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Supplementary Materials: Non-Covalent Interactions of the Lewis Acids Cu–X, Ag–X, and Au–X (X = F and Cl) with Nine Simple Lewis Bases B: A Systematic Investigation of Coinage–Metal Bonds by ab initio Calculations

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Table S1. Optimized geometry (Å) and electronic energy (Hartree) at CCSD(T)/aug-cc-pVTZ/aug-cc-pVTZ-PP computational level.

	FCu complexes				ClCu complexes			
	CCSD(T)/AVTZ ENERGY=-1739.22063466				CCSD(T)/AVTZ ENERGY=-2099.25035766			
-	Cu	0.0000000000	0.0000000000	-0.4076144976	Cl	0.0000000000	0.0000000000	-1.3391794445
	F	0.0000000000	0.0000000000	1.3633920106	Cu	0.0000000000	0.0000000000	0.7471426816
	CCSD(T)/AVTZ ENERGY=-1848.64280386				CCSD(T)/AVTZ ENERGY=-2208.66614901			
	F	0.0000000000	0.0000000000	-2.0463515847	Cl	0.0000000000	0.0000000000	-2.0250926222
N_2	Cu	0.0000000000	0.0000000000	-0.2998597591	Cu	0.0000000000	0.0000000000	0.0478092023
	N	0.0000000000	0.0000000000	1.5150580377	N	0.0000000000	0.0000000000	1.9020103187
	N	0.0000000000	0.0000000000	2.6209840233	N	0.0000000000	0.0000000000	3.0068922184
	CCSD(T)/AVTZ ENERGY=-1852.44890984				CCSD(T)/AVTZ ENERGY=-2212.46969761			
	F	0.0000000000	0.0000000000	-2.0622149677	Cl	0.0000000000	0.0000000000	-2.0409992233
CO	Cu	0.0000000000	0.0000000000	-0.3165771964	Cu	0.0000000000	0.0000000000	0.0363404298
	C	0.0000000000	0.0000000000	1.4683711945	C	0.0000000000	0.0000000000	1.8531807863
	O	0.0000000000	0.0000000000	2.6038100885	O	0.0000000000	0.0000000000	2.9870933963
	CCSD(T)/AVTZ ENERGY=-1816.47147670				CCSD(T)/AVTZ ENERGY=-2176.49428454			
	F	0.0000000000	0.0000000000	-1.9055580675	Cl	0.0000000000	0.0000000000	-1.8986809128
	Cu	0.0000000000	0.0000000000	-0.1464608795	Cu	0.0000000000	0.0000000000	0.1898927665
C_2H	C	0.0000000000	0.6187735019	1.7277271810	C	0.0000000000	0.6164775715	2.1049420105
2	C	0.0000000000	-0.6187735019	1.7277271810	C	0.0000000000	-0.6164775715	2.1049420105
	H	0.0000000000	1.6571300539	1.9872714712	H	0.0000000000	1.6640789015	2.3226043650
	H	0.0000000000	-1.6571300539	1.9872714712	H	0.0000000000	-1.6640789015	2.3226043650
	CCSD(T)/AVTZ ENERGY=-1817.72612778				CCSD(T)/AVTZ ENERGY=-2177.74923853			
	F	0.0000000000	0.0000000000	-1.9426762710	Cl	0.0000000000	0.0000000000	-1.9358289589
	Cu	0.0000000000	0.0000000000	-0.1820468187	Cu	0.0000000000	0.0000000000	0.1531001992
	C	0.0000000000	0.6883417031	1.7128971892	C	0.0000000000	0.6857479369	2.0868544286
C_2H	C	0.0000000000	-0.6883417031	1.7128971892	C	0.0000000000	-0.6857479369	2.0868544286
4	H	-0.9237943648	1.2476533687	1.8177861674	H	-0.9246727634	1.2461433366	2.1756309247
	H	0.9237943648	1.2476533687	1.8177861674	H	0.9246727634	1.2461433366	2.1756309247
	H	0.9237943648	-1.2476533687	1.8177861674	H	0.9246727634	-1.2461433366	2.1756309247
	H	-0.9237943648	-1.2476533687	1.8177861674	H	-0.9246727634	-1.2461433366	2.1756309247
	CCSD(T)/AVTZ ENERGY=-2081.98184952				CCSD(T)/AVTZ ENERGY=-2442.00534725			
	F	-0.0000000000	0.0000000000	-2.1159864828	Cl	-0.0000000000	0.0000000000	-2.1038311260
	Cu	-0.0000000000	0.0000000000	-0.3527947111	Cu	-0.0000000000	0.0000000000	-0.0119361716
PH_3	P	0.0000000000	0.0000000000	1.7811754861	P	0.0000000000	0.0000000000	2.1556866015
	H	1.2317118206	0.0000000000	2.4635575624	H	1.2325550024	0.0000000000	2.8361150594
	H	-0.6158559103	1.0666937268	2.4635575624	H	-0.6162775012	1.0674239436	2.8361150594
	H	-0.6158559103	-1.0666937268	2.4635575624	H	-0.6162775012	-1.0674239436	2.8361150594
	CCSD(T)/AVTZ ENERGY=-2138.21486131				CCSD(T)/AVTZ ENERGY=-2498.23962746			
	Cu	0.0000000000	0.0014540758	0.3470652976	Cu	0.0000000000	0.0072797066	0.0084873674
SH_2	F	0.0000000000	-0.0091511349	2.1091899304	Cl	0.0000000000	-0.0096138270	2.0961970823
	S	0.0000000000	0.0546357876	-1.8060982537	S	0.0000000000	0.0490977528	-2.1812166491

	H	0.9755055556	-0.8285052190	-2.0945401955	H	0.9756055687	-0.8412361760	-2.4436016234
	H	-0.9755055556	-0.8285052190	-2.0945401955	H	-0.9756055687	-0.8412361760	-2.4436016234

		CCSD(T)/AVTZ ENERGY=-1832.56279003				CCSD(T)/AVTZ ENERGY=-2192.58704189		
	F	0.0000000000	0.0000000000	-2.0465377086	Cl	0.0000000000	0.0000000000	-2.0205395562
	Cu	0.0000000000	0.0000000000	-0.2914478353	Cu	0.0000000000	0.0000000000	0.0608848476
NCH	N	0.0000000000	0.0000000000	1.5278180790	N	0.0000000000	0.0000000000	1.9115406461
	C	0.0000000000	0.0000000000	2.6825951347	C	0.0000000000	0.0000000000	3.0657924058
	H	0.0000000000	0.0000000000	3.7511683603	H	0.0000000000	0.0000000000	4.1347614013

		CCSD(T)/AVTZ ENERGY=-1815.60958471				CCSD(T)/AVTZ ENERGY=-2175.63571624		
	Cu	0.0000000000	0.0056656416	0.0201394684	Cu	0.0000000000	0.0118652762	-0.3227032525
	F	0.0000000000	-0.0142597323	1.7745017606	Cl	0.0000000000	-0.0124873788	1.7535805592
OH_2	O	0.0000000000	0.0414794942	-1.8971262450	O	0.0000000000	0.0274057180	-2.2657377596
	H	0.7706264433	-0.3734169408	-2.3015261744	H	0.7704886019	-0.3719223584	-2.6850536609
	H	-0.7706264433	-0.3734169408	-2.3015261744	H	-0.7704886019	-0.3719223584	-2.6850536609

		CCSD(T)/AVTZ ENERGY=-1795.77049708				CCSD(T)/AVTZ ENERGY=-2155.79573068		
	F	-0.0000000000	0.0000000000	-1.7613556283	Cl	-0.0000000000	0.0000000000	-1.7402799892
	Cu	-0.0000000000	0.0000000000	-0.0027716683	Cu	-0.0000000000	0.0000000000	0.3426488403
NH_3	N	0.0000000000	0.0000000000	1.9079124805	N	0.0000000000	0.0000000000	2.2767777692
	H	0.9433596271	0.0000000000	2.2870127005	H	0.9428409644	0.0000000000	2.6569174343
	H	-0.4716798136	0.8169734020	2.2870127005	H	-0.4714204822	0.8165242269	2.6569174343
	H	-0.4716798136	-0.8169734020	2.2870127005	H	-0.4714204822	-0.8165242269	2.6569174343

	FAg complexes				**ClAg complexes**			
	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-246.20662653				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-606.24295525			
	F	0.0000000000	0.0000000000	-1.6939621032	Cl	0.0000000000	0.0000000000	-1.7302153023
-	Ag	0.0000000000	0.0000000000	0.2983509014	Ag	0.0000000000	0.0000000000	0.5686692010

	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-355.60992318				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-715.64340555			
	F	0.0000000000	0.0000000000	-2.1916724959	Cl	0.0000000000	0.0000000000	-2.2415723603
	Ag	0.0000000000	0.0000000000	-0.2373241172	Ag	0.0000000000	0.0000000000	0.0291819313
N_2	N	0.0000000000	0.0000000000	1.8487341057	N	0.0000000000	0.0000000000	2.1731515131
	N	0.0000000000	0.0000000000	2.9516830272	N	0.0000000000	0.0000000000	3.2758594950

	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-359.41469527				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-719.44478363			
	F	0.0000000000	0.0000000000	-2.1765659010	Cl	0.0000000000	0.0000000000	-2.2327840222
	Ag	0.0000000000	0.0000000000	-0.2350799534	Ag	0.0000000000	0.0000000000	0.0332343624
CO	C	0.0000000000	0.0000000000	1.7351795106	C	0.0000000000	0.0000000000	2.0521742606
	O	0.0000000000	0.0000000000	2.8668379111	O	0.0000000000	0.0000000000	3.1829503637

	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-323.43896493				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-683.47173101			
	F	0.0000000000	0.0000000000	-2.0856548043	Cl	0.0000000000	0.0000000000	-2.1426358421
	Ag	0.0000000000	0.0000000000	-0.1226205961	Ag	0.0000000000	0.0000000000	0.1387983337
C_2H_2	C	0.0000000000	0.6136572908	2.0162025636	C	0.0000000000	0.6122266223	2.3311609647
	C	0.0000000000	-0.6136572908	2.0162025636	C	0.0000000000	-0.6122266223	2.3311609647
	H	0.0000000000	1.6675588894	2.1914774143	H	0.0000000000	1.6706705166	2.4762353878
	H	0.0000000000	-1.6675588894	2.1914774143	H	0.0000000000	-1.6706705166	2.4762353878

