Supporting Information

Halogen bonding in the complexes of brominated electrophiles with chloride anion: from a weak supramolecular interaction to a covalent Br-Cl bond

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Content

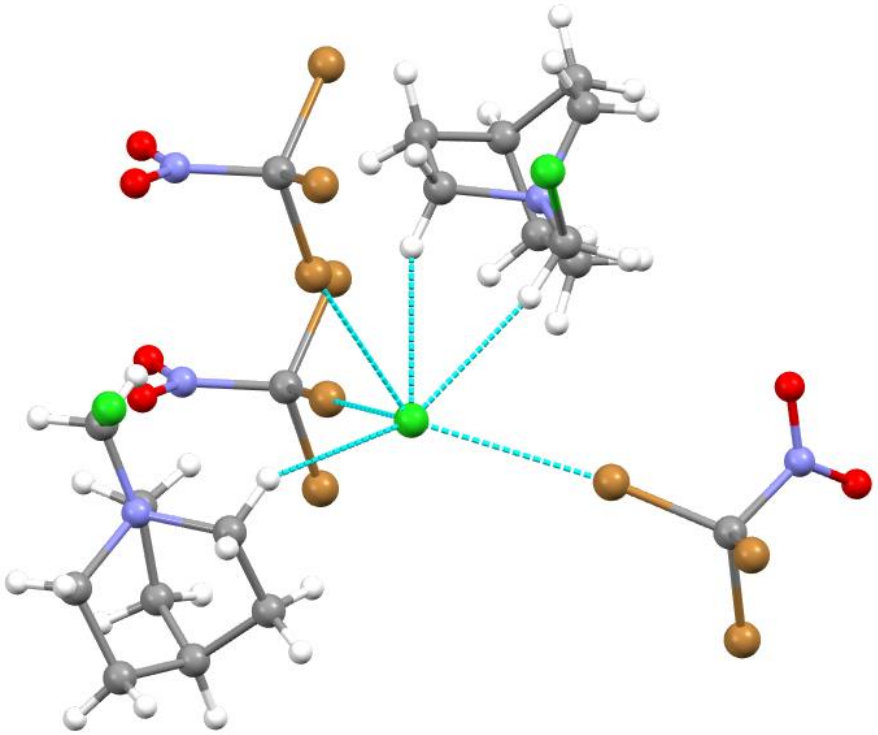

Figure S1: Fragment of the X-ray structure of (DABCO-CH_2Cl)Cl ·CBr_3NO_2 showing hydrogen and halogen bonds (blue lines) involving Cl^- anions. .

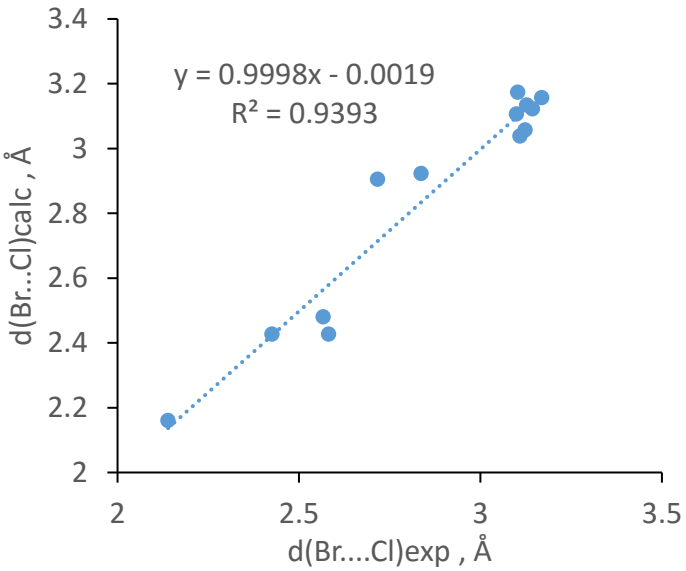

Figure S2: Correlation between calculated and experimental Br···Cl distances.

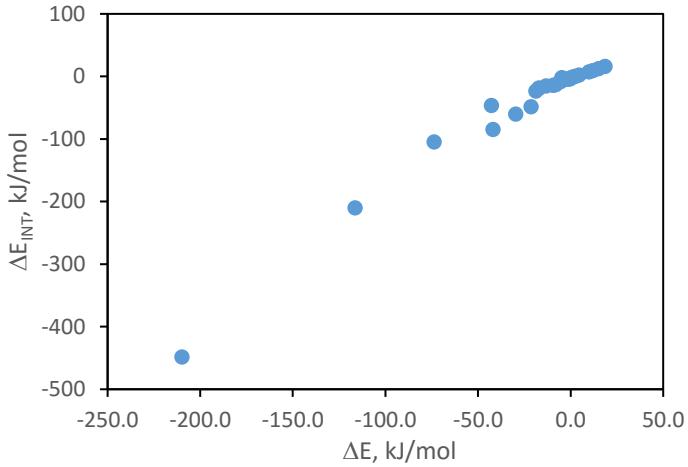

Figure S3. Correlation between calculated values of ΔE and ΔE_{INT}.

