Supplementary Materials: Non-Covalent Interactions Involving Alkaline-Earth Atoms and Lewis Bases B: An ab Initio Investigation of Beryllium and Magnesium Bonds, B···MR_2 (M = Be or Mg, and R = H, F or CH_3)

Ibon Alkorta and Anthony C. Legon

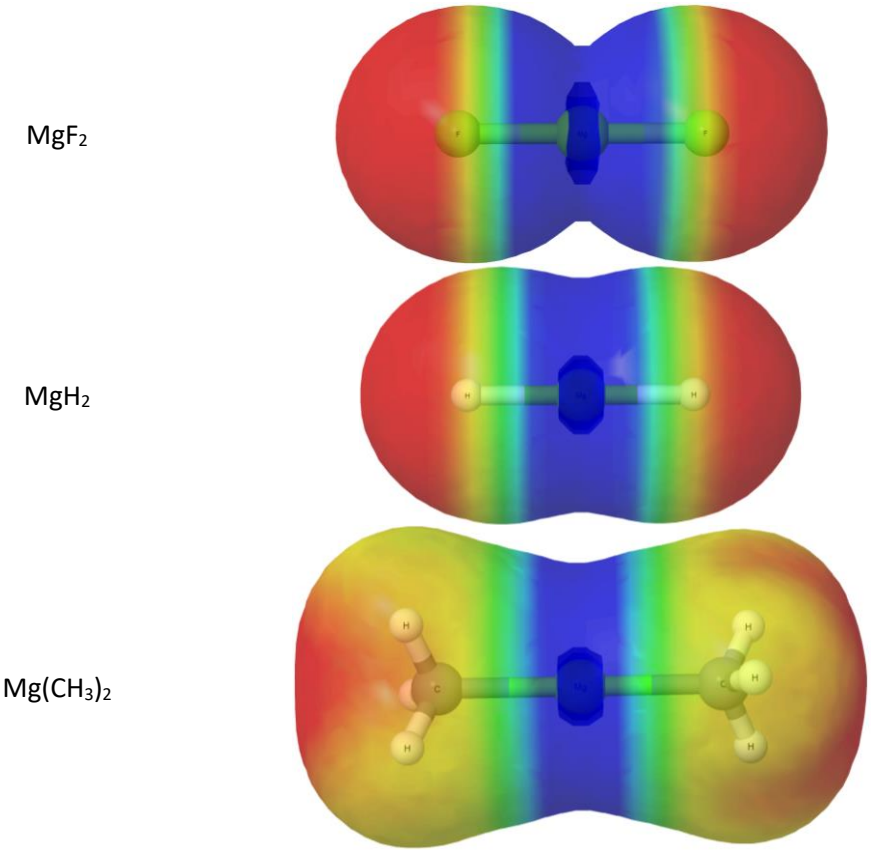
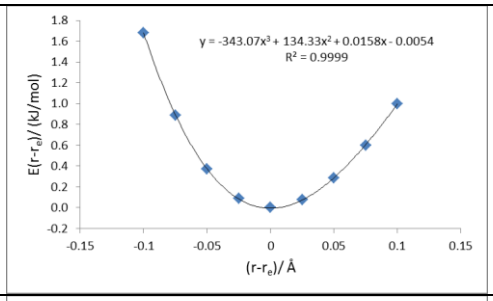
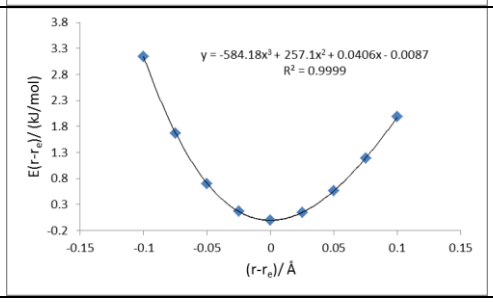
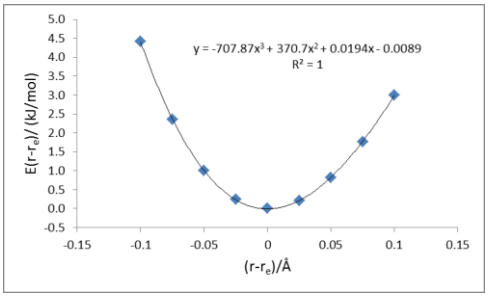
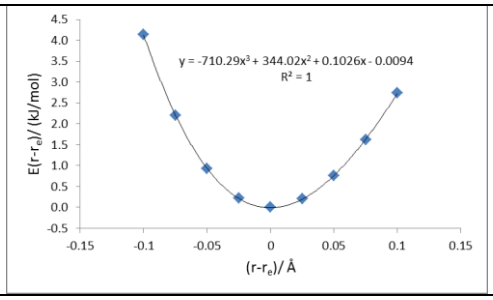


Fig. S1. Molecular electrostatic surface potentials of the linear, non-polar molecules, MgF_2, MgH_2 and $Mg(CH_3)_2$ calculated at the 0.001 e $bohr^{-3}$ electron density isosurface at the CCSD/aug-cc-pVTZ//CCSD(T)/aug-cc-pVTZ level of theory. The surface has been cut away to reveal the molecular model within. The most intense blue (and therefore the most electrophilic) belts centred on Be correspond to positive electrostatic potential energies of 753, 321 and 280 kJ mol^{-1} for MgF_2, MgH_2 and $Mg(CH_3)_2$, respectively, and confirm expectations based on the inductive effects of CH_3 and F relative to H.

Table S1. Optimized geometry, electronic energy and Variation of the energy E(r-r_e) as a function of the displacement (r-r_e) from the global minimum at r_e at the CCSD(T)/aug-cc-pVTZ computational level.

