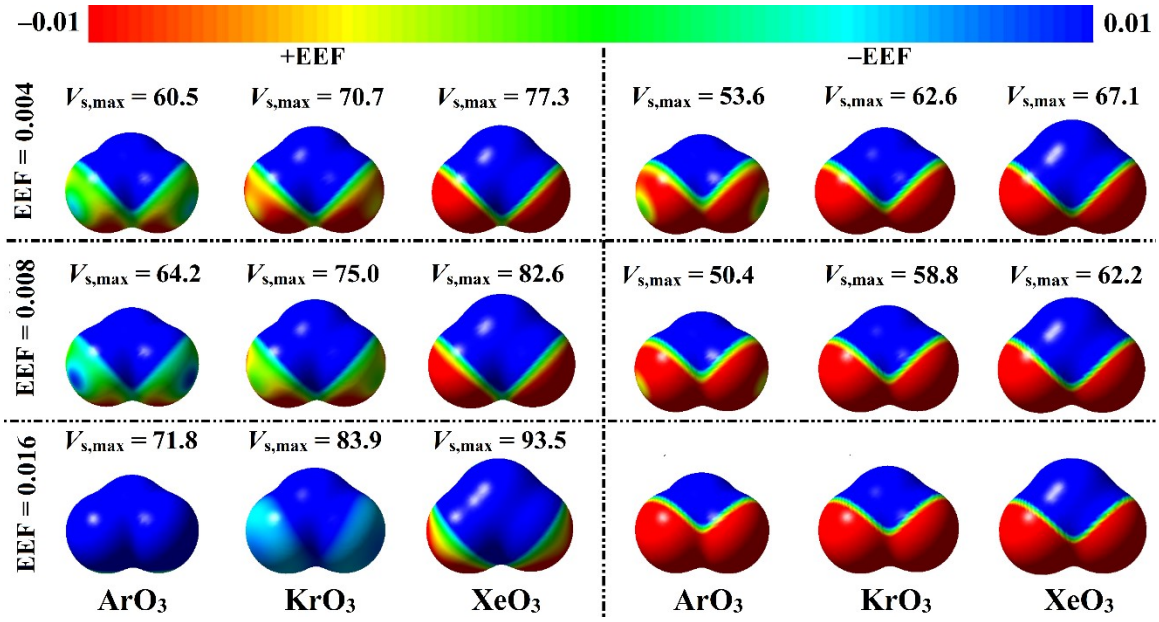

Figure S1. MEP maps of the optimized ZO_3 monomers under the positively- and negatively-oriented EEF with magnitudes of 0.004-0.016 au. $V_{s,max}$ values at the aerogen σ-hole site of the optimized ZO_3 monomers are in kcal/mol.

