Supplementary Information

Factors Contributing to Halogen Bond Strength and Stretch or Contraction of Internal Covalent Bond

Mariusz Michalczyk*,[1] Beata Kizior,[1] Wiktor Zierkiewicz,[1] and Steve Scheiner[2*]

[1] Faculty of Chemistry, Wrocław University of Science and Technology, Wybrzeże Wyspiańskiego 27, 50-370 Wrocław, Poland

[2] Department of Chemistry and Biochemistry, Utah State University Logan, Utah 84322-0300, United States

Corresponding authors: mariusz.michalczyk@pwr.edu.pl, steve.scheiner@usu.edu.

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Table 1SI. XYZ coordinates of optimized geometries for investigated monomers.

Monomer	
F3C-Cl	C -1.58112000 -3.05396800 -0.75604600 F -1.14990000 -2.44368800 0.33415000 F -2.90270100 -3.06328700 -0.73933200 F -1.14974800 -4.30323800 -0.73922000 Cl -0.99563100 -2.22539100 -2.19071700
F3C-Br	C -1.59256500 -3.06995700 -0.72814900 F -1.16119500 -2.45982200 0.36178700 F -2.91389500 -3.07937200 -0.71162500 F -1.16103700 -4.31899900 -0.71165200 Br -0.95040900 -2.16142200 -2.30152300
F3C-I	C -1.60560400 -3.08827500 -0.69629100 F -1.17597100 -2.48123100 0.39954900 F -2.92976700 -3.10127600 -0.67442100 F -1.17636400 -4.34070200 -0.67423400 I -0.89139400 -2.07808800 -2.44576800
F3Si-Cl	Si -1.57935000 -3.05144800 -0.76046900 F -1.07039900 -2.33022800 0.53700000 F -3.14837500 -3.06506300 -0.73532900 F -1.06946700 -4.53547500 -0.73651100 Cl -0.91151100 -2.10735700 -2.39585400
F3Si-Br	Si -1.58976700 -3.06546300 -0.73560400 F -1.08049900 -2.34630600 0.56478100 F -3.16026700 -3.08191100 -0.70825700 F -1.08102500 -4.55140800 -0.70847400 Br -0.86754200 -2.04448400 -2.50361000
F3Si-I	Si -1.60214200 -3.08351500 -0.70462300 F -1.09740800 -2.36937700 0.60314700 F -3.17482700 -3.10354400 -0.66934900 F -1.09613600 -4.57283700 -0.67096200 I -0.80858800 -1.96029900 -2.64937700
F3Ge-Cl	Ge -1.57249700 -3.04134900 -0.77708800 F -1.03166000 -2.27733400 0.63700700 F -3.26754800 -3.06806100 -0.73251900 F -1.03251000 -4.64840500 -0.73186900 Cl -0.87488600 -2.05442400 -2.48669500
F3Ge-Br	Ge -1.57979600 -3.05230700 -0.75913200 F -1.04641600 -2.29532500 0.66469600 F -3.27697100 -3.08450200 -0.70099000 F -1.04472700 -4.66335100 -0.70356300 Br -0.83119000 -1.99408600 -2.59217400

Table 1SI (Continuation). XYZ coordinates of the optimized geometries for the investigated monomers.

F3Ge-I	Ge -1.59006600 -3.06617300 -0.73416900 F -1.06390200 -2.32064600 0.70287600 F -3.29022800 -3.10800400 -0.66068000 F -1.06179800 -4.68289100 -0.66412600 I -0.77310600 -1.91185600 -2.73506500
F3Sn-Cl	Sn -1.56841900 -3.03575900 -0.78871700 F -0.97307700 -2.19564100 0.79446800 F -3.45569600 -3.06834200 -0.72704300 F -0.97009600 -4.82602800 -0.72488000 Cl -0.81181400 -1.96380000 -2.64499100
F3Sn-Br	Sn -1.57369200 -3.04370300 -0.77516600 F -0.98659000 -2.21734100 0.82130700 F -3.46268600 -3.08696500 -0.69708800 F -0.98548400 -4.83923900 -0.69139400 Br -0.77065000 -1.90232400 -2.74882300
F3Sn-I	Sn -1.58182700 -3.05400300 -0.75679000 F -1.00739000 -2.24532600 0.85784900 F -3.47319500 -3.11230400 -0.65237200 F -1.00475700 -4.85582600 -0.65117500 I -0.71193200 -1.82211200 -2.88867500
F3Pb-Cl	Pb -1.55760900 -3.02024400 -0.81462300 F -0.95524800 -2.16926600 0.87334300 F -3.53806900 -3.07950800 -0.70894700 F -0.95253200 -4.90680200 -0.70951000 Cl -0.77564200 -1.91375200 -2.73142700
F3Pb-Br	Pb -1.55967100 -3.02437200 -0.80799500 F -0.97259300 -2.19532500 0.90044600 F -3.54157900 -3.10037600 -0.67448200 F -0.97014000 -4.91774400 -0.67431900 Br -0.73511800 -1.85175500 -2.83481400
F3Pb-I	Pb -1.56414500 -3.02999800 -0.79799000 F -0.99596800 -2.22802000 0.93636200 F -3.54806800 -3.12808900 -0.62681900 F -0.99345200 -4.93233500 -0.62856100 I -0.67746900 -1.77112900 -2.97415500