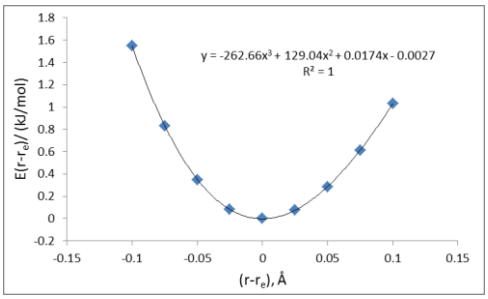
BeH_2 complexes

Optimized geometry and energy at CCSD(T)/aug-cc-pVTZ level.	Variation of the energy E(r-r_e) as a function of the displacement (r-r_e) from the global minimum at r_e
BeH_2 CCSD(T)/AVTZ ENERGY=-15.84934381 Be 0.0000000000 0.0000000000 0.0000000000 H 0.0000000000 0.0000000000 1.3333483359 H 0.0000000000 0.0000000000 -1.3333483359	
OC···BeH_2 CCSD(T)/AVTZ ENERGY=-129.02025196 Be 0.0000000000 0.0000000000 -1.8368632325 H 0.0000000000 1.2977816259 -2.2147053227 H 0.0000000000 -1.2977816259 -2.2147053227 C 0.0000000000 0.0000000000 0.1054055652 O 0.0000000000 0.0000000000 1.2345897977	
HCN···BeH_2 CCSD(T)/AVTZ ENERGY=-109.15108893 Be 0.0000000000 0.0000000000 -1.6704262314 H 0.0000000000 1.2843860233 -2.1141411831 H 0.0000000000 -1.2843860233 -2.1141411831 N 0.0000000000 0.0000000000 0.1198239787 C 0.0000000000 0.0000000000 1.2720076447 H 0.0000000000 0.0000000000 2.3410267074	
H_3N···BeH_2 CCSD(T)/AVTZ ENERGY=-72.36813735 Be 0.0000000000 -0.0007067290 -1.0881968228 H 0.0000000000 1.2949225521 -1.5315219638 H 0.0000000000 -1.2681666948 -1.5999707412 N 0.0000000000 -0.0058891673 0.6952020249 H -0.8118708221 0.4970039398 1.0453837795 H 0.8118708221 0.4970039398 1.0453837795 H 0.0000000000 -0.9326067350 1.1097167921	
H_2O···BeH_2 CCSD(T)/AVTZ ENERGY=-92.22198109 Be -0.0062242383 0.0000000000 -1.0519129312 H -0.0277344728 1.2962865524 -1.4718827872 H -0.0277344728 -1.2962865524 -1.4718827872 O 0.0340620274 0.0000000000 0.6359952010 H -0.2147789931 0.7892897213 1.1268657527 H -0.2147789931 -0.7892897213 1.1268657527	

$H_3P\cdots BeH_2$

CCSD(T)/AVTZ ENERGY=-358.55828624

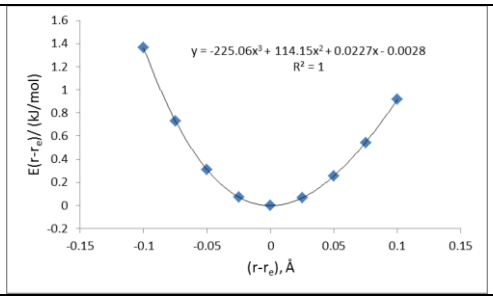
Be	0.0000000000	-0.0012172929	-1.7682148970
H	0.0000000000	1.3266507421	-2.0559747362
H	0.0000000000	-1.2581800857	-2.2691666617
P	0.0000000000	-0.0095366235	0.5362885751
H	-1.0620498074	0.6913112833	1.1431736518
H	1.0620498074	0.6913112833	1.1431736518
H	0.0000000000	-1.1471509735	1.3687118619



$H_2S\cdots BeH_2$

CCSD(T)/AVTZ ENERGY=-414.80319322

Be	-0.0190799313	0.0000000000	-1.7104801354
H	-0.0151476945	1.3015024460	-2.0824240185
H	-0.0151476945	-1.3015024460	-2.0824240185
S	0.0572556041	0.0000000000	0.5585161520
H	-0.8101310378	0.9836248559	0.8467984035
H	-0.8101310378	-0.9836248559	0.8467984035



BeF_2 complexes

BeF_2

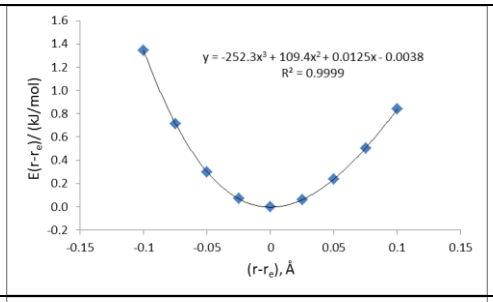
CCSD(T)/AVTZ ENERGY=-214.35237239

Be	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	0.0000000000	1.3838289558
F	0.0000000000	0.0000000000	-1.3838289558

$OC\cdots BeF_2$

CCSD(T)/AVTZ ENERGY=-327.52570958

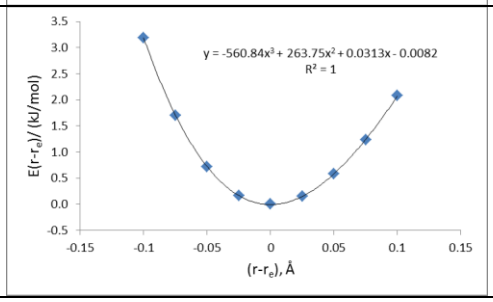
Be	0.0000000000	0.0000000000	-0.8173463350
F	0.0000000000	1.3593162274	-1.1821113695
F	0.0000000000	-1.3593162274	-1.1821113695
C	0.0000000000	0.0000000000	1.2223940479
O	0.0000000000	0.0000000000	2.3501102393



