**A Holistic View on the Interactions between Electron-deficient systems: Clustering of Beryllium and Magnesium Hydrides and Halides.**

Otilia Mó[1], M. Merced Montero-Campillo[1]\*, Manuel Yáñez[1]\*, Ibon Alkorta[2]\*, José Elguero[2].

[1] Departamento de Química, Módulo 13, Facultad de Ciencias, and Institute of Advanced Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, Campus de Excelencia UAM-CSIC, Cantoblanco, 28049 Madrid, Spain.

[2] Instituto de Química Médica, IQM-CSIC, Juan de la Cierva, 3. 28006 Madrid, Spain.

mm.montero@uam.es, manuel.yanes@uam.es, ibon@iqm.csic.es

## CONTENTS

**Table S7.** MBIE analysis of linear heterotrimer complexes formed by $BeX_2$ and $MgX_2$ (X = H, F, Cl).

**Figure S5**. Bond paths for the stable hexagonal heterotrimers $BeCl_2$ and $MgCl_2$ homotrimers, showing their stabilization and relative enthalpies with respect to the corresponding linear heterotrimer in $kJ \cdot mol^{-1}$.

**Table S8.** MBIE analysis of $BeBeMgH_6$ and $BeMgMgH_6$ heterotrimer complexes.

**Table S9.** Molecular graphs of cycles **C**-**G** of $BeX_2BX_2MgX_2$ and $BeX_2MgX_2Mgx_2$ (X = F, Cl) and their stabilization enthalpies

**Table S10 .** MBIE analysis of heterotrimer complexes for fluorides and chlorides.



**Figure S1**. Correlation between the interaction enthalpies calculated at the G4 and M06-2X levels of theory for $BeBeX_4$, $MgMgX_4$, $BeMgX_4$, $BeBeBeX_6$, $MgMgMgX_6$, $BeBeMgX_6$, and $BeMgMgX_6$ (X = H, F, Cl) clusters ($\Delta H$ G4 = 1.0735 $\Delta H$ M062X - 13.890; $R^2$ = 0.991).
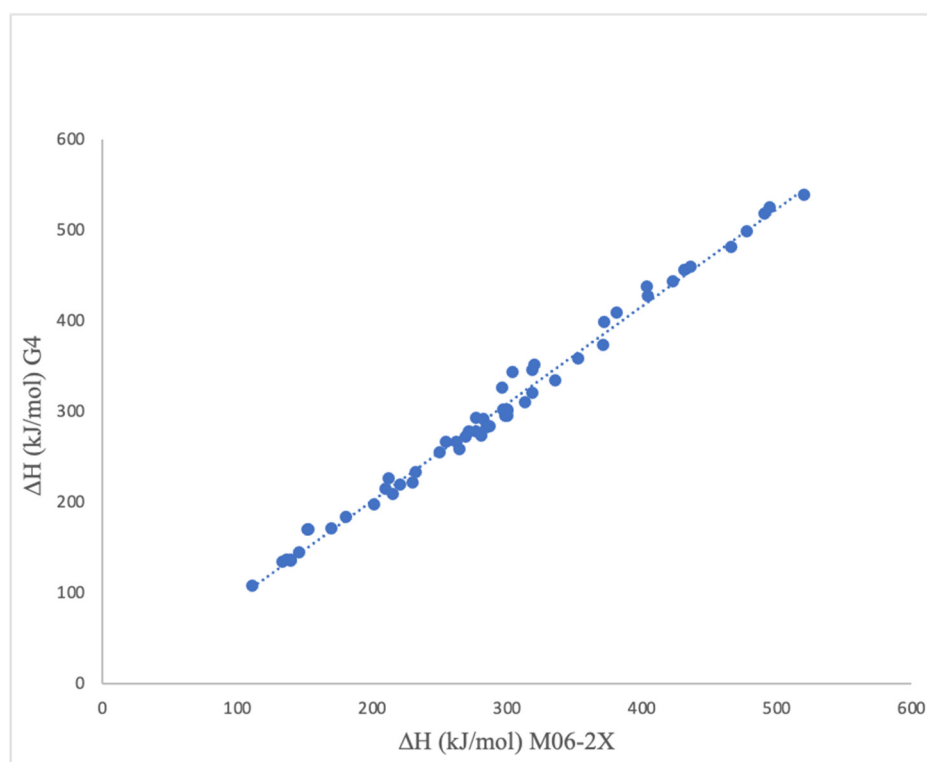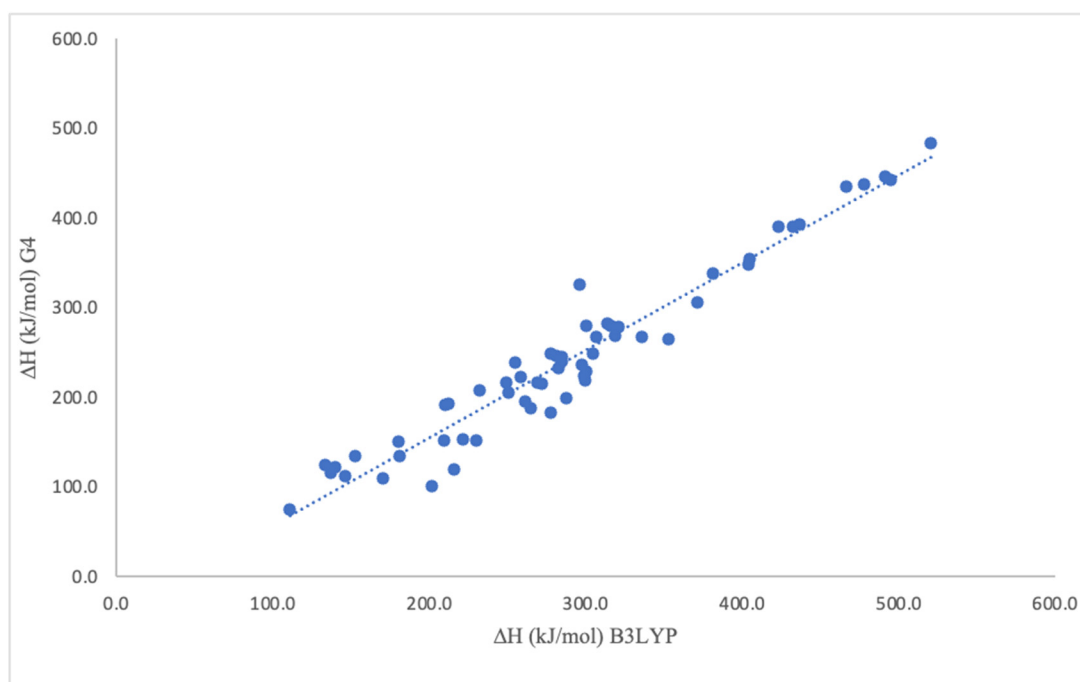
**Figure S2**. Correlation between the interaction enthalpies calculated at the G4 and B3LYP levels of theory for $BeBeX_4$, $MgMgX_4$, $BeMgX_4$, $BeBeBeX_6$, $MgMgMgX_6$, $BeBeMgX_6$, and $BeMgMgX_6$ (X = H, F, Cl) clusters ($\Delta H$ G4 = 0.9777 $\Delta H$ B3LYP - 40.213; $R^2$ = 0.9399).