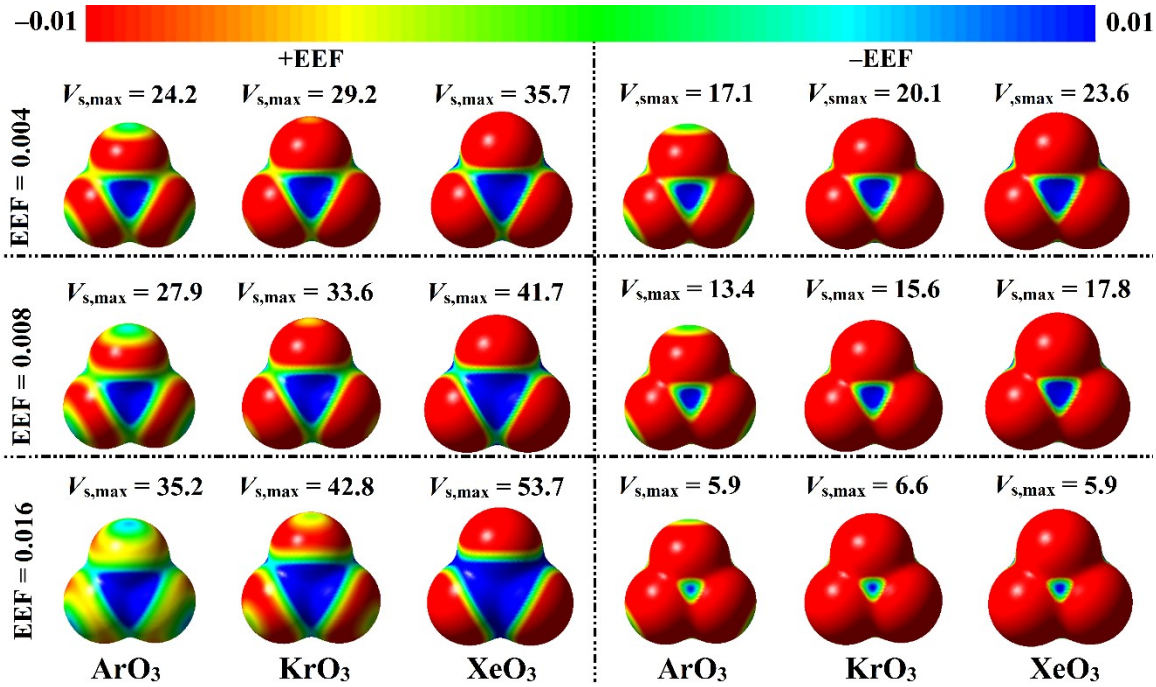

Figure S2. MEP maps of the optimized ZO_3 monomers under the positively- and negatively-oriented EEF with magnitudes of 0.004-0.016 au. $V_{s,max}$ values at the aerogen lp-hole site of the optimized ZO_3 monomers are in kcal/mol.

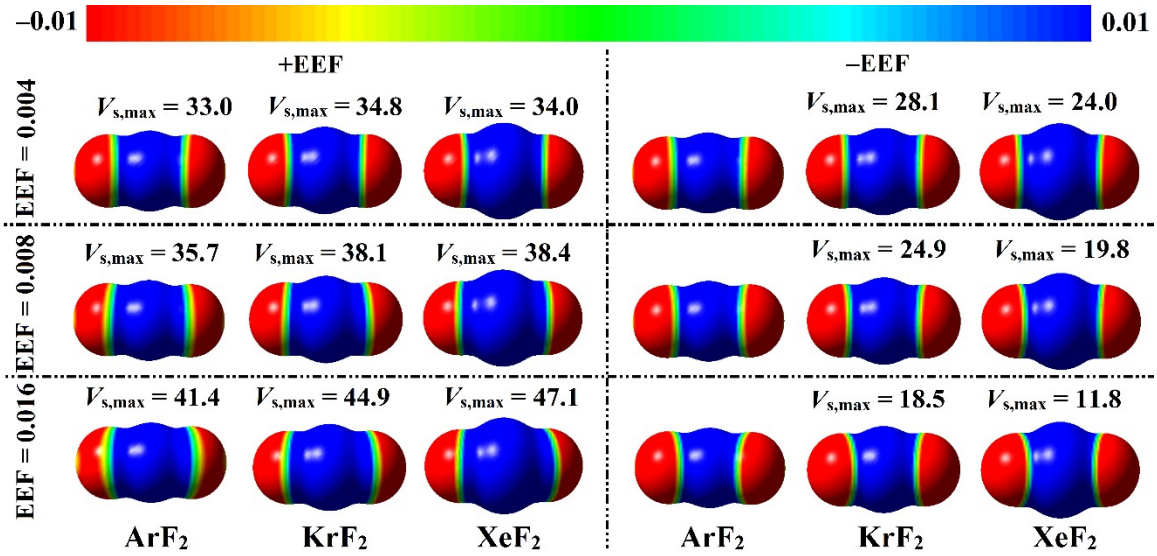

Figure S3. MEP maps of the optimized ZF_2 monomers under the positively- and negatively-oriented EEF with magnitudes of 0.004-0.016 au. $V_{s,max}$ values at the aerogen π-hole site of the optimized ZF_2 monomers are in kcal/mol.

Cartesian atomic coordinates

EEF=0.000 au

$ArO_3\cdots NH_3$:

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –6.56 kcal/mol

Cartesian atomic coordinates:

O	1.72749800	0.83369500	0.00188800
O	0.87792500	-1.06455400	1.20169300
O	1.72972700	0.83425500	2.39862700
Ar	0.98866200	0.40671800	1.20101000
N	-0.37252500	2.91653000	1.20024700
H	-0.90560500	3.20820500	2.01075800
H	-0.89691100	3.21379900	0.38612300
H	0.48119300	3.46281200	1.20678100

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.30 kcal/mol

Cartesian atomic coordinates:

O	-1.32863200	0.45039700	-0.00487800
O	-1.32990100	-1.63510200	1.19920600
O	-1.32943800	0.45042000	2.40325600
Ar	-1.80564600	-0.24456200	1.19903400
N	1.75766300	-0.24606000	1.20037300
H	2.13772400	0.69228300	1.20057000
H	2.13762900	-0.71539400	0.38779300
H	2.13690900	-0.71544000	2.01326300

