NICS(0),ppm), atomic charges (Q_K, NPA) and Fukui function (fk^+, fk^-, eV, (NPA)) values for nucleophilic and electrophilic attacks respectively of two different Be_6-Mg isomers.

Isomers	Unit	NICS(0)	Atomic Charges (Q_K)	fk^+ (NPA)	fk^- (NPA)
Be_6-Mg (I) (C_6v)	Be_6	0.93	-0.042, -0.042, -0.042 -0.042, -0.042, -0.042	0.115, 0.156, 0.157 0.115, 0.154, 0.154	0.155, 0.155, 0.155 0.155, 0.155, 0.155
	Mg		0.252	0.148	0.069
Be_6-Mg (II) (C_6v)	Be_6	1.00	-0.042, -0.041, -0.041 -0.041, -0.042, -0.042	0.155, 0.1185, 0.159 0.156, 0.1516, 0.112	0.156, 0.1536, 0.153, 0.154, 0.157, 0.157
	Mg		0.250	0.148	0.069