**Table S1.** LMO-EDA analysis for the $BeBeX_4$, $MgMgX_4$ and $BeMgX_4$ (X = H, F, Cl) dimers (all values in $kJ \cdot mol^{-1}$)

a) Hydrides

| | Energies ($kJ \cdot mol^{-1}$) of the different components | | | % of the attractive components to the total E | | |
|---|---|---|---|---|---|---|
| | $BeBeH_4$ | $MgMgH_4$ | $BeMgH_4$ | $BeBeH_4$ | $MgMgH_4$ | $BeMgH_4$ |
| Electrostatic | -425.1 | -376.6 | -384.4 | 34.5 | 39.4 | 35.4 |
| Exchange | -388.7 | -301.5 | -342.7 | 31.5 | 31.6 | 31.6 |
| Repulsion | 972.6 | 738.9 | 841.6 | | | |
| Polarization | -351.1 | -218.0 | -293.0 | 28.5 | 22.8 | 27.0 |
| Dispersion | -69.0 | -59.4 | -64.8 | 5.6 | 6.2 | 6.0 |
| Total E | -261.4 | -216.6 | -243.4 | 34.5 | 39.4 | 35.4 |

b) Fluorides

|  | BeBeF$_4$ | MgMgF$_4$ | BeMgF$_4$ | BeBeF$_4$ | MgMgF$_4$ | BeMgF$_4$ |
|---|---|---|---|---|---|---|
| Electrostatic | -494.2 | -498.0 | -497.9 | 42.4 | 56.9 | 48.3 |
| Exchange | -263.0 | -157.2 | -211.6 | 22.6 | 18.0 | 20.5 |
| Repulsion | 823.9 | 521.7 | 673.2 |  |  |  |
| Polarization | -311.9 | -146.1 | -235.8 | 26.8 | 16.7 | 22.9 |
| Dispersion | -95.4 | -73.3 | -85.6 | 8.2 | 8.4 | 8.3 |
| Total E | -340.7 | -352.9 | -357.6 | 42.4 | 56.9 | 48.3 |