Table 2SI. XYZ coordinates of the optimized geometries for the investigated dimers.

Dimer	
F3C-Cl···NH3	C -1.54294100 -3.09763500 -0.48738000 F -1.07976900 -2.42280800 0.55557100 F -2.86373800 -3.15518500 -0.38900200 F -1.06935600 -4.33425300 -0.42289300 Cl -1.06549600 -2.32815100 -1.98562700 N -0.22145700 -1.01389300 -4.58144500 H -0.52509400 -0.05038800 -4.64696600 H 0.78642500 -1.01678800 -4.67663100 H -0.59882200 -1.50150000 -5.38438600
F3C-Br···NH3	C -1.56458400 -3.13467000 -0.41414800 F -1.17252000 -2.41792000 0.63108100 F -2.88406500 -3.25925700 -0.35586600 F -1.03178500 -4.34500400 -0.30639000 Br -1.02829000 -2.29447900 -2.06035500 N -0.20102900 -0.98617300 -4.63714300 H -0.38697000 0.00899000 -4.63722100 H 0.78815300 -1.10709100 -4.81558400 H -0.69915500 -1.38499600 -5.42313300
F3C-I···NH3	C -1.59561400 -3.18446600 -0.31769600 F -1.04805200 -2.57720000 0.73297000 F -2.91702900 -3.15040000 -0.15943200 F -1.21886700 -4.46095800 -0.28739500 I -1.00715000 -2.24231100 -2.15553200 N -0.17745200 -0.94368000 -4.71854300 H -0.59179300 -0.02737100 -4.83651700 H 0.82774600 -0.82919500 -4.76130800 H -0.45203700 -1.50502100 -5.51530700
F3Si-Cl···NH3	Si -1.61014000 -3.20547900 -0.27714300 F -1.06058800 -2.40716400 0.96013400 F -3.17623600 -3.26573300 -0.15967700 F -1.05969700 -4.67504800 -0.19028100 Cl -1.05649300 -2.33673100 -1.98921700 N -0.13503200 -0.87788300 -4.84907900 H -0.44797900 0.08268800 -4.91336900 H 0.87261300 -0.86922900 -4.94583100 H -0.50669500 -1.36602200 -5.65429500

Table 2SI (Continuation). XYZ coordinates of the optimized geometries for the investigated dimers.

F3Si-Br···NH3	Si -1.62485800 -3.22933700 -0.23047000 F -1.03581900 -2.46059900 1.01004000 F -3.19209600 -3.23818000 -0.08706300 F -1.12864500 -4.72055600 -0.14897700 Br -1.01542200 -2.30244100 -2.08612600 N -0.12118100 -0.87041600 -4.87939400 H -0.51501800 0.05975900 -4.94856500 H 0.88387700 -0.77350700 -4.95400200 H -0.43108500 -1.38532500 -5.69420100
F3Si-I···NH3	Si -1.65883600 -3.28134700 -0.12434900 F -1.19715200 -2.44662800 1.13178900 F -3.22504100 -3.43937000 -0.03070500 F -1.03431800 -4.72277000 0.01661200 I -1.00118100 -2.23610200 -2.16254100 N -0.09360300 -0.81760000 -4.96898000 H -0.28091500 0.17751500 -4.97742000 H 0.89655700 -0.93506600 -5.14555400 H -0.58575600 -1.21923400 -5.75761200
F3Ge-Cl···NH3	Ge -1.59864400 -3.18627500 -0.31335800 F -1.17253400 -2.25580100 1.04301600 F -3.27949300 -3.42484900 -0.24420500 F -0.87123300 -4.70956700 -0.11935100 Cl -1.01729600 -2.26991200 -2.09829300 N -0.13665100 -0.88986000 -4.82856100 H -0.18037200 0.12023500 -4.77503600 H 0.81139400 -1.13225900 -5.08840200 H -0.73541900 -1.17231400 -5.59456900
F3Ge-Br···NH3	Ge -1.61927300 -3.21960300 -0.25107800 F -0.87413900 -2.50855900 1.10453000 F -3.29731800 -3.12466900 0.01749600 F -1.21789300 -4.87335000 -0.20935200 Br -1.00419400 -2.24047500 -2.17323000 N -0.12041400 -0.86048700 -4.88494300 H -0.73907800 -0.10097600 -5.14127900 H 0.81400600 -0.47496600 -4.82546900 H -0.12194700 -1.51751600 -5.65543400

