Supplementary Information

Noble Gas Insertion Compounds of Hydrogenated and Lithiated Hyperhalogens

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Table S1 Symmetry Point Group, NPA charge on H, Li and M atoms (q, |e|) for the $H/LiBO_2$ and $H/LiM(BO_2)_2$ (M = Cu, Ag, Au) compounds at the ωB97X-D/def2-TZVPP level.

isomers	*symmetry*	q(H)	q(M)	isomers	*symmetry*	q(Li)	q(M)
HBO_2	C_s	0.52		**$LiBO_2$**	$C_{\infty v}$	0.98	
a1	C_s	0.55	0.87	**A1**	C_{2v}	0.97	0.84
a2	C_s	0.54	0.80	**A2**	C_s	0.97	0.86
a3	C_s	0.55	0.80	**A3**	C_{2v}	0.97	0.92
a4	C_{2v}	0.10	1.23				
b1	C_s	0.54	0.90	**B1**	C_{2v}	0.96	0.86
b2	C_1	0.54	0.82	**B2**	C_s	0.97	0.90
b3	C_s	0.55	0.82	**B3**	C_{2v}	0.97	0.92
b4	C_2	0.15	1.17				
c1	C_s	0.56	0.75	**C1**	C_{2v}	0.96	0.67
c2	C_1	0.54	0.64	**C2**	C_s	0.96	0.74
c3	C_1	0.56	0.63	**C3**	C_s	0.97	0.59
c4	C_1	0.17	1.10	**C4**	C_{2v}	0.97	0.85

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Table S2 NPA charge on H, M and Ng (Ng = Xe, Ar, Kr) atoms (q, |e|), Symmetry Point Group, ZPE-corrected dissociation energy (E_{dis}, kcal/mol), reaction enthalpy (ΔH, kcal/mol), and reaction Gibbs free energy (ΔG, kcal/mol) at 298.15 K for dissociation channels of high-lying Ng (Ng = Xe, Ar, Kr) insertion compounds of HBO_2 and $HM(BO_2)_2$ (M = Cu, Ag, Au) at the ωB97X-D/def2-TZVPP level. BSSE-corrected binding energy (E_b, kcal/mol) of these species at the CCSD (T)/def2-TZVPP level.

isomers	*symmetry*	dissociation channel	E_{dis}	ΔH	ΔG	E_b	q(H)	q(Ng)	q(M)
ii-Xe	C_s	HO+Xe+BO	14.5	16.0	-0.9	-4.5	0.45	0.83	
ii-Ar	C_s	HO+Ar+BO	-31.4	-29.9	-46.5	-44.1	0.43	0.51	
ii-Kr	C_s	HO+Kr+BO	-11.5	-63.3	-26.9	-26.7	0.44	0.66	
iii-Xe	C_1	HOB +XeO	5.6	5.2	-0.8	34.9	0.55	0.87	
iii-Ar	C_s	HOB +ArO	3.1	2.7	-3.4	5.7	0.55	0.55	
iii-Kr	C_s	HOB +KrO	4.0	3.7	-2.9	17.4	0.55	0.69	
d2-Xe	C_1	$Xe+HCu(BO_2)_2$	-53.6	-53.9	-58.3	33.0	0.55	0.26	0.66
		$HBO_2+Xe+Cu+BO_2$	65.1	65.1	44.7				
d3-Xe	C_s	$Xe+HCu(BO_2)_2$	-75.9	-75.9	-82.2	37.1	0.56	0.29	0.62
		$HBO_2+Xe+Cu+BO_2$	42.8	43.1	20.9				
e2-Xe	C_s	$Xe+HAg(BO_2)_2$	-45.2	-45.5	-50.7	27.2	0.55	0.24	0.67
		$HBO_2+Xe+Ag+BO_2$	47.8	47.7	27.5				
e3-Xe	C_s	$Xe+HAg(BO_2)_2$	-63.8	-63.9	-70.1	30.7	0.55	0.27	0.63
		$HBO_2+Xe+Ag+BO_2$	29.2	29.3	8.1				
f2-Xe	C_s	$Xe+HAu(BO_2)_2$	-46.2	-46.6	-51.4	49.6	0.55	0.41	0.44
		$HBO_2+Xe+Au+BO_2$	42.4	42.4	21.0				
f3-Xe	C_s	$Xe+HAu(BO_2)_2$	-64.3	-64.5	-70.3	59.5	0.55	0.46	0.36
		$HBO_2+Xe+Au+BO_2$	24.3	24.5	2.1				
f4-Xe	C_s	$Xe+HAu(BO_2)_2$	-63.0	-62.7	-69.9	3.3	0.15	0.77	0.60
		$H+Xe+Au(BO_2)_2$	20.8	22.0	7.9				

Table S3 NPA charge on Li, M and Xe atoms (q, |e|), Symmetry Point Group, ZPE-corrected dissociation energy (E_{dis}, kcal/mol), reaction enthalpy (ΔH, kcal/mol), and reaction Gibbs free energy (ΔG, kcal/mol) at 298.15 K for dissociation channels of high-lying Xe insertion compounds of $LiBO_2$ and $LiM(BO_2)_2$ (M = Cu, Ag, Au) at the ωB97X-D/def2-TZVPP level. BSSE-corrected binding energy (E_b, kcal/mol) of these species at the CCSD (T)/def2-TZVPP level.

isomers	*symmetry*	dissociation channel	E_{dis}	ΔH	ΔG	E_b	q(Li)	q(Xe)	q(M)
D2-Xe	C_1	Xe+$LiCu(BO_2)_2$	-79.6	-80.6	-81.4	29.9	0.99	0.24	0.67
		$LiBO_2$+$CuXeBO_2$	54.5	54.2	46.8				
E2-Xe	C_1	Xe+$LiAg(BO_2)_2$	-73.6	-74.6	-76.0	23.6	0.99	0.22	0.68
		$LiBO_2$+$AgXeBO_2$	42.2	41.9	34.3				
F2-Xe	C_1	Xe+$LiAu(BO_2)_2$	-71.0	-71.8	-73.6	44.8	0.99	0.37	0.45
		$LiBO_2$+$AuXeBO_2$	45.7	45.4	37.7				
F3-Xe	C_s	Xe+$LiAu(BO_2)_2$	-50.1	-50.5	-55.6	38.8	0.98	0.41	0.38
		$LiBO_2$+$AuXeBO_2$	31.6	31.3	23.2				

Table S4 Electron density descriptors (au.) at the bond critical points (BCPs) and Wiberg bond indices (WBI) of important bonds at the ωB97X-D/def2-TZVPP level.