$HCN\cdots BeF_2$

CCSD(T)/AVTZ ENERGY=-307.65973720

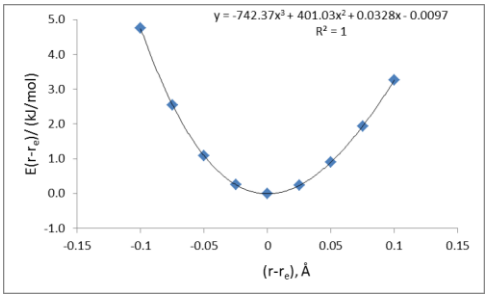
Be	0.0000000000	0.0000000000	-0.6408668317
F	0.0000000000	1.3393628423	-1.1079212437
F	0.0000000000	-1.3393628423	-1.1079212437
N	0.0000000000	0.0000000000	1.1771623889
C	0.0000000000	0.0000000000	2.3279268961
H	0.0000000000	0.0000000000	3.3972115613



$H_3N\cdots BeF_2$

CCSD(T)/AVTZ ENERGY=-270.87914706

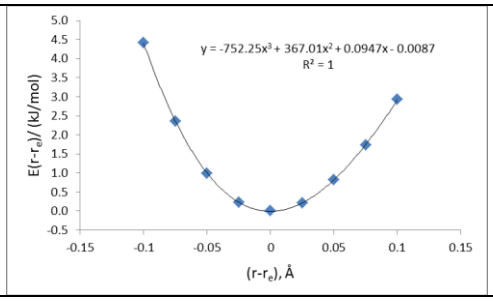
Be	-0.1855157370	-0.0018406339	0.0000000000
F	-0.6987172329	0.0003715135	1.3339707836
F	-0.6987172329	0.0003715135	-1.3339707836
N	1.5911314077	-0.0015895005	0.0000000000
H	1.9647908750	-0.4610450356	0.8254948186
H	1.9647908750	-0.4610450356	-0.8254948186
H	1.9580941779	0.9466306746	0.0000000000



$H_2O\cdots BeF_2$

CCSD(T)/AVTZ ENERGY=-290.73100187

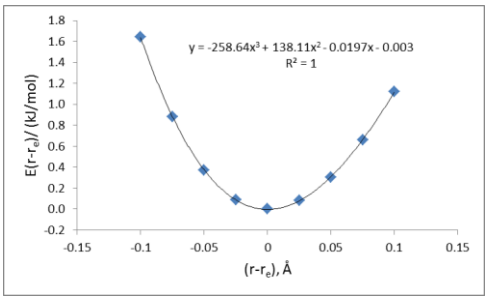
Be	-0.2178681766	0.0201323399	0.0000000000
F	-0.6738690307	-0.0068185019	1.3480560121
F	-0.6738690307	-0.0068185019	-1.3480560121
O	1.4789133295	0.0388799869	0.0000000000
H	1.9379189876	-0.2700614316	0.7878147844
H	1.9379189876	-0.2700614316	-0.7878147844



$H_3P\cdots BeF_2$

CCSD(T)/AVTZ ENERGY=-557.06475168

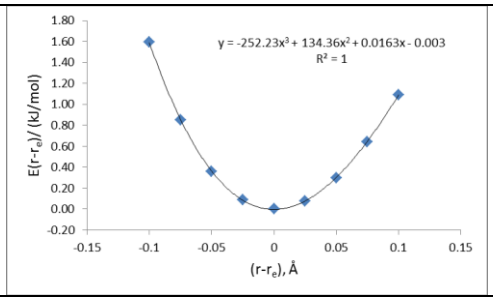
Be	0.0000000000	0.0074442472	-0.8050867402
F	0.0000000000	1.3759422612	-1.1689803644
F	0.0000000000	-1.3181736799	-1.2971745245
P	0.0000000000	-0.0364965831	1.5310306742
H	-1.0634879430	0.6070039920	2.1934271783
H	1.0634879430	0.6070039920	2.1934271783
H	0.0000000000	-1.2479021411	2.2472849807



$H_2S\cdots BeF_2$

CCSD(T)/AVTZ ENERGY=-613.31005979

Be	0.0072276710	0.0000000000	-0.7748524042
F	-0.0045930845	1.3527289296	-1.1838871439
F	-0.0045930845	-1.3527289296	-1.1838871439
S	0.0562677894	0.0000000000	1.5138068707
H	-0.8406055215	0.9820491846	1.7036684727
H	-0.8406055215	-0.9820491846	1.7036684727



$Be(CH_3)_2$ complexes

$Be(CH_3)_2$

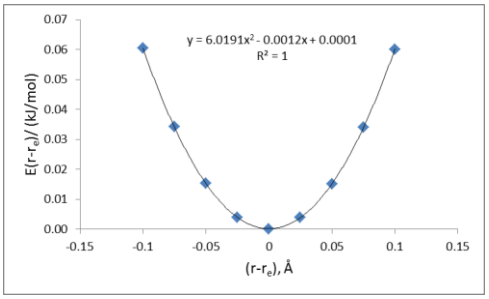
CCSD(T)/AVTZ ENERGY=-94.37442242

Be	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	1.6928515366
C	0.0000000000	0.0000000000	-1.6928515366
H	1.0162576054	0.0000000000	2.1048814395
H	-0.5081288027	0.8801049031	2.1048814395
H	-0.5081288027	-0.8801049031	2.1048814395
H	-1.0162576054	0.0000000000	-2.1048814395
H	0.5081288027	-0.8801049031	-2.1048814395
H	0.5081288027	0.8801049031	-2.1048814395