c) Chlorides

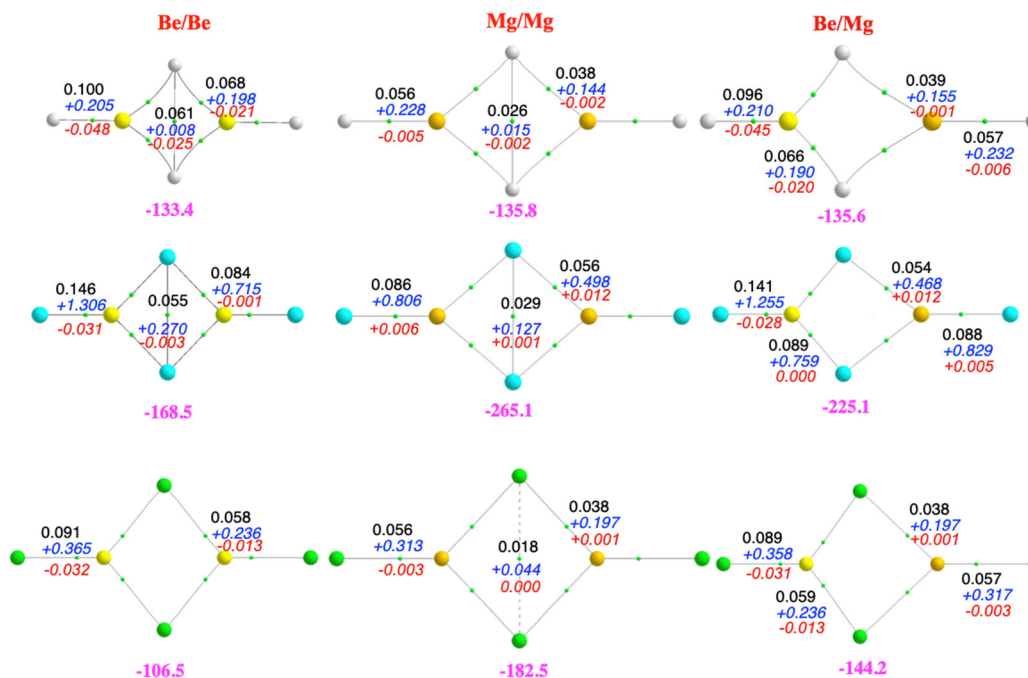|  | BeBeCl$_4$ |  | BeMgCl$_4$ | BeBeCl$_4$ |  | BeMgCl$_4$ |
|---|---|---|---|---|---|---|
| Electrostatic | -355.5 |  | -343.8 | 30.3 |  | 35.0 |
| Exchange | -322.0 |  | -249.4 | 27.5 |  | 25.4 |
| Repulsion | 900.9 |  | 705.7 |  |  |  |
| Polarization | -386.9 |  | -292.8 | 33.0 |  | 29.8 |
| Dispersion | -107.2 |  | -95.0 | 9.1 |  | 9.7 |
| Total E | -270.5 |  | -275.3 |  |  |  |



**Figure S3**. Molecular graphs of the homo and heterodimers involving BeX$_2$ and MgX$_2$ (X = H, F, Cl) monomers. The electron density (black), its Laplacian (blue italic) and the energy density (red italic) at the bond critical points (BCPs) are in

a.u. The numbers in magenta are the stabilization enthalpies in kJ·mol$^{-1}$.

**Table S2.** AdNPD orbital list for the BeBeX$_4$, MgMgX$_4$ and BeMgX$_4$ dimers


**Be$_2$H$_4$:**
```
                ---- AdNDP orbital list ----
#   1 Occ: 1.9918 Atom:  1Be   2H
#   2 Occ: 1.9918 Atom:  4Be   5H
#   3 Occ: 1.9642 Atom:  3H   4Be   6H
#   4 Occ: 1.9642 Atom:  1Be   3H   6H
Total occupation number in above orbitals:   7.9119
```

Residual valence electrons of all atoms in the search list:   0.088505


**Mg$_2$H$_4$:**
```
                ---- AdNDP orbital list ----
#   1 Occ: 1.9959 Atom:  1Mg   3H
#   2 Occ: 1.9959 Atom:  4Mg   6H
#   3 Occ: 1.9894 Atom:  1Mg   2H   5H
#   4 Occ: 1.9894 Atom:  2H   4Mg   5H
Total occupation number in above orbitals:   7.9707
```

Residual valence electrons of all atoms in the search list:   0.030936


**BeMgH$_4$:**
```
                ---- AdNDP orbital list ----
#   1 Occ: 1.9975 Atom:  4Mg   5H
#   2 Occ: 1.9895 Atom:  1Be   3H
#   3 Occ: 1.9925 Atom:  1Be   2H   6H
#   4 Occ: 1.9562 Atom:  1Be   4Mg   6H
Total occupation number in above orbitals:   7.9357
```

Residual valence electrons of all atoms in the search list:   0.064916


**Be$_2$F$_4$:**
```
                ---- AdNDP orbital list ----
#   1 Occ: 1.9964 Atom:  2F
#   2 Occ: 1.9964 Atom:  5F
#   3 Occ: 1.9951 Atom:  3F
#   4 Occ: 1.9951 Atom:  6F
#   5 Occ: 1.9909 Atom:  5F
#   6 Occ: 1.9909 Atom:  2F
#   7 Occ: 1.9867 Atom:  3F
```

# 8 Occ: 1.9867 Atom:  6F
# 9 Occ: 1.9993 Atom:  1Be   3F
# 10 Occ: 1.9993 Atom:  4Be   6F
# 11 Occ: 1.9992 Atom:  1Be   3F
# 12 Occ: 1.9992 Atom:  4Be   6F
# 13 Occ: 1.9986 Atom:  1Be   2F
# 14 Occ: 1.9986 Atom:  1Be   5F
# 15 Occ: 1.9986 Atom:  4Be   5F
# 16 Occ: 1.9986 Atom:  2F    4Be
Total occupation number in above orbitals:  31.9295

Residual valence electrons of all atoms in the search list:  0.070317

**$Mg_2F_4$**
---- AdNDP orbital list ----
# 1 Occ: 1.9992 Atom:  3F
# 2 Occ: 1.9992 Atom:  5F
# 3 Occ: 1.9980 Atom:  2F
# 4 Occ: 1.9980 Atom:  6F
# 5 Occ: 1.9964 Atom:  2F
# 6 Occ: 1.9964 Atom:  6F
# 7 Occ: 1.9949 Atom:  3F
# 8 Occ: 1.9949 Atom:  5F
# 9 Occ: 1.9944 Atom:  3F
# 10 Occ: 1.9944 Atom:  5F
# 11 Occ: 1.9991 Atom:  1Mg   3F
# 12 Occ: 1.9991 Atom:  4Mg   5F
# 13 Occ: 1.9989 Atom:  2F    4Mg
# 14 Occ: 1.9989 Atom:  1Mg   6F
# 15 Occ: 1.9989 Atom:  1Mg   2F
# 16 Occ: 1.9989 Atom:  4Mg   6F
Total occupation number in above orbitals:  31.9600