	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-324.69665032				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-684.72901337			
C_2H_4	F	0.0000000000	0.0000000000	-2.1104781811	Cl	0.0000000000	0.0000000000	-2.1679628928
	Ag	0.0000000000	0.0000000000	-0.1461858054	Ag	0.0000000000	0.0000000000	0.1150150625
					C	0.0000000000	0.6819135318	2.2873224023

	C	0.0000000000	0.6836868463	1.9793144427	C	0.0000000000	-0.6819135318	2.2873224023
	C	0.0000000000	-0.6836868463	1.9793144427	H	-0.9256029010	1.2422699971	2.3583402609
	H	-0.9249609855	1.2432789962	2.0629757622	H	0.9256029010	1.2422699971	2.3583402609
	H	0.9249609855	1.2432789962	2.0629757622	H	0.9256029010	-1.2422699971	2.3583402609
	H	0.9249609855	-1.2432789962	2.0629757622	H	-0.9256029010	-1.2422699971	2.3583402609
	H	-0.9249609855	-1.2432789962	2.0629757622				
	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-588.95746405				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-948.98891289			
	F	-0.0000000000	0.0000000000	-2.2282010640	Cl	-0.0000000000	0.0000000000	-2.2876110363
	Ag	-0.0000000000	0.0000000000	-0.2642807506	Ag	-0.0000000000	0.0000000000	-0.0013139475
PH_3	P	0.0000000000	0.0000000000	2.0231609285	P	0.0000000000	0.0000000000	2.3292740084
	H	1.2315221723	0.0000000000	2.7034842003	H	1.2321539727	0.0000000000	3.0087879280
	H	-0.6157610862	1.0665294866	2.7034842003	H	-0.6160769863	1.0670766417	3.0087879280
	H	-0.6157610862	-1.0665294866	2.7034842003	H	-0.6160769863	-1.0670766417	3.0087879280
	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-645.18889184				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-1005.22216679			
	Ag	0.0000000000	0.0031777572	0.2694958914	Ag	0.0000000000	0.0079186742	0.0071271636
	F	0.0000000000	-0.0149798502	2.2363676918	Cl	0.0000000000	-0.0146874979	2.2912384550
SH_2	S	0.0000000000	0.0511951083	-2.0852287811	S	0.0000000000	0.0434636962	-2.3930699758
	H	0.9739172976	-0.8430565752	-2.3339765523	H	0.9740539462	-0.8566498866	-2.6183343414
	H	-0.9739172976	-0.8430565752	-2.3339765523	H	-0.9740539462	-0.8566498866	-2.6183343414
	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-339.52898512				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-699.56277901			
	F	0.0000000000	0.0000000000	-2.1851466408	Cl	0.0000000000	0.0000000000	-2.2306955345
	Ag	0.0000000000	0.0000000000	-0.2244211848	Ag	0.0000000000	0.0000000000	0.0459491509
NCH	N	0.0000000000	0.0000000000	1.8363533420	N	0.0000000000	0.0000000000	2.1473350279
	C	0.0000000000	0.0000000000	2.9897472213	C	0.0000000000	0.0000000000	3.3008375468
	H	0.0000000000	0.0000000000	4.0588740551	H	0.0000000000	0.0000000000	4.3702594130
	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-322.57928636				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-682.61485251			
	Ag	0.0000000000	0.0064936536	0.0190298368	Ag	0.0000000000	0.0109759649	-0.2486204079
	F	0.0000000000	-0.0233798633	1.9877791460	Cl	0.0000000000	-0.0185015351	2.0296860337
OH_2	O	0.0000000000	0.0317038767	-2.1640324131	O	0.0000000000	0.0154198571	-2.4583406633
	H	0.7676140288	-0.3787535316	-2.5766034394	H	0.7676667683	-0.3843141032	-2.8812466300
	H	-0.7676140288	-0.3787535316	-2.5766034394	H	-0.7676667683	-0.3843141032	-2.8812466300
	CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-302.73924730				CCSD(T)/AVTZ,AG=AVTZ-PP ENERGY=-662.77337063			
	F	-0.0000000000	0.0000000000	-1.9635476055	Cl	-0.0000000000	0.0000000000	-2.0100900123
	Ag	-0.0000000000	0.0000000000	-0.0000736027	Ag	-0.0000000000	0.0000000000	-0.2677065908
NH_3	N	0.0000000000	0.0000000000	2.1232435804	N	0.0000000000	0.0000000000	2.4220219795
	H	0.9431248329	0.0000000000	2.4990553228	H	0.9429500618	0.0000000000	2.7984992070
	H	-0.4715624164	0.8167700642	2.4990553228	H	-0.4714750309	0.8166187080	2.7984992070
	H	-0.4715624164	-0.8167700642	2.4990553228	H	-0.4714750309	-0.8166187080	2.7984992070

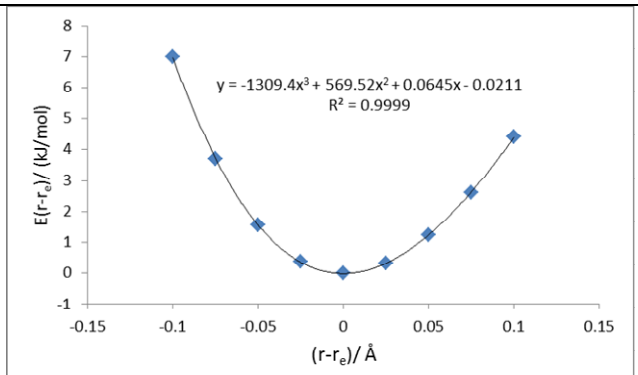
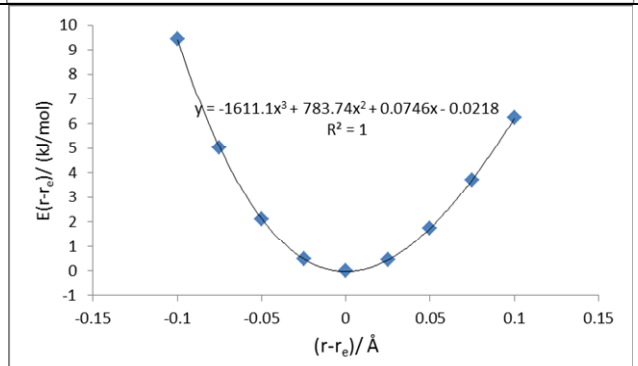
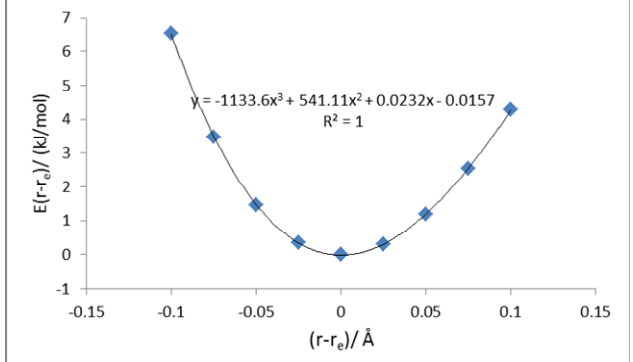
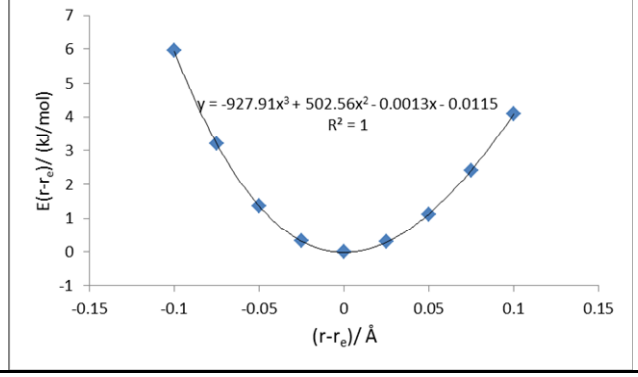
	FAu complexes				ClAu complexes			
-	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-234.89453117				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-594.93936142			
	F	0.0000000000	0.0000000000	-1.7711816311	Cl	0.0000000000	0.0000000000	-1.8896414550
	Au	0.0000000000	0.0000000000	0.1708393174	Au	0.0000000000	0.0000000000	0.3401261560
N_2	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-344.32765756				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-704.36028386			
	F	0.0000000000	0.0000000000	-2.0462240612	Cl	0.0000000000	0.0000000000	-2.1907149642
	Au	0.0000000000	0.0000000000	-0.1368958540	Au	0.0000000000	0.0000000000	0.0285339037
	N	0.0000000000	0.0000000000	1.7972539286	N	0.0000000000	0.0000000000	2.0193618386
	N	0.0000000000	0.0000000000	2.9032741450	N	0.0000000000	0.0000000000	3.1244046792
CO	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-348.15296533				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-708.18045244			
	F	0.0000000000	0.0000000000	-2.0539634336	Cl	0.0000000000	0.0000000000	-2.2040354257
	Au	0.0000000000	0.0000000000	-0.1388827244	Au	0.0000000000	0.0000000000	0.0304379249
	C	0.0000000000	0.0000000000	1.7204043159	C	0.0000000000	0.0000000000	1.9269987151
	O	0.0000000000	0.0000000000	2.8572004550	O	0.0000000000	0.0000000000	3.0625670242
C_2H_2	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-312.16494904				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-672.19671008			
	F	0.0000000000	0.0000000000	-2.0024615128	Cl	0.0000000000	0.0000000000	-2.1469096443
	Au	0.0000000000	0.0000000000	-0.0660243513	Au	0.0000000000	0.0000000000	0.1001415693
	C	0.0000000000	0.6233903642	1.9360643673	C	0.0000000000	0.6212641569	2.1434885886
	C	0.0000000000	-0.6233903642	1.9360643673	C	0.0000000000	-0.6212641569	2.1434885886
	H	0.0000000000	1.6458549101	2.2521270968	H	0.0000000000	1.6520255323	2.4301894668
	H	0.0000000000	-1.6458549101	2.2521270968	H	0.0000000000	-1.6520255323	2.4301894668
C_2H_4	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-313.42492706				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-673.45652246			
	F	0.0000000000	0.0000000000	-2.0224490527	Cl	0.0000000000	0.0000000000	-2.1676672769
	Au	0.0000000000	0.0000000000	-0.0818038858	Au	0.0000000000	0.0000000000	0.0841384901
	C	0.0000000000	0.6970932352	1.9223872690	C	0.0000000000	0.6941949426	2.1293997593
	C	0.0000000000	-0.6970932352	1.9223872690	C	0.0000000000	-0.6941949426	2.1293997593
	H	-0.9211313783	1.2486666259	2.0726283946	H	-0.9225732162	1.2474560119	2.2633795272
	H	0.9211313783	1.2486666259	2.0726283946	H	0.9225732162	1.2474560119	2.2633795272
	H	0.9211313783	-1.2486666259	2.0726283946	H	0.9225732162	-1.2474560119	2.2633795272
	H	-0.9211313783	-1.2486666259	2.0726283946	H	-0.9225732162	-1.2474560119	2.2633795272
PH_3	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-577.69149465				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-937.72188796			
	F	-0.0000000000	0.0000000000	-2.1049999272	Cl	-0.0000000000	0.0000000000	-2.2530746289
	Au	-0.0000000000	0.0000000000	-0.1575262154	Au	-0.0000000000	0.0000000000	0.0098910790
	P	0.0000000000	0.0000000000	2.0302542644	P	0.0000000000	0.0000000000	2.2334102116
	H	1.2409454097	0.0000000000	2.6901124778	H	1.2404241643	0.0000000000	2.8946603085
	H	-0.6204727048	1.0746902495	2.6901124778	H	-0.6202120821	1.0742388377	2.8946603085
	H	-0.6204727048	-1.0746902495	2.6901124778	H	-0.6202120821	-1.0742388377	2.8946603085
SH_2	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-633.91105280				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-993.94422670			
	Au	0.0000000000	-0.0005117749	0.1602130546	Au	0.0000000000	0.0006988309	-0.0047731966
	F	0.0000000000	-0.0037529523	2.0998452059				
	S	0.0000000000	0.0569293527	-2.0780650643	Cl	0.0000000000	-0.0050097038	2.2439013896
	H	0.9741760448	-0.8200152927	-2.3947576780	S	0.0000000000	0.0534279186	-2.2896427502
	H	-0.9741760448	-0.8200152927	-2.3947576780	H	0.9745887441	-0.8298789240	-2.5829561103

