

Concerning the Role of σ -hole in Non-Covalent Interactions: Insights from the Study of the Complexes of ArBeO with Simple Ligands

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Supplementary Information

Table S1. MP2/aVTZ and CCSDT(T)/aVTZ Ar-X distances (Å) and harmonic vibrational frequencies (cm⁻¹) of the LAr and L-ArBeO.

Ar-X ^a		Frequencies				
		MP2	CCSD(T)		MP2	CCSD(T)
HeAr	Ar-He	3.5421	3.4973	σ_g	30.8	34.2
NeAr	Ar-Ne	3.5441	3.5178	σ_g	26.2	27.6
ArAr	Ar-Ar	3.7657	3.8134	σ_g	32.0	29.6
NN-Ar	Ar-N	3.6139	3.6498	σ_g/π	37.0, 2185.5/6.2	35.1, 2339.3/12.6
N ₂ -Ar (T ^b)	Ar-CM	3.6062	3.6801	a_1/b_2	41.2, 2185.4/12.1	36.4, 2339.5/6.0
OC-Ar	Ar-C	3.8424	3.8424	σ_g/π	30.8, 2109.4/ <u>11.9i</u>	31.1, 2144.2/ <u>7.3i</u>
CO-Ar	Ar-O	3.4496	3.4833	σ_g/π	39.3, 2108.5/1.5	36.9, 2143.8/6.6
FF-Ar	Ar-F	3.1061	3.1628	σ_g/π	43.9, 998.5/37.0	39.8, 915.2/31.1
F ₂ -Ar (T)	Ar-CM	3.4263	3.4263	a_1/b_2	34.5, 1002.7/31.6	34.4, 916.4/31.6
ClCl-Ar	Ar-Cl	3.3886	3.4699	σ_g/π	45.2, 571.8/27.6	40.3, 541.5/23.4
Cl ₂ -Ar (T)	Ar-CM	3.6191	3.6853	a_1/b_2	43.0, 573.6/37.6	38.9, 542.1/33.2
FCl-Ar	Ar-Cl	3.2467	3.3251	σ_g/π	52.8, 795.5/51.0	47.6, 770.5/43.6
ClF-Ar	Ar-F	3.1953	3.2287	σ_g/π	38.1, 797.7/19.4	36.1, 771.7/16.9
FH-Ar	Ar-H	2.5109	2.5048	σ_g/π	69.6, 4099.8/196.4	71.7, 4105.7/195.2
HF-Ar	Ar-F	3.3392	3.3415	σ_g/π	40.7, 4119.9/70.9	40.8, 4122.6/67.7
ClH-Ar	Ar-H	2.6663	2.7113	σ_g/π	52.4, 3037.9/97.7	49.3, 2989.8/90.3
HCl-Ar	Ar-Cl	3.5919	3.6533	σ_g/π	42.6, 3041.5/78.3	38.7, 2989.5/69.2
H ₃ N-Ar	Ar-N	3.7809	3.7655	a_1	40.4, 1041.7, 3501.6	41.6, 1066.8, 3463.0
				e	<u>17.0i</u> , 1669.1, 3648.3	<u>10.5i</u> , 1672.9, 3591.4
He-ArBeO	Ar-He	3.2431	3.2167	σ_g/π	51.3, 269.5, 1490.4/6.8, 163.4	54.7, 272.6, 1536.4/7.4, 156.4
Ne-ArBeO	Ar-Ne	3.2991	3.2740	σ_g/π	36.2, 270.1, 1490.4/5.1, 163.9	38.1, 273.4, 1536.5/4.8, 156.6
Ar-ArBeO	Ar-Ar	3.5759	3.6065	σ_g/π	38.6, 271.6, 1490.4/6.7, 164.8	36.9, 274.7, 1536.3/6.1, 157.9
HF-ArBeO	Ar-F	2.9032	2.9040	σ_g	89.3, 288.0, 1492.2, 4099.8	89.8, 291.3, 1536.9, 4106.3
				π	13.4, 122.9, 175.1	12.6, 118.8, 169.5
		MP2				
NN-ArBeO	Ar-N	3.2775		σ_g/π	57.3, 277.4, 1490.7, 2187.7/9.7, 58.0, 167.2	
N ₂ -ArBeO (T)	Ar-CM	3.5420		$a_1/b_1/b_2$	38.5, 269.0, 1489.9, 2183.6/5.6, 161.4/ <u>52.5i</u> , 5.3, 191.2	
OC-ArBeO	Ar-C	3.3811		σ_g/π	60.4, 281.2, 1490.3, 2120.3/10.8, 74.4, 169.7	
CO-ArBeO	Ar-O	3.1894		σ_g/π	54.9, 274.9, 1491.6, 2104.8/8.6, 44.9, 165.1	
FF-ArBeO	Ar-F	3.1745		σ_g/π	30.5, 267.1, 1006.1, 1489.9/ <u>32.1i</u> , <u>2.4i</u> , 159.3	
F ₂ -ArBeO (T)	Ar-CM	3.1795		$a_1/b_1/b_2$	47.0, 273.5, 999.1/7.4, 163.5/4.8, 45.9, 163.7	
ClCl-ArBeO	Ar-Cl	3.6223		σ_g/π	22.8, 265.1, 574.9, 1489.1/ <u>29.6i</u> , <u>2.3i</u> , 158.7	
Cl ₂ -ArBeO (T)	Ar-CM	3.4276		$a_1/b_1/b_2$	50.1, 277.3, 571.6, 1490.4/7.6, 166.0/ <u>3.7i</u> , 45.3, 166.2	
ClF-ArBeO	Ar-F	2.9614		σ_g/π	52.2, 277.4, 796.6, 1491.2/5.6, 10.0, 166.0	
HCl-ArBeO	Ar-Cl	3.4929		σ_g/π	44.4, 272.2, 1489.9, 3034.3/ <u>122.0i</u> , 6.0, 163.5	
H ₃ N-ArBeO	Ar-N	3.1286		a_1	104.9, 300.6, 1105.4, 1492.8, 3494.5	
				e	19.6, 183.4, 209.7, 1671.4, 3633.2	