Residual valence electrons of all atoms in the search list:  0.040214

**$BeMgF_4$**
---- AdNDP orbital list ----
# 1 Occ: 1.9992 Atom:  6F
# 2 Occ: 1.9962 Atom:  5F
# 3 Occ: 1.9962 Atom:  2F
# 4 Occ: 1.9952 Atom:  3F
# 5 Occ: 1.9946 Atom:  6F
# 6 Occ: 1.9942 Atom:  6F

\#   7 Occ: 1.9919 Atom:  5F
\#   8 Occ: 1.9919 Atom:  2F
\#   9 Occ: 1.9998 Atom:  1Be   3F
\#  10 Occ: 1.9996 Atom:  1Be   3F
\#  11 Occ: 1.9993 Atom:  1Be   3F
\#  12 Occ: 1.9991 Atom:  4Mg   6F
\#  13 Occ: 1.9989 Atom:  1Be   2F
\#  14 Occ: 1.9989 Atom:  1Be   5F
\#  15 Occ: 1.9974 Atom:  2F   4Mg
\#  16 Occ: 1.9974 Atom:  4Mg   5F
Total occupation number in above orbitals:   31.9498

Residual valence electrons of all atoms in the search list:    0.049794

## Be$_2$Cl$_4$
                ---- AdNDP orbital list ----
\#   1 Occ: 1.9950 Atom:  2Cl
\#   2 Occ: 1.9950 Atom:  5Cl
\#   3 Occ: 1.9945 Atom:  3Cl
\#   4 Occ: 1.9945 Atom:  6Cl
\#   5 Occ: 1.9859 Atom:  5Cl
\#   6 Occ: 1.9859 Atom:  2Cl
\#   7 Occ: 1.9835 Atom:  3Cl
\#   8 Occ: 1.9835 Atom:  6Cl
\#   9 Occ: 1.9995 Atom:  1Be   2Cl
\#  10 Occ: 1.9995 Atom:  4Be   5Cl
\#  11 Occ: 1.9984 Atom:  1Be   2Cl
\#  12 Occ: 1.9984 Atom:  4Be   5Cl
\#  13 Occ: 1.9973 Atom:  1Be   6Cl
\#  14 Occ: 1.9973 Atom:  1Be   3Cl
\#  15 Occ: 1.9973 Atom:  3Cl   4Be
\#  16 Occ: 1.9973 Atom:  4Be   6Cl
Total occupation number in above orbitals:   31.9028

Residual valence electrons of all atoms in the search list:    0.096778

## Mg$_2$Cl$_4$
                ---- AdNDP orbital list ----
\#   1 Occ: 1.9987 Atom:  3Cl
\#   2 Occ: 1.9987 Atom:  6Cl
\#   3 Occ: 1.9983 Atom:  5Cl

\#   4 Occ: 1.9983 Atom:   2Cl
\#   5 Occ: 1.9943 Atom:   3Cl
\#   6 Occ: 1.9943 Atom:   6Cl
\#   7 Occ: 1.9880 Atom:   2Cl
\#   8 Occ: 1.9880 Atom:   5Cl
\#   9 Occ: 1.9856 Atom:   2Cl
\#  10 Occ: 1.9856 Atom:   5Cl
\#  11 Occ: 1.9995 Atom:   1Mg   2Cl
\#  12 Occ: 1.9995 Atom:   4Mg   5Cl
\#  13 Occ: 1.9989 Atom:   1Mg   6Cl
\#  14 Occ: 1.9989 Atom:   1Mg   3Cl
\#  15 Occ: 1.9989 Atom:   4Mg   6Cl
\#  16 Occ: 1.9989 Atom:   3Cl   4Mg
Total occupation number in above orbitals:   31.9243

Residual valence electrons of all atoms in the search list:   0.075740

**BeMgCl$_4$**
                 ---- AdNDP orbital list ----
\#   1 Occ: 1.9983 Atom:   5Cl
\#   2 Occ: 1.9967 Atom:   3Cl
\#   3 Occ: 1.9967 Atom:   6Cl
\#   4 Occ: 1.9948 Atom:   2Cl
\#   5 Occ: 1.9888 Atom:   3Cl
\#   6 Occ: 1.9888 Atom:   6Cl
\#   7 Occ: 1.9874 Atom:   5Cl
\#   8 Occ: 1.9871 Atom:   2Cl
\#   9 Occ: 1.9996 Atom:   4Mg   5Cl
\#  10 Occ: 1.9994 Atom:   4Mg   5Cl
\#  11 Occ: 1.9994 Atom:   1Be   2Cl
\#  12 Occ: 1.9987 Atom:   1Be   3Cl
\#  13 Occ: 1.9987 Atom:   1Be   6Cl
\#  14 Occ: 1.9985 Atom:   1Be   2Cl
\#  15 Occ: 1.9976 Atom:   3Cl   4Mg
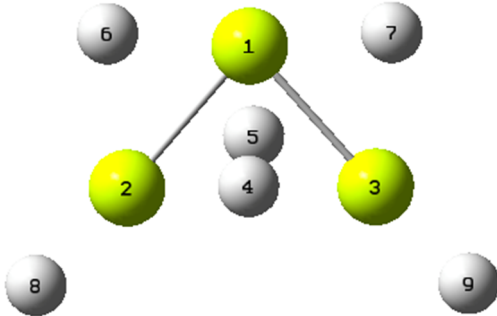\#  16 Occ: 1.9976 Atom:   4Mg   6Cl
Total occupation number in above orbitals:   31.9282