$OC\cdots Be(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-207.53955461

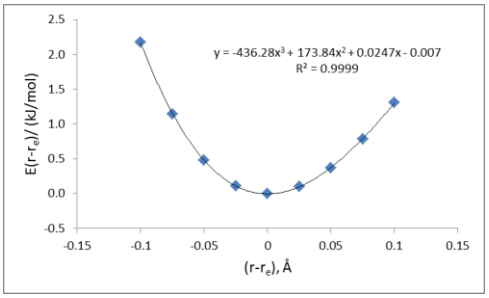
Be	0.0000000000	0.0000000000	-1.4469532658
C	0.0000000000	1.6938948146	-1.5411964569
C	0.0000000000	-1.6938948146	-1.5411964569
H	0.0000000000	2.0612133092	-2.5740138300
H	0.8792243487	2.1290262660	-1.0495075893
H	-0.8792243487	2.1290262660	-1.0495075893
H	0.0000000000	-2.0612133092	-2.5740138300
H	-0.8792243487	-2.1290262660	-1.0495075893
H	0.8792243487	-2.1290262660	-1.0495075893
C	0.0000000000	0.0000000000	1.4754897483
O	0.0000000000	0.0000000000	2.6101593137



$HCN\cdots Be(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-187.66881839

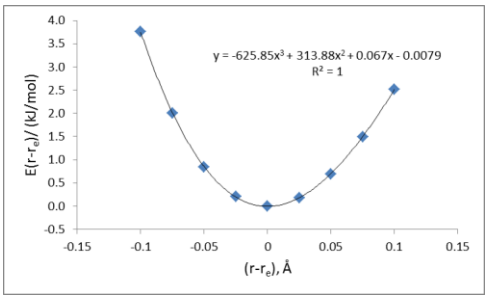
Be	0.0000000000	0.0000000000	-0.7416237785
C	0.0000000000	1.6425252395	-1.2789638564
C	0.0000000000	-1.6425252395	-1.2789638564
H	0.0000000000	1.7406322432	-2.3702940671
H	0.8754952665	2.1998498627	-0.9135762734
H	-0.8754952665	2.1998498627	-0.9135762734
H	0.0000000000	-1.7406322432	-2.3702940671
H	-0.8754952665	-2.1998498627	-0.9135762734
H	0.8754952665	-2.1998498627	-0.9135762734
N	0.0000000000	0.0000000000	1.1019095895
C	0.0000000000	0.0000000000	2.2549128872
H	0.0000000000	0.0000000000	3.3241955759



$H_3N\cdots Be(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-150.88460520

Be	-0.0036636666	-0.2366206922	0.0000000000
C	0.0016270061	-0.8300184897	1.6339335901
C	0.0016270061	-0.8300184897	-1.6339335901
H	0.1062123481	-1.9181777915	1.7094978011
H	-0.9302015841	-0.5762681277	2.1649942554
H	0.8088171533	-0.3991342655	2.2474896046
H	0.1062123481	-1.9181777915	-1.7094978011
H	-0.9302015841	-0.5762681277	-2.1649942554

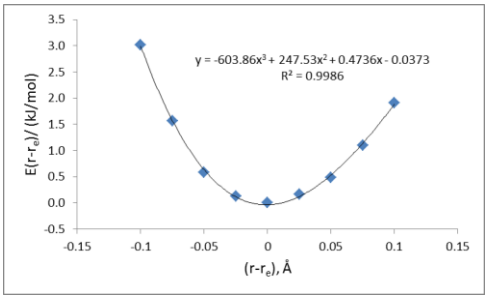


H	0.8088171533	-0.3991342655	-2.2474896046
N	-0.0028219121	1.5722771416	0.0000000000
H	0.9589265739	1.9050276861	0.0000000000
H	-0.4476933124	1.9652533913	-0.8248867929
H	-0.4476933124	1.9652533913	0.8248867929

$H_2O\cdots Be(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-170.73886992

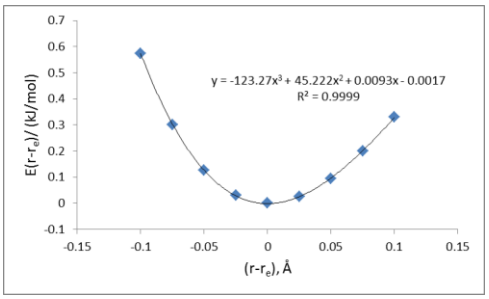
Be	0.0363530268	-0.2512746236	0.0000000000
C	-0.0068295568	-0.8063486536	1.6413604508
C	-0.0068295568	-0.8063486536	-1.6413604508
H	0.4461652610	-1.7978850235	1.7591290917
H	-1.0424106090	-0.9105384596	1.9998540775
H	0.4976942992	-0.1507362660	2.3668161218
H	0.4461652610	-1.7978850235	-1.7591290917
H	-1.0424106090	-0.9105384596	-1.9998540775
H	0.4976942992	-0.1507362660	-2.3668161218
O	0.0349985211	1.4682612904	0.0000000000
H	-0.2603570945	1.9381425279	-0.7870146660
H	-0.2603570945	1.9381425279	0.7870146660



$H_3P\cdots Be(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-437.07674622

