

Supplementary Information

Does a Halogen Bond Require Positive Potential on the Acid and Negative Potential on the Base?

Steve Scheiner*

Department of Chemistry and Biochemistry
Utah State University
Logan, Utah 84322-0300

email: steve.scheiner@usu.edu

Table of contents:

Tables S1-S3. SAPT decompositions of various complexes.

Table S4. Cartesian coordinates of complexes.

Table S1. SAPT decomposition of the interaction energy of each base with ICCH; all in kcal/mol.

	ES	EX	IND	DISP	TOT	%ES ^a
Me ₂ CS	-4.74	8.28	-2.08	-5.90	-4.44	37.3
Me ₂ CTe	-5.27	9.64	-2.53	-6.80	-4.96	36.1

^aES/(ES+IND+DISP)

Table S2. SAPT decomposition of the interaction energy of each base with ICCH; all in kcal/mol.

	ES	EX	IND	DISP	TOT	%ES
NH ₃	-11.49	11.96	-3.66	-3.62	-6.82	61.2
NCF	-5.18	5.42	-1.60	-2.90	-4.23	53.5
NCNO ₂	-3.27	3.95	-1.00	-2.55	-2.88	47.9
NF ₃	-1.51	3.08	-0.61	-2.04	-1.09	36.3
N(NO ₂) ₃	-0.94	4.43	-0.82	-4.41	-1.74	15.2
PF ₃	-2.51	4.81	-1.20	-2.46	-1.36	40.7

Table S3. SAPT decomposition of the interaction energy of each Lewis acid with NH₃; all in kcal/mol.

	ES	EX	IND	DISP	TOT	%ES
--	----	----	-----	------	-----	-----

GeH ₃ I	-3.65	5.69	-1.36	-2.18	-1.50	50.8
GeH ₃ Br	-1.07	2.91	-0.66	-1.34	-0.17	34.9
C ₆ Me ₅ Br	-3.00	5.29	-1.13	-2.07	-0.91	48.4
C ₆ Me ₅ Cl	-1.42	3.71	-0.88	-1.60	-0.19	36.4

Table S4. CARTESIAN COORDINATES OF COMPLEXES

COMPLEXES WITH ICCH

C₂H₂

6	-3.331468000	0.000017000	0.000546000
6	-2.132459000	-0.000004000	0.000291000
53	-0.138727000	-0.000020000	-0.000207000
1	-4.395498000	0.000074000	0.000768000
6	3.180049000	-0.597830000	0.000370000
6	3.179775000	0.597957000	0.000371000
1	3.185917000	1.662701000	0.000370000
1	3.186757000	-1.662571000	0.000372000

C₂F₂

6	-3.863985000	-0.000141000	-0.000524000
6	-2.665415000	-0.000020000	-0.000267000
53	-0.675576000	0.000151000	0.000196000
1	-4.928100000	-0.000265000	-0.000743000
6	2.660747000	0.590951000	-0.000154000
6	2.660657000	-0.591490000	-0.000171000
9	2.665103000	-1.871027000	-0.000162000
9	2.666186000	1.870632000	-0.000166000

C₂H₄

6	-3.410102000	0.000734000	0.000097000
6	-2.211025000	0.000375000	-0.000022000
53	-0.215587000	-0.000307000	-0.000025000
1	-4.474143000	0.001093000	0.000157000
6	3.101481000	-0.661909000	0.000044000
1	3.103742000	-1.229275000	-0.922672000
1	3.103708000	-1.229265000	0.922769000
6	3.100903000	0.662968000	0.000043000
1	3.102643000	1.230338000	-0.922673000
1	3.102605000	1.230353000	0.922755000

C₂F₄

6	-4.296375000	0.000249000	0.000211000
6	-3.098079000	0.000102000	0.000083000
53	-1.110507000	-0.000123000	-0.000154000
1	-5.360555000	0.000368000	0.000340000
6	2.260573000	-0.659578000	0.000062000
9	2.263193000	-1.378539000	-1.094798000
9	2.262476000	-1.378540000	1.095009000
6	2.260465000	0.659760000	0.000149000
9	2.262959000	1.378793000	-1.094726000
9	2.262250000	1.378616000	1.095051000

C₆H₆

6	-4.126278000	0.572394000	-0.005497000
6	-2.959972000	0.293703000	-0.003384000
53	-1.023421000	-0.170292000	0.000695000
1	-5.161026000	0.819854000	-0.007268000
6	2.596065000	1.286826000	-0.649896000
6	2.440496000	0.121172000	-1.387814000
6	2.582571000	1.238013000	0.738112000
1	2.445504000	0.159686000	-2.469352000
1	2.698612000	2.147716000	1.312680000
6	2.272063000	-1.095446000	-0.737561000
6	2.413573000	0.023399000	1.389020000
1	2.148455000	-2.004332000	-1.312445000
1	2.397787000	-0.014328000	2.470498000
6	2.258840000	-1.144433000	0.651550000
1	2.125194000	-2.091535000	1.158538000
1	2.722616000	2.234637000	-1.156654000