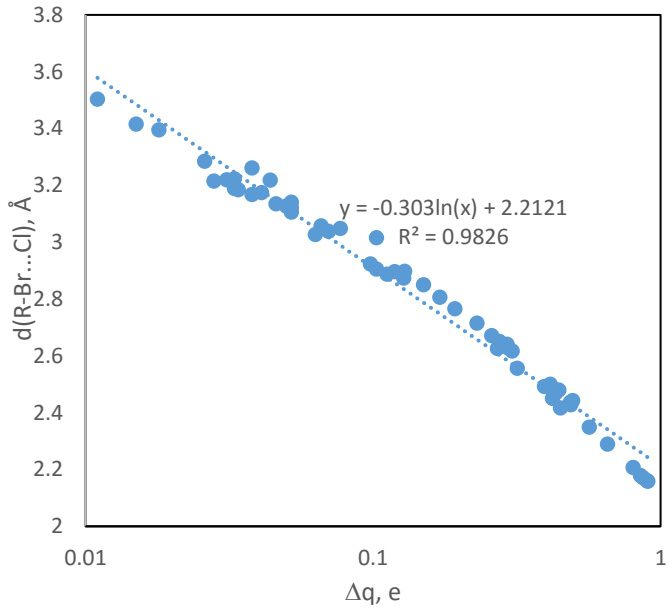

Figure S4. Correlation between calculated values of charge transfer (Δq) and intermolecular distances, d(R-Br…Cl).

Table S1: Characteristics of the R-Br·Cl^- complexes calculated (M062X/6-311+G(d,p)) in the gas phase.

R-Br[1]	$d_{Br\cdots Cl}$, Å	ΔE, kJ mol^{-1}	R [3]	$d_{X\cdots Br}^{com}$/ $d_{X\cdots Br}^{sep}$ [4]	$q(Cl)$,[5]
$CH_2Br(NH_2)$	3.261	-0.4	0.89	0.97	-0.962
CH_3Br	3.219	-1.5	0.88	1.00	-0.956
CH_2BrF	3.141	-5.5	0.86	1.00	-0.948
CH_2Br_2	3.048	-7.8	0.83	1.01	-0.923
BrCCH	3.016	-9.6	0.82	1.01	-0.897
$C_6Br_2F_4$	2.896	-15.3	0.79	1.02	-0.881
$C_2Br_2F_4$	2.874	-15.7	0.79	1.01	-0.872
$CHBr_3$	2.897	-12.8	0.79	1.01	-0.871
CBr_3CONH_2	2.850	-17.7	0.78	1.01	-0.850
CBr_3F	2.806	-16.5	0.77	1.00	-0.829
CBr_3COCBr_3	2.640	-20.9	0.72	1.06	-0.707
$CBrCl_3$	2.765	-16.7	0.76	1.02	-0.807
CBr_4	2.714	-17.6	0.74	1.03	-0.77
CBr_3CN	2.651	-21.8	0.72	1.05	-0.725
CBr_3NO_2	2.627	-22.4	0.72	1.02	-0.704
$CBr(NO_2)_3$	2.500	-33.2	0.68	1.11	-0.586
BrSIM	2.491	-22.0	0.68	1.12	-0.605
BrPIM	2.469	-23.1	0.67	1.12	-0.59
Br_2	2.443	-31.1	0.67	1.12	-0.505
BrSAC[2]	2.349	-32.5	0.64	1.20	-0.435
BrCl	2.436	-32.1	0.67	1.13	-0.514
BrF	2.451	-37.6	0.67	1.10	-0.579
pyrazine-Br^+	2.207	-136.3	0.60	1.36	-0.196
F_5Pyr-Br^+	2.171	-161.0	0.59	1.52	-0.129
Br^+	2.158	-277.8	0.59	N/A	-0.095
$C_4H_8Br_2N^+$	2.617	-68.2	0.71	1.05	-0.695
3-BrPYR$^+$	2.626	-73.7	0.72	1.04	-0.729
4-BrPYR$^+$	2.656	-73.8	0.73	1.03	-0.882
$C_{12}H_8BrF_2^+$	2.671	-98.5	0.73	1.03	-0.741

1) See Table 2 for R-Br abbreviations. 2) N-bromosaccharin. 3) $R = d_{Br\cdots Cl}/(r_{Br} + r_{Cl^-})$, where r_{Br} and r_{Cl^-} are van der Waals radii of bromine and chloride or 1.85 Å and 1.81 Å, respectively [37]. 4) Ratio of X–Br bond lengths (where X – C, N, Cl, F or Br) in the separate and halogen-bonded R-Br electrophile. 5) Charge on halogen-bonded chloride, from NBO analysis [41].

