

Supplementary Information

Comparison of π -Hole Tetrel Bonding with σ -Hole Halogen Bonds

in Complexes of XCN (X = F, Cl, Br, I) and NH₃

Vincent de Paul N. Nziko and Steve Scheiner

Cartesian Coordinates of Optimized Heterodimers

π -hole XCN \cdots NH₃

F

6	0.000000000	0.937176225	0.000000000
7	-1.159571464	1.191976167	0.000000000
9	1.263709330	0.727888179	0.000000000
7	-0.250224146	-1.961764606	0.000000000
1	-0.140555849	-2.565736388	0.815386062
1	-0.140555849	-2.565736388	-0.815386062
1	-1.223707227	-1.654060161	0.000000000

Cl

6	0.000000000	0.912699058	0.000000000
7	-1.038174931	1.495525399	0.000000000
17	1.446246294	0.126086014	0.000000000
7	-1.615202018	-1.794317418	0.000000000
1	-1.946996178	-2.311144238	0.815265877
1	-1.946996178	-2.311144238	-0.815265877
1	-2.118546460	-0.905827162	0.000000000

Br

6	0.000000000	-1.055925125	0.000000000
7	0.624853072	-2.070556430	0.000000000
35	-0.950619903	0.465064285	0.000000000
7	2.784341449	0.507631836	0.000000000
1	3.346701329	0.754999993	0.815228306
1	3.346701329	0.754999993	-0.815228306
1	2.713943407	-0.511213837	0.000000000

I

6	0.949907072	-0.896359068	0.000000000
7	1.528173115	-1.939837147	0.000000000
53	0.000000000	0.867594065	0.000000000
7	-1.654707125	-2.584828195	0.000000000
1	-1.134707086	-2.923324221	0.810927062
1	-1.134707086	-2.923324221	-0.810927062
1	-2.544288192	-3.085036233	0.000000000

σ -hole NCX $\cdot\cdot$ NH₃

F

6	-0.000285000	-0.009247001	-1.519953115
7	0.000762000	-0.016056001	-2.707448205
9	-0.001280000	-0.001840000	-0.237864018
7	-0.000278000	0.017614001	2.903076220
1	-0.392147030	0.874534066	3.294621249
1	0.940687071	-0.064287005	3.289144249
1	-0.538688041	-0.749111057	3.307339250

Cl

6	-1.675669127	0.000017000	-0.000069000
7	-2.866491217	-0.000082000	-0.000100000
17	-0.020846002	0.000107000	0.000067000
7	2.929450222	0.000182000	0.000237000
1	3.324668251	0.925504070	-0.170528013
1	3.319470251	-0.611255046	-0.717830054
1	3.323545251	-0.316864024	0.886669067

Br

6	-1.777501134	-0.000110000	0.000031000
7	-2.969213225	-0.001031000	0.000455000
35	0.032862002	0.000460000	-0.000207000
7	2.912524220	-0.000607000	0.000185000
1	3.304298250	-0.522670039	-0.784460059

1	3.301705250	-0.420791032	0.844988064
1	3.305663250	0.939484071	-0.057949005
I			
6	1.968385149	-0.000355000	0.000232000
7	3.161306239	-0.000989000	0.000682000
53	-0.067534005	0.000349000	-0.00030100
7	-2.919755221	-0.000782000	0.000931000
1	-3.306380250	-0.452970034	0.830457063
1	-3.306976250	-0.493777037	-0.804722061
1	-3.308504250	0.942800071	-0.022449002