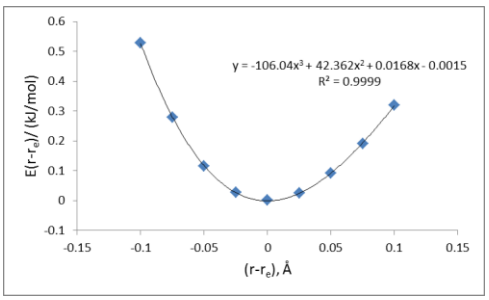
Be	0.0000000000	-0.0167126089	-0.9828549596
C	1.6632647464	0.0028757961	-1.4215151731
C	-1.6632647464	0.0028757961	-1.4215151731
H	1.8148346213	0.0658795057	-2.5054517504
H	2.1910994420	-0.8998152637	-1.0816211332
H	2.2079327820	0.8494726269	-0.9790310529
H	-1.8148346213	0.0658795057	-2.5054517504
H	-2.1910994420	-0.8998152637	-1.0816211332
H	-2.2079327820	0.8494726269	-0.9790310529
P	0.0000000000	-0.0055786214	1.4730392077
H	0.0000000000	1.2845638877	2.0499158640
H	-1.0616160370	-0.5316577591	2.2413366937
H	1.0616160370	-0.5316577591	2.2413366937



$H_2S\cdots Be(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-493.32223054

Be	0.0000000000	0.0045264726	-0.9560950439
C	1.6667273165	-0.0043719212	-1.3735741662
C	-1.6667273165	-0.0043719212	-1.3735741662
H	1.8331492509	0.0812898474	-2.4536109430
H	2.1655995981	-0.9314600767	-1.0554770868
H	2.2282800195	0.8152615648	-0.9035691401
H	-1.8331492509	0.0812898474	-2.4536109430
H	-2.1655995981	-0.9314600767	-1.0554770868
H	-2.2282800195	0.8152615648	-0.9035691401
S	0.0000000000	0.0565185481	1.4681921809
H	-0.9787345301	-0.8320852770	1.7052826910
H	0.9787345301	-0.8320852770	1.7052826910



MgH_2 complexes

MgH_2

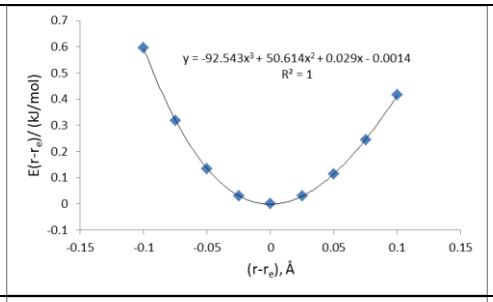
CCSD(T)/AVTZ ENERGY=-200.81325416

Mg	0.0000000000	0.0000000000	0.0000000000
H	0.0000000000	0.0000000000	1.7133968314
H	0.0000000000	0.0000000000	-1.7133968314

$OC\cdots MgH_2$

CCSD(T)/AVTZ ENERGY=-313.98309809

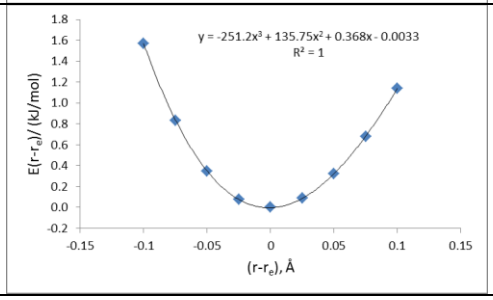
Mg	0.0000000000	0.0000000000	-1.6483382733
H	0.0000000000	1.7067287175	-1.8742958729
H	0.0000000000	-1.7067287175	-1.8742958729
C	0.0000000000	0.0000000000	0.9191045057
O	0.0000000000	0.0000000000	2.0501926997



$HCN\cdots MgH_2$

CCSD(T)/AVTZ ENERGY=-294.11342726

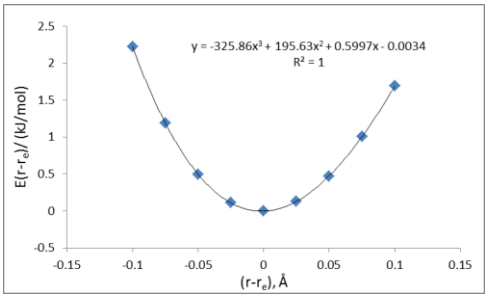
Mg	0.0000000000	0.0000000000	-1.4366857931
H	0.0000000000	1.6881735848	-1.8266429330
H	0.0000000000	-1.6881735848	-1.8266429330
N	0.0000000000	0.0000000000	0.8322706562
C	0.0000000000	0.0000000000	1.9867885427
H	0.0000000000	0.0000000000	3.0559939796



$H_3N\cdots MgH_2$

CCSD(T)/AVTZ ENERGY=-257.32423556

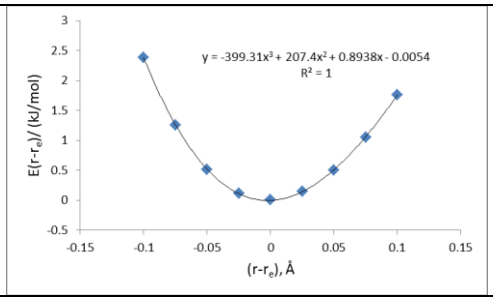
Mg	0.0001385776	0.0000000000	-0.8844900006
H	-0.0001997936	1.6899060247	-1.3045929351
H	-0.0001997936	-1.6899060247	-1.3045929351
N	-0.0011742249	0.0000000000	1.3486389753
H	-0.4634718582	0.8201561397	1.7316107168
H	-0.4634718582	-0.8201561397	1.7316107168
H	0.9403191631	0.0000000000	1.7329715297