Residual valence electrons of all atoms in the search list:   0.071941

**Table S3**. Wiberg bond indexes for $Be_2X_4$, $Mg_2X_4$, $BeMgX_4$ (X = H, F, Cl)

| Cluster | Bonds | Wiberg indexes |
|---------|-------|----------------|
| $Be_2H_4$ | Be-H | 0.600 / 0.228 |
| $Mg_2H_4$ | Mg-H | 0.518 / 0.154 |
| $BeMgH_4$ | Be-H | 0.570 / 0.274 |
| | Mg-H | 0.536 / 0.126 |
| $Be_2F_4$ | Be-F | 0.256 / 0.125 |
| $Mg_2F_4$ | Mg-F | 0.109 / 0.055 |
| $BeMgF_4$ | Be-F | 0.242 / 0.146 |
| | Mg-F | 0.111 / 0.052 |
| $Be_2Cl_4$ | Be-Cl | 0.445 / 0.268 |
| $Mg_2Cl_4$ | Mg-Cl | 0.315 / 0.152 |
| $BeMgCl_4$ | Be-Cl | 0.434 / 0.300 |
| | Mg-Cl | 0.320 / 0.148 |

**Table S4.** Interatomic distances in the cycles **A** of $Be_2X_4$ and $Mg_2X_4$ (X = H, Cl). All values are in Å. The atoms numbering is shown in the attached figure.



| $Be_2X_4$  and $Mg_2X_4$ / Cycle **A** | | |
|---|---|---|
| **X = H** | | |
| Atoms involved | **1-2** and **1-3** | **2-3** |
| Be-Be distances | 1.860 | 2.416 |
| Mg-Mg distances | 2.603 | 3.124 |
| Atoms involved | **1-6** and **1-7** / **2-6** and **3-7** | **2-4** and **3-4** / **2-8** and **3-9** |

| | | |
|---|---|---|
| Be-H distances | 1.386 / 1.553 | 1.581 / 1.320 |
| Mg-H distances | 1.756/ 1.984 | 1.988 / 1.687 |
| Atoms involved | 4-5 | |
| H-H (in Be cycle) | 1.972 | |
| H-H (in Mg cycle) | 2.295 | |
| **X = Cl** | | |
| Atoms involved | **1-2** and **1-3** | **2-3** |
| Be-Be distances | 2.280 | 3.167 |
| Mg-Mg distances | 2.924 | 3.739 |

**Table S5.** LMO-EDA analysis for the $BeBeBeF_6$ trimers (all values in $kJ \cdot mol^{-1}$)

| | Energies ($kJ \cdot mol^{-1}$) of the different components | | | % of the attractive components to the total E | | |
|---|---|---|---|---|---|---|
| | Cycle **A** | Cycle **B** | linear | Cycle **A** | Cycle **B** | linear |
| Electrostatic | -993.4 | -873.7 | -991.6 | 39.7 | 40.5 | 41.9 |
| Exchange | -652.8 | -470.5 | -540.3 | 26.1 | 21.8 | 22.8 |
| Repulsion | **1934.2** | **1468.7** | **1672.5** | | | |
| Polarization | -608.6 | -604.3 | -638.3 | 24.3 | 28.0 | 27.0 |
| Dispersion | -250.6 | -208.3 | -196.5 | 10.0 | 9.7 | 8.3 |
| Total E | -571.1 | -688.0 | -694.2 | | | |

**Table S6.** Relative stabilities ($kJ \cdot mol^{-1}$) for the $MgF_2$ trimers obtained by different theoretical approaches.

| | GA/DFT[a] | M06-2X | G4 |
|---|---|---|---|
| Linear | 0.0 | 0.0 | 0.0 |
| Hexagonal cycle | 40.2 | 56.9 | 54.1 |
| cycle | 32.2 | 20.7 | 29.4 |
| cycle | 43.1 | 13.8 | 25.4 |

**Table S7.** MBIE analysis of linear heterotrimer complexes formed by BeX$_2$ and MgX$_2$ (X = H, F, Cl). All values in kJ·mol$^{-1}$.