isomers	bond	WBI	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$
ii-Xe	Xe-O	0.34	0.105	0.158	0.081	-0.122	-0.041
	Xe-B	0.83	0.105	-0.085	0.030	-0.081	-0.051
iii-Xe	Xe-O	1.06	0.169	0.108	0.127	-0.227	-0.100
	Xe-B	0.06	0.015	0.034	0.008	-0.007	0.001
d2-Xe	Xe-O	0.05	0.035	0.116	0.029	-0.030	0.000
	Xe-Cu	0.58	0.073	0.150	0.060	-0.083	-0.023
d3-Xe	Xe-O	0.07	0.040	0.125	0.033	-0.035	-0.002
	Xe-Cu	0.61	0.074	0.144	0.059	-0.083	-0.023
e2-Xe	Xe-O	0.05	0.035	0.114	0.029	-0.030	-0.001
	Xe-Ag	0.51	0.064	0.131	0.048	-0.062	-0.015
e3-Xe	Xe-O	0.07	0.040	0.123	0.033	-0.035	-0.022
	Xe-Ag	0.53	0.063	0.127	0.046	-0.060	-0.014
f2-Xe	Xe-O	0.08	0.044	0.133	0.036	-0.039	-0.003
	Xe-Au	0.66	0.088	0.103	0.056	-0.086	-0.030
f3-Xe	Xe-O	0.11	0.052	0.143	0.042	-0.048	-0.006
	Xe-Au	0.70	0.087	0.097	0.053	-0.082	-0.029
f4-Xe	Xe-O	0.08	0.044	0.133	0.036	-0.040	-0.033
	Xe-H	0.90	0.167	-0.300	0.057	-0.189	-0.132
D2-Xe	Xe-O	0.04	0.031	0.107	0.026	-0.026	0.000
	Xe-Cu	0.56	0.072	0.156	0.061	-0.083	-0.022
E2-Xe	Xe-O	0.04	0.031	0.101	0.025	-0.025	0.000
	Xe-Ag	0.48	0.062	0.137	0.048	-0.062	-0.014
F2-Xe	Xe-O	0.07	0.039	0.122	0.032	-0.034	-0.001
	Xe-Au	0.62	0.086	0.115	0.058	-0.087	-0.029
F3-Xe	Xe-O	0.09	0.045	0.131	0.036	-0.040	-0.003
	Xe-Au	0.65	0.087	0.103	0.055	-0.085	-0.030

Table S5 Electron density descriptors (au.) at the bond critical points (BCPs) and Wiberg bond indices (WBI) of important bonds at the ωB97X-D /def2-TZVPP level.

isomers	bond	WBI	$\rho(r_c)$	$\nabla^2\rho(r_c)$	$G(r_c)$	$V(r_c)$	$H(r_c)$
ii-Ar	Ar-O	0.28	0.106	0.250	0.087	-0.111	-0.024
	Ar-B	0.68	0.126	-0.203	0.037	-0.125	-0.088
iii-Ar	Ar-O	0.88	0.176	0.294	0.153	-0.233	-0.080
	Ar-B	0.01	0.009	0.028	0.005	-0.004	0.002
ii-Kr	Kr-O	0.30	0.107	0.201	0.083	-0.115	-0.032
	Kr-B	0.76	0.119	-0.140	0.031	-0.097	-0.066
iii-Kr	Kr-O	0.98	0.176	0.156	0.129	-0.220	-0.090
	Kr-B	0.03	0.012	0.031	0.007	-0.006	0.001

Table S6 Approximate energy barrier ($\Delta E^{\ddagger}$, kcal/mol) for the isomerization $HXeM(BO_2)_2/LiXeM(BO_2)_2$ (M = Cu, Ag, Au) ⟶ $XeHM(BO_2)_2/XeLiM(BO_2)_2$ at the ωB97X-D/def2-TZVPP level.

isomers	$\Delta E^{\ddagger}$	isomers	$\Delta E^{\ddagger}$
d1-Xe	0.66	**D1-Xe**	1.56
d2-Xe	2.82	**D2-Xe**	3.70
d3-Xe	3.43		
e1-Xe	0.70	**E1-Xe**	1.27
e2-Xe	2.73	**E2-Xe**	0.67
e3-Xe	3.74		
f1-Xe	1.54	**F1-Xe**	2.81
f2-Xe	13.62	**F2-Xe**	4.61
f3-Xe	19.41	**F3-Xe**	4.30
f4-Xe	17.72		

Cartesian coordinates of the optimized isomeric structures and transition states.

##########

HBO_2 charge=0 spin=1

O	0.14626400	1.32369700	0.00000000
B	0.00000000	0.12325600	0.00000000
O	-0.21501600	-1.18140900	0.00000000
H	0.55002000	-1.75458300	0.00000000

##########

i-Xe charge=0 spin=1

O	-0.68967800	-3.36651100	0.00000000
B	0.01756300	-2.36472600	0.00000000
O	0.73709800	-1.29206300	0.00000000
H	-0.46717000	2.44491800	0.00000000
Xe	0.00000000	0.86383900	0.00000000

##########

i-Xe-TS charge=0 spin=1

O	-0.68967800	-3.36651100	0.00000000
B	0.01756300	-2.36472600	0.00000000
O	0.73709800	-1.29206300	0.00000000
H	-0.46717000	2.44491800	0.00000000
Xe	0.00000000	0.86383900	0.00000000

##########

ii-Xe charge=0 spin=1

O	-0.02122400	-3.18866900	0.00000000
B	-0.03287400	-1.98943000	0.00000000
O	-0.06073300	2.38362800	0.00000000
H	0.82002200	2.76256500	0.00000000
Xe	0.00000000	0.25231300	0.00000000

##########

iii-Xe charge=0 spin=1

O	2.46534600	-0.04478500	0.02082100
B	-2.71998800	0.02789200	-0.01415900
O	-4.00662400	0.06504500	0.01560000
H	-4.60988600	-0.67975400	-0.00416700
Xe	0.56555600	0.00700400	-0.00400800

##########

$LiBO_2$ charge=0 spin=1

O	0.00000000	0.00000000	1.61299800
B	0.00000000	0.00000000	0.38490000
O	0.00000000	0.00000000	-0.89736200
Li	0.00000000	0.00000000	-2.54986200

##########

I-Xe charge=0 spin=1

O	0.00000000	0.00000000	-3.00168600

B 0.00000000 0.00000000 -4.28295900
O 0.00000000 0.00000000 -5.51187100
Li 0.00000000 0.00000000 -1.34077800
Xe 0.00000000 0.00000000 1.73232600
##
II-Xe charge=0 spin=1
O 0.00000000 0.00000000 -3.36863800
B 0.00000000 0.00000000 -2.16333400
O 0.00000000 0.00000000 2.17924200
Li 0.00000000 0.00000000 3.80336200
Xe 0.00000000 0.00000000 0.16521800
##
III-Xe charge=0 spin=1
O -2.57775700 0.04856300 0.00268200
B 2.39777000 -0.05332500 -0.00184300
O 3.64358000 -0.02114000 0.00354600
Li 5.33059400 0.12702100 -0.00296500
Xe -0.67606000 -0.00618200 -0.00058700
##
i-Ar charge=0 spin=1
O 2.46694400 0.45810300 0.00000000
B 1.26679100 0.73023100 0.00000000
O 0.00000000 0.95862300 0.00000000
H -2.18394300 -1.73163100 0.00000000
Ar -1.32697600 -0.73629600 0.00000000
##
i-Ar-TS charge=0 spin=1
O -2.98958600 -0.03882200 -0.02459800
B -1.75398500 0.02174400 0.00910300
O -0.47978000 0.08427100 0.04081500
H 2.33724500 1.10230200 -0.04326600
Ar 1.89931200 -0.08747900 -0.00733300
##
ii-Ar charge=0 spin=1
O -0.01217400 -2.71325600 0.00000000
B -0.02943300 -1.51765700 0.00000000
O -0.07395200 2.41124200 0.00000000
H 0.83617200 2.71851000 0.00000000
Ar 0.00000000 0.40477100 0.00000000
##
iii-Ar charge=0 spin=1
O 0.03246600 2.84791900 0.00000000
B -0.01496600 -2.18347500 0.00000000
O -0.10200100 -3.47125300 0.00000000