$ArF_2\cdots NH_3$

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –2.76 kcal/mol

Cartesian atomic coordinates:

Ar	0.03105400	1.43979100	0.36069700
F	0.02549400	3.29636600	0.37077300
F	0.02549400	-0.41678500	0.37077300
N	1.43503300	1.43979100	-2.48444900
H	1.18047800	0.62708200	-3.03235000
H	2.44572500	1.43979100	-2.42233400
H	1.18047700	2.25250000	-3.03234900

KrO_3···NH_3

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –8.87 kcal/mol

Cartesian atomic coordinates:

O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.57818845
O	2.23311055	0.00000000	1.28960538
Kr	0.74545609	0.58732873	1.28747984
N	1.77140315	2.48901744	-0.49106127
H	2.57534881	3.05186569	-0.23888581
H	1.15816493	3.08104883	-1.03893104
H	2.11002053	1.76689124	-1.11739207

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.92 kcal/mol

Cartesian atomic coordinates:

O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.60523724
O	2.25625216	0.00000000	1.30262700
Kr	0.75210751	0.53659174	1.30261417
N	0.75267634	-2.83867824	1.30544959
H	-0.18649459	-3.21688234	1.30650352
H	1.22195206	-3.21511413	2.11979728
H	1.22206625	-3.21999881	0.49343683

KrF_2···NH_3

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –3.01 kcal/mol

Cartesian atomic coordinates:

F	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	3.76175515
Kr	0.00977963	0.00000000	1.88086136
N	3.27364636	0.19044078	1.88166251
H	3.71998013	-0.71858855	1.88249915
H	3.62275026	0.68252821	2.69509073
H	3.62602449	0.68264904	1.06972445

XeO_3···NH_3

σ-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –11.65 kcal/mol**

Cartesian atomic coordinates:

O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.79037558
O	2.42196118	0.00000000	1.38559579
Xe	0.80985655	0.69839902	1.39655599
N	1.98072863	2.20070988	3.41366349
H	2.79648974	2.77373681	3.23021521
H	2.30816180	1.36865392	3.89367206
H	1.39405574	2.70574641	4.06804119

lp-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –3.50 kcal/mol**

Cartesian atomic coordinates:

O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.87383705
O	2.48857202	0.00000000	1.43694319
Xe	0.82943870	0.57787825	1.43690519
N	0.82637494	-2.43445826	1.43714778
H	-0.11550408	-2.80653659	1.43731447
H	1.29652407	-2.80784869	2.25269768
H	1.29662888	-2.80877471	0.62208324

XeF_2···NH_3

π-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –2.74 kcal/mol**

Cartesian atomic coordinates:

F	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	3.98438202
Xe	0.01038501	0.00000000	1.99217404
N	3.47922734	0.28073207	1.99193812
H	3.95182377	-0.61507121	1.99277119
H	3.81624419	0.78269124	2.80459390
H	3.81896154	0.78259070	1.18034790

ArO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –5.10 kcal/mol

Cartesian atomic coordinates:

O	2.00003000	0.12714000	0.00101600
O	0.92954100	-1.65728600	1.19893300
O	2.00134600	0.12497500	2.39889400
Ar	1.21910800	-0.21167300	1.20009000
C	-0.52917900	3.41265200	1.20032300
H	-0.82279200	4.43699500	1.19908300
N	-0.20546500	2.29292900	1.20177200

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.17 kcal/mol

Cartesian atomic coordinates:

O	1.00090600	0.44851700	-0.00354500
O	1.00088300	-1.63457000	1.19912500
O	1.00596400	0.44853300	2.40182500
Ar	0.52265200	-0.24524000	1.20016500
C	5.21440500	-0.24521300	1.20030400
H	6.27940900	-0.24463500	1.20132600
N	4.04700200	-0.24582500	1.19922100

ArF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –2.28 kcal/mol

Cartesian atomic coordinates:

Ar	0.12521300	1.43979700	0.30106500
F	0.12190800	3.29754100	0.31280500
F	0.12191600	-0.41795300	0.31277900
C	1.28015500	1.43978600	-3.82875400
H	1.56701800	1.43978900	-4.85451500
N	0.96594600	1.43978500	-2.70521100

KrO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –6.42 kcal/mol

Cartesian atomic coordinates:

O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.58208089
O	2.23490657	0.00000000	1.28883756
Kr	0.74580035	0.57752446	1.28887301
C	2.14398782	3.43969651	-1.13961293
H	2.59262838	4.00963763	-1.92049610
N	1.65450932	2.81250186	-0.28843298

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.36 kcal/mol

Cartesian atomic coordinates:

O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.59773172
O	2.24980290	0.00000000	1.29887009
Kr	0.74998909	0.54624601	1.29886520
C	0.76021092	-4.04096162	1.29918475
H	0.76328687	-5.10600448	1.29937640
N	0.75688279	-2.87365806	1.29897675

KrF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –2.48 kcal/mol

Cartesian atomic coordinates:

F	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	3.76110200
Kr	0.01132893	0.00000000	1.88055100
C	4.40158227	-0.00076980	1.88055217
H	5.46688260	-0.00095611	1.88055245
N	3.23513113	-0.00056580	1.88055186

XeO_3···NCH

σ-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –7.67 kcal/mol**

Cartesian atomic coordinates:

O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.79970160
O	2.42510204	0.00000000	1.39899199
Xe	0.80954714	0.68252173	1.40160836
C	2.48685228	2.90745402	4.30250745
H	2.99994905	3.20123547	5.18942948
N	1.92717104	2.58073377	3.33480067

lp-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –0.93 kcal/mol**

Cartesian atomic coordinates:

O	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	2.83741985
O	2.45764008	0.00000000	1.41872904
Xe	0.81933549	0.62474572	1.41870905
C	0.83120610	-3.84612169	1.41914430
H	0.83505354	-4.91110653	1.41941922
N	0.82703413	-2.67917932	1.41886508

XeF_2···NCH

π-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –2.33 kcal/mol**

Cartesian atomic coordinates:

F	0.00000000	0.00000000	0.00000000
F	0.00000000	0.00000000	3.98277000
Xe	0.01298594	0.00000000	1.99138325
C	4.61890242	-0.04444053	1.99149266
H	5.68416810	-0.05472943	1.99151387
N	3.45243697	-0.03317704	1.99147152

EEF=0.004 au

$ArO_3\cdots NH_3$:

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –7.23 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.48259500
O	1.39261300	0.00000000	-0.46764000
O	-0.67309800	-1.21917000	-0.46760400
N	-0.71649500	1.21522100	-2.45584100
H	-1.20758100	0.45801200	-2.91847600
H	0.18380300	1.28342400	-2.91775000
H	-1.21869800	2.06200800	-2.69624700

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.57 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Ar	0.00000000	0.00000000	3.51413400
O	1.39255800	0.00000000	3.04533800
O	-0.69588400	1.20470000	3.04158700
O	-0.69493300	-1.20628500	3.04388700
H	0.44957800	0.81549000	-0.39940900
H	-0.93562000	-0.02167700	-0.38833900
H	0.48213000	-0.80273200	-0.38708700

$ArF_2\cdots NH_3$

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –3.14 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
F	1.85692000	0.00000000	0.03395200
F	-1.85684600	-0.00058400	0.03437100
N	-0.01840500	0.01661000	-3.15864900
H	-0.02353400	0.95040100	-3.55217300
H	-0.82942700	-0.45088600	-3.54718900
H	0.78961900	-0.44669800	-3.55825100

KrO_3···NH_3

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –10.08 kcal/mol

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.60889400
O	1.53188600	0.00000000	-0.45292700
O	-0.64731600	1.38841500	-0.45290600
N	-0.50128200	-0.78770000	-2.60238300
H	-1.00427800	-1.56804300	-3.00940200
H	0.43867400	-0.82541200	-2.98233900
H	-0.92347200	0.05276300	-2.98278300

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –1.47 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Kr	0.00000000	0.00000000	3.31408500
O	1.51128700	0.00000000	2.79896100
O	-0.75591600	1.29678900	2.76742800
O	-0.74663400	-1.31514100	2.80219800
H	0.91763300	0.01481100	-0.42959600
H	-0.46330500	0.85200600	-0.29366800
H	-0.50424700	-0.76163400	-0.43871400

KrF_2···NH_3

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –3.49 kcal/mol

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
F	1.88114400	0.00000000	0.02900800
F	-1.88119400	-0.00079400	0.03532100
N	0.00467200	0.00378200	-3.24673200
H	0.00706600	0.93407700	-3.64892300
H	-0.80635800	-0.46268200	-3.63652300
H	0.81265700	-0.46718700	-3.63735200