$H_2O\cdots MgH_2$

CCSD(T)/AVTZ ENERGY=-277.18165798

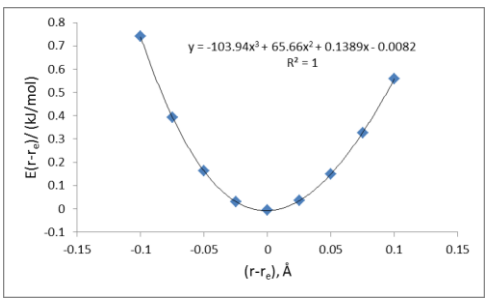
Mg	-0.0000815477	0.0000000000	-0.8679434273
H	-0.0025975048	1.7026230508	-1.2063821241
H	-0.0025975048	-1.7026230508	-1.2063821241
O	0.0023374113	0.0000000000	1.2428971472
H	-0.0149705854	0.7793199973	1.8064954170
H	-0.0149705854	-0.7793199973	1.8064954170



$H_3P\cdots MgH_2$

CCSD(T)/AVTZ ENERGY=-543.52091340

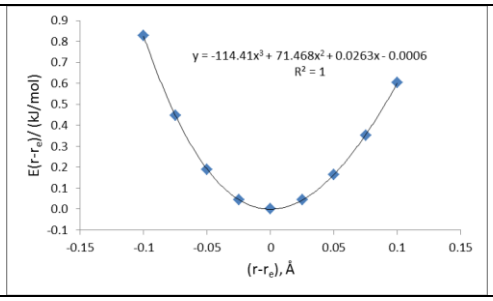
Mg	0.0000000000	0.0030120826	-1.6341017812
H	0.0000000000	1.7277664862	-1.7769747282
H	0.0000000000	-1.6642173177	-2.0811163806
P	0.0000000000	-0.0124678408	1.2197901350
H	-1.0524306396	0.6889967298	1.8483632259
H	1.0524306396	0.6889967298	1.8483632259
H	0.0000000000	-1.1310407720	2.0814758761



$H_2S\cdots MgH_2$

CCSD(T)/AVTZ ENERGY=-599.76662683

Mg	0.0000000000	0.0032496922	-1.5639203024
S	0.0000000000	-0.0565680845	1.2125840933
H	1.7035120722	0.0224607214	-1.8533520849
H	-1.7035120722	0.0224607214	-1.8533520849
H	-0.9791650532	0.8380017171	1.4245750344
H	0.9791650532	0.8380017171	1.4245750344



MgF_2 complexes

MgF_2

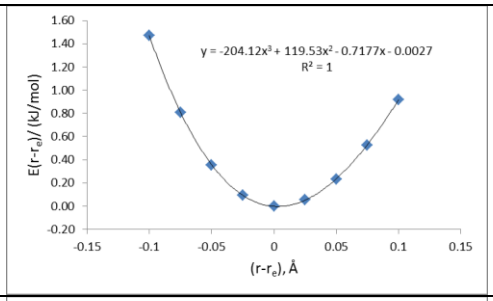
CCSD(T)/AVTZ ENERGY=-399.29088334

Mg	0.0000000000	0.0000000000	0.0000000000
F	0.0000000000	0.0000000000	1.7626908782
F	0.0000000000	0.0000000000	-1.7626908782

$OC\cdots MgF_2$

CCSD(T)/AVTZ ENERGY=-512.46879614

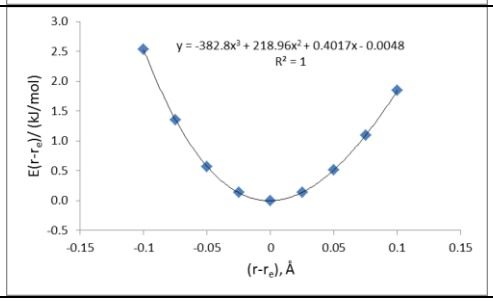
Mg	0.0000000000	0.0000000000	-0.8299221439
F	0.0000000000	1.7530317629	-1.0986331646
F	0.0000000000	-1.7530317629	-1.0986331646
C	0.0000000000	0.0000000000	1.5658763582
O	0.0000000000	0.0000000000	2.6943552875



$HCN\cdots MgF_2$

CCSD(T)/AVTZ ENERGY=-492.60296586

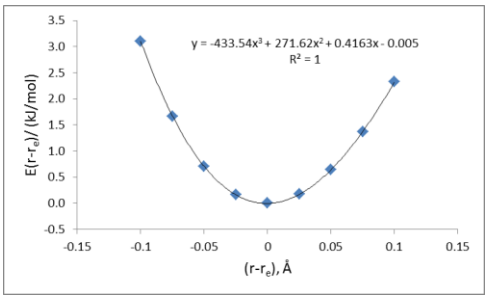
Mg	0.0000000000	0.0000000000	-0.6552219839
F	0.0000000000	1.7281061833	-1.0873662492
F	0.0000000000	-1.7281061833	-1.0873662492
N	0.0000000000	0.0000000000	1.5228081997
C	0.0000000000	0.0000000000	2.6756372525
H	0.0000000000	0.0000000000	3.7452805602