H 0.63110600 -4.08925000 0.00000000
Ar 0.00000000 1.11073900 0.00000000
##
I-Ar charge=0 spin=1
O 0.00000000 0.00000000 -1.37451800
B 0.00000000 0.00000000 -2.65613700
O 0.00000000 0.00000000 -3.88464400
Li 0.00000000 0.00000000 0.28276100
Ar 0.00000000 0.00000000 3.02809500
##
II-Ar charge=0 spin=1
O 0.00000000 0.00000000 -2.99933500
B 0.00000000 0.00000000 -1.79605800
O 0.00000000 0.00000000 2.12519500
Li 0.00000000 0.00000000 3.74375400
Ar 0.00000000 0.00000000 0.26345200
##
III-Ar charge=0 spin=1
O 0.05071400 3.02964700 0.00000000
B -0.06064700 -1.80008700 0.00000000
O -0.04723000 -3.04913300 0.00000000
Li 0.09178800 -4.73166300 0.00000000
Ar 0.00000000 1.29729500 0.00000000
##
i-Kr charge=0 spin=1
O -0.75983100 -2.94691200 0.00000000
B 0.02134500 -1.99849600 0.00000000
O 0.80532000 -0.97453300 0.00000000
H -0.47064100 2.46578300 0.00000000
Kr 0.00000000 1.08050700 0.00000000
##
i-Kr-TS charge=0 spin=1
O -0.06407700 3.64975600 0.00000000
B -0.03387700 2.41290800 0.00000000
O 0.00000000 1.13626500 0.00000000
H 1.36398600 -1.63502800 0.00000000
Kr -0.01894400 -1.35326900 0.00000000
##
ii-Kr charge=0 spin=1
O -0.01183800 -2.95706100 0.00000000
B -0.02672000 -1.75981200 0.00000000
O -0.07457800 2.36150500 0.00000000
H 0.82493000 2.69684700 0.00000000
Kr 0.00000000 0.30185200 0.00000000

##

iii-Kr charge=0 spin=1

O	0.01993400	2.56177400	0.00000000
B	-0.01112800	-2.52114000	0.00000000
O	-0.09263900	-3.80775000	0.00000000
H	0.63727800	-4.42939200	0.00000000
Kr	0.00000000	0.75008000	0.00000000

##

I-Kr charge=0 spin=1

O	0.00000000	0.00000000	-2.36625600
B	0.00000000	0.00000000	-3.64773800
O	0.00000000	0.00000000	-4.87641800
Li	0.00000000	0.00000000	-0.70771400
Kr	0.00000000	0.00000000	2.17509000

##

II-Kr charge=0 spin=1

O	0.00000000	0.00000000	-3.17828900
B	0.00000000	0.00000000	-1.97404000
O	0.00000000	0.00000000	2.12157500
Li	0.00000000	0.00000000	3.74087500
Kr	0.00000000	0.00000000	0.19725800

##

III-Kr charge=0 spin=1

O	0.04215300	2.70922500	0.00000000
B	-0.04998800	-2.20093800	0.00000000
O	-0.03943200	-3.44882200	0.00000000
Li	0.07605700	-5.13531400	0.00000000
Kr	0.00000000	0.89798400	0.00000000

##

a1 charge=0 spin=1

Cu	0.00000000	1.10224400	0.00000000
O	-1.82048600	0.54013600	0.00000000
O	1.85346400	0.49726300	0.00000000
B	1.57579000	-0.72213200	0.00000000
B	-1.60999500	-0.71561300	0.00000000
O	1.23103100	-1.95471400	0.00000000
O	-1.26558700	-1.91910200	0.00000000
H	0.18364700	-2.08500600	0.00000000

##

a2 charge=0 spin=1

Cu	0.00000000	0.36496700	0.00000000
O	-1.56006300	-0.67838800	0.00000000
O	1.48190300	1.39718800	0.00000000
B	2.73010900	1.07736200	0.00000000

B -2.50023700 -1.44648900 0.00000000
O 3.92414000 0.79290800 0.00000000
O -3.55520500 -2.20863900 0.00000000
H -3.47555400 -3.16295900 0.00000000
##
a3 charge=0 spin=1
O 0.27822300 -1.87863300 0.00000000
O -0.26886100 1.85020100 0.00000000
B 0.61309200 2.79580900 0.00000000
B -0.68435400 -2.81953100 0.00000000
O 1.44081600 3.69840300 0.00000000
O -1.55438000 -3.64587800 0.00000000
H 1.18992700 -2.18383800 0.00000000
Cu 0.00000000 0.07274800 0.00000000
##
a4 charge=0 spin=1
Cu 0.00000000 0.00000000 0.41773500
O 0.00000000 1.74008000 0.54475700
O 0.00000000 -1.74008000 0.54475700
B 0.00000000 -2.74546000 -0.29558200
B 0.00000000 2.74546000 -0.29558200
O 0.00000000 -3.69158700 -1.05499800
O 0.00000000 3.69158700 -1.05499800
H 0.00000000 0.00000000 -0.99463400
##
b1 charge=0 spin=1
Ag 0.00000000 1.08821500 0.00000000
O 1.96696000 -0.00513600 0.00000000
O -1.95235800 0.10164500 0.00000000
B -1.65253900 -1.12612000 0.00000000
B 1.63682600 -1.20348700 0.00000000
O -1.24083500 -2.31151100 0.00000000
O 1.21715900 -2.41135700 0.00000000
H 0.15115800 -2.48717500 0.00000000
##
b2 charge=0 spin=1
Ag 0.16214700 -0.29139900 -0.02251500
O -1.97222000 -0.01109900 -0.10843200
O 2.16176200 -0.58665400 0.16517800
B 3.05964900 0.33100600 0.05304300
B -3.14437100 0.29326300 -0.01772900
O 3.92338200 1.19894700 -0.05099000
O -4.41904000 0.56187300 0.03117700
H -4.74839000 1.26986700 0.58618400

##

b3 charge=0 spin=1

Ag	0.00000000	0.13185500	0.00000000
O	0.86973200	-1.97590200	0.00000000
O	-0.87154000	1.95822400	0.00000000
B	-2.15159500	2.13708000	0.00000000
B	2.16315000	-2.33094500	0.00000000
O	-3.36646600	2.30587500	0.00000000
O	3.33285300	-2.60568100	0.00000000
H	0.22559400	-2.68797300	0.00000000

##

b4 charge=0 spin=1

Ag	0.00000000	0.00000000	0.38228200
O	-0.19259600	-1.92108500	0.49600700
O	0.19259600	1.92108500	0.49600700
B	0.09197900	2.84076500	-0.43040100
B	-0.09197900	-2.84076500	-0.43040100
O	0.00000000	3.70518000	-1.27940300
O	0.00000000	-3.70518000	-1.27940300
H	0.00000000	0.00000000	-1.12889100