^a X = closest atom/center-of-mass (CM) of X₂ for linear/T-shaped species. ^b T-shaped.

Data S1. Cartesian coordinates (Å) of the *L*Ar and *L*-ArBeO**HeAr**

MP2/aVTZ

Ar 0.000000 0.000000 0.000000

He 3.542092 0.000000 0.000000

CCSD(T)/aVTZ

Ar 0.000000 0.000000 0.000000

He 3.497343 0.000000 0.000000

NeAr

MP2/aVTZ

Ar 0.000000 0.000000 0.000000

Ne 3.544096 0.000000 0.000000

CCSD(T)/aVTZ

Ar 0.000000 0.000000 0.000000

Ne 3.517812 0.000000 0.000000

ArAr

MP2/aVTZ

Ar 0.000000 0.000000 0.000000

Ar 3.765654 0.000000 0.000000

CCSD(T)/aVTZ

Ar 0.000000 0.000000 0.000000

Ar 3.813444 0.000000 0.000000

N₂-Ar

MP2/aVTZ

Ar 0.000000 0.000000 0.000000

N 3.613868 0.000000 0.000000

N 4.728054 0.000000 0.000000

CCSD(T)/aVTZ

Ar 0.000000 0.000000 0.000000

N 3.649789 0.000000 0.000000

N 4.753769 0.000000 0.000000

N₂-Ar (T-shaped)

MP2/aVTZ

Ar 0.000000 0.000000 0.000000

N 3.606201 0.000000 0.5570995

N 3.606201 0.000000 -0.5570995

CCSD(T)/aVTZ

Ar 0.000000 0.000000 0.000000

N 3.680109 0.000000 0.551983

N 3.680109 0.000000 -0.551983

OC-Ar

MP2/aVTZ

Ar 0.000000 0.000000 0.000000

C 3.842395 0.000000 0.000000

O 4.981386 0.000000 0.000000

CCSD(T)/aVTZ

Ar 0.000000 0.000000 0.000000

C 3.842397 0.000000 0.000000

O 4.978383 0.000000 0.000000

CO-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
O	3.449593	0.000000	0.000000
C	4.588669	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
O	3.483322	0.000000	0.000000
C	4.619335	0.000000	0.000000