C₆F₆

6	4.755384000	-1.002244000	-0.009235000
6	3.641899000	-0.559973000	-0.005713000
53	1.795242000	0.171382000	0.000094000
1	5.744661000	-1.394547000	-0.012166000
6	-1.881291000	-1.232776000	-0.558172000
6	-1.711110000	-0.128783000	-1.376622000
6	-1.854752000	-1.085819000	0.819298000
9	-1.728889000	-0.269506000	-2.691115000
9	-2.011217000	-2.141553000	1.599628000

6	-1.515067000	1.124112000	-0.817593000
6	-1.657945000	0.165458000	1.378948000
9	-1.346075000	2.178773000	-1.598322000
9	-1.624032000	0.305825000	2.693293000
6	-1.488751000	1.271425000	0.560636000
9	-1.295495000	2.466606000	1.094422000
9	-2.063482000	-2.428712000	-1.091474000

Me₂CS

16	-2.427266000	1.223437000	0.001273000
6	-2.450829000	-0.396624000	0.000696000
6	-2.454717000	-1.204893000	1.261982000
1	-1.585103000	-1.868674000	1.270247000
1	-2.439505000	-0.573009000	2.144894000
1	-3.339594000	-1.847359000	1.282496000
6	-2.464598000	-1.203814000	-1.261205000
1	-1.600153000	-1.874151000	-1.273405000
1	-3.354390000	-1.839608000	-1.278739000
1	-2.448730000	-0.571333000	-2.143672000
6	4.020817000	-0.691665000	-0.000633000
6	2.874684000	-0.339868000	-0.000569000
53	0.970055000	0.245702000	-0.000436000
1	5.038685000	-1.001864000	-0.000687000

Me₂CTe

52	-2.149544000	-0.662371000	0.000391000
6	-1.562080000	1.224458000	0.000920000
6	-1.319479000	1.992676000	1.256875000
1	-1.980891000	2.865808000	1.279616000
1	-1.476857000	1.397811000	2.151273000
1	-0.295737000	2.382700000	1.253698000
6	-1.329904000	1.996581000	-1.254584000
1	-1.989559000	2.871232000	-1.268104000
1	-0.305382000	2.384586000	-1.259596000
1	-1.496777000	1.405186000	-2.149549000
6	4.835074000	0.111791000	0.000974000
6	3.642144000	-0.008308000	0.000130000
53	1.657226000	-0.207245000	-0.001042000
1	5.893996000	0.216724000	0.001700000

NH₃

7	3.038936000	-0.000349000	-0.001195000
1	3.402855000	-0.144792000	-0.935546000
1	3.408580000	-0.736487000	0.588497000
1	3.408858000	0.879326000	0.338835000
6	-3.144728000	-0.000428000	-0.001515000
6	-1.944685000	-0.000140000	-0.000663000
53	0.061363000	0.000160000	0.000603000
1	-4.208584000	-0.000658000	-0.002302000

NCF

6	3.883069000	0.086015000	0.000477000
6	2.684486000	0.043146000	-0.000355000
53	0.691655000	-0.022946000	-0.000153000
1	4.946241000	0.124182000	0.001851000
9	-4.787830000	0.077569000	-0.000132000
6	-3.531773000	0.005883000	-0.000202000
7	-2.389738000	-0.059488000	0.001131000

NCNO₂

6	4.688249000	0.019354000	0.033822000
6	3.489442000	0.010334000	0.018864000
53	1.498830000	-0.005062000	-0.008038000
1	5.752107000	0.026837000	0.049192000
6	-2.806930000	-0.005867000	-0.011387000
7	-1.665016000	-0.014671000	-0.027765000
7	-4.239956000	0.005826000	0.008792000
8	-4.763813000	-1.073691000	0.017220000
8	-4.746171000	1.093745000	0.015511000

NF₃

7	-2.345533000	0.007609000	0.000282000
9	-2.872002000	-0.936799000	-0.809889000
9	-3.009582000	1.120219000	-0.382030000
9	-2.919334000	-0.278205000	1.189512000
6	4.099843000	-0.058129000	-0.001351000
6	2.901780000	-0.025898000	-0.000628000
53	0.914220000	0.026236000	0.000633000
1	5.163576000	-0.086554000	-0.002016000

N(NO₂)₃

7	-1.440993000	0.001095000	-0.000359000
7	-1.982008000	0.072703000	-1.400813000
8	-1.442253000	-0.697050000	-2.119896000
8	-2.837028000	0.871823000	-1.600009000
7	-1.985164000	1.174952000	0.765381000
8	-2.836328000	0.943006000	1.559618000
8	-1.451050000	2.185152000	0.457433000
7	-1.972655000	-1.252679000	0.636912000
8	-2.823037000	-1.830935000	0.043919000
8	-1.431189000	-1.486712000	1.662899000
6	4.988300000	-0.002764000	0.000665000
6	3.789925000	-0.000294000	0.000330000
53	1.802094000	0.003177000	-0.000874000
1	6.052462000	-0.004830000	0.000774000