XeO_3···NH_3

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –13.78 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.76529500
O	1.70475200	0.00000000	-0.42041400
O	-0.61119600	-1.59138200	-0.42044000
N	-0.21532900	0.31722300	-2.70097300
H	-0.69498900	1.01312200	-3.26168800
H	-0.57774200	-0.58957200	-2.97867200
H	0.76165900	0.33536600	-2.97649400

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –6.81 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	1.69215400	0.00000000	-0.48773900
O	-0.82259700	1.47429800	-0.50114500
O	-0.84154100	-1.44064100	-0.56327000
N	0.04801600	0.05691300	-2.77598600
H	0.73342700	-0.58793800	-3.15239200
H	0.27700800	0.97861500	-3.12996300
H	-0.85114700	-0.19981200	-3.16699600

XeF_2···NH_3

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –3.32 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
F	1.99285400	0.00000000	0.03306600
F	-1.99263700	-0.00108200	0.04783100
N	0.01319000	0.00544000	-3.44253000
H	0.00036000	0.93253700	-3.85213300
H	-0.78190500	-0.48140300	-3.84049800
H	0.83579500	-0.45035700	-3.82089600

ArO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –5.69 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.48150300
O	1.38963300	0.00000000	-0.47163900
O	-0.68092700	1.21133500	-0.47171100
C	-0.88778400	-1.51810700	-3.51777200
H	-0.96615400	-1.65250100	-4.57343099
N	-0.79957700	-1.36665600	-2.36553299

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.42 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Ar	0.00000000	0.00000000	3.47206600
O	1.38992700	0.00000000	2.99667000
O	-0.69531300	1.20421100	2.99852300
O	-0.69564200	-1.20367300	2.99749700
C	0.00182000	-0.00127700	-1.16711400
H	0.00284300	-0.00284700	-2.23355300

ArF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –2.67 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
F	1.85759600	0.00000000	0.03895200
F	-1.85772700	0.00000000	0.03074400
C	0.00425500	0.00000000	-4.26671000
H	0.00397200	0.00000000	-5.33335200
N	0.00425200	0.00000000	-3.10042500

KrO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –7.36 kcal/mol

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.60717900
O	1.52521900	0.00000000	-0.46594600
O	-0.66282800	1.37355500	-0.46631800
C	-0.72386700	-1.12649100	-3.71055200
H	-0.77103100	-1.18343900	-4.77541800
N	-0.67062400	-1.05819900	-2.54885000

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.76 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Kr	0.00000000	0.00000000	3.36099700
O	1.50219100	0.00000000	2.82209600
O	-0.75248800	1.30221900	2.82700400
O	-0.75305200	-1.30167200	2.82656300
C	0.00329900	0.00591100	-1.16693100
H	0.00590600	0.01061900	-2.23341200

KrF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –2.96 kcal/mol

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
F	1.88061600	0.00000000	0.03135100
F	-1.88067000	0.00000000	0.03390500
C	-0.00114300	0.00000000	-4.36454300
H	-0.00451700	0.00000000	-5.43137100
N	0.00298000	0.00000000	-3.19832800

XeO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –9.05 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.76249800
O	1.69381400	0.00000000	-0.44736300
O	-0.63126600	-1.57172800	-0.44755100
C	-0.43025600	0.61628700	-3.93016000
H	-0.40239300	0.56406100	-4.99633000
N	-0.45875500	0.66818500	-2.76728000

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –1.73 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Xe	0.00000000	0.00000000	3.20780000
O	1.64681300	0.00000000	2.60556700
O	-0.82294700	1.42705900	2.60707400
O	-0.82397500	-1.42558800	2.60501900
C	0.00633000	0.00034600	-1.16640300
H	0.01205400	-0.00139500	-2.23287500

XeF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –2.90 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
F	1.99181600	0.00000000	0.04414300
F	-1.99154000	0.00000000	0.04070000
C	-0.00899200	0.00000000	-4.56337600
H	0.00200600	0.00000000	-5.63021300
N	-0.02128800	0.00000000	-3.39714800

EEF=0.008 au

$ArO_3\cdots NH_3$:

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –7.94 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.49109000
O	1.39434200	0.00000000	-0.45358600
O	-0.67233900	-1.22085900	-0.45456000
N	-0.68575400	1.11916000	-2.48355900
H	-1.59182400	0.83652900	-2.84218300
H	-0.00966200	0.58562700	-3.02133000
H	-0.56429800	2.08045400	-2.78372900