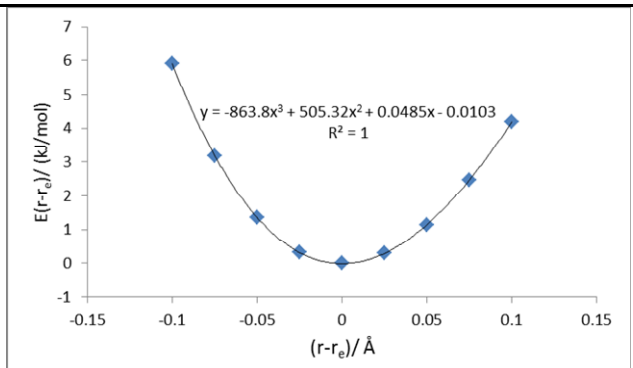
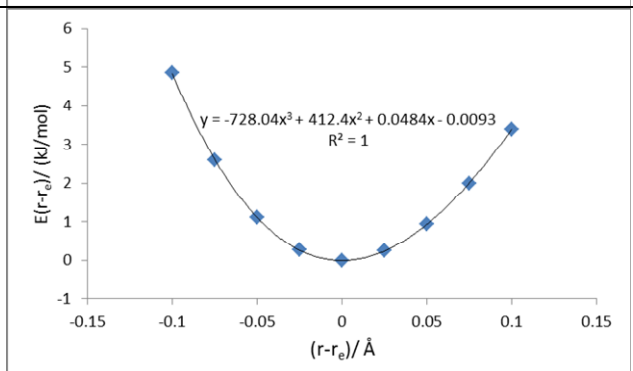
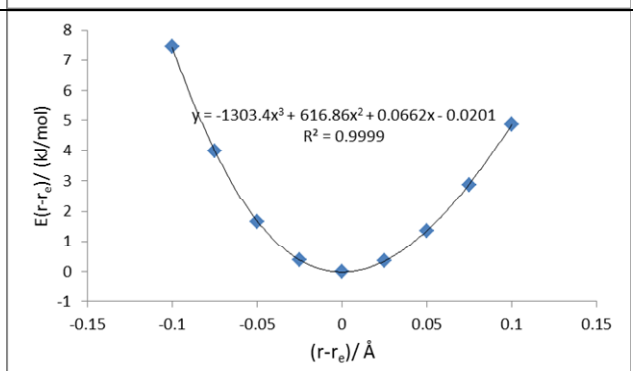
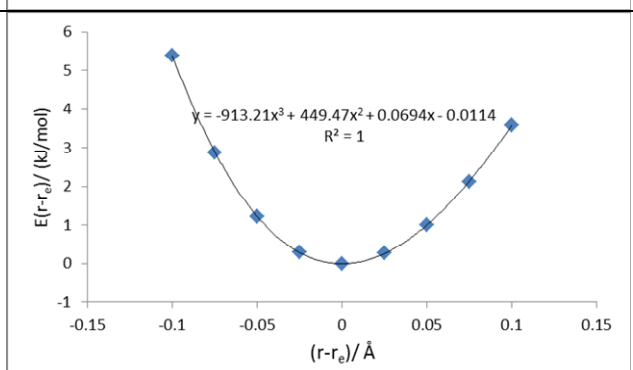
					H	-0.9745887441	-0.8298789240	-2.5829561103
	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-328.24902941				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-688.28185997			
NCH	F	0.0000000000	0.0000000000	-2.0521339649	Cl	0.0000000000	0.0000000000	-2.1933201706
	Au	0.0000000000	0.0000000000	-0.1318217111	Au	0.0000000000	0.0000000000	0.0355850537
	N	0.0000000000	0.0000000000	1.8081395835	N	0.0000000000	0.0000000000	2.0226971102
	C	0.0000000000	0.0000000000	2.9609861946	C	0.0000000000	0.0000000000	3.1755375173
	H	0.0000000000	0.0000000000	4.0292628954	H	0.0000000000	0.0000000000	4.2443238561

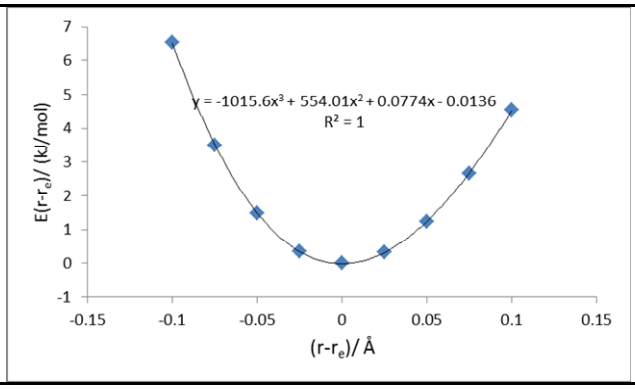
	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-311.28845946				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-671.32527470			
	Au	0.0000000000	0.0020072277	0.0075146351	Au	0.0000000000	0.0038151880	-0.1582495531
	F	0.0000000000	-0.0146597814	1.9275043806	Cl	0.0000000000	-0.0123379461	2.0627806106
OH_2	O	0.0000000000	0.0460508356	-2.0766771403	O	0.0000000000	0.0346238369	-2.2903140603
	H	0.7716686168	-0.4234527479	-2.4178265296	H	0.7708237686	-0.4305849784	-2.6381776717
	H	-0.7716686168	-0.4234527479	-2.4178265296	H	-0.7708237686	-0.4305849784	-2.6381776717

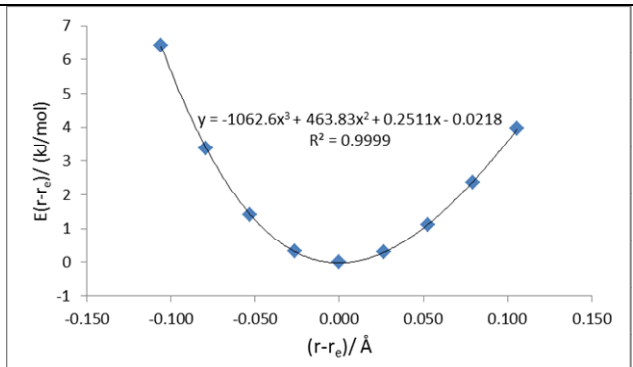
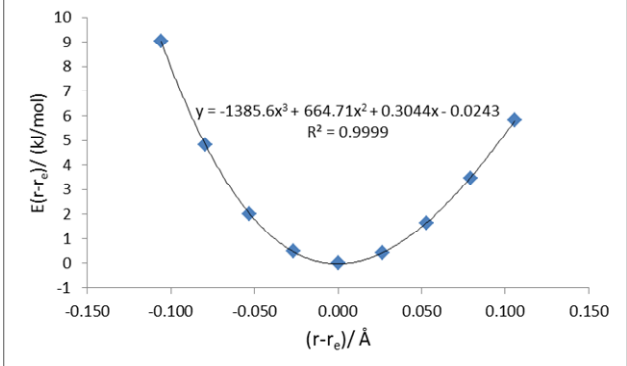
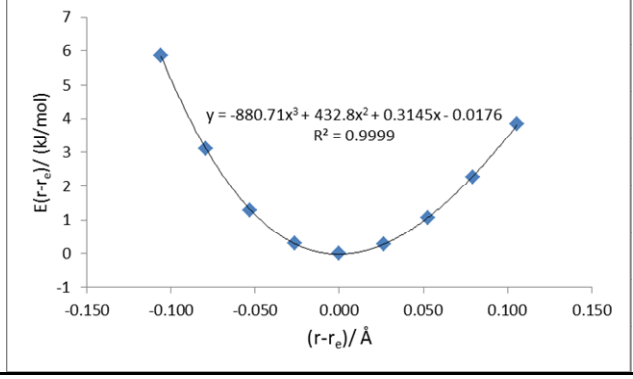
	CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-291.46071659				CCSD(T)/AVTZ,AU=AVTZ-PP ENERGY=-651.49445669			
	F	-0.0000000000	0.0000000000	-1.9272116452	Cl	-0.0000000000	0.0000000000	-2.0656104086
	Au	-0.0000000000	0.0000000000	0.0036413975	Au	-0.0000000000	0.0000000000	0.1716891717
NH_3	N	0.0000000000	0.0000000000	2.0424569844	N	0.0000000000	0.0000000000	2.2490700553
	H	0.9473434155	0.0000000000	2.4104040396	H	0.9470356197	0.0000000000	2.6168955244
	H	-0.4736717078	0.8204234640	2.4104040396	H	-0.4735178099	0.8201569050	2.6168955244
	H	-0.4736717078	-0.8204234640	2.4104040396	H	-0.4735178099	-0.8201569050	2.6168955244