F₂-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
F	3.106127	0.000000	0.000000
F	4.508576	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
F	3.162790	0.000000	0.000000
F	4.581308	0.000000	0.000000

F₂-Ar (T-shaped)

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
F	3.426341	0.000000	0.700749
F	3.426341	0.000000	-0.700749

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
F	3.426298	0.000000	0.709056
F	3.426298	0.000000	-0.709056

Cl₂-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Cl	3.388634	0.000000	0.000000
Cl	5.388335	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
Cl	3.469899	0.000000	0.000000
Cl	5.489794	0.000000	0.000000

Cl₂-Ar (T-shaped)

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Cl	3.619097	0.000000	0.999162
Cl	3.619097	0.000000	-0.999162

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
Cl	3.685349	0.000000	1.009552
Cl	3.685349	0.000000	-1.009552

FCI-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Cl	3.246687	0.000000	0.000000
F	4.886555	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
Cl	3.325118	0.000000	0.000000
F	4.972285	0.000000	0.000000

ClF-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
F	3.195294	0.000000	0.000000
Cl	4.834456	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
F	3.228704	0.000000	0.000000
Cl	4.875472	0.000000	0.000000

FH-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
H	2.510865	0.000000	0.000000
F	3.433739	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
H	2.504846	0.000000	0.000000
F	3.426750	0.000000	0.000000

HF-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
F	3.339206	0.000000	0.000000
H	4.261224	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
F	3.341485	0.000000	0.000000
H	4.262585	0.000000	0.000000

ClH-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
H	2.666308	0.000000	0.000000
Cl	3.941738	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
H	2.711337	0.000000	0.000000
Cl	3.990636	0.000000	0.000000

HCl-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Cl	3.591854	0.000000	0.000000
H	4.866893	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
Cl	3.653298	0.000000	0.000000
H	4.932325	0.000000	0.000000

H₃N-Ar

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
N	3.780873	0.000000	0.000000
H	4.161841	0.000000	0.937834
H	4.161841	0.812188	-0.468917
H	4.161841	-0.812188	-0.468917

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
N	3.765453	0.000000	0.000000
H	4.152642	0.000000	0.938226
H	4.152642	0.812527	-0.469113
H	4.152642	-0.812527	-0.469113

He-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.078054	0.000000	0.000000
O	3.429223	0.000000	0.000000
He	-3.243142	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.074342	0.000000	0.000000
O	3.415667	0.000000	0.000000
He	-3.216686	0.000000	0.000000

Ne-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.077510	0.000000	0.000000
O	3.428697	0.000000	0.000000
Ne	-3.299058	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.073680	0.000000	0.000000
O	3.415018	0.000000	0.000000
Ne	-3.273997	0.000000	0.000000

Ar-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.076147	0.000000	0.000000
O	3.427404	0.000000	0.000000
Ar	-3.575896	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.072500	0.000000	0.000000
O	3.413916	0.000000	0.000000
Ar	-3.606492	0.000000	0.000000

N₂-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.069828	0.000000	0.000000
O	3.421416	0.000000	0.000000

N	-3.277501	0.000000	0.000000
N	-4.391416	0.000000	0.000000

N₂-ArBeO (T-shaped)

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.078273	0.000000	0.000000
O	3.429536	0.000000	0.000000
N	-3.541996	0.000000	0.557212
N	-3.541996	0.000000	-0.557212

OC-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.065773	0.000000	0.000000
O	3.417668	0.000000	0.000000
C	-3.381107	0.000000	0.000000
O	-4.518611	0.000000	0.000000

CO-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.072712	0.000000	0.000000
O	3.423965	0.000000	0.000000
O	-3.189422	0.000000	0.000000
C	-4.329420	0.000000	0.000000

F₂-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.080132	0.000000	0.000000
O	3.431308	0.000000	0.000000
F	-3.174483	0.000000	0.000000
F	-4.574741	0.000000	0.000000

F₂-ArBeO (T-shaped)

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.073693	0.000000	0.000000
O	3.425128	0.000000	0.000000
F	-3.179484	0.000000	0.701473
F	-3.179484	0.000000	-0.701473

Cl₂-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.082255	0.000000	0.000000
O	3.433453	0.000000	0.000000
Cl	-3.622299	0.000000	0.000000
Cl	-5.619307	0.000000	0.000000