##

c1 charge=0 spin=1

O	-1.31676800	-2.34465100	0.00000000
O	-2.01568700	0.08957300	0.00000000
O	2.08907200	0.10538100	0.00000000
O	1.26445400	-2.30492300	0.00000000
B	-1.71824800	-1.16539500	0.00000000
B	1.63422500	-1.07165700	0.00000000
Au	0.00000000	0.62385500	0.00000000
H	0.25153600	-2.46236500	0.00000000

##

c2 charge=0 spin=1

O	-3.79009500	1.26309300	-0.05441600
O	-2.04851100	-0.54078100	0.21096200
O	1.91519300	0.09416200	-0.21075500
O	4.36008900	0.59510100	0.08604700
B	-2.92899700	0.40244600	0.06868600
B	3.08565700	0.36092100	-0.03507800
Au	-0.11344800	-0.20668000	-0.01467300
H	4.68566700	1.21827100	0.73642000

##

c3 charge=0 spin=1

O	3.98533800	-0.60983700	0.64760800
O	1.95873300	0.77045200	-0.03570100

O	-1.86881500	-0.74255700	-0.31799600
O	-3.83425700	0.33840600	0.84041700
B	3.03206700	0.04457200	0.32598200
B	-2.87350400	-0.17357600	0.28850000
Au	-0.06091000	0.01143100	-0.15023000
H	2.09112500	1.69022700	-0.27885400

##

c4 charge=0 spin=1

O	3.69567200	1.32835800	-0.17058900
O	1.93023900	-0.43494700	0.22137300
O	-1.91506700	-0.40857900	-0.27755500
O	-3.73266300	1.29680700	0.12526400
B	2.84124000	0.48584000	0.01331500
B	-2.85386500	0.48141000	-0.06641200
Au	0.00358500	-0.25616600	0.00660800
H	-0.04555400	1.14774000	0.55550500

##

d1-Xe charge=0 spin=1

Cu	1.83016700	-0.28700800	0.04606600
O	-3.84079900	0.22349700	-0.01679100
O	3.63793400	-0.39646900	0.14836700
B	4.55820900	0.50134500	0.04349800
B	-5.04112800	0.37782200	0.04943600
O	5.44524900	1.34230800	-0.05414700
O	-6.35050100	0.48296100	0.12981300
H	-6.74646000	1.35004600	0.05168800
Xe	-0.64905300	-0.19705600	-0.06500400

##

d2-Xe charge=0 spin=1

Cu	-1.45064500	-0.07602700	0.00673300
O	-3.33720700	0.15960100	0.01008900
O	3.59942400	-0.52216700	-0.01099900
B	4.37738700	0.48605000	-0.00441700
B	-4.53820200	0.36048700	-0.00266900
O	5.10004200	1.49660200	0.00226400
O	-5.82785300	0.49214200	-0.01919100
H	-6.25598900	1.34882600	0.00896500
Xe	0.97876900	-0.30344700	-0.00048400

##

d3-Xe charge=0 spin=1

B	1.47885300	4.01157900	0.00000000
O	2.64109600	4.44336300	0.00000000
O	0.30377100	3.51347200	0.00000000
B	-1.29473400	-4.27762700	0.00000000

O	-0.19598500	-3.49454700	0.00000000
O	-2.29570700	-4.93749900	0.00000000
Xe	0.00000000	0.95865000	0.00000000
H	0.65349100	-3.94673000	0.00000000
Cu	-0.17929300	-1.47201400	0.00000000

##

e1-Xe charge=0 spin=1

Ag	1.69259000	-0.25146600	0.05291200
O	-4.23012400	0.32075600	0.06346000
O	3.68876100	-0.52886900	0.33706000
B	4.61628400	0.35780900	0.20596800
B	-5.42483000	0.22295000	0.24162000
O	5.50510600	1.19589900	0.08313300
O	-6.71276100	0.05427000	0.45525900
H	-7.30723000	0.78026700	0.27050700
Xe	1.00388100	-0.00373300	-0.23160400

##

e2-Xe charge=0 spin=1

Ag	0.00000000	1.32373600	0.00000000
O	0.43940400	3.45532000	0.00000000
O	-0.74480900	-3.89562300	0.00000000
B	0.27717000	-4.65624100	0.00000000
B	0.70283900	4.64349600	0.00000000
O	1.30193900	-5.35826600	0.00000000
O	0.90511700	5.92736900	0.00000000
H	1.78810600	6.29848500	0.00000000
Xe	-0.40558100	-1.28668000	0.00000000

##

e3-Xe charge=0 spin=1

Ag	-0.15436700	-1.34002600	0.00000000
O	-0.08353400	-3.69324200	0.00000000
O	0.24280400	3.86081100	0.00000000
B	1.42731500	4.33863500	0.00000000
B	-1.14197900	-4.52007800	0.00000000
O	2.59643300	4.74956100	0.00000000
O	-2.12497000	-5.20990000	0.00000000
H	0.78269300	-4.10906000	0.00000000
Xe	0.00000000	1.30258600	0.00000000

##

f1-Xe charge=0 spin=1

O	4.98609300	1.38746800	0.06672400
O	3.29814200	-0.47309000	0.28351200
O	-4.38260500	0.28856200	-0.02327100
O	-6.84813400	0.17830300	0.51936100

B	4.15329100	0.49746700	0.16815100
B	-5.57171200	0.24344200	0.20764900
Au	1.33450300	-0.20994600	0.03918700
H	-7.49780700	0.33750900	-0.16417500
Xe	-1.24562600	0.02766200	-0.21446700

##

f2-Xe charge=0 spin=1

O	1.19108300	-5.61611900	0.00000000
O	-0.71602500	-3.97487900	0.00000000
O	0.31859400	3.15599800	0.00000000
O	0.78968200	5.62459900	0.00000000
B	0.24072300	-4.82276300	0.00000000
B	0.58546100	4.34206800	0.00000000
Au	0.00000000	1.05333100	0.00000000
H	1.67327500	5.99459000	0.00000000
Xe	-0.34205300	-1.48742600	0.00000000

##

f3-Xe charge=0 spin=1

O	-2.03927000	4.83741500	0.00000000
O	0.03398500	3.36173400	0.00000000
O	-0.08230400	-3.92202500	0.00000000
O	2.07924600	-5.21198600	0.00000000
B	-1.04970800	4.15793300	0.00000000
B	1.00932800	-4.59808800	0.00000000
Au	0.00000000	1.08848500	0.00000000
H	0.89568100	3.78706700	0.00000000
Xe	-0.01161200	-1.48329000	0.00000000

##

f4-Xe charge=0 spin=1

O	3.91457100	-0.15724700	0.00000000
O	1.39832800	-0.31768900	0.00000000
O	-1.46149600	2.55003400	0.00000000
O	-3.77214600	1.53291200	0.00000000
B	2.69824800	-0.18719600	0.00000000
B	-2.65059600	2.02838600	0.00000000
Au	0.00000000	1.19665300	0.00000000
H	-0.93912500	-3.70194400	0.00000000
Xe	0.00123700	-2.38710500	0.00000000