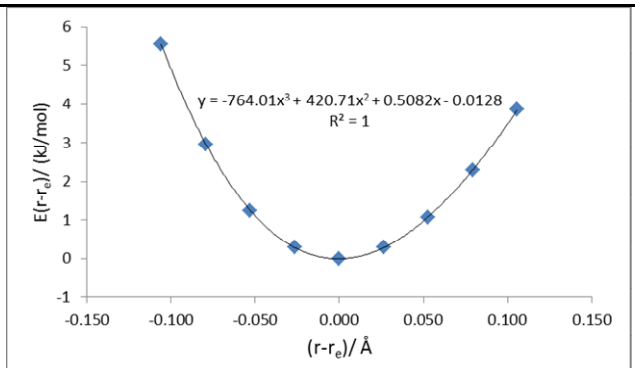
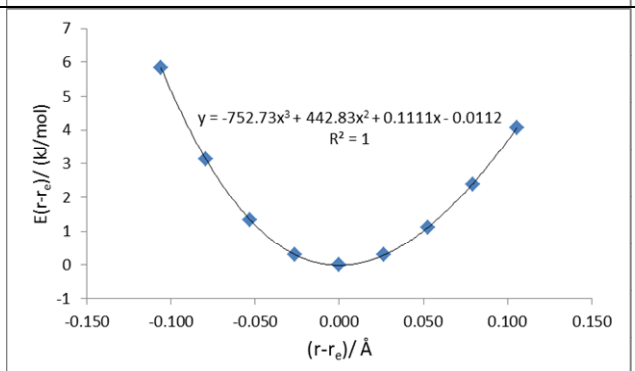
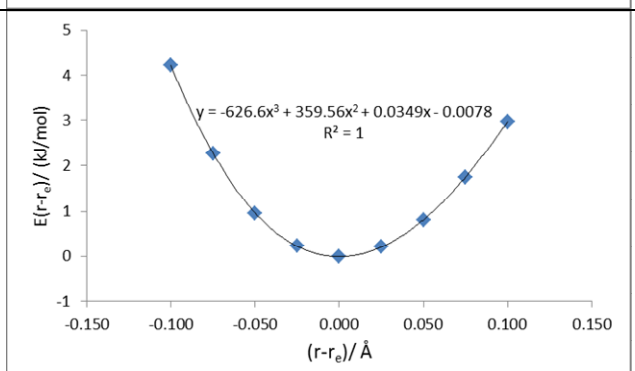
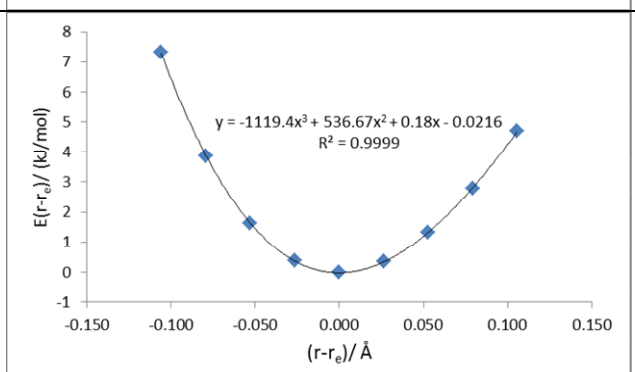
Table S2. Intermolecular stretching quadratic force constants k_σ calculations.

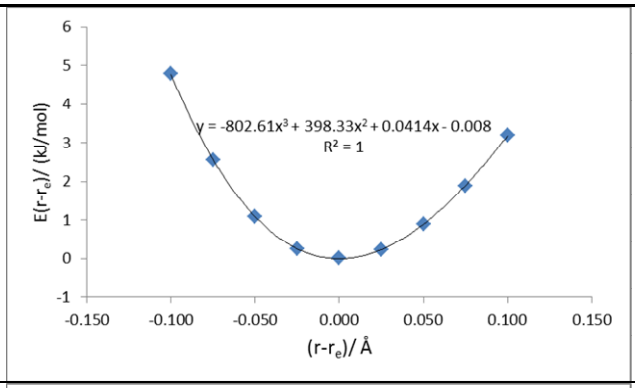
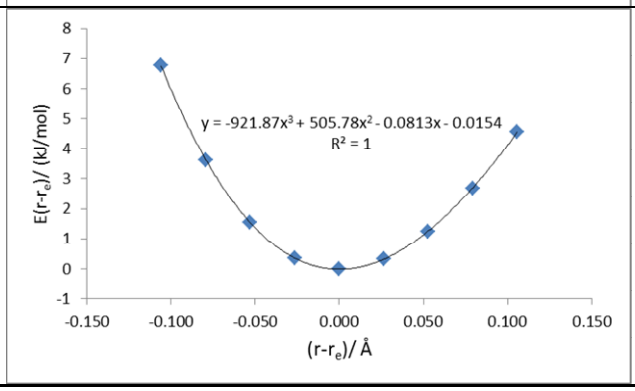
FCu:Base	r-r_e/ Å	E(r-r_e)/ (kJ/mol)	Fitted Curve
FCu:N_2	-0.1	6.99	
	-0.075	3.70	
	-0.05	1.55	
	-0.025	0.37	
	0	0.00	
	0.025	0.33	
	0.05	1.23	
	0.075	2.61	
	0.1	4.39	
FCu:CO	-0.1	9.44	
	-0.075	5.03	
	-0.05	2.12	
	-0.025	0.50	
	0	0.00	
	0.025	0.45	
	0.05	1.73	
	0.075	3.69	
	0.1	6.23	
FCu:HCCH	-0.1	6.54	
	-0.075	3.49	
	-0.05	1.47	
	-0.025	0.35	
	0	0.00	
	0.025	0.31	
	0.05	1.19	
	0.075	2.53	
	0.1	4.28	
FCu:H_2CCH_2	-0.1	5.95	
	-0.075	3.19	
	-0.05	1.35	
	-0.025	0.32	
	0	0.00	
	0.025	0.29	
	0.05	1.12	
	0.075	2.41	
	0.1	4.09	

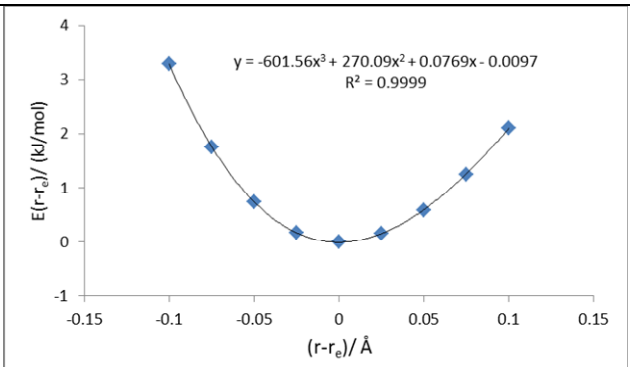
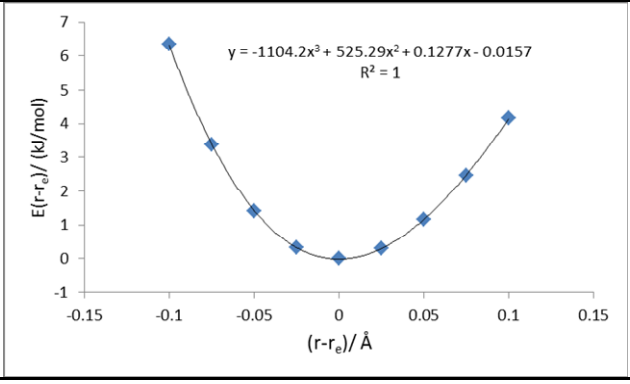
$FCu:PH_3$	-0.1	5.91	
	-0.075	3.18	
	-0.05	1.35	
	-0.025	0.32	
	0	0.00	
	0.025	0.30	
	0.05	1.14	
	0.075	2.46	
	0.1	4.19	
$FCu:SH_2$	-0.1	4.85	
	-0.075	2.60	
	-0.05	1.10	
	-0.025	0.26	
	0	0.00	
	0.025	0.24	
	0.05	0.93	
	0.075	2.00	
	0.1	3.40	
FCu:NCH	-0.1	7.46	
	-0.075	3.97	
	-0.05	1.67	
	-0.025	0.40	
	0	0.00	
	0.025	0.36	
	0.05	1.35	
	0.075	2.88	
	0.1	4.87	
$FCu:OH_2$	-0.1	5.40	
	-0.075	2.88	
	-0.05	1.21	
	-0.025	0.29	
	0	0.00	
	0.025	0.27	
	0.05	0.99	
	0.075	2.12	
	0.1	3.59	