Cl₂-ArBeO (T-shaped)

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.070047	0.000000	0.000000

O	3.421661	0.000000	0.000000
Cl	-3.427555	0.000000	1.000297
Cl	-3.427555	0.000000	-1.000297

ClF-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.070024	0.000000	0.000000
O	3.421507	0.000000	0.000000
F	-2.961366	0.000000	0.000000
Cl	-4.604040	0.000000	0.000000

HF-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.060280	0.000000	0.000000
O	3.412135	0.000000	0.000000
F	-2.903182	0.000000	0.000000
H	-3.826560	0.000000	0.000000

CCSD(T)/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.056844	0.000000	0.000000
O	3.398998	0.000000	0.000000
F	-2.904036	0.000000	0.000000
H	-3.826362	0.000000	0.000000

HCl-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.075010	0.000000	0.000000
O	3.426486	0.000000	0.000000
Cl	-3.492872	0.000000	0.000000
H	-4.768685	0.000000	0.000000

H₃N-ArBeO

MP2/aVTZ

Ar	0.000000	0.000000	0.000000
Be	2.046988	0.000000	0.000000
O	3.399617	0.000000	0.000000
N	-3.128550	0.000000	0.000000
H	-3.519296	0.000000	0.934951
H	-3.519296	0.809691	-0.467475
H	-3.519296	-0.809691	-0.467475

Table S2. MP2/aVTZ and CCSD(T)/aVTZ properties of the nCov(C) bonds of the LAr and L-ArBeO. $N(\Omega_s)$, $\rho_s(\text{ave})$, and $H_s(\text{ave/max/min})$ are, respectively, the total electronic charge (me), the average electron density ($e \text{ a}_0^{-3}$), and the average, maximum and minimum of $H(r)$ (hartree a_0^{-3}) over the volume $\Omega_s (\text{a}_0^3)$ enclosed by the $s(r) = 0.4$ isosurface at around the BCP.

Bond	LAr		Ω_s	$N(\Omega_s)$	$\rho_s(\text{ave})$	$H_s(\text{ave/max/min})$
He-Ar	HeAr	MP2	0.0212	0.024	0.0011	0.00040/0.00042/0.00038
		CCSD(T)	0.0215	0.025	0.0011	0.00040/0.00042/0.00038
Ne-Ar	NeAr	MP2	0.0316	0.063	0.0020	0.00059/0.00061/0.00057
		CCSD(T)	0.0313	0.062	0.0020	0.00058/0.00060/0.00057
Ar-Ar	ArAr	MP2	0.0948	0.27	0.0029	0.00074/0.00078/0.00069
		CCSD(T)	0.0946	0.27	0.0029	0.00073/0.00077/0.00068
N-Ar	N ₂ -Ar	MP2	0.0788	0.22	0.0028	0.00076/0.00080/0.00071
		CCSD(T)	0.0780	0.22	0.0028	0.00076/0.00080/0.00071
	N ₂ -Ar (T ^a)	MP2	0.1570	0.46	0.0029	0.00075/0.00082/0.00067
		CCSD(T)	0.1525	0.45	0.0030	0.00075/0.00081/0.00068
C-Ar	OC-Ar	MP2	0.0914	0.21	0.0023	0.00060/0.00063/0.00056
		CCSD(T)	0.0901	0.21	0.0023	0.00059/0.00062/0.00055
O-Ar	CO-Ar	MP2	0.0736	0.24	0.0032	0.00086/0.00091/0.00080
		CCSD(T)	0.0729	0.23	0.0032	0.00086/0.00091/0.00080
F-Ar	F ₂ -Ar	MP2	0.0966	0.46	0.0047	0.00154/0.00176/0.00137
		CCSD(T)	0.0952	0.45	0.0047	0.00154/0.00176/0.00136
	F ₂ -Ar (T)	MP2	0.2052	0.59	0.0029	0.00068/0.00076/0.00058
		CCSD(T)	0.2024	0.57	0.0028	0.00067/0.00075/0.00058
Cl-Ar	Cl ₂ -Ar	MP2	0.1687	0.90	0.0053	0.00153/0.00165/0.00139
		CCSD(T)	0.1651	0.87	0.0053	0.00153/0.00164/0.00139
	Cl ₂ -Ar (T)	MP2	0.4444	1.56	0.0035	0.00088/0.00095/0.00076
		CCSD(T)	0.4398	1.53	0.0035	0.00087/0.00094/0.00076
Cl-Ar	FCl-Ar	MP2	0.2167	1.44	0.0067	0.00184/0.00199/0.00165
		CCSD(T)	0.2119	1.41	0.0066	0.00184/0.00198/0.00164
F-Ar	ClF-Ar	MP2	0.0866	0.38	0.0043	0.00121/0.00132/0.00111
		CCSD(T)	0.0852	0.37	0.0043	0.00121/0.00131/0.00111
H-Ar	FH-Ar	MP2	0.0777	0.65	0.0084	0.00148/0.00158/0.00134
		CCSD(T)	0.0765	0.64	0.0084	0.00149/0.00158/0.00136
F-Ar	HF-Ar	MP2	0.0700	0.23	0.0032	0.00092/0.00097/0.00086
		CCSD(T)	0.0687	0.22	0.0032	0.00092/0.00097/0.00086
H-Ar	ClH-Ar	MP2	0.0922	0.64	0.0069	0.00129/0.00140/0.00123
		CCSD(T)	0.0921	0.64	0.0070	0.00130/0.00141/0.00123
Cl-Ar	HCl-Ar	MP2	0.1268	0.46	0.0037	0.00112/0.00120/0.00102
		CCSD(T)	0.1263	0.46	0.0036	0.00111/0.00119/0.00102
N-Ar	H ₃ N-Ar	MP2	0.1113	0.31	0.0028	0.00055/0.00063/0.00051
		CCSD(T)	0.1073	0.30	0.0028	0.00055/0.00063/0.00051