##

A1 charge=0 spin=1

Cu	0.00000000	0.00000000	1.10215400
O	0.00000000	1.84758000	0.68553200
O	0.00000000	-1.84758000	0.68553200
B	0.00000000	-1.78717800	-0.58257900

B 0.00000000 1.78717800 -0.58257900
O 0.00000000 -1.64983500 -1.82698900
O 0.00000000 1.64983500 -1.82698900
Li 0.00000000 0.00000000 -2.62445000
##
A2 charge=0 spin=1
Cu 0.00000000 0.84799200 0.00000000
O -1.88202300 1.34800600 0.00000000
O 0.95333400 -0.81844900 0.00000000
B 2.24112000 -1.00237600 0.00000000
B -2.18921800 0.11549800 0.00000000
O 3.44333100 -1.20420500 0.00000000
O -2.31443500 -1.13450100 0.00000000
Li -0.62039000 -1.89473200 0.00000000
##
A3 charge=0 spin=1
Cu 0.00000000 0.00000000 0.80823300
O 0.00000000 1.44101100 -0.56132300
O 0.00000000 -1.44101100 -0.56132300
B 0.00000000 -2.73186600 -0.42882400
B 0.00000000 2.73186600 -0.42882400
O 0.00000000 -3.94654000 -0.31204900
O 0.00000000 3.94654000 -0.31204900
Li 0.00000000 0.00000000 -1.72551900
##
B1 charge=0 spin=1
Ag 0.00000000 0.00000000 1.02212300
O 0.00000000 2.04704200 0.31092600
O 0.00000000 -2.04704200 0.31092600
B 0.00000000 -1.88768300 -0.94251400
B 0.00000000 1.88768300 -0.94251400
O 0.00000000 -1.65030700 -2.17354700
O 0.00000000 1.65030700 -2.17354700
Li 0.00000000 0.00000000 -2.93756400
##
B2 charge=0 spin=1
Ag 0.00000000 0.87502700 0.00000000
O 1.01264500 -1.11692300 0.00000000
O -2.22248800 0.80310900 0.00000000
B -2.28008700 -0.45789800 0.00000000
B 2.30771600 -1.18377900 0.00000000
O -2.17359400 -1.70992400 0.00000000
O 3.52842700 -1.24060900 0.00000000
Li -0.43268900 -2.26771300 0.00000000

##

B3 charge=0 spin=1

Ag	0.00000000	0.00000000	0.83319600
O	0.00000000	1.46027100	-0.90585800
O	0.00000000	-1.46027100	-0.90585800
B	0.00000000	-2.74977600	-0.79293000
B	0.00000000	2.74977600	-0.79293000
O	0.00000000	-3.96638600	-0.67327100
O	0.00000000	3.96638600	-0.67327100
Li	0.00000000	0.00000000	-1.98828500

##

C1 charge=0 spin=1

O	0.00000000	1.73383700	-2.20355800
O	0.00000000	2.05419000	0.30659000
O	0.00000000	-2.05419000	0.30659000
O	0.00000000	-1.73383700	-2.20355800
B	0.00000000	1.92173900	-0.96695400
B	0.00000000	-1.92173900	-0.96695400
Au	0.00000000	0.00000000	0.61529600
Li	0.00000000	0.00000000	-2.86243800

##

C2 charge=0 spin=1

O	-2.39851600	-1.41108300	0.00000000
O	-2.06735900	1.10347400	0.00000000
O	1.08064800	-1.31191900	0.00000000
O	3.58629700	-1.59258100	0.00000000
B	-2.29468000	-0.15835200	0.00000000
B	2.37791200	-1.44141500	0.00000000
Au	0.00000000	0.51028000	0.00000000
Li	-0.67490500	-2.20546300	0.00000000

##

C3 charge=0 spin=1

B	-2.61939700	1.13327800	0.00000000
O	-3.77453600	0.72914300	0.00000000
O	-1.38938600	1.55587300	0.00000000
B	2.62732500	-1.27704500	0.00000000
O	1.32932200	-1.44420500	0.00000000
O	3.83789800	-1.18275600	0.00000000
Au	0.00000000	0.14253700	0.00000000
Li	-0.02200900	-2.60201900	0.00000000

##

C4 charge=0 spin=1

O	0.00000000	3.95513800	-0.81662200
O	0.00000000	1.45636600	-1.13496100

O 0.00000000 -1.45636600 -1.13496100
O 0.00000000 -3.95513800 -0.81662200
B 0.00000000 2.74432800 -0.96990300
B 0.00000000 -2.74432800 -0.96990300
Au 0.00000000 0.00000000 0.60312200
Li 0.00000000 0.00000000 -2.24077400
##
D1-Xe charge=0 spin=1
Cu 1.91778300 -0.27552300 0.05458900
O 3.72933700 -0.38464200 0.15024500
O -3.55656700 0.11531900 -0.17406600
B -4.76866100 0.28797400 -0.03162800
B 4.66193800 0.49740300 0.03975900
O -6.02170600 0.46722500 0.11795400
O 5.56489200 1.32218600 -0.06245700
Li -7.65491700 0.72643200 0.31570500
Xe -0.55268500 -0.19031000 -0.05230100
##
D2-Xe charge=0 spin=1
Cu -1.35734500 -0.10926300 -0.12108600
O 3.74024400 -0.45725500 0.25845300
O -3.21150300 0.04329100 -0.19717200
B -4.41790800 0.26510500 -0.01052900
B 4.58821800 0.47437000 0.08587800
O -5.64182800 0.48373400 0.16779300
O 5.39308800 1.40705900 -0.08943500
Li -7.29314000 0.80107800 0.41851800
Xe 1.07686800 -0.27308500 0.01411300
##
E1-Xe charge=0 spin=1
Ag 1.77948300 -0.22163500 0.06724000
O -3.94787700 0.13044400 -0.03596000
O 3.78953200 -0.44228900 0.33533500
B 4.70636100 0.43927200 0.12919800
B -5.16857900 0.23132800 0.09931000
O 5.58915400 1.27205900 -0.06311800
O -6.43135400 0.33672500 0.24081200
Li -8.07538800 0.50503700 0.44509100
Xe -0.90915000 -0.08938500 -0.17508700
##
E2-Xe charge=0 spin=1
Ag -1.24187400 -0.49606600 -0.03500700
O -3.35849300 -0.29360500 -0.04589600
O 4.06533900 0.03253800 0.13520000