Table 2SI (Continuation). XYZ coordinates of the optimized geometries for the investigated dimers.

F3Ge-I···NH3	Ge -1.64743200 -3.26264800 -0.16306200 F -1.22428100 -2.35212800 1.21803700 F -3.33311500 -3.50928800 -0.04935400 F -0.94334300 -4.80070200 0.06985500 I -0.96580200 -2.19662100 -2.26761200 N -0.09417100 -0.82253900 -4.96541500 H -0.15415600 0.18690400 -4.90935500 H 0.86116800 -1.05069700 -5.21231400 H -0.67911500 -1.11288400 -5.73953900
F3Sn-Cl···NH3	Sn -1.62004400 -3.21378300 -0.26135500 F -0.84613400 -2.37574700 1.24817400 F -3.49143100 -3.18764300 0.01683800 F -1.09619000 -5.03038900 -0.18076400 Cl -1.01349100 -2.22242500 -2.21093200 N -0.10801900 -0.84573400 -4.91693900 H -0.65003100 -0.01285100 -5.11080200 H 0.86517100 -0.56759000 -4.89251000 H -0.22008000 -1.46444000 -5.71046800
F3Sn-Br···NH3	Sn -1.63184300 -3.24241600 -0.20767900 F -0.86254300 -2.43330800 1.32421900 F -3.50429900 -3.20299200 0.08430600 F -1.14634500 -5.07208400 -0.10676800 Br -0.96529600 -2.18865900 -2.27757700 N -0.09546900 -0.81848800 -4.96801500 H -0.64761600 0.00760900 -5.16294800 H 0.87464300 -0.52927800 -4.94474600 H -0.20147900 -1.44098600 -5.75955000
F3Sn-I···NH3	Sn -1.65550400 -3.28028600 -0.13369700 F -0.89121800 -2.49353900 1.41924500 F -3.52863200 -3.23999900 0.18925300 F -1.20087400 -5.12084800 0.00357600 I -0.92713000 -2.14658700 -2.38013800 N -0.07079100 -0.78358700 -5.03922200 H -0.63687700 0.03266700 -5.23673600 H 0.89449400 -0.47835800 -5.01152100 H -0.16371600 -1.41006600 -5.82951800

Table 2SI (Continuation). XYZ coordinates of the optimized geometries for the investigated dimers.

F3Pb-Cl···NH3	Pb -1.58512000 -3.17470600 -0.34863300 F -0.79717500 -2.33642800 1.27726900 F -3.54811200 -3.14445700 -0.01411200 F -1.09623400 -5.09795400 -0.18708100 Cl -0.93256600 -2.16307000 -2.36572700 N -0.13071900 -0.87554200 -4.85882000 H -0.69895600 -0.05860600 -5.04457900 H 0.83448000 -0.57217400 -4.82539000 H -0.22584500 -1.49766500 -5.65168700
F3Pb-Br···NH3	Pb -1.59373700 -3.19089700 -0.30746700 F -0.85908500 -2.34587400 1.34697000 F -3.55893700 -3.23952900 0.04774600 F -1.05920300 -5.10406700 -0.09996600 Br -0.91684900 -2.10577800 -2.44772000 N -0.12506300 -0.85422300 -4.90447200 H 0.87313200 -0.68590200 -4.92091000 H -0.35206000 -1.43170300 -5.70446600 H -0.58844500 0.03737100 -5.02847500
F3Pb-I···NH3	Pb -1.61261900 -3.21648100 -0.25949400 F -0.88056800 -2.43511500 1.44036600 F -3.58043000 -3.24499200 0.14309100 F -1.14559200 -5.15534300 -0.02186300 I -0.85952100 -2.04017500 -2.57406900 N -0.09891400 -0.82664300 -4.95310700 H -0.65935400 -0.00191500 -5.13137200 H 0.87289800 -0.54221300 -4.92559200 H -0.21615000 -1.45772500 -5.73671900