| Ternary complex | E$_R$(A) | E$_R$(B) | E$_R$(C) | D$^2$E(AB) | D$^2$E(AC) | D$^2$E(BC) | D$^3$E(ABC) | E$_{total}$ |
|---|---|---|---|---|---|---|---|---|
| | | | | | | | | |
| BeBeMgH$_6$ | 58.5 | 110.2 | 32.7 | -262.8 | 8.6 | -247.0 | -33.2 | -333.0 |
| BeMgBeH$_6$ | 67.4 | 57.2 | 67.4 | -240.5 | -0.3 | -240.5 | -4.0 | -293.2 |
| BeMgMgH$_6$ | 67.2 | 62.0 | 37.8 | -241.6 | -0.3 | -214.6 | -8.3 | -297.8 |
| MgBeMgH$_6$ | 31.6 | 117.5 | 31.6 | -247.1 | 11.2 | -247.3 | -31.5 | -333.8 |
| | | | | | | | | |
| BeBeMgF$_6$ | 82.6 | 172.4 | 42.6 | -347.7 | -1.9 | -364.7 | 0.4 | -416.4 |
| BeMgBeF$_6$ | 86.6 | 80.7 | 86.6 | -358.0 | -2.4 | -358.0 | 0.5 | -464.1 |
| BeMgMgF$_6$ | 86.2 | 81.5 | 43.1 | -359.8 | -2.6 | -355.2 | 0.5 | -506.3 |
| MgBeMgF$_6$ | 40.9 | 176.1 | 40.9 | -365.3 | 0.6 | -365.3 | 4.8 | -467.2 |
| | | | | | | | | |
| BeBeMgCl$_6$ | 80.3 | 168.3 | 39.7 | -276.8 | -0.5 | -2821 | 7.9 | -263.1 |
| BeMgBeCl$_6$ | 88.6 | 77.0 | 88.6 | -276.9 | -1.9 | -276.9 | 0.4 | -301.1 |
| BeMgMgCl$_6$ | 88.5 | 81.2 | 44.5 | -277.5 | -2.5 | -276.0 | 1.3 | -340.4 |
| MgBeMgCl$_6$ | 39.3 | 175.9 | 39.3 | -282.1 | -1.0 | -282.1 | 10.8 | -299.7 |
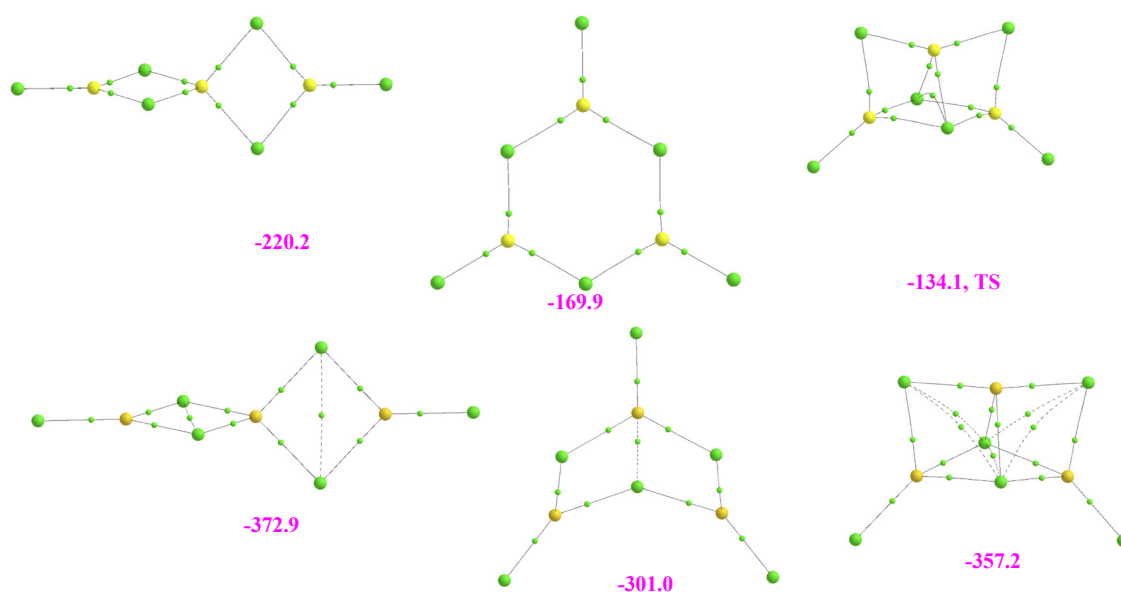