^a T-shaped.

Table S3. Values of the MEP of L (kcal mol⁻¹) at the points of minimum ($V_{S,Min}$) or maximum ($V_{S,Max}$) calculated at the experimental (Exp.^a), and at the CCSD(T)/aVTZ and MP2/aVTZ optimized geometries (Å and °). The mapped isodensity surfaces are 0.0005, 0.0010, 0.0015, and 0.0020 e ao^{-3} .

L	MEP points	R/θ	Level	0.0005	0.0010	0.0015	0.0020
N₂	$V_{S,Min}(N)/V_{S,Max}(\text{perp})$	1.0977 (Exp)	CCSD(T)/aVTZ	-7.26/5.40	-8.46/7.40	-9.08/9.16	-9.44/10.79
		1.1040 [CCSD(T)/aVTZ]	CCSD(T)/aVTZ	-7.21/5.29	-8.38/7.27	-8.99/9.01	-9.33/10.63
		1.1141 (MP2/aVTZ)	CCSD(T)/aVTZ	-7.06 /5.17	-8.20/7.11	-8.78/8.84	-9.10/10.44
			MP2/aVTZ	-7.34/5.72	-8.53/7.82	-9.15/9.66	-9.49/11.37
CO	$V_{S,Min}(C)/V_{S,Min}(O)$	1.1283 (Exp)	CCSD(T)/aVTZ	-10.80/-5.25	-12.83/-5.85	-13.99/-6.04	-14.75/-6.05
		1.1360 [CCSD(T)/aVTZ]	CCSD(T)/aVTZ	-10.51/-5.41	-12.50/-6.02	-13.62/-6.21	-14.36/-6.22
		1.1390 (MP2/aVTZ)	CCSD(T)/aVTZ	-10.40/-5.47	-12.36/-6.08	-13.48/-6.28	-14.21/-6.28
			MP2/aVTZ	-11.87/-3.75	-14.04/-4.12	-15.29/-4.17	-16.08/-4.04
F₂	$V_{S,Max}(F)/V_{S,Max}(\text{perp})$	1.4119 (Exp)	CCSD(T)/aVTZ	12.44/-0.23	16.36/0.90	19.54/2.10	22.39/3.33
		1.4181 [CCSD(T)/aVTZ]	CCSD(T)/aVTZ	12.55/-0.32	16.50/0.80	19.68/1.98	22.55/3.21
		1.4014 (MP2/aVTZ)	CCSD(T)/aVTZ	12.25/-0.09	16.14/1.07	19.29/2.30	22.11/3.56
			MP2/aVTZ	12.59/-0.34	16.57/0.76	19.80/1.93	22.67/3.14
Cl₂	$V_{S,Max}(Cl)/V_{S,Max}(\text{perp})$	1.9879 (Exp)	CCSD(T)/aVTZ	19.02/-0.28	25.02/1.73	29.54/3.75	33.63/5.71
		2.0194 [CCSD(T)/aVTZ]	CCSD(T)/aVTZ	19.32/-0.61	25.34/1.32	29.97/3.27	34.0/5.20