Table S2. Calcualted energies of the R-Br$^-$ electrophiles and R-Br·Cl$^-$complexes.[a]

	R-Br$^-$		R-Br·Cl$^-$		
R-Br[1]	E , Hartree	ZPE, Hartree	E , Hartree	ZPE, Hartree	BSSE, Hartree
			Gas phase		
$CH_2Br(NH_2)$	-2669.4201408	0.056169	-3129.689657	0.056545	0.000415427
CH_3Br	-2614.065904	0.037553	-3074.336912	0.037644	0.000390679
CH_2BrF	-2713.29989080	0.030887	-3173.577386	0.031081	0.000425571
CH_2Br_2	-5187.63098812	0.02859	-5647.912143	0.028743	0.00045232
BrCCH	-2650.87915188	0.01902	-3111.167543	0.019269	0.004695068
$C_6Br_2F_4$	-5776.27253676	0.048683	-6236.565756	0.048800	0.000587208
$C_2Br_2F_4$	-5623.90003370	0.024972	-6084.193893	0.02503	0.000578067
$CHBr_3$	-7761.190639	0.018454	-8221.479862	0.018593	0.000506982
CBr_3CONH_2	-7929.87664825	0.044194	-8390.174311	0.044956	0.000557236
CBr_3F	-7860.42272335	0.009678	-8320.717868	0.009784	0.000549739
CBr_3COCBr_3	-15634.4799836	0.024436	-16094.78177	0.024486	0.000228616
$CBrCl_3$	-3992.82887673	0.009201	-4453.124541	0.009365	0.000777465
CBr_4	-10334.7426779	0.007299	-10795.03953	0.007401	0.000610334
CBr_3CN	-7853.40483413	0.016089	-8313.708461	0.016281	0.000617545
CBr_3NO_2	-7965.65170545	0.020003	-8425.956481	0.020205	0.000668701
$CBr(NO_2)_3$	-3227.45880632	0.045549	-3687.781123	0.045987	0.000903861
BrSIM	-2934.159517	0.082078	-3394.463568	0.082178	0.00069493
BrPIM	-3086.561089	0.106143	-3546.866783	0.106127	0.000699079
Br_2	-5148.32323095	0.000775	-5608.642147	0.001465	0.00060096
BrSAC[2]	-3521.764115	0.106317	-3982.084736	0.106277	0.00077148
BrCl	-3034.33527463	0.001026	-3494.65706	0.001701	0.000728262
BrF	-2673.93466191	0.001596	-3134.263781	0.00202	0.000651507
pyrazine-Br$^+$	-2838.136582	0.079482	-3298.622688	0.079479	0.000710274
F_5Pyr-Br$^+$	-3318.240613	0.05132	-3778.766127	0.05118	0.000983688
Br^+	-2573.62272309	0	-3034.335274	0.001026	0.000713179
$C_4H_8Br_2N^+$	-5360.04110055	0.126016	-5820.418142	0.125209	0.000955119
3-BrPYR$^+$	-2822.162357	0.093022	-3282.548258	0.092801	0.000607057
4-BrPYR$^+$	-2822.16692	0.093055	-3282.553049	0.092799	0.000605473
$C_{12}H_8BrF_2{}^+$	-3235.53411637	0.165352	-3695.961541	0.166533	0.001095163

a) From M062X/6-311+G(dp) calculations

Table S2 (cont). Calcualted energies of the R-Br$^-$ electrophiles and R-Br·Cl$^-$ complexes.

