Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supporting Information belonging to the manuscript:

Neutral Noble Gas Compounds Exhibiting a Xe–Xe Bond: Structure, Stability and Bonding Situation

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Cartesian coordinates (in Å) and total energies (in a.u., zero point energy included) of all stationary points discussed in the text. All calculations have been performed at the M05-2X/def2-TZVPP level of theory. See text for computational details.

HXeXeX series (X = F to I)

HXeXeF, E = -758.867104

Xe	1.818088000	0.000020000	-0.000039000
Xe	-1.287427000	-0.000184000	0.000053000
H	3.578632000	0.002385000	0.000667000
F	-3.581589000	0.000721000	-0.000158000

HXeXeCl, E = -1119.238277

Xe	2.172566000	0.015726000	0.000005000
Xe	-1.012642000	-0.037729000	-0.000006000
H	3.934166000	0.094867000	0.000023000
Cl	-3.915889000	0.064312000	0.000001000

HXeXeBr, E = -3233.149486

Xe	-2.718396000	-0.020193000	-0.000001000
Xe	0.491464000	0.046498000	0.000001000
H	-4.483475000	-0.107380000	0.000027000
Br	3.563937000	-0.037516000	0.000000000

HXeXeI, E = -956.721798

Xe	3.217674000	-0.013973000	-0.000029000
Xe	-0.037788000	0.030995000	0.000019000
H	5.006463000	-0.068799000	0.000843000
I	-3.334345000	-0.016045000	-0.000005000

TS1-F, E = -758.850351

Xe	-0.404351000	-1.683217000	0.000000000

Xe	0.000000000	1.425737000	0.000000000
H	-0.368539000	-3.344221000	0.000000000
F	2.467055000	1.916459000	0.000000000

TS1-Cl, E = -1119.228154

Xe	-0.965469000	-1.777392000	0.000000000
Xe	0.000000000	1.348323000	0.000000000
H	-1.153901000	-3.461256000	0.000000000
Cl	3.134661000	1.566527000	0.000000000

TS1-Br, E = -3233.141014

Xe	-2.023096000	-1.398295000	0.000000000
Xe	0.000000000	1.220601000	0.000000000
H	-2.801133000	-2.913081000	0.000000000
Br	3.201380000	0.357388000	0.000000000

TS1-I, E = -381.167688

Xe	-2.834243000	-0.566977000	0.000000000
Xe	0.000000000	1.266654000	0.000000000
H	-4.066018000	-1.783298000	0.000000000
I	2.964437000	-0.679231000	0.000000000

HXeF, E = -429.642483

Xe	0.000096000	-0.269190000	0.000000000
H	-0.006076000	-1.937360000	0.000000000
F	0.000096000	1.830401000	0.000000000

HXeCl, E = -789.994825

Xe	0.000099000	-0.593482000	0.000000000
H	-0.007030000	-2.285421000	0.000000000
Cl	0.000099000	2.019616000	0.000000000

HXeBr, E = -2903.900839

Xe	0.000099000	-1.062373000	0.000000000
H	-0.008786000	-2.761700000	0.000000000
Br	0.000099000	1.717996000	0.000000000

HXeI, E = -627.467686

Xe	0.000042000	1.449463000	0.000000000
H	-0.004520000	3.167379000	0.000000000
I	0.000042000	-1.536573000	0.000000000

TS2-F, E = -555.207667

Xe	0.024359000	-0.330187000	0.000000000
H	-1.534641000	-0.618187000	0.000000000
F	0.024359000	2.049812000	0.000000000

TS2-Cl, E = -789.940935

Xe	0.021931000	-0.695475000	0.000000000
H	-1.557088000	-0.909148000	0.000000000
Cl	0.021931000	2.262634000	0.000000000

TS2-Br, E = -2903.849300

Xe	0.017603000	-1.218663000	0.000000000
H	-1.566643000	-1.413678000	0.000000000
Br	0.017603000	1.920613000	0.000000000

TS2-I, E = -627.417214

Xe	0.014757000	-1.650445000	0.000000000
H	-1.578981000	-1.807028000	0.000000000
I	0.014757000	1.715680000	0.000000000