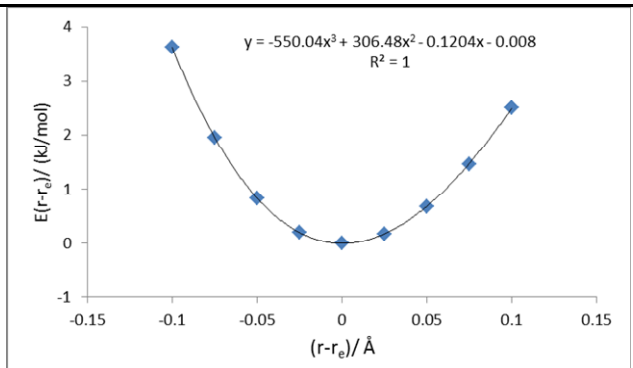
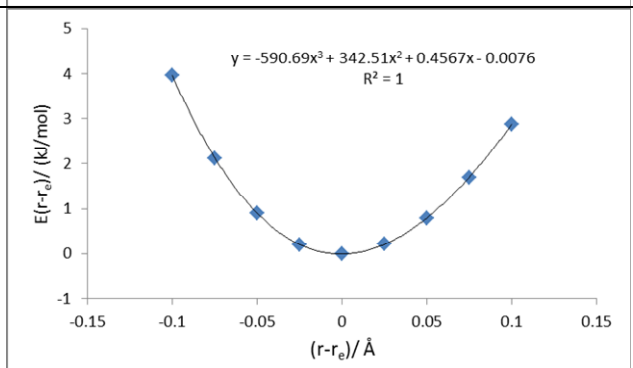
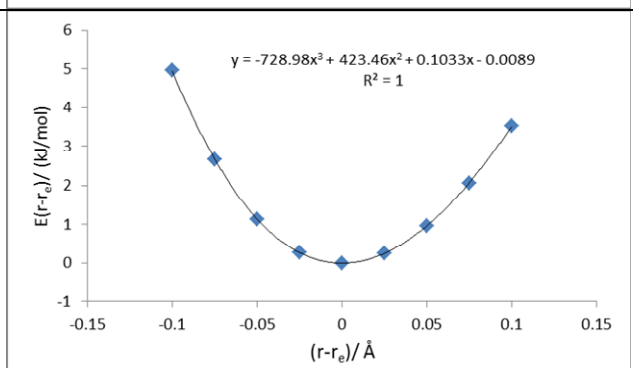
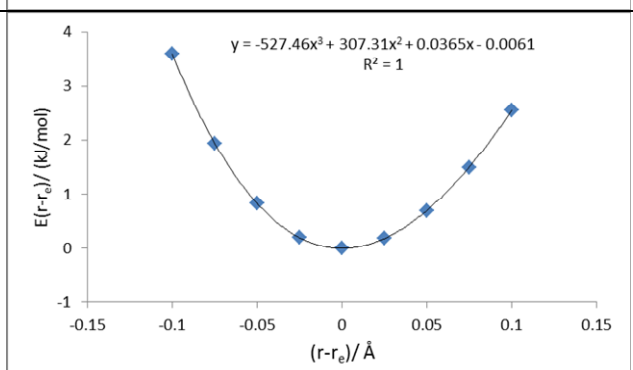
FCu:NH_3	-0.1	6.55	
	-0.075	3.51	
	-0.05	1.49	
	-0.025	0.35	
	0	0.00	
	0.025	0.32	
	0.05	1.24	
	0.075	2.66	
	0.1	4.53	

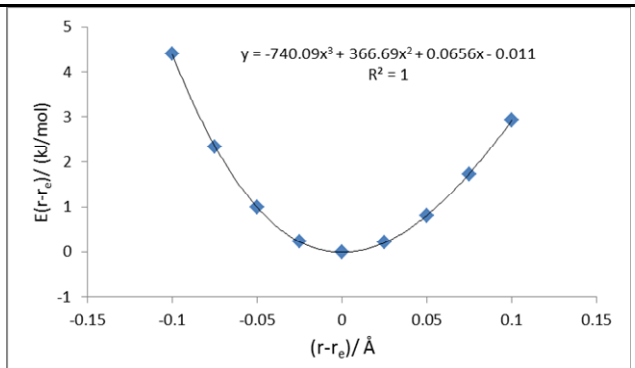
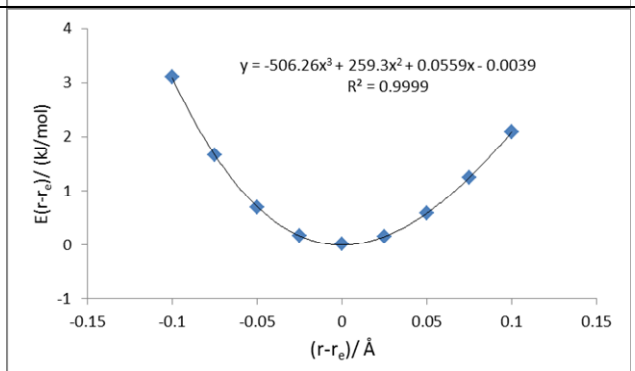
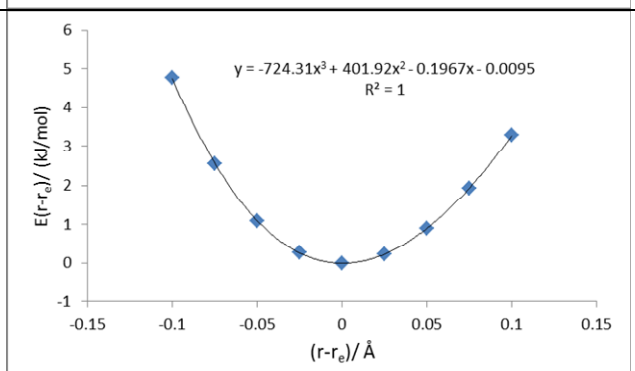
ClCu:Base	r-r_e/ Å	E(r-r_e)/ (kJ/mol)	Fitted Curve
ClCu:N_2	-0.106	6.42	
	-0.079	3.39	
	-0.053	1.41	
	-0.026	0.33	
	0.000	0.00	
	0.026	0.30	
	0.053	1.12	
	0.079	2.37	
	0.106	3.96	
ClCu:CO	-0.106	9.05	
	-0.079	4.80	
	-0.053	2.01	
	-0.026	0.47	
	0.000	0.00	
	0.026	0.43	
	0.053	1.63	
	0.079	3.47	
	0.106	5.83	
ClCu:HCCH	-0.106	5.85	
	-0.079	3.10	
	-0.053	1.30	
	-0.026	0.30	
	0.000	0.00	
	0.026	0.29	
	0.053	1.07	
	0.079	2.27	
	0.106	3.83	

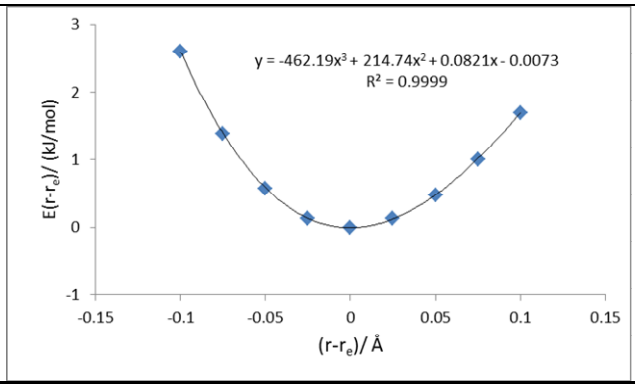
ClCu:H_2CCH_2	-0.106	5.56	
	-0.079	2.96	
	-0.053	1.24	
	-0.026	0.29	
	0.000	0.00	
	0.026	0.29	
	0.053	1.07	
	0.079	2.28	
	0.106	3.86	
ClCu:PH_3	-0.106	5.84	
	-0.079	3.13	
	-0.053	1.33	
	-0.026	0.32	
	0.000	0.00	
	0.026	0.29	
	0.053	1.12	
	0.079	2.40	
	0.106	4.08	
ClCu:SH_2	-0.1	4.22	
	-0.075	2.27	
	-0.05	0.96	
	-0.025	0.23	
	0	0.00	
	0.025	0.21	
	0.05	0.81	
	0.075	1.74	
	0.1	2.97	
ClCu:NCH	-0.106	7.31	
	-0.079	3.88	
	-0.053	1.62	
	-0.026	0.38	
	0.000	0.00	
	0.026	0.35	
	0.053	1.31	
	0.079	2.79	
	0.106	4.70	

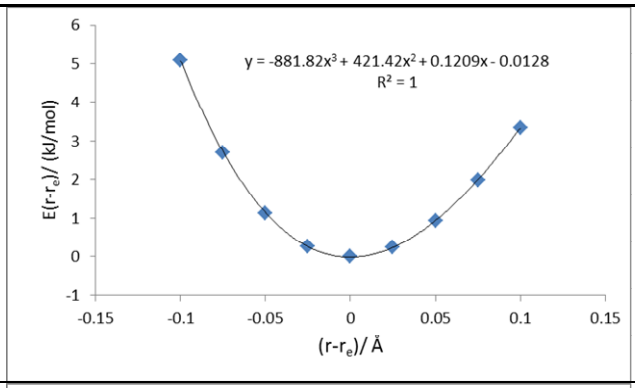
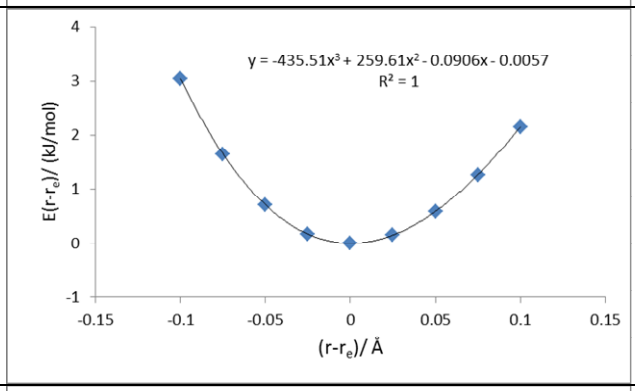
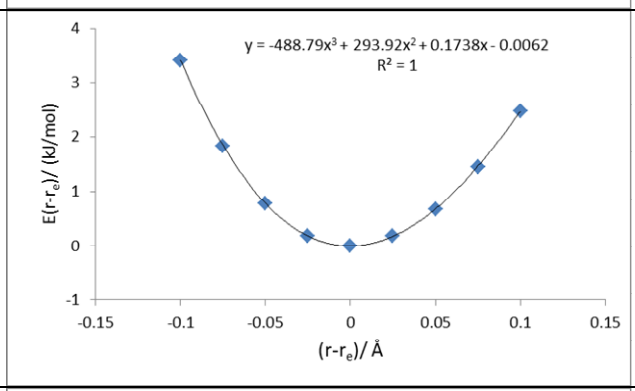
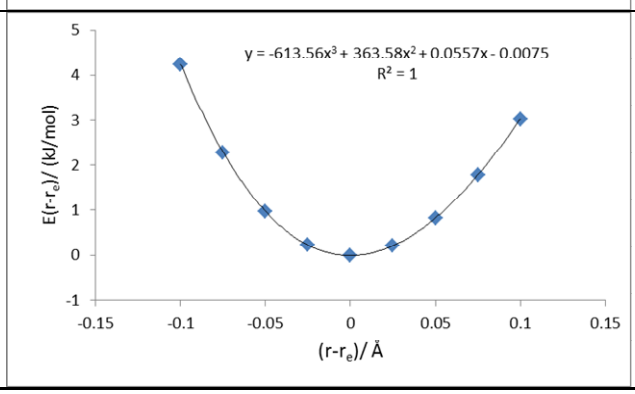
ClCu:OH_2	-0.1	4.78	
	-0.075	2.56	
	-0.05	1.08	
	-0.025	0.26	
	0	0.01	
	0.025	0.23	
	0.05	0.88	
	0.075	1.88	
	0.1	3.19	
ClCu:NH_3	-0.106	6.76	
	-0.079	3.62	
	-0.053	1.53	
	-0.026	0.37	
	0.000	0.00	
	0.026	0.33	
	0.053	1.25	
	0.079	2.69	
	0.106	4.56	