B 4.34795600 1.26525400 0.00948300
B -4.24441000 0.57950300 0.00517700
O 4.56454500 2.48506800 -0.11812500
O -5.15005700 1.45036800 0.05592900
Li -6.27484600 2.72009000 0.13251600
Xe 1.40193000 -0.43451600 0.01773400
##########
F1-Xe charge=0 spin=1
O 6.58271200 0.10810900 0.31779800
O 4.12148300 0.35311400 -0.09044600
O -3.37089000 -0.50669300 0.24641900
O -5.10042900 1.32420500 0.14923100
B 5.33213900 0.23379900 0.10966100
B -4.24524500 0.44921500 0.19283700
Au -1.40427100 -0.21414500 0.02407200
Li 8.21722900 -0.05861800 0.59648200
Xe 1.16644900 0.06385800 -0.18866100
##########
F2-Xe charge=0 spin=1
O 4.09415500 -0.06382000 -0.00056300
O -3.12583600 -0.32261600 0.00036400
B -3.84264900 0.70337800 -0.00003800
B 4.62300700 1.09608800 0.00003900
O -4.58375500 1.71446700 -0.00043800
O 5.09666700 2.24362800 0.00064100
Li -5.36603900 3.22843600 -0.00040200
Xe 1.52680600 -0.31428000 -0.00015600
Au -1.03925400 -0.38335200 0.00012100
##########
F3-Xe charge=0 spin=1
B 4.64129900 0.35999000 -0.00002200
O 5.23779600 1.44497400 -0.00002000
O 3.96473100 -0.72500600 -0.00001300
B -4.04210900 -0.07967400 -0.00000800
O -3.06512400 0.79519700 0.00001300
O -4.97874600 -0.85088200 -0.00003900
Au -1.05198600 0.09769500 0.00000300
Li -2.80812900 2.54145100 -0.00000400
Xe 1.46789000 -0.40848300 0.00000700
##########
d1-Ar charge=0 spin=1
Cu -1.42699200 -0.36040300 -0.00340800
O 3.81836200 0.10738500 0.05478200
O -3.22942100 -0.46665300 -0.04196400

B -4.12749300 0.46118600 -0.01727000
B 5.01499300 0.28669500 -0.00506800
O -4.99332600 1.32796300 0.00568200
O 6.32171000 0.42527300 -0.09630900
H 6.71634200 1.23795800 0.21745200
Ar 0.82724100 -0.31541300 0.03419700
##########
e1-Ar charge=0 spin=1
Ag -1.28299100 -0.24172500 0.00464300
O 4.36392900 0.13151500 0.03298900
O -3.27906800 -0.51748700 -0.27445500
B -4.19337000 0.38053800 -0.11680500
B 5.56795700 0.21111100 -0.07204300
O -5.06775800 1.22868200 0.03066500
O 6.88217300 0.23988700 -0.16696800
H 7.29714900 1.04489600 -0.47399200
Ar 1.27423700 -0.07238100 0.23456500
##########
f1-Ar charge=0 spin=1
O 4.52827300 1.47063600 -0.02199600
O 2.90737400 -0.44774200 0.22197400
O -4.46691100 0.13710700 -0.13747900
O -6.93931400 0.39090900 0.32367900
B 3.72738100 0.55546900 0.09193000
B -5.65623900 0.26489900 0.05403700
Au 0.95317300 -0.20733500 0.00282900
H -7.53637600 0.60914700 -0.39071800
Ar -1.46418800 -0.04104600 -0.20289200
##########
D1-Ar charge=0 spin=1
Cu 1.55794900 -0.43247700 -0.00065000
O 3.36104200 -0.28924700 0.00015600
O -3.51289200 -0.28347300 0.00535300
B -4.63959900 0.21351100 0.00231100
B 4.13054300 0.74641100 0.00058900
O -5.80582900 0.73230500 -0.00086500
O 4.87891000 1.71768500 0.00099000
Li -7.30251600 1.45954900 -0.00557400
Ar -0.67208500 -0.64747600 -0.00133400
##########
E1-Ar charge=0 spin=1
Ag -1.39277700 -0.23227900 -0.00679900
O 4.04739700 -0.00891400 0.11358200
O -3.39332500 -0.48808700 -0.28800700

B -4.31117000 0.40124300 -0.11260600
B 5.26079000 0.15139500 -0.01781600
O -5.19277200 1.24008100 0.05081000
O 6.51936200 0.31918400 -0.15557600
Li 8.15245600 0.55849000 -0.34714500
Ar 1.13387600 -0.11220400 0.23592500
##########
F1-Ar charge=0 spin=1
O 6.66160000 0.35140800 0.14345600
O 4.18915200 0.05547000 -0.15310600
O -3.00563300 -0.42829400 0.23216800
O -4.63732900 1.47600400 -0.03983400
B 5.40331700 0.20007800 -0.00839300
B -3.82900400 0.56784500 0.08705900
Au -1.04787900 -0.20356000 0.00817000
Li 8.29635300 0.56023000 0.36219000
Ar 1.35330600 -0.05976700 -0.19926900
##########
d1-Kr charge=0 spin=1
Cu 1.63449200 -0.31450700 0.03700200
O -3.79499400 0.17800200 -0.03945400
O 3.43689600 -0.42239900 0.15233400
B 4.34629500 0.48752200 0.04441500
B -4.99259600 0.34512700 0.03815100
O 5.22265600 1.33853900 -0.05567400
O -6.30061000 0.46469900 0.13005200
H -6.68478700 1.33857000 0.07151700
Kr -0.72209900 -0.24588500 -0.08487500
##########
e1-Kr charge=0 spin=1
Ag 1.49391000 -0.24730100 0.03212400
O -4.24596200 0.21618700 0.03153500
O 3.48623600 -0.53344200 0.32379300
B 4.40982500 0.35571800 0.17452400
B -5.44867900 0.20317400 0.17576500
O 5.29367900 1.19574400 0.03478800
O -6.75609200 0.12719400 0.31827100
H -7.23410700 0.91741700 0.56642800
Kr -1.11134000 -0.00372700 -0.26374400
##########
f1-Kr charge=0 spin=1
O 4.77106200 1.38978700 0.04304900
O 3.09395600 -0.47965100 0.27847500
O -4.37481400 0.21407000 -0.07320100

O	-6.84422900	0.24856800	0.46454800
B	3.94346100	0.49722200	0.15300700
B	-5.56457100	0.23708200	0.15518200
Au	1.14214400	-0.20580900	0.02365300
H	-7.48140100	0.41888300	-0.22793300
Kr	-1.32806100	0.03295300	-0.24679400

##########

D1-Kr charge=0 spin=1

Cu	-1.74026500	-0.29860400	0.04112600
O	-3.54513200	-0.41809100	0.15123800
O	3.51787900	0.05643900	-0.11522900
B	4.73152700	0.24142800	-0.01414500
B	-4.47262900	0.47114300	0.04270600
O	5.98805700	0.43420400	0.09258300
O	-5.37015000	1.30116800	-0.05740000
Li	7.62202600	0.70920600	0.24389900
Kr	0.59949700	-0.22279800	-0.07324200

##########

E1-Kr charge=0 spin=1

Ag	1.59249200	-0.23181900	0.04415400
O	-3.96614400	0.06580200	-0.05931200
O	3.59312500	-0.48491600	0.33007800
B	4.51371800	0.39881200	0.14490800
B	-5.18420800	0.17721000	0.08357800
O	5.39854500	1.23290800	-0.02772100
O	-6.44627000	0.29451300	0.23342800
Li	-8.08629500	0.46717000	0.44888400
Kr	-0.99638500	-0.06257100	-0.23266900