**Figure S4**. Bond paths and stabilization enthalpies (kJ·mol$^{-1}$) for the BeCl$_2$ and MgCl$_2$ homotrimers.
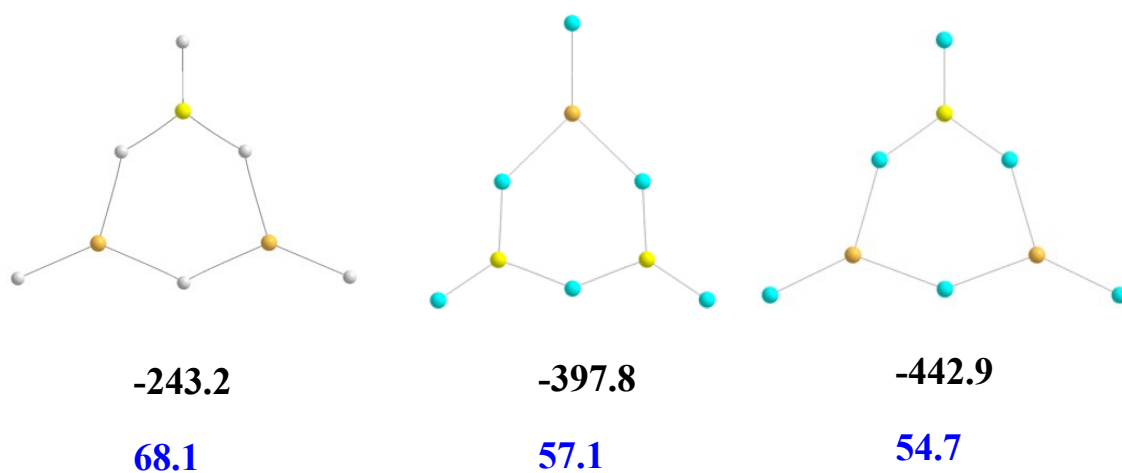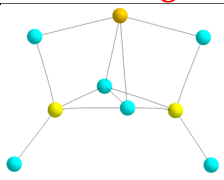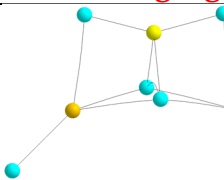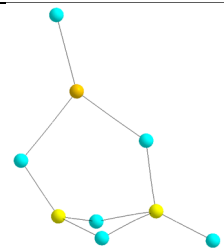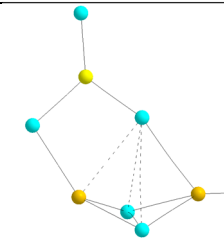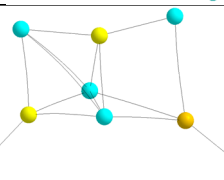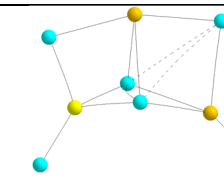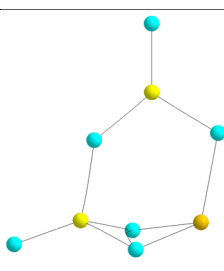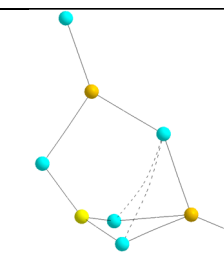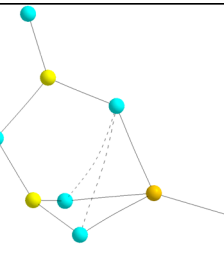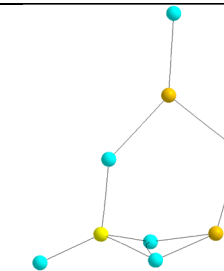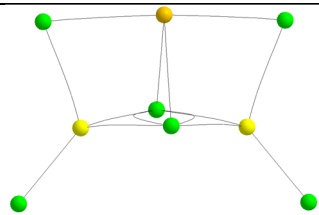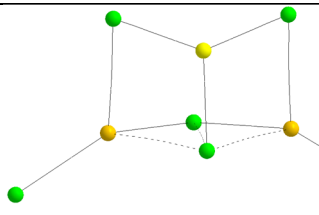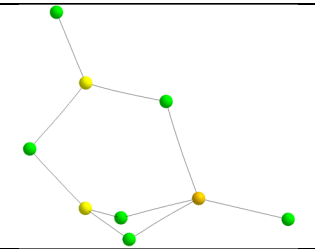
**-243.2**

**68.1**

**-397.8**

**57.1**

**-442.9**

**54.7**

**Figure S5**. Bond paths for the stable hexagonal heterotrimers $BeCl_2$ and $MgCl_2$ homotrimers, showing their stabilization (black) and relative enthalpies (blue) with respect to the corresponding linear heterotrimer in $kJ \cdot mol^{-1}$.

**Table S8.** MBIE analysis of $BeBeMgH_6$ and $BeMgMgH_6$ heterotrimer complexes. All values in $kJ \cdot mol^{-1}$.

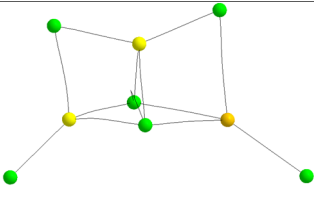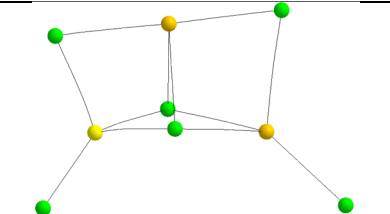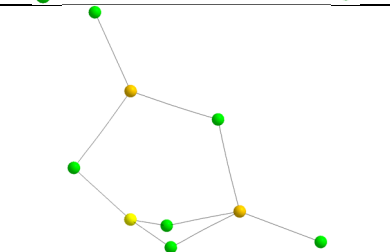| BeBeMgH$_6$ | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Ternary complex | $E_R(A)$ | $E_R(B)$ | $E_R(C)$ | $\Delta^2E(AB)$ | $\Delta^2E(AC)$ | $\Delta^2E(BC)$ | $\Delta^3E(ABC)$ | $E_{total}$ |
| linear | 58.5 | 110.2 | 32.7 | -262.8 | 8.6 | -247.0 | -33.2 | -333.0 |
| Cycle **E** | 18.1 | 89.47 | 54.4 | -143.41 | -115.49 | -182.33 | -59.1 | -338.36 |
| BeMgMgH$_6$ | | | | | | | | |
| Ternary complex | | | | | | | | |
| linear | 67.2 | 62.0 | 37.8 | -241.6 | -0.3 | -214.6 | -8.3 | -297.8 |
| Cycle **C** | 36.5 | 60.2 | 60.2 | -152.8 | -152.7 | -147.5 | -45.8 | -341.9 |