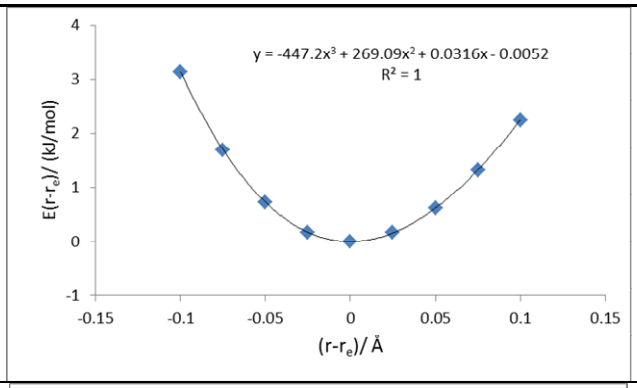
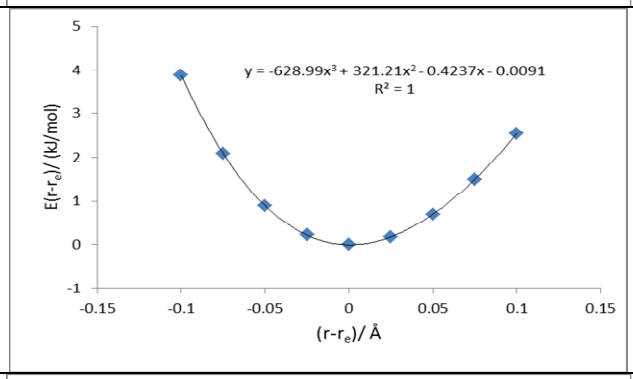
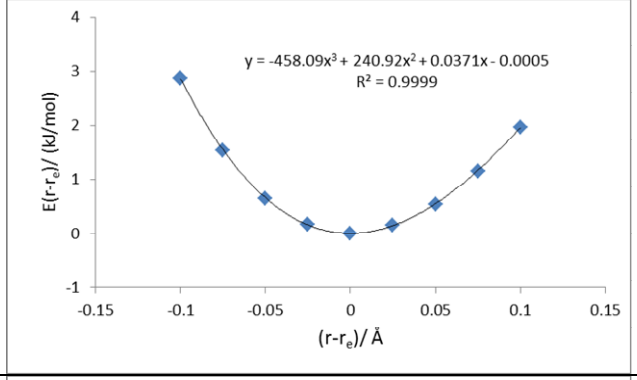
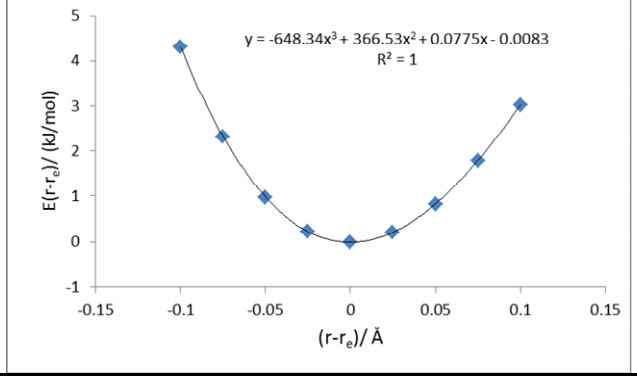
FAg:Base	**r-r_e/ Å**	**E(r-r_e)/ (kJ/mol)**	**Fitted Curve**
FAg:N_2	-0.1	3.29	
	-0.075	1.75	
	-0.05	0.73	
	-0.025	0.17	
	0	0.00	
	0.025	0.16	
	0.05	0.59	
	0.075	1.25	
	0.1	2.10	
FAg:CO	-0.1	6.34	
	-0.075	3.38	
	-0.05	1.42	
	-0.025	0.34	
	0	0.00	
	0.025	0.31	
	0.05	1.16	
	0.075	2.47	
	0.1	4.16	

FAg:HCCH	-0.1	3.63	
	-0.075	1.95	
	-0.05	0.83	
	-0.025	0.20	
	0	0.00	
	0.025	0.18	
	0.05	0.68	
	0.075	1.47	
	0.1	2.50	
$FAg:H_2CCH_2$	-0.1	3.97	
	-0.075	2.12	
	-0.05	0.90	
	-0.025	0.21	
	0	0.00	
	0.025	0.21	
	0.05	0.79	
	0.075	1.70	
	0.1	2.88	
$FAg:PH_3$	-0.1	4.95	
	-0.075	2.66	
	-0.05	1.13	
	-0.025	0.27	
	0	0.00	
	0.025	0.25	
	0.05	0.96	
	0.075	2.06	
	0.1	3.51	
$FAg:SH_2$	-0.1	3.60	
	-0.075	1.93	
	-0.05	0.82	
	-0.025	0.20	
	0	0.00	
	0.025	0.18	
	0.05	0.69	
	0.075	1.50	
	0.1	2.55	

FAg:NCH	-0.1	4.40	
	-0.075	2.35	
	-0.05	0.99	
	-0.025	0.23	
	0	0.00	
	0.025	0.21	
	0.05	0.81	
	0.075	1.73	
	0.1	2.93	
FAg:OH_2	-0.1	3.10	
	-0.075	1.65	
	-0.05	0.70	
	-0.025	0.17	
	0	0.01	
	0.025	0.15	
	0.05	0.58	
	0.075	1.24	
	0.1	2.09	
FAg:NH_3	-0.1	4.76	
	-0.075	2.56	
	-0.05	1.09	
	-0.025	0.26	
	0	0.00	
	0.025	0.23	
	0.05	0.89	
	0.075	1.92	
	0.1	3.27	

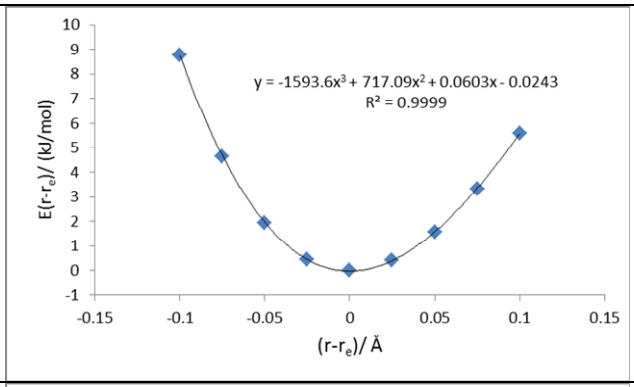
ClAg:Base	**r-re/ Å**	**E(r-re)/ (kJ/mol)**	**Fitted Curve**
ClAg:N_2	-0.1	2.60	
	-0.075	1.38	
	-0.05	0.58	
	-0.025	0.14	
	0	0.00	
	0.025	0.13	
	0.05	0.47	
	0.075	1.00	
	0.1	1.69	

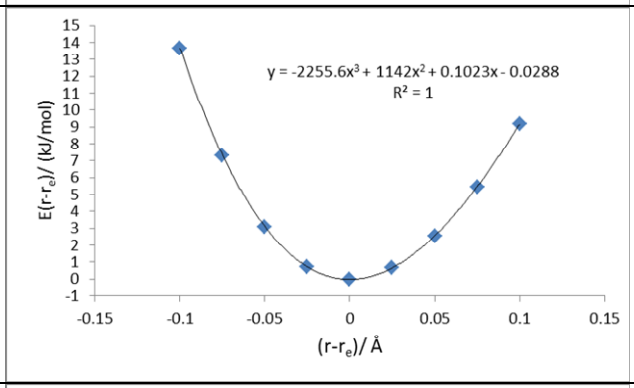
ClAg:CO	-0.1	5.08	
	-0.075	2.70	
	-0.05	1.14	
	-0.025	0.27	
	0	0.00	
	0.025	0.25	
	0.05	0.93	
	0.075	1.98	
	0.1	3.34	
ClAg:HCCH	-0.1	3.04	
	-0.075	1.64	
	-0.05	0.70	
	-0.025	0.17	
	0	0.00	
	0.025	0.15	
	0.05	0.58	
	0.075	1.26	
	0.1	2.15	
ClAg:H_2CCH_2	-0.1	3.41	
	-0.075	1.83	
	-0.05	0.78	
	-0.025	0.18	
	0	0.00	
	0.025	0.18	
	0.05	0.67	
	0.075	1.45	
	0.1	2.47	
ClAg:PH_3	-0.1	4.24	
	-0.075	2.28	
	-0.05	0.97	
	-0.025	0.23	
	0	0.00	
	0.025	0.22	
	0.05	0.82	
	0.075	1.77	
	0.1	3.03	

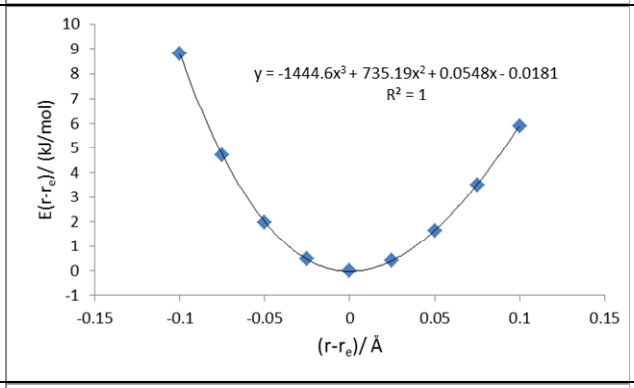
ClAg:SH_2	-0.1	3.13	
	-0.075	1.69	
	-0.05	0.72	
	-0.025	0.17	
	0	0.00	
	0.025	0.16	
	0.05	0.61	
	0.075	1.32	
	0.1	2.25	
ClAg:NCH	-0.1	3.88	
	-0.075	2.08	
	-0.05	0.89	
	-0.025	0.22	
	0	0.00	
	0.025	0.18	
	0.05	0.69	
	0.075	1.49	
	0.1	2.54	
ClAg:OH_2	-0.1	2.87	
	-0.075	1.54	
	-0.05	0.65	
	-0.025	0.16	
	0	0.01	
	0.025	0.15	
	0.05	0.54	
	0.075	1.16	
	0.1	1.96	
ClAg:NH_3	-0.1	4.30	
	-0.075	2.31	
	-0.05	0.98	
	-0.025	0.23	
	0	0.00	
	0.025	0.22	
	0.05	0.83	
	0.075	1.78	
	0.1	3.02	