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.89 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Ar	0.00000000	0.00000000	3.46899500
O	1.39390900	0.00000000	3.00489100
O	-0.69620400	1.20780500	3.00536400
O	-0.69710900	-1.20618800	3.00255300
H	0.45481700	0.80952500	-0.40757200
H	-0.93176100	-0.01336700	-0.39991800
H	0.47424400	-0.80273100	-0.39875900

$ArF_2\cdots NH_3$

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –3.55 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
F	1.85629800	0.00000000	0.05559200
F	-1.85625900	-0.00124400	0.05604900
N	-0.01157500	0.02231300	-3.14276500
H	-0.01406700	0.95305700	-3.54570000
H	-0.82023300	-0.44133400	-3.54262500
H	0.79280800	-0.44088400	-3.55166800

KrO_3···NH_3

σ-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –11.40 kcal/mol**

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.61692200
O	1.53644100	0.00000000	-0.43027100
O	-0.64486300	1.39457000	-0.43026000
N	-0.46267200	-0.72399400	-2.58721300
H	-0.96606400	-1.50792300	-2.98909000
H	0.47178400	-0.76478200	-2.98232500
H	-0.88860600	0.10874200	-2.98233600

lp-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –2.05 kcal/mol**

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Kr	0.00000000	0.00000000	3.24248200
O	1.51141100	0.00000000	2.72649600
O	-0.75586200	1.31351500	2.73865500
O	-0.75986500	-1.30683200	2.72716700
H	0.54618600	-0.76521300	-0.38033700
H	0.38953300	0.84042000	-0.41296200
H	-0.92283500	-0.09812400	-0.40905300

KrF_2···NH_3

π-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –4.01 kcal/mol**

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
F	1.88132600	0.00000000	0.05075000
F	-1.88123400	-0.00083300	0.05973700
N	0.00116500	0.00516300	-3.22561600
H	-0.00416600	0.93261700	-3.63627100
H	-0.80164800	-0.46656100	-3.62796400
H	0.81145200	-0.45609700	-3.62510300

XeO_3···NH_3

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –15.98 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.77319700
O	1.71200800	0.00000000	-0.38456100
O	-0.61040100	-1.59938600	-0.38487500
N	-0.17108700	0.25550000	-2.64673700
H	0.28084500	1.04895700	-3.09135500
H	-1.07241800	0.13955100	-3.10025700
H	0.37919500	-0.56088200	-2.89944900

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –14.17 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	1.71318100	0.00000000	-0.44690200
O	-0.85303700	1.49926600	-0.40039300
O	-0.87077400	-1.47262300	-0.45560200
N	-0.01792600	0.04614100	-2.49264000
H	0.44493900	-0.77383100	-2.87070200
H	0.46330900	0.87043500	-2.83670600
H	-0.97017300	0.06400200	-2.84241900

XeF_2···NH_3

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –3.97 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
F	1.99284500	0.00000000	0.05980600
F	-1.99258700	-0.00096400	0.07827300
N	0.00814000	0.00829300	-3.41222700
H	0.00204100	0.93354100	-3.82828200
H	-0.79008600	-0.46808800	-3.81875300
H	0.82191200	-0.45201700	-3.80618700

ArO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –6.39 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.48961700
O	1.39072700	0.00000000	-0.45928100
O	-0.68065100	1.21273000	-0.45939800
C	-0.79062900	-1.36092500	-3.57509900
H	-0.83907500	-1.44746100	-4.63934900
N	-0.73581600	-1.26145800	-2.41517400

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –0.72 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Ar	0.00000000	0.00000000	3.42404800
O	1.39160300	0.00000000	2.95457000
O	-0.69741500	1.20286100	2.95111400
O	-0.69462000	-1.20783600	2.95946400
C	0.00108300	0.00025200	-1.16694900
H	0.00176600	-0.00098700	-2.23500600

ArF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –3.11 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
F	1.85725900	0.00000000	0.06089800
F	-1.85745800	0.00000000	0.05279800
C	0.00501200	0.00000000	-4.24542300
H	0.00560600	0.00000000	-5.31374500
N	0.00406900	0.00000000	-3.07926900