**Table S9.** Molecular graphs of cycles **C-G** of $BeX_2BX_2MgX_2$ and $BeX_2MgX_2Mgx_2$ (X = F, Cl) and their stabilization enthalpies (bold numbers). In blue their relative stabilities with respect to the corresponding linear trimer are also given. All values in kJ·mol$^{-1}$.

| *Fluorides* | **BeBeMg** | | **BeMgMg** | |
|---|---|---|---|---|
| **C** |  | **-342.5** <br><br> 112.4 |  | **-426.6** <br><br> 71.0 |
| **D** |  | **-360.6** <br><br> 94.3 |  | **-466.0** <br><br> 31.6 |
| **E** |  | **TS** |  | **-437.3** <br><br> 60.3 |
| **F** |  | **-372.4** <br><br> 82.5 |  | **-455.0** <br><br> 42.6 |
| **G** |  | **-398.4** <br><br> 56.5 |  | **-423.0** <br><br> 74.6 |
| *Chlorides* | | | | |
| **C** |  | **-197.1** <br> 97.5 |  | **-283.3** <br> 50.5 |
| **D** | | **TS** | **Does not exist**[a] | |

| | | | | |
|---|---|---|---|---|
| E |  | -207.7 <br> 86.9 |  | -277.5 <br> 56.3 |
| F | **Does not exist**[a] | |  | -289.8 |
| G |  | -241.0 <br> 53.6 | **Does not exist**[a] | 44.0 |

[a] These structures are not stable as they collapse to the global minimum.

**Table S10.** MBIE analysis of heterotrimer complexes for fluorides and chlorides. All values in kJ·mol$^{-1}$.

| Ternary complex | $E_R(A)$ | $E_R(B)$ | $E_R(C)$ | $\Delta^2E(AB)$ | $\Delta^2E(AC)$ | $\Delta^2E(BC)$ | $\Delta^3E(ABC)$ | $E_{total}$ |
|---|---|---|---|---|---|---|---|---|
| BeBeMgF$_6$_linear | 82.6 | 172.4 | 42.6 | -347.7 | -1.9 | -364.7 | 0.4 | -416.4 |
| BeMgBeF$_6$_linear | 86.6 | 80.7 | 86.6 | -358.0 | -2.4 | -358.0 | 0.5 | -464.1 |
| BeMgMgF$_6$_cyc_hexagonal | 94.2 | 44.6 | 50.5 | -139.2 | -224.0 | -195.8 | -81.6 | -451.4 |
| BeBeMgF$_6$ cycle **E** | 39.5 | 171.0 | 86.6 | -184.4 | -171.1 | -353.9 | 83.0 | -329.2 |
| BeBeMgF$_6$ cycle **C** | 27.8 | 176.7 | 176.6 | -209.9 | -209.5 | -367.9 | 57.3 | -348.9 |
| BeMgMgF$_6$_linear | 86.2 | 81.5 | 43.1 | -359.8 | -2.6 | -355.2 | 0.5 | -506.3 |
| MgBeMgF$_6$_linear | 40.9 | 176.1 | 40.9 | -365.3 | 0.6 | -365.3 | 4.8 | -467.2 |
| BeMgMgF6_cyc_hexagonal | 94.2 | 44.6 | 50.48 | -139.2 | -224.0 | -195.8 | -81.6 | -451.4 |
| BeMgMgF6 cycle **E** | 21.9 | 182.5 | 84.8 | -232.4 | -188.5 | -367.2 | 54.1 | -444.6 |
| BeMgMgF6 cycle **C** | 51.1 | 92.6 | 92.4 | -207.2 | -207.2 | -336.4 | 80.9 | -433.9 |
| BeBeMgCl6_linear | 80.3 | 168.3 | 39.7 | -276.8 | -0.5 | -282.1 | 7.9 | -263.1 |
| BeMgBeCl6_linear | 88.6 | 77.0 | 88.6 | -276.9 | -1.9 | -276.9 | 0.4 | -301.1 |
| BeBeMgCl6_cyc_hexagonal_NP | 126.6 | 63.7 | 62.1 | -89.9 | -291.3 | -63.7 | -31.4 | -223.9 |
| BeBeMgCl6 cycle **E** | 54.2 | 151.4 | 73.0 | -167.1 | -149.0 | -264.9 | 90.0 | -212.3 |
| BeBeMgCl6 cycle **C** | 14.0 | 158.2 | 157.9 | -162.7 | -162.5 | -278.2 | 72.0 | -201.4 |
| BeMgMgCl6_linear | 88.5 | 81.2 | 44.5 | -277.5 | -2.57 | -276.0 | 1.3 | -340.4 |
| MgBeMgCl6_linear | 39.3 | 175.9 | 39.35 | -282.1 | -1.0 | -282.1 | 10.8 | -299.7 |
| BeBeMgCl6_cyc_hexagonal_NP | 133.7 | 48.3 | 87.7 | -116.7 | -292.0 | -117.2 | -50.0 | -306.2 |
| BeMgMgCl6 cycle **E** | 14.9 | 166.5 | 77.5 | -182.7 | -149.3 | -275.6 | 66.0 | -282.7 |
| BeMgMgCl6 cycle **C** | 65.6 | 76.9 | 76.9 | -168.5 | -168.5 | -258.1 | 86.8 | -288.8 |