		1.9987 (MP2/aVTZ)	CCSD(T)/aVTZ	19.11/-0.40	25.13/1.59	29.69/3.58	33.74/5.52
			MP2/aVTZ	19.38/-0.64	25.50/1.26	30.14/3.19	34.24/5.09
ClF	$V_{S,Max}(Cl)/V_{S,Max}(F)$	1.6281 (Exp ^b)	CCSD(T)/aVTZ	31.56/-3.25	39.89/-2.23	46.33/-1.16	51.33/-0.05
		1.6463 [CCSD(T)/aVTZ]	CCSD(T)/aVTZ	32.00/-3.37	40.38/-2.34	46.85/-1.21	51.88/-0.12
		1.6385 (MP2/aVTZ)	CCSD(T)/aVTZ	31.82/-3.32	40.17/-2.30	46.63/-1.19	51.65/-0.09
			MP2/aVTZ	32.38/-2.97	40.94/-1.86	47.56/-0.68	52.69/0.47
HF	$V_{S,Max}(H)/V_{S,Max}(F)$	0.9168 (Exp)	CCSD(T)/aVTZ	55.15/-17.92	68.19/-18.97	77.96/-19.38	85.96/-19.45
		0.9210 [CCSD(T)/aVTZ]	CCSD(T)/aVTZ	55.18/-17.94	68.23/-18.98	78.03/-19.39	86.08/-19.46
		0.9218 (MP2/aVTZ)	CCSD(T)/aVTZ	55.18/-17.94	68.24/-18.99	78.04/-19.39	86.10/-19.46
			MP2/aVTZ	55.56/-17.87	68.78/-18.91	78.71/-19.28	86.90/-19.36
HCl	$V_{S,Max}(H)/V_{S,Max}(Cl)$	1.2746 (Exp)	CCSD(T)/aVTZ	35.55/5.66	43.92/9.26	50.30/12.28	55.95/14.93
		1.2789 [CCSD(T)]	CCSD(T)/aVTZ	35.60/5.66	44.0/9.27	50.37/12.28	56.07/14.94
		1.2747 (MP2/aVTZ)	CCSD(T)/aVTZ	35.55/5.66	43.93/9.26	50.30/12.28	55.95/14.93
			MP2/aVTZ	36.70/5.39	45.38/9.00	52.08/11.93	57.90/14.63
NH₃	$V_{S,Min}(N)$	1.0124/106.67 (Exp ^c)	CCSD(T)/aVTZ	-32.88	-38.64	-42.28	-44.93
		1.0149/106.40 [CCSD(T)/aVTZ]	CCSD(T)/aVTZ	-31.59	-37.30	-41.17	-44.10
		1.0121/106.77 (MP2/aVTZ)	CCSD(T)/aVTZ	-31.53	-37.24	-41.12	-44.06
			MP2/aVTZ	-31.52	-37.25	-41.13	-44.11

^a Unless stated otherwise, all experimental values are from Ref. [1]. ^b Ref. [2]. ^c Ref. [3].

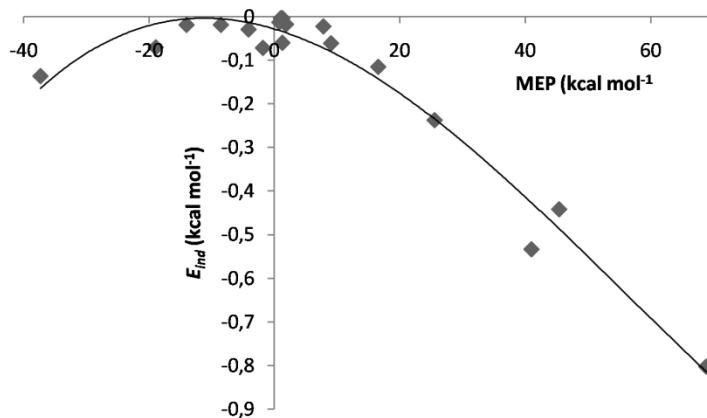


Figure S1. E_{ind} of the LAr vs. MEP at the $V_{S,max}/V_{S,min}$ of L .