$H_3N\cdots MgF_2$

CCSD(T)/AVTZ ENERGY=-455.81592664

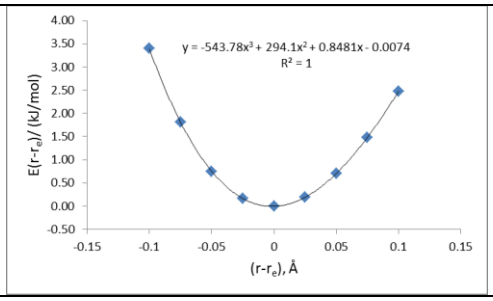
Mg	-0.2666250748	-0.0000607359	-0.0507582028
F	-0.8827145219	0.0000317761	1.6282492252
F	-0.5139304025	0.0000325483	-1.8190746964
N	1.8718592830	0.0000124615	0.2724618193
H	2.0541049056	0.0000810556	1.2727450269
H	2.3440878070	-0.8102195975	-0.1190445670
H	2.3440480420	0.8102174955	-0.1191484431



$H_2O\cdots MgF_2$

CCSD(T)/AVTZ ENERGY=-475.67144873

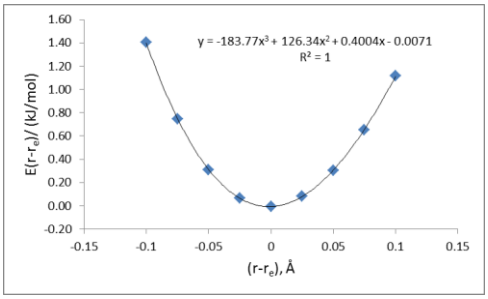
Mg	-0.3066007384	0.0012974939	0.0000000000
F	-0.6584453172	-0.0008611588	1.7482003808
F	-0.6584453172	-0.0008611588	-1.7482003808
O	1.7397577314	0.0016303809	0.0000000000
H	2.2995764025	-0.0123516392	0.7815667200
H	2.2995764025	-0.0123516392	-0.7815667200



$H_3P\cdots MgF_2$

CCSD(T)/AVTZ ENERGY=-742.00834965

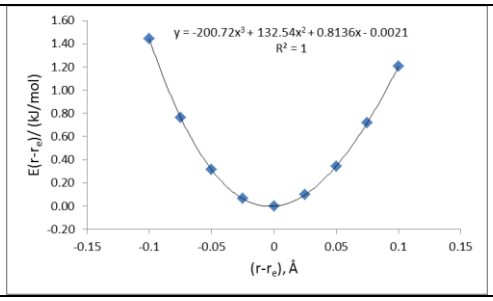
Mg	0.0000000000	0.0762914255	-0.8307108802
F	0.0000000000	1.8575506222	-0.8309558773
F	0.0000000000	-1.5552805510	-1.5363187984
P	0.0000000000	-0.2225284689	1.8553180405
H	-1.0596288625	0.3831938643	2.5598309440
H	1.0596288625	0.3831938643	2.5598309440
H	0.0000000000	-1.4652074358	2.5183825734



$H_2S\cdots MgF_2$

CCSD(T)/AVTZ ENERGY=-798.25402967

Mg	0.0255280730	0.0000000000	-0.8030954692
F	-0.0168552579	1.7476604000	-1.1335192880
F	-0.0168552579	-1.7476604000	-1.1335192880
S	0.0540354892	0.0000000000	1.8276366528
H	-0.8494511738	0.9827731535	1.9819219274
H	-0.8494511738	-0.9827731535	1.9819219274



$Mg(CH_3)_2$ complexes

$Mg(CH_3)_2$

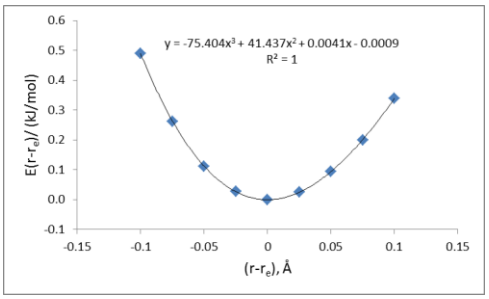
CCSD(T)/AVTZ ENERGY=-279.31929961

Mg	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	2.1049185670
C	0.0000000000	0.0000000000	-2.1049185670
H	1.0169598583	0.0000000000	2.5154878600
H	-0.5084799291	0.8807130719	2.5154878600
H	-0.5084799291	-0.8807130719	2.5154878600
H	-1.0169598583	0.0000000000	-2.5154878600
H	0.5084799291	-0.8807130719	-2.5154878600
H	0.5084799291	0.8807130719	-2.5154878600

$OC\cdots Mg(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-392.48859508

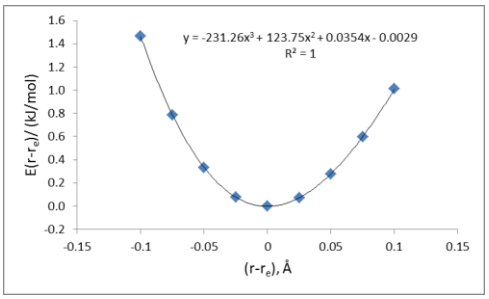
Mg	0.0000000000	0.0000000000	-1.0165206286
C	0.0000000000	2.0974788967	-1.2556066805
C	0.0000000000	-2.0974788967	-1.2556066805
H	0.0000000000	2.4134895570	-2.3056892336
H	0.8790872832	2.5623471251	-0.7889895170
H	-0.8790872832	2.5623471251	-0.7889895170
H	0.0000000000	-2.4134895570	-2.3056892336
H	-0.8790872832	-2.5623471251	-0.7889895170
H	0.8790872832	-2.5623471251	-0.7889895170
C	0.0000000000	0.0000000000	1.5920030095
O	0.0000000000	0.0000000000	2.7236132978