KrO_3···NCH

σ-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –8.45 kcal/mol**

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.61450300
O	1.52854400	0.00000000	-0.44711600
O	-0.66048900	1.37845700	-0.44720500
C	-0.64734900	-1.02906400	-3.72093900
H	-0.67605900	-1.07519600	-4.78891800
N	-0.61350700	-0.97499800	-2.55780900

lp-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –1.24 kcal/mol**

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Kr	0.00000000	0.00000000	3.30351400
O	1.50747100	0.00000000	2.77989900
O	-0.75287100	1.30511400	2.77769400
O	-0.75302300	-1.30510900	2.77796000
C	-0.00518300	0.00567800	-1.16670800
H	-0.01030500	0.00903400	-2.23482700

KrF_2···NCH

π-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –3.50 kcal/mol**

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
F	1.88080200	0.00000000	0.05561900
F	-1.88083100	0.00000000	0.05932200
C	-0.00026100	0.00000000	-4.33227500
H	-0.00365400	0.00000000	-5.40082700
N	0.00323700	0.00000000	-3.16618400

XeO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –10.67 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.76902800
O	1.69975300	0.00000000	-0.41734600
O	-0.62672500	-1.58002100	-0.41720300
C	-0.39190100	0.57278100	-3.90402400
H	-0.37137100	0.54202800	-4.97332100
N	-0.41348100	0.60105800	-2.74028800

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –2.77 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Xe	0.00000000	0.00000000	3.11235300
O	1.65583200	0.00000000	2.53444400
O	-0.82714700	1.43513500	2.53625000
O	-0.82891900	-1.43333400	2.53436600
C	0.00903100	0.00533500	-1.16593000
H	0.01969900	0.00960600	-2.23410600

XeF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –3.56 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
F	1.99191500	0.00000000	0.07389800
F	-1.99165500	0.00000000	0.07069700
C	-0.00736900	0.00000000	-4.52206400
H	0.00314500	0.00000000	-5.59067000
N	-0.01938200	0.00000000	-3.35594500

EEF=0.016 au

$ArO_3\cdots NH_3$:

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –9.72 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.51083200
O	1.39770100	0.00000000	-0.42572500
O	-0.67166500	-1.22531100	-0.42656600
N	-0.58505400	0.96340100	-2.51279600
H	-1.52220600	0.83166500	-2.88295600
H	-0.01840900	0.29944000	-3.03519700
H	-0.29588700	1.86901900	-2.87137800

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –1.65 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Ar	0.00000000	0.00000000	3.38555800
O	1.39781000	0.00000000	2.93372700
O	-0.69847000	1.21003300	2.93196100
O	-0.69821800	-1.21044300	2.93238800
H	0.45608700	0.80203800	-0.42466600
H	-0.92481500	-0.00864200	-0.41981600
H	0.46781500	-0.79922700	-0.41711100

$ArF_2\cdots NH_3$

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –4.46 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
F	1.85564800	0.00000000	0.10127000
F	-1.85569200	-0.00092600	0.10012200
N	-0.00001300	0.02134500	-3.11529400
H	-0.00295700	0.94387600	-3.54050500
H	-0.79991400	-0.44389200	-3.53441800
H	0.80271200	-0.43886800	-3.53456800

KrO_3···NH_3

σ-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –14.93 kcal/mol**

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.63712400
O	1.54706500	0.00000000	-0.37988200
O	-0.64181800	1.40802600	-0.37908000
N	-0.35294200	-0.56258900	-2.53432000
H	-1.27975500	-0.65888500	-2.94136100
H	0.19408300	-1.31987700	-2.93587700
H	0.02700300	0.28186800	-2.95635800

lp-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –3.71 kcal/mol**

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Kr	0.00000000	0.00000000	3.10081000
O	1.52374100	0.00000000	2.61918100
O	-0.75979900	1.32267000	2.62367600
O	-0.76349500	-1.31629200	2.61267300
H	0.37295000	-0.85081800	-0.41145300
H	0.54713000	0.74249500	-0.42623800
H	-0.91978500	0.09677700	-0.42064600

KrF_2···NH_3

π-Hole Interactions

***E*$_{MP2/aug-cc-pVTZ(PP)}$ = –5.17 kcal/mol**

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
F	1.88146400	0.00000000	0.09571100
F	-1.88136100	-0.00066900	0.10758300
N	-0.00189700	0.00625400	-3.18387300
H	-0.00631300	0.92864700	-3.60980600
H	-0.80329600	-0.45876900	-3.60084700
H	0.79926200	-0.45415900	-3.60620800