PF₃

15	2.344490000	0.011794000	-0.004183000
9	3.062429000	-0.515560000	1.279892000
9	3.202222000	1.302183000	-0.208538000
9	3.079786000	-0.895943000	-1.042223000
6	-4.459113000	-0.068940000	0.015641000
6	-3.261219000	-0.031436000	0.007249000
53	-1.272124000	0.028511000	-0.006793000
1	-5.522733000	-0.101876000	0.023234000

COMPLEXES WITH NH₃

GeH₃I

32	-1.957173000	0.002845000	0.001672000
53	0.565724000	-0.003491000	-0.002051000
1	-2.437062000	1.056323000	-1.013781000
1	-2.435127000	0.358286000	1.421646000
1	-2.442512000	-1.402233000	-0.399972000
7	3.886009000	0.005915000	0.003812000
1	4.237997000	0.397424000	0.868716000
1	4.247915000	0.567697000	-0.756837000
1	4.272875000	-0.924910000	-0.091237000

GeH₃Br

32	1.722132000	0.035528000	0.001464000
----	-------------	-------------	-------------

35	-0.595942000	-0.064105000	-0.002751000
1	2.192251000	0.046476000	-1.463836000
1	2.242893000	-1.209138000	0.741550000
1	2.136561000	1.328069000	0.727068000
7	-3.977938000	0.058632000	0.000432000
1	-4.512872000	-0.281420000	-0.788774000
1	-4.022492000	1.069977000	-0.012786000
1	-4.441022000	-0.257637000	0.843192000

C₆Me₅Br

6	0.510082000	1.223861000	-0.043088000
6	-0.156145000	-0.001238000	-0.054882000
6	1.909095000	1.213386000	0.015103000
35	-2.068660000	-0.003935000	-0.016221000
6	0.513261000	-1.224622000	-0.043040000
6	2.608112000	0.002327000	-0.001271000
6	1.912224000	-1.210550000	0.015257000
6	-0.230113000	-2.533205000	-0.098782000
1	-1.163608000	-2.429256000	-0.644743000
1	0.363792000	-3.300473000	-0.590444000
1	-0.479115000	-2.890809000	0.904436000
6	4.117450000	0.004296000	-0.056582000
1	4.492753000	-0.870297000	-0.583552000
1	4.490456000	0.879816000	-0.583641000
1	4.564561000	0.004933000	0.942275000
6	2.660036000	2.519065000	0.127121000
1	3.606380000	2.386739000	0.646589000
1	2.878247000	2.950415000	-0.854595000
1	2.086317000	3.254440000	0.687267000
6	-0.236438000	2.530653000	-0.098833000
1	0.354499000	3.298466000	-0.593265000
1	-1.171146000	2.423825000	-0.642110000
1	-0.483376000	2.889328000	0.904517000
6	2.666577000	-2.514237000	0.127603000
1	2.094970000	-3.250771000	0.688390000
1	2.885488000	-2.945546000	-0.853971000
1	3.612778000	-2.379205000	0.646623000
7	-5.227655000	0.003988000	0.107788000
1	-5.664635000	0.063153000	-0.803534000
1	-5.541594000	0.798859000	0.650619000

1	-5.574940000	-0.832220000	0.560702000
---	--------------	--------------	-------------

C₆Me₅Br

6	0.122787000	1.222366000	-0.025385000
6	-0.544346000	-0.002299000	-0.033495000
6	1.521497000	1.212848000	0.013883000
17	-2.289872000	-0.005599000	-0.013417000
6	0.127285000	-1.224505000	-0.025386000
6	2.221757000	0.002787000	-0.008766000
6	1.525939000	-1.209850000	0.013911000
6	-0.616697000	-2.533157000	-0.065180000
1	-1.615322000	-2.407699000	-0.472091000
1	-0.087731000	-3.260795000	-0.678936000
1	-0.720687000	-2.958665000	0.936898000
6	3.730241000	0.005638000	-0.075445000
1	4.102927000	-0.869105000	-0.604231000
1	4.099566000	0.881785000	-0.604278000
1	4.183573000	0.006546000	0.920657000
6	2.270545000	2.520677000	0.101356000
1	3.208603000	2.403559000	0.639923000
1	2.506224000	2.920277000	-0.889821000
1	1.687890000	3.274211000	0.626736000
6	-0.626002000	2.528277000	-0.065257000
1	-0.100047000	3.257623000	-0.679578000
1	-1.624363000	2.398998000	-0.471617000
1	-0.730995000	2.953801000	0.936712000
6	2.279694000	-2.514962000	0.101548000
1	1.699698000	-3.270496000	0.627005000
1	2.516805000	-2.913849000	-0.889574000
1	3.217303000	-2.394424000	0.640129000
7	-5.438923000	0.000798000	0.052543000
1	-5.867979000	0.065679000	-0.862115000
1	-5.758671000	0.792384000	0.596718000
1	-5.792703000	-0.837160000	0.497061000