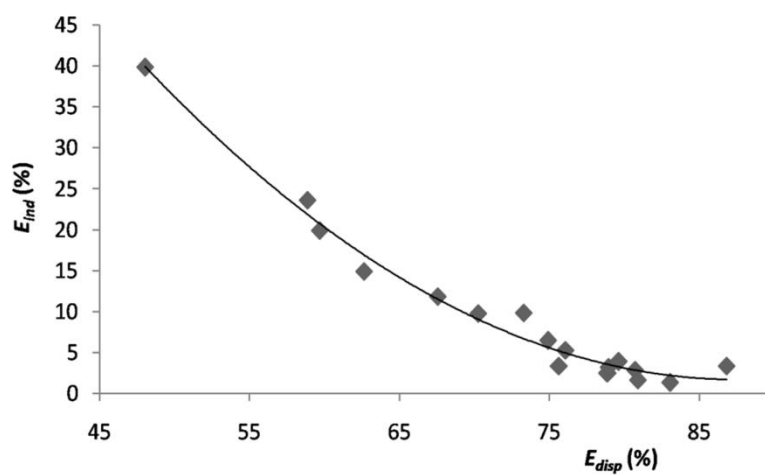


Figure S2. $E_{ind}(\%)$ vs. $E_{disp}(\%)$ of the LAr.

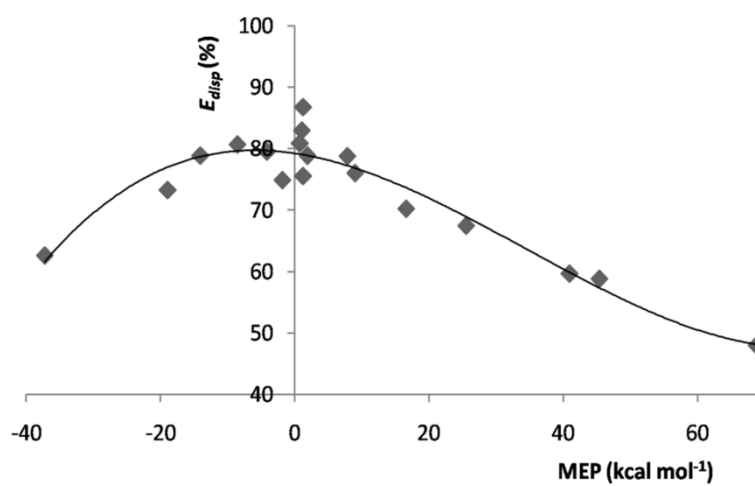


Figure S3. $E_{disp}(\%)$ of the LAr vs. MEP at the $V_{S,max}/V_{S,min}$ of L .

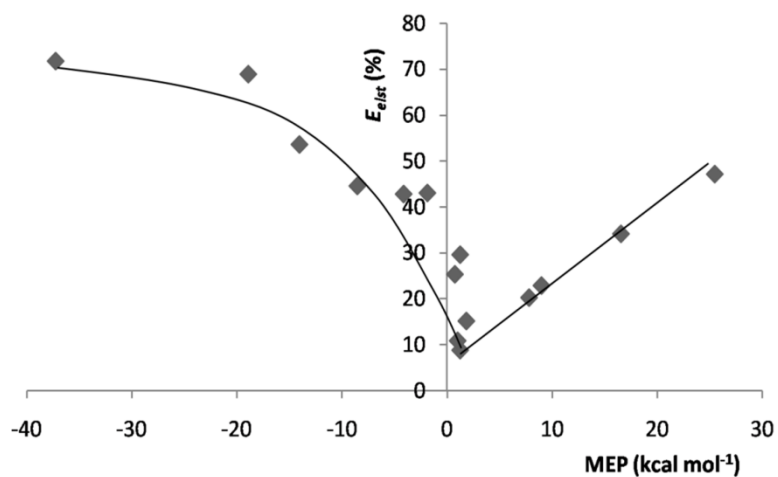


Figure S4. E_{elst} (%) of the L -ArBeO vs. MEP at the $V_{S,max}/V_{S,min}$ of L .