XeO_3···NH_3

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –22.07 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.79187100
O	1.72626400	0.00000000	-0.31256400
O	-0.61410600	-1.61342500	-0.31204600
N	-0.08771300	0.13319600	-2.55563600
H	0.38760700	0.91626900	-2.99992000
H	-0.99093500	0.04559300	-3.01729500
H	0.43944800	-0.69652300	-2.82238600

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –26.85 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	1.73880700	0.00000000	-0.37905700
O	-0.88011200	1.50177700	-0.37095200
O	-0.87096000	-1.51551900	-0.33681400
N	-0.02064400	-0.02294200	-2.34229400
H	0.44770400	-0.85598800	-2.69186000
H	0.46149400	0.79842100	-2.70073500
H	-0.97834300	-0.01652200	-2.68615100

XeF_2···NH_3

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –5.46 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
F	1.99301200	0.00000000	0.11453800
F	-1.99235900	-0.00086100	0.14206600
N	0.00131200	0.01189000	-3.34519300
H	-0.00020600	0.93311000	-3.77397800
H	-0.79769200	-0.45408100	-3.76599000
H	0.80440000	-0.44991900	-3.76281100

ArO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –8.12 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.50867400
O	1.39291200	0.00000000	-0.43475200
O	-0.68074900	1.21503800	-0.43516600
C	-0.67412400	-1.17090000	-3.62583400
H	-0.70555000	-1.23251200	-4.69674100
N	-0.63972700	-1.10117200	-2.46273200

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –1.48 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Ar	0.00000000	0.00000000	3.33765200
O	1.39453300	0.00000000	2.87808100
O	-0.69804100	1.20847900	2.88104000
O	-0.69833800	-1.20787200	2.87993100
C	0.00014300	0.00172400	-1.16689200
H	0.00052900	0.00339100	-2.23876500

ArF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –4.10 kcal/mol

Cartesian atomic coordinates:

Ar	0.00000000	0.00000000	0.00000000
F	1.85643000	0.00000000	0.10637100
F	-1.85678700	0.00000000	0.09807800
C	0.00668900	0.00000000	-4.20478100
H	0.00868900	0.00000000	-5.27706200
N	0.00421300	0.00000000	-3.03848700

KrO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –11.12 kcal/mol

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.63172800
O	1.53512400	0.00000000	-0.40874800
O	-0.65637300	1.38788200	-0.40836700
C	-0.53349900	-0.86401300	-3.71643400
H	-0.54728300	-0.89616700	-4.78984000
N	-0.51721700	-0.82745200	-2.55194800

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –2.48 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Kr	0.00000000	0.00000000	3.18843800
O	1.51486800	0.00000000	2.68634000
O	-0.75690400	1.31230700	2.68662100
O	-0.75758800	-1.31142100	2.68534500
C	0.00072800	-0.00400200	-1.16661100
H	0.00301600	-0.00690000	-2.23864400

KrF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –4.74 kcal/mol

Cartesian atomic coordinates:

Kr	0.00000000	0.00000000	0.00000000
F	1.88127700	0.00000000	0.10160300
F	-1.88127100	0.00000000	0.10751800
C	0.00182600	0.00000000	-4.27756600
H	-0.00198900	0.00000000	-5.35017400
N	0.00580600	0.00000000	-3.11131800

XeO_3···NCH

σ-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –14.78 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.78475900
O	1.71105800	0.00000000	-0.35562000
O	-0.61862300	-1.59526400	-0.35593300
C	-0.29782000	0.43117200	-3.83928000
H	-0.28447200	0.40891400	-4.91405300
N	-0.31362000	0.45314100	-2.67513400

lp-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –5.99 kcal/mol

Cartesian atomic coordinates:

N	0.00000000	0.00000000	0.00000000
Xe	0.00000000	0.00000000	2.90437400
O	1.67724900	0.00000000	2.38582200
O	-0.83779700	1.45351000	2.38709200
O	-0.83936400	-1.45169500	2.38466900
C	-0.00045000	-0.00112200	-1.16532600
H	-0.00208500	-0.00264300	-2.23798100

XeF_2···NCH

π-Hole Interactions

$E_{MP2/aug-cc-pVTZ(PP)}$ = –5.12 kcal/mol

Cartesian atomic coordinates:

Xe	0.00000000	0.00000000	0.00000000
F	1.99187500	0.00000000	0.13460700
F	-1.99166800	0.00000000	0.13118700
C	-0.00701500	0.00000000	-4.44272300
H	0.00322000	0.00000000	-5.51550700
N	-0.01805100	0.00000000	-3.27647100