##########

F1-Kr charge=0 spin=1

O	6.60078100	0.29720400	0.22935100
O	4.12388700	0.12234900	-0.11841600
O	-3.18906600	-0.44395700	0.27191400
O	-4.86325600	1.42111800	-0.00589200
B	5.34100500	0.20817200	0.05124000
B	-4.03467500	0.53071400	0.12390900
Au	-1.22898700	-0.19978100	0.02948200
Li	8.24083100	0.42126300	0.48430600
Kr	1.23491900	-0.00970200	-0.21315000

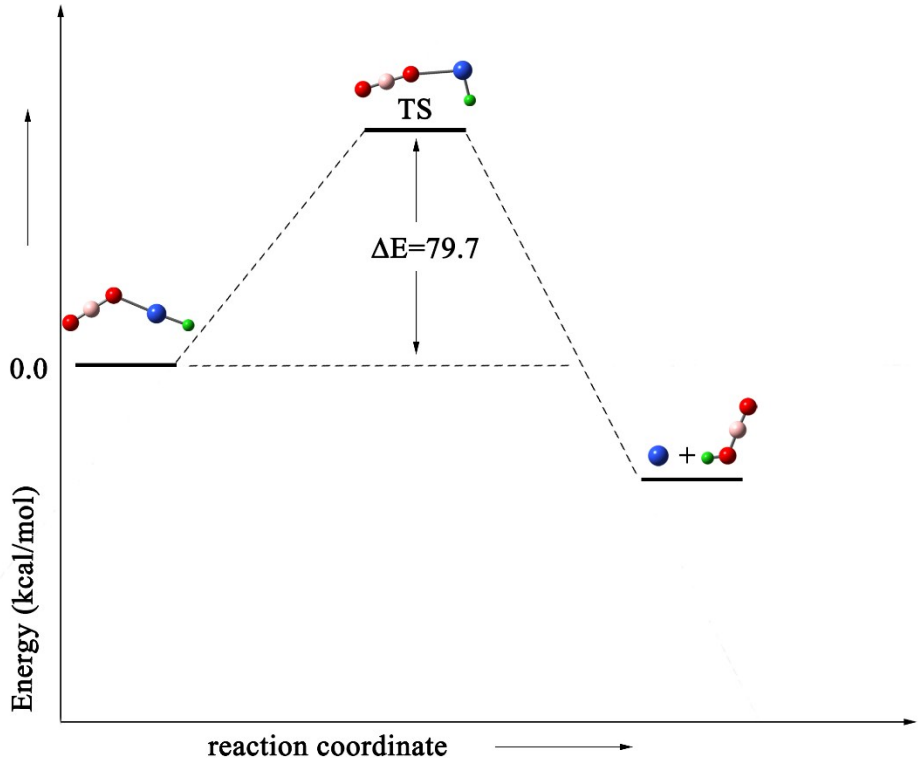

Figure S1. Energetics of fragmentation of structure **i-Xe**.

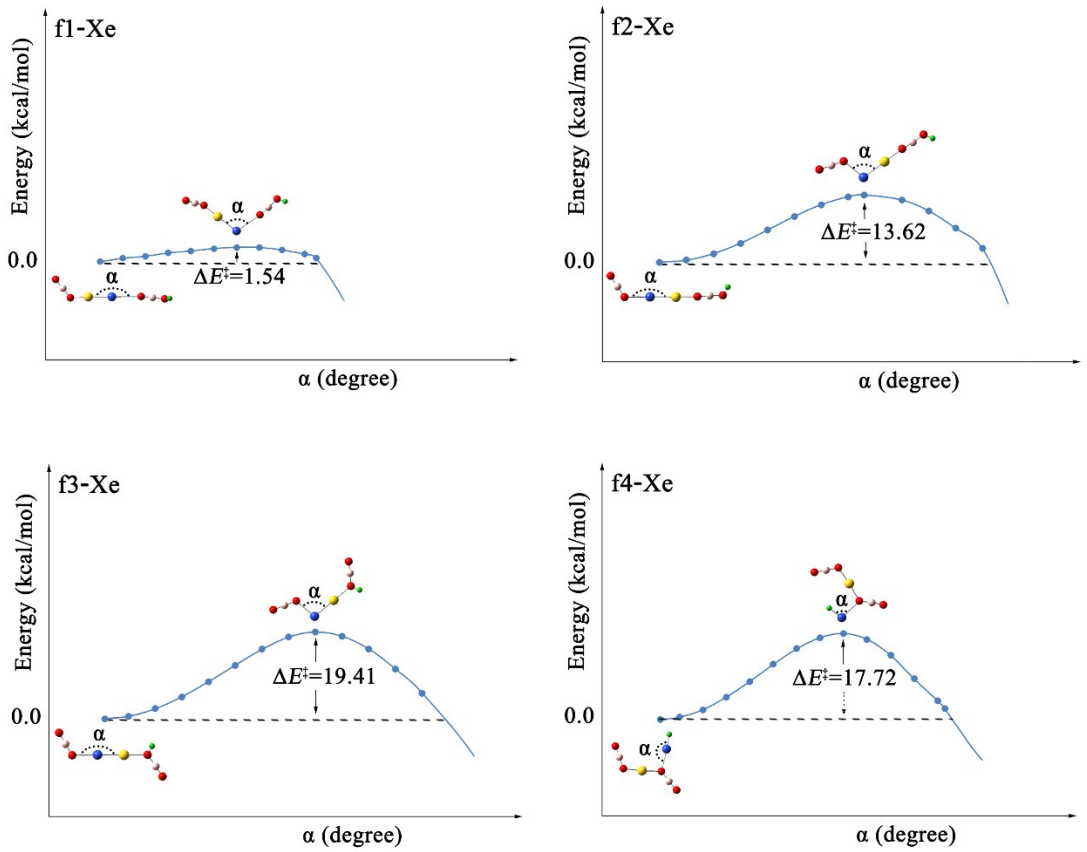

Fig. S2 Energy scan for the formation of Au-O bond (H-O bond in the case of **f4-Xe**) at the ωB97X-D/def2-TZVPP level, using as approximate reaction coordinate for the isomerization $HXeAu(BO_2)_2 \longrightarrow XeHAu(BO_2)_2$.