HF, E = -100.468748

H	0.000000000	0.000000000	-0.827531000
F	0.000000000	0.000000000	0.091948000

HCl, E = -460.800243

H	0.000000000	0.000000000	-1.202608000
Cl	0.000000000	0.000000000	0.070742000

HBr, E = -2574.692995

H	0.000000000	0.000000000	-1.379654000
Br	0.000000000	0.000000000	0.039419000

HI, E = -298.252604

H	0.000000000	0.000000000	-1.573712000
I	0.000000000	0.000000000	0.029693000

RXeXeR' series (R = halogen atom)

FXeXeF, E = -858.155740

Xe	0.000000000	1.443284000	0.000000000
Xe	-0.000198000	-1.443301000	0.000000000
F	0.000630000	3.529462000	0.000000000
F	0.000556000	-3.529362000	0.000000000

FXeXeCl, E = -1218.520748

Xe	-0.000468000	-1.757835000	0.000000000
F	-0.000152000	-3.858887000	0.000000000
Xe	0.000000000	1.204015000	0.000000000
Cl	0.001567000	3.802133000	0.000000000

ClXeXeCl, E = -1578.890404

Xe	-1.530202000	-0.000363000	-0.000316000
Xe	1.530342000	-0.000756000	0.000248000
Cl	-4.161378000	0.001548000	0.000437000
Cl	4.160933000	0.002008000	-0.000221000

BrXeXeBr, E = -5806.712762

Xe	-0.000702000	-1.565182000	0.000000000
Xe	0.000000000	1.565183000	0.000000000
Br	0.000175000	-4.378329000	0.000000000
Br	0.000908000	4.378328000	0.000000000

TS1-F,F, E = -858.096324

Xe	0.000000000	1.328646000	0.000000000
Xe	-0.405603000	-1.507598000	0.000000000
F	0.463654000	3.238948000	0.000000000
F	1.969962000	-2.165236000	0.000000000

TS1-F,Cl, E = -1218.475240

Xe	0.000000000	1.585214000	0.000000000
Xe	-0.823884000	-1.460859000	0.000000000
F	0.621166000	3.504686000	0.000000000
Cl	2.288192000	-2.250432000	0.000000000

TS1-Cl,Cl, E = -1578.858998

Xe	0.000000000	1.516684000	0.000000000
Xe	-1.015523000	-1.845730000	0.000000000
Cl	1.238783000	3.804671000	0.000000000
Cl	1.986995000	-2.759465000	0.000000000

TS1-Br,Br, E = -5806.690964

Xe	-1.881850000	-1.065573000	0.000000000
Xe	0.000000000	2.103734000	0.000000000
Br	2.938154000	1.789645000	0.000000000

Br	-0.034728000	-3.391379000	0.000000000

FXeF, E = -528.921098

Xe	0.000000000	0.001460000	0.000000000
F	1.966724000	0.089735000	0.000000000
F	-1.966724000	-0.098494000	0.000000000

FXeCl, E = -889.276709

Xe	0.000000000	0.289072000	0.000000000
F	0.031615000	2.291802000	0.000000000
Cl	-0.016737000	-2.131535000	0.000000000

ClXeCl, E = -1249.635757

Xe	0.000000000	0.000022000	0.000000000
Cl	2.135395000	1.255138000	0.000000000
Cl	-2.135395000	-1.255207000	0.000000000

TS2-F,F, E = -528.787911

Xe	0.000000000	0.345412000	0.000000000
F	1.605035000	-0.661827000	0.000000000
F	-1.605035000	-1.410643000	0.000000000

TS2-F,Cl, E = -889.161788

Xe	0.000000000	0.636547000	0.000000000
F	1.924519000	0.278803000	0.000000000
Cl	-1.018863000	-2.169575000	0.000000000

TS2-Cl,Cl, E = -1249.542240 (geometry optimized at the wB97XD/def2-TZVPP level)

Xe	0.000000000	0.718194000	0.000000000
Cl	1.994569000	-0.676871000	0.000000000
Cl	-1.994569000	-1.604451000	0.000000000

F_2, E = -199.558711

F	0.000000000	0.000000000	0.680028000
F	0.000000000	0.000000000	-0.680028000

FCl, E = -559.990579

F	0.000000000	0.000000000	-1.056453000
Cl	0.000000000	0.000000000	0.559299000

Cl_2, E = -920.370278

Cl	0.000000000	0.000000000	0.996689000
Cl	0.000000000	0.000000000	-0.996689000

Br_2, E = 5148.186559

Br	0.000000000	0.000000000	1.144520000
Br	0.000000000	0.000000000	-1.144520000