$HCN\cdots Mg(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-372.61802729

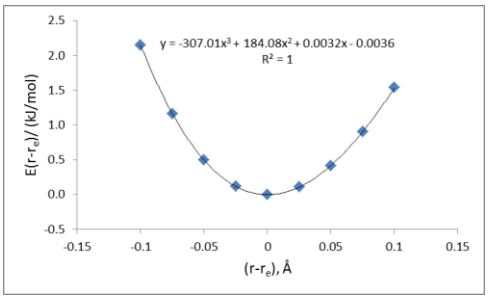
Mg	0.0000000000	0.0000000000	-0.7862510698
C	0.0000000000	2.0728385186	-1.2319497597
C	0.0000000000	-2.0728385186	-1.2319497597
H	0.0000000000	2.2898716379	-2.3075061251
H	0.8783161484	2.5832518663	-0.8118096608
H	-0.8783161484	2.5832518663	-0.8118096608
H	0.0000000000	-2.2898716379	-2.3075061251
H	-0.8783161484	-2.5832518663	-0.8118096608
H	0.8783161484	-2.5832518663	-0.8118096608
N	0.0000000000	0.0000000000	1.4991220586
C	0.0000000000	0.0000000000	2.6540452908
H	0.0000000000	0.0000000000	3.7233522012



$H_3N\cdots Mg(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-335.82801800

Mg	0.0017920165	-0.3347546874	0.0000000000
N	-0.0013642919	1.9101101150	0.0000000000
H	0.9387308851	2.2976389143	0.0000000000
C	-0.0007886023	-0.8316688403	2.0694264295
C	-0.0007886023	-0.8316688403	-2.0694264295
H	0.0307524084	-1.9114449100	2.2624470007
H	-0.8961586509	-0.4552624626	2.5863112966
H	0.8586754609	-0.3997971515	2.6033131468

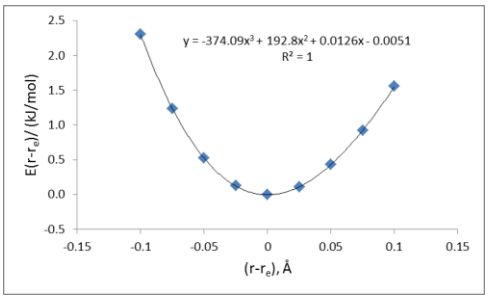


H	0.0307524084	-1.9114449100	-2.2624470007
H	-0.8961586509	-0.4552624626	-2.5863112966
H	0.8586754609	-0.3997971515	-2.6033131468
H	-0.4653639558	2.2924386295	-0.8196053667
H	-0.4653639558	2.2924386295	0.8196053667

$H_2O\cdots Mg(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-355.68553896

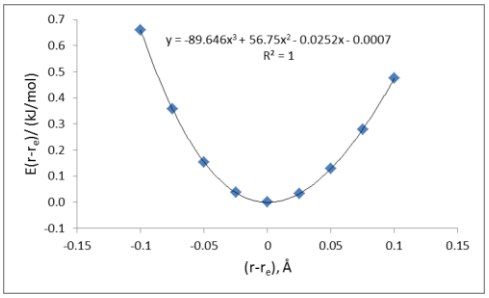
Mg	-0.0003626328	-0.3680007417	0.0000000000
O	-0.0004360469	1.7559539941	0.0000000000
C	0.0002616463	-0.7770213721	2.0842123015
C	0.0002616463	-0.7770213721	-2.0842123015
H	-0.0032925219	-1.8499251660	2.3143511764
H	-0.8767826686	-0.3528187245	2.5941028601
H	0.8813725937	-0.3590761993	2.5922569986
H	-0.0032925219	-1.8499251660	-2.3143511764
H	-0.8767826686	-0.3528187245	-2.5941028601
H	0.8813725937	-0.3590761993	-2.5922569986
H	0.0034176648	2.3215553384	-0.7780898608
H	0.0034176648	2.3215553384	0.7780898608



$H_3P\cdots Mg(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-622.02616478

Mg	0.0000000000	-0.0107085779	-1.0221501134
P	0.0000000000	-0.0033340468	1.8695628503
H	0.0000000000	1.2580168360	2.5083505646
C	2.0911409331	0.0067193865	-1.3488034791
C	-2.0911409331	0.0067193865	-1.3488034791
H	2.3675070497	0.0487479315	-2.4095331425
H	2.5755624613	-0.8880075283	-0.9338556271
H	2.5724091784	0.8686106313	-0.8658989480
H	-2.3675070497	0.0487479315	-2.4095331425
H	-2.5755624613	-0.8880075283	-0.9338556271
H	-2.5724091784	0.8686106313	-0.8658989480
H	-1.0563032892	-0.5580921495	2.6261864328
H	1.0563032892	-0.5580921495	2.6261864328



$H_2S\cdots Mg(CH_3)_2$

CCSD(T)/AVTZ ENERGY=-678.27189066

Mg	0.0000000000	0.0160785449	-0.9765703278
S	0.0000000000	0.0551831617	1.8315786997
C	2.0930648106	-0.0134822421	-1.2885930713
C	-2.0930648106	-0.0134822421	-1.2885930713
H	2.3810493479	0.0625632467	-2.3442075636
H	2.5471478326	-0.9398267029	-0.9091321809
H	2.5966942350	0.8123204204	-0.7671749069
H	-2.3810493479	0.0625632467	-2.3442075636
H	-2.5471478326	-0.9398267029	-0.9091321809
H	-2.5966942350	0.8123204204	-0.7671749069
H	-0.9780272129	-0.8458704933	2.0212445876
H	0.9780272129	-0.8458704933	2.0212445876