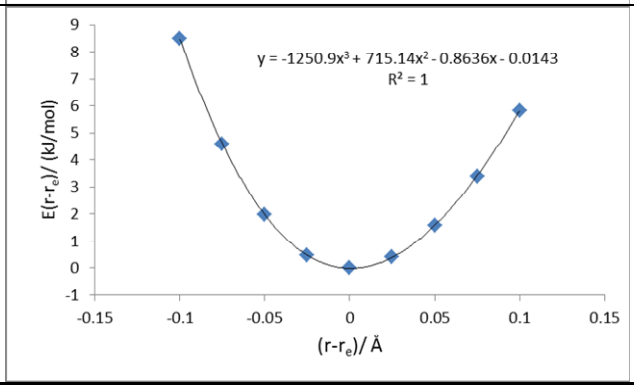
FAu:Base	**r-r_e/ Å**	**E(r-r_e)/ (kJ/mol)**	**Fitted Curve**

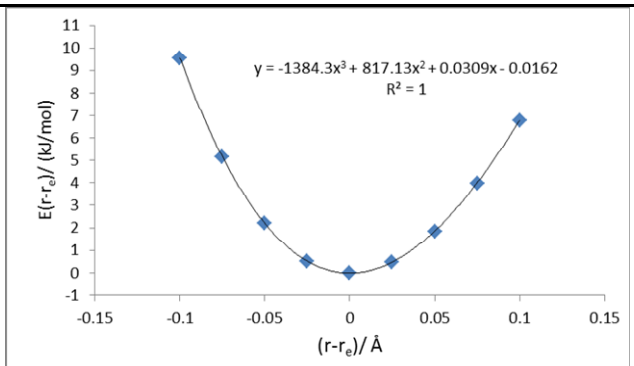
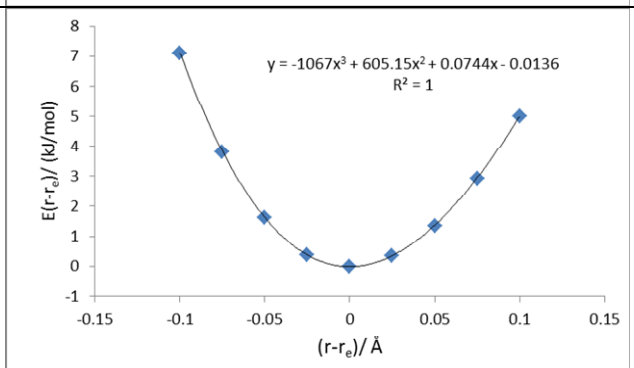
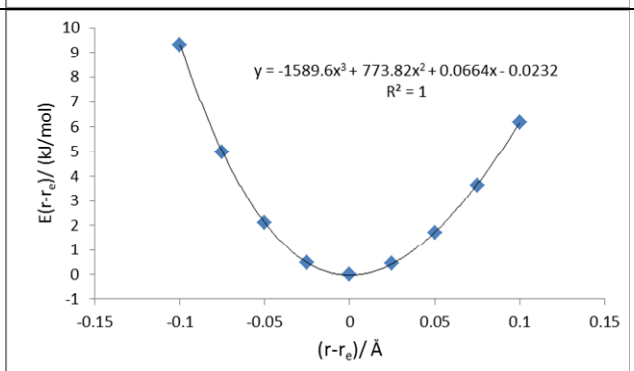
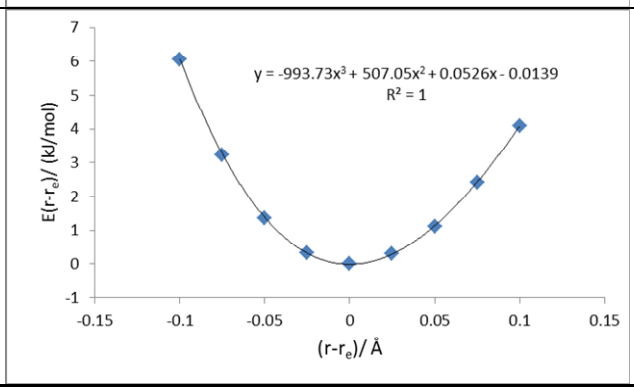
FAu:N_2	-0.1	8.75
	-0.075	4.65
	-0.05	1.95
	-0.025	0.46
	0	0.00
	0.025	0.41
	0.05	1.56
	0.075	3.31
	0.1	5.58
FAu:CO	-0.1	13.66
	-0.075	7.30
	-0.05	3.09
	-0.025	0.73
	0	0.00
	0.025	0.67
	0.05	2.53
	0.075	5.42
	0.1	9.17
FAu:HCCH	-0.1	8.79
	-0.075	4.70
	-0.05	1.99
	-0.025	0.47
	0	0.00
	0.025	0.43
	0.05	1.63
	0.075	3.49
	0.1	5.91
FAu:H_2CCH_2	-0.1	8.49
	-0.075	4.58
	-0.05	1.96
	-0.025	0.48
	0	0.00
	0.025	0.40
	0.05	1.57
	0.075	3.40
	0.1	5.81

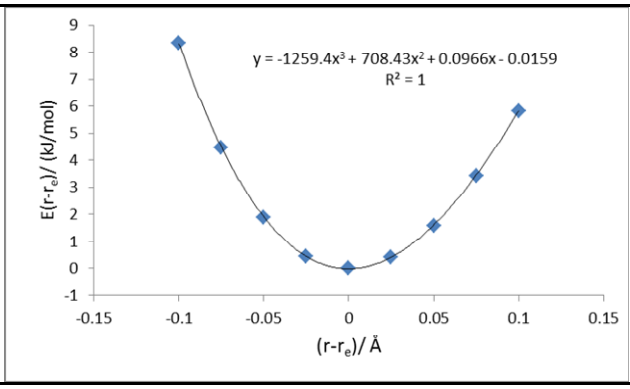


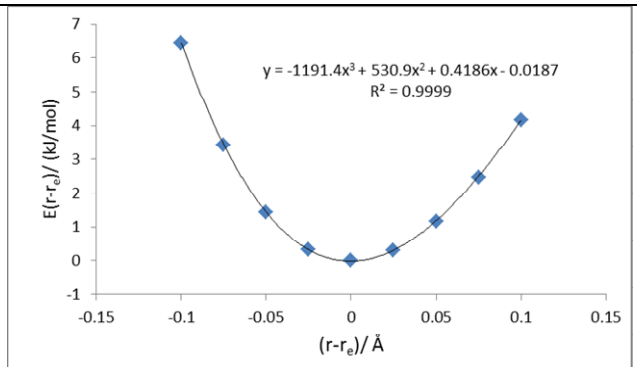
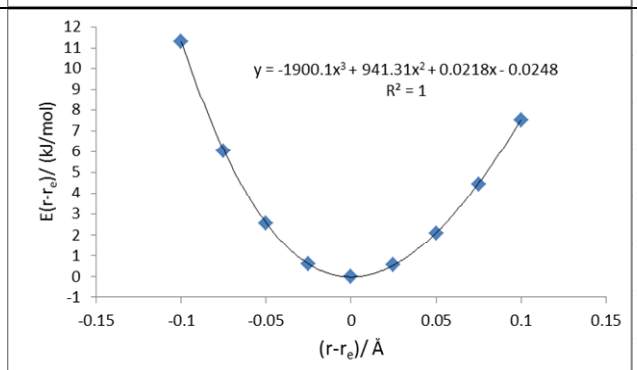
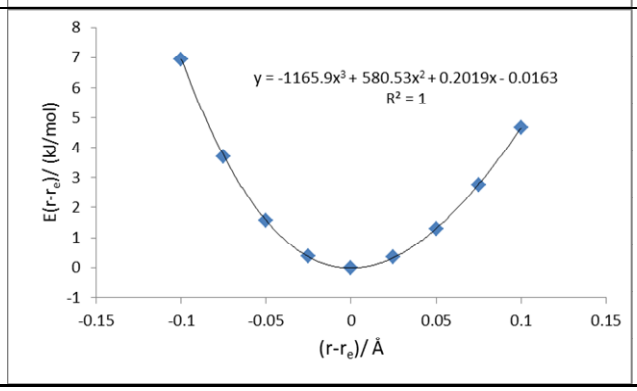


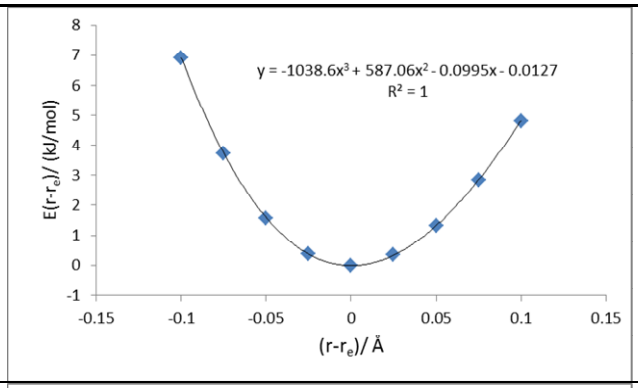
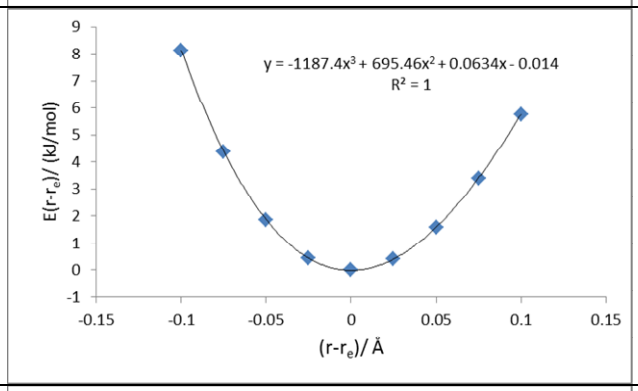
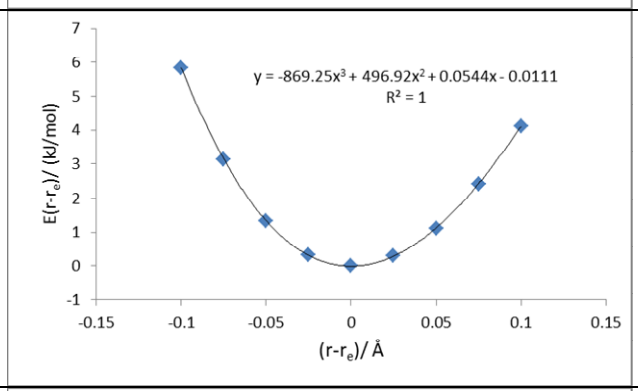
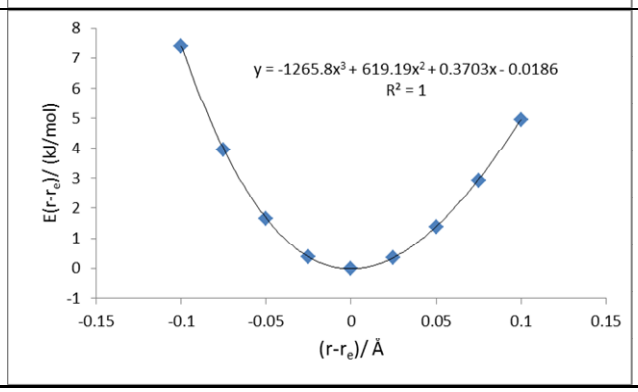