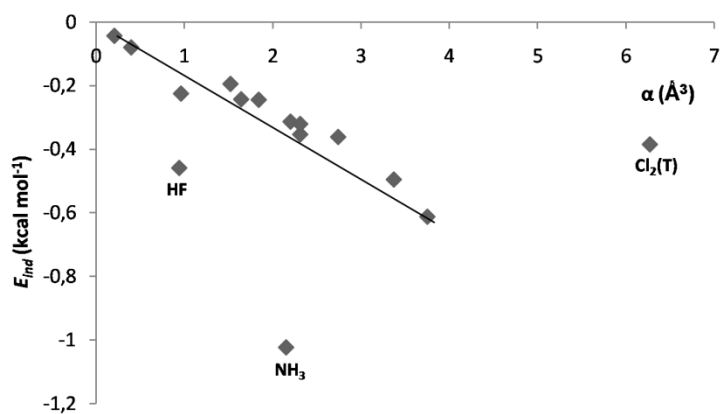


Figure S5. E_{ind} of the L -ArBeO vs. polarizability α of L .

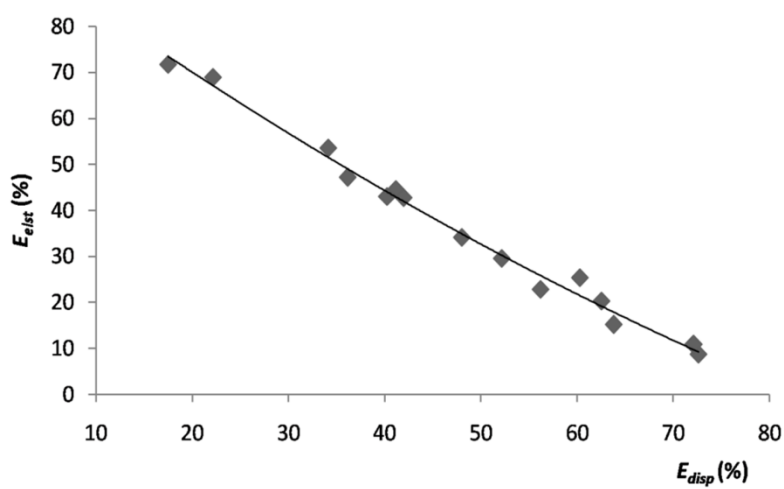


Figure S6. E_{elst} (%) vs. E_{disp} (%) of the L -ArBeO.

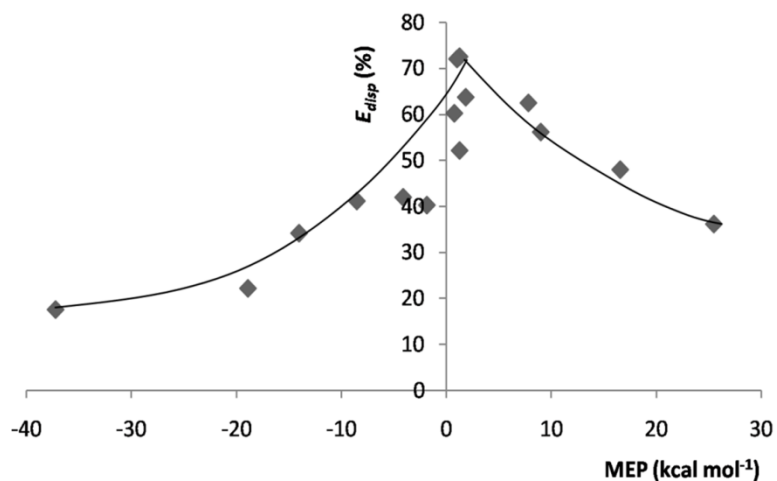


Figure S7. E_{disp} (%) of the L -ArBeO vs. MEP at the $V_{S,max}/V_{S,min}$ of L .

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