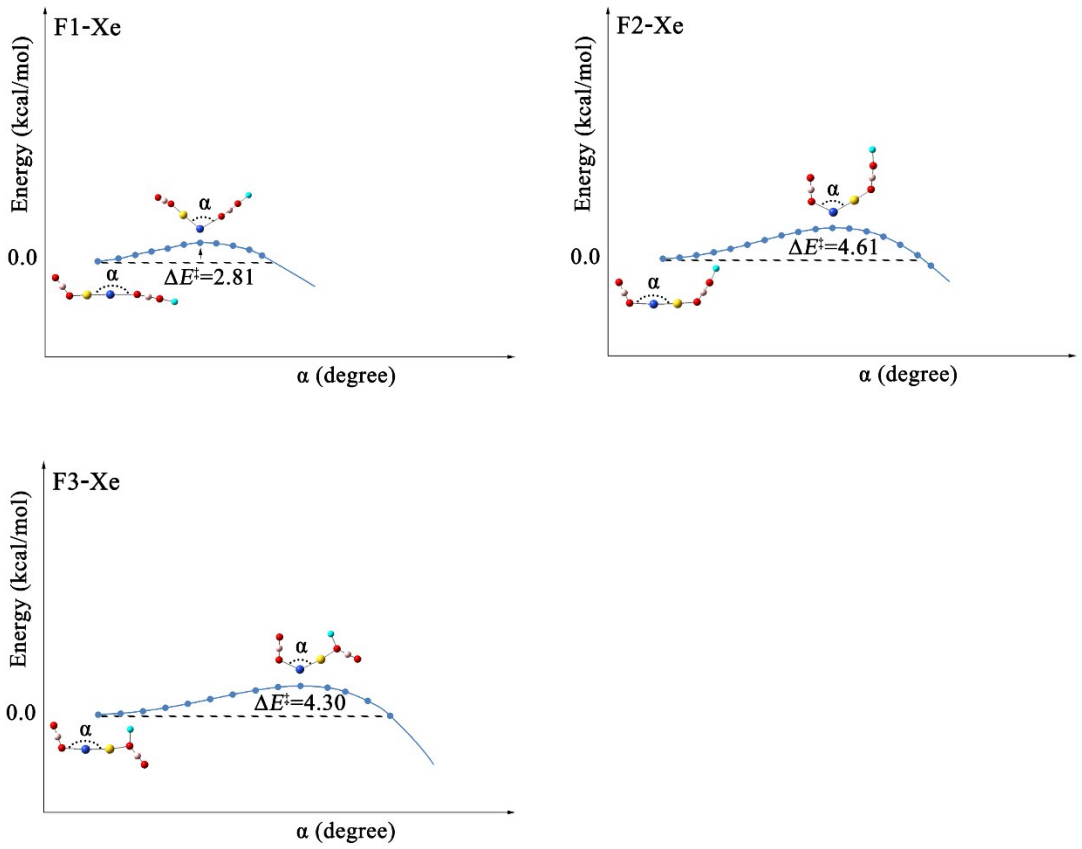

Fig. S3 Energy scan for the formation of Au-O bond at the ωB97X-D/def2-TZVPP level, using as approximate reaction coordinate for the isomerization $LiXeAu(BO_2)_2 \longrightarrow XeLiAu(BO_2)_2$.

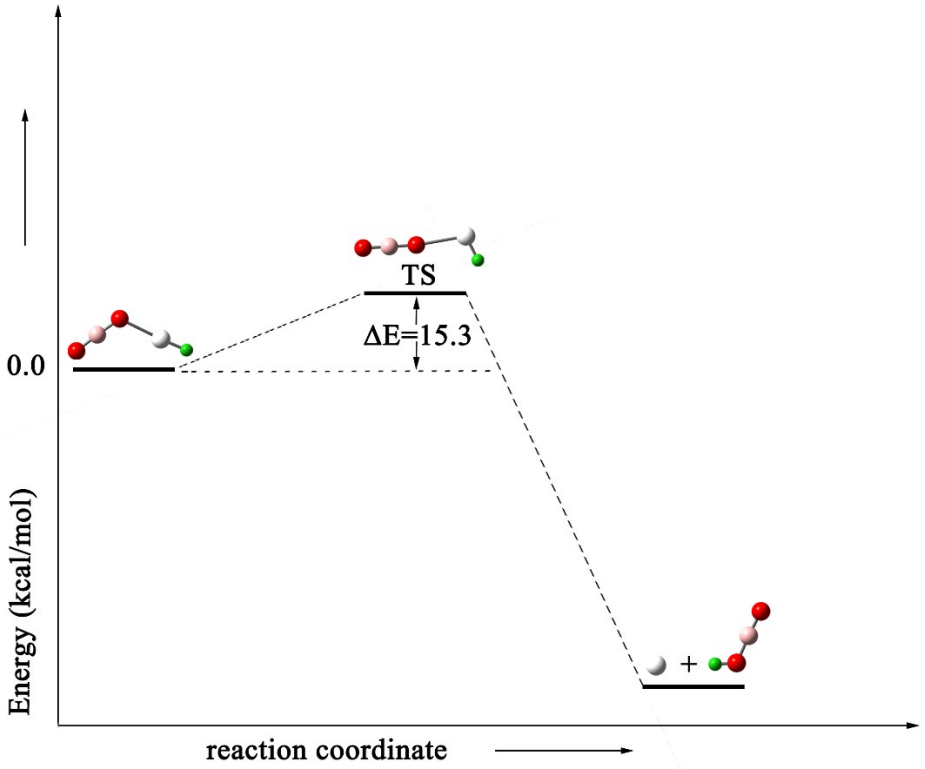

Figure S4. Energetics of fragmentation of structure **i-Ar**.

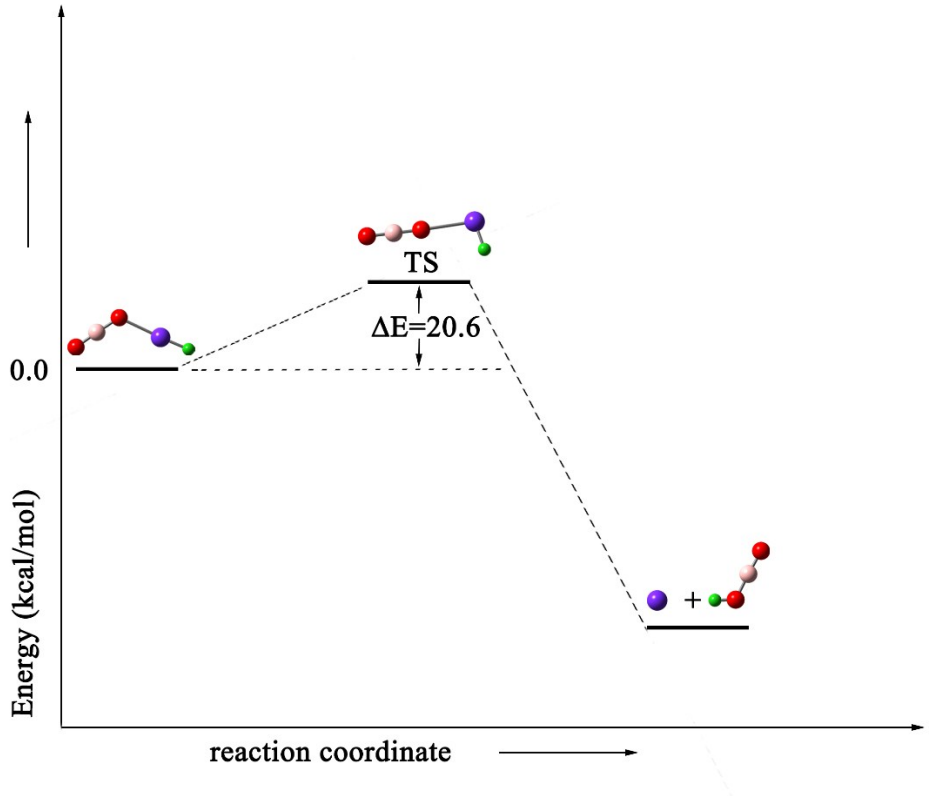

Figure S5. Energetics of fragmentation of structure **i-Kr**.