FAu:PH_3	-0.1	9.55	
	-0.075	5.14	
	-0.05	2.19	
	-0.025	0.52	
	0	0.00	
	0.025	0.48	
	0.05	1.85	
	0.075	3.98	
	0.1	6.79	
FAu:SH_2	-0.1	7.11	
	-0.075	3.82	
	-0.05	1.62	
	-0.025	0.39	
	0	0.00	
	0.025	0.36	
	0.05	1.36	
	0.075	2.93	
	0.1	4.99	
FAu:NCH	-0.1	9.32	
	-0.075	4.97	
	-0.05	2.09	
	-0.025	0.50	
	0	0.00	
	0.025	0.45	
	0.05	1.70	
	0.075	3.64	
	0.1	6.15	
FAu:OH_2	-0.1	6.06	
	-0.075	3.24	
	-0.05	1.37	
	-0.025	0.32	
	0	0.00	
	0.025	0.30	
	0.05	1.12	
	0.075	2.41	
	0.1	4.08	

FAu:NH_3	-0.1	8.33	
	-0.075	4.47	
	-0.05	1.90	
	-0.025	0.45	
	0	0.00	
	0.025	0.42	
	0.05	1.59	
	0.075	3.43	
	0.1	5.83	

ClAu:Base	r-r_e/ Å	E(r-r_e)/ (kJ/mol)	Fitted Curve
ClAu:N_2	-0.1	6.45	
	-0.075	3.42	
	-0.05	1.43	
	-0.025	0.33	
	0	0.00	
	0.025	0.31	
	0.05	1.17	
	0.075	2.48	
	0.1	4.15	
ClAu:CO	-0.1	11.31	
	-0.075	6.04	
	-0.05	2.55	
	-0.025	0.61	
	0	0.00	
	0.025	0.55	
	0.05	2.08	
	0.075	4.44	
	0.1	7.51	
ClAu:HCCH	-0.1	6.95	
	-0.075	3.71	
	-0.05	1.56	
	-0.025	0.37	
	0	0.00	
	0.025	0.34	
	0.05	1.29	
	0.075	2.75	
	0.1	4.66	

ClAu:H_2CCH_2	-0.1	6.92	
	-0.075	3.72	
	-0.05	1.58	
	-0.025	0.38	
	0	0.00	
	0.025	0.34	
	0.05	1.31	
	0.075	2.83	
	0.1	4.82	
ClAu:PH_3	-0.1	8.13	
	-0.075	4.38	
	-0.05	1.86	
	-0.025	0.45	
	0	0.00	
	0.025	0.41	
	0.05	1.57	
	0.075	3.39	
	0.1	5.77	
ClAu:SH_2	-0.1	5.83	
	-0.075	3.13	
	-0.05	1.33	
	-0.025	0.32	
	0	0.00	
	0.025	0.29	
	0.05	1.12	
	0.075	2.41	
	0.1	4.10	
ClAu:NCH	-0.1	7.42	
	-0.075	3.95	
	-0.05	1.66	
	-0.025	0.39	
	0	0.00	
	0.025	0.37	
	0.05	1.38	
	0.075	2.94	
	0.1	4.96	

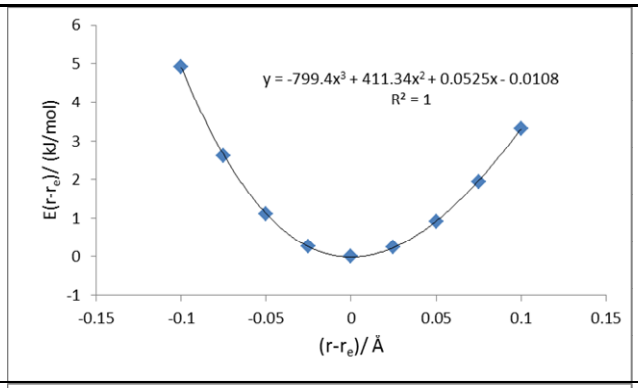
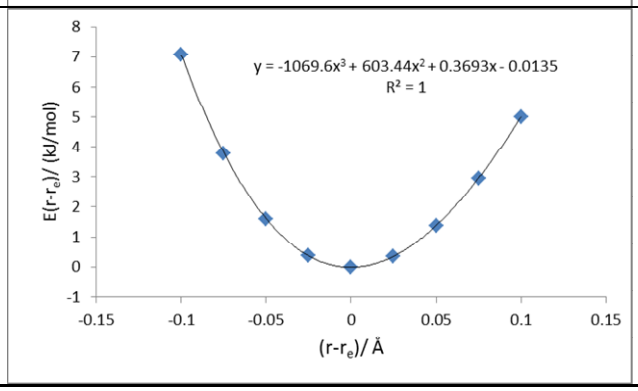
ClAu:OH_2	-0.1	4.91	
	-0.075	2.62	
	-0.05	1.11	
	-0.025	0.26	
	0	0.00	
	0.025	0.24	
	0.05	0.91	
	0.075	1.96	
	0.1	3.32	
ClAu:NH_3	-0.1	7.06	
	-0.075	3.79	
	-0.05	1.60	
	-0.025	0.38	
	0	0.00	
	0.025	0.36	
	0.05	1.37	
	0.075	2.94	
	0.1	5.00	

Table S3. Dipole Moment (debye) computed at MP2/aug-cc-pVTZ/aug-cc-pVTZ-PP computational level.

	Base	**FCu:base**	**ClCu:base**	**FAg:Base**	**ClAg:Base**	**FAu:Base**	**ClAu:Base**
-		6.24	6.34	6.79	6.87	5.34	3.58
N_2	0.00	4.83	5.19	6.33	6.54	4.27	4.25
CO	0.25	4.22	4.54	5.79	6.11	3.83	3.75
HCCH	0.00	5.35	5.64	7.02	7.35	5.62	5.59
H_2CCH_2	0.00	5.17	5.59	6.93	7.26	5.55	5.53
PH_3	0.63	7.02	7.44	8.13	8.49	7.18	7.24
SH_2	1.01	7.04	7.39	7.96	8.22	7.06	7.07
NCH	3.02	8.89	9.41	10.22	10.59	8.55	8.74
OH_2	1.86	8.03	8.38	8.77	8.95	7.59	7.49
NH_3	1.52	8.42	8.81	9.28	9.56	8.56	8.63

Table S4. D_e [CCSD(T)] and fitted using Eq. 2 (kJ mol^{-1}). The residuals (kJ mol^{-1}) of the fitting are also included.

Complex	D_e CCSD(T)	D_e fitted	Residual
fcu:n2	107.58	96.19	11.39
fcu:co	173.08	175.77	-2.69
fcu:hcch	154.52	151.23	3.28
fcu:h2cch2	161.23	165.02	-3.79
fcu:ph3	177.95	196.21	-18.25
fcu:sh2	145.23	150.89	-5.66
fcu:nch	160.28	149.00	11.27
fcu:oh2	123.43	111.01	12.42
fcu:nh3	183.96	179.03	4.93
clcu:n2	90.17	86.35	3.82
clcu:co	149.39	157.79	-8.40
clcu:hcch	136.09	135.77	0.33
clcu:h2cch2	143.33	148.14	-4.81
clcu:ph3	161.20	176.14	-14.94
clcu:sh2	132.08	135.46	-3.38
clcu:nch	145.12	133.76	11.36
clcu:oh2	114.01	99.65	14.36
clcu:nh3	171.93	160.72	11.22
fag:n2	58.92	70.84	-11.92
fag:co	120.85	129.44	-8.59
fag:hcch	107.27	111.37	-4.10
fag:h2cch2	121.82	121.53	0.29
fag:ph3	150.97	144.49	6.47
fag:sh2	114.05	111.12	2.93
fag:nch	109.27	109.73	-0.47
fag:oh2	82.69	81.75	0.94
fag:nh3	140.13	131.84	8.29
clag:n2	51.52	65.18	-13.66
clag:co	104.34	119.10	-14.76
clag:hcch	97.95	102.47	-4.52
clag:h2cch2	111.44	111.82	-0.38
clag:ph3	137.40	132.95	4.45
clag:sh2	105.46	102.24	3.22
clag:nch	102.91	100.96	1.94
clag:oh2	80.76	75.22	5.55
clag:nh3	134.66	121.31	13.35
fau:n2	138.57	132.20	6.37
fau:co	256.18	241.58	14.60
fau:hcch	209.77	207.86	1.91
fau:h2cch2	229.87	226.81	3.06
fau:ph3	277.87	269.67	8.20
fau:sh2	208.85	207.39	1.46
fau:nch	195.65	204.79	-9.14
fau:oh2	139.14	152.57	-13.43

fau:nh3	229.58	246.06	-16.47
clau:n2	106.43	111.23	-4.80
clau:co	208.88	203.25	5.63
clau:hcch	174.78	174.88	-0.10
clau:h2cch2	194.23	190.82	3.41
clau:ph3	237.79	226.89	10.90
clau:sh2	176.52	174.49	2.03
clau:nch	163.76	172.30	-8.54
clau:oh2	118.59	128.37	-9.77
clau:nh3	200.52	207.02	-6.50