	R-Br$^-$		R-Br·Cl$^-$		
R-Br[1]	E , Hartree	ZPE, Hartree	E , Hartree	ZPE, Hartree	BSSE, Hartree
			In dichloromethane		
$CH_2Br(NH_2)$	-2669.426973	0.055689	-3129.794516	0.055983	0.000235391
CH_3Br	-2614.068788	0.037509	-3074.437803	0.037867	0.000347042
CH_2BrF	-2713.303875	0.030809	-3173.674181	0.031219	0.000376868
CH_2Br_2	-5187.634477	0.028545	-5648.005544	0.028942	0.000385773
BrCCH	-2650.881501	0.018992	-3111.255874	0.019379	0.000431743
$C_6Br_2F_4$	-5776.275799	0.048534	-6236.649796	0.048905	0.000514039
$C_2Br_2F_4$	-5623.901446	0.02681	-6084.275985	0.024946	0.000499259
$CHBr_3$	-7761.193561	0.018387	-8221.56659974	0.018627	0.000436646
CBr_3CONH_2	-7929.885021	0.0442	-8390.260225	0.044791	0.000496504
CBr_3F	-7860.424334	0.009509	-8320.799222550	0.009916	0.000462261
CBr_3COCBr_3	-15634.48402	0.024325	-16094.85966	0.024726	0.000594991
$CBrCl_3$	-3992.830218	0.009051	-4453.205653	0.009525	0.000662333
CBr_4	-10334.74457	0.007185	-10795.11982	0.007675	0.000486398
CBr_3CN	-7853.408728	0.01605	-8313.785552	0.016399	0.000495259
CBr_3NO_2	-7965.656118	0.019901	-8426.033184	0.020191	0.00054686
$CBr(NO_2)_3$	-3227.465036	0.045271	-3687.84738	0.045728	0.000693846
BrSIM	-2934.170983	0.081712	-3394.549302	0.08235	0.000545789
BrPIM	-3086.570197	0.105954	-3546.948916	0.106452	0.000529502
Br_2	-5148.324441	0.000771	-5608.711016	0.001352	0.000596274
BrSAC[2]	-3521.777092	0.106041	-3982.160217	0.106206	0.000736862
BrCl	-3034.3364	0.001021	-3494.727763	0.001576	0.000730952
BrF	-2673.93718	0.001596	-3134.340312	0.0019	0.000663688
pyrazine-Br^+	-2838.212376	0.079715	-3298.631525	0.079752	0.000686536
F_5Pyr-Br^+	-3318.316905	0.051317	-3778.771671	0.051023	0.001010588
Br^+	-2573.728843	0	-3034.3364	0.001021	0.000711901
$C_4H_8Br_2N^+$	-5360.126067	0.126806	-5820.505978	0.127157	0.000473695
3-$BrPYR^+$	-2822.238898	0.093173	-3282.620395	0.093605	0.000447993
4-$BrPYR^+$	-2822.242812	0.093397	-3282.624224	0.093766	0.000454159
$C_{12}H_8BrF_2{}^+$	-3235.60112	0.165799	-3695.993151	0.166423	0.001056171

Table S3. Atomic coordinates of the calculated R-Br·Cl^- compleses (M062X/6-311+G(dp)).

R-Br	In the gas phase				In dichloromethane			
$CH_2Br(NH_2)$	C	-2.13442000	-0.44424800	-0.07488800	C	-2.52200900	-0.43011000	0.00165500
	H	-2.32642600	-0.91149700	-1.04451900	H	-2.66882600	-1.01673200	-0.89741700
	H	-2.42271900	-1.13056200	0.71986300	H	-2.66715000	-1.01357400	0.90305100
	Br	-0.20329800	-0.20172200	0.02269500	Br	-0.46889600	-0.16980300	-0.00067300
	N	-2.81119000	0.83038800	0.12070600	N	-3.26486100	0.74473200	0.00030300
	H	-2.38182700	1.53898000	-0.46467800	H	-3.15926200	1.30775400	-0.83341700
	H	-3.78857200	0.75463800	-0.14430400	H	-3.15783200	1.31058000	0.83192100
	Cl	2.97175400	0.21538200	-0.01507800	Cl	3.88532500	0.16015400	0.00043200
CH_3Br	C	2.54239800	0.00045300	0.00006400	C	2.62182000	0.00024100	0.00066100
	H	2.89681000	0.69113500	-0.76151500	H	2.95498400	0.82004100	0.62856900
	H	2.89680900	0.31492000	0.97891200	H	2.95563100	-0.95316000	0.39678200
	H	2.89744100	-1.00427000	-0.21710300	H	2.95605600	0.13418600	-1.02288500
	Br	0.59175100	-0.00020700	-0.00003100	Br	0.67217700	-0.00011100	-0.00028600
	Cl	-2.62686600	0.00016000	0.00002400	Cl	-2.83081100	0.00008000	0.00021000
	Br	-0.20039600	-0.13843200	0.00003800	Br	-0.27496200	-0.17258900	0.00020900
	C	-2.10836200	-0.43611800	-0.00007000	C	-2.20084100	-0.40280300	-0.00046900
	H	-2.38026100	-0.98367700	0.89993600	H	-2.47405600	-0.93620300	0.90435500
	H	-2.38010500	-0.98321200	-0.90039900	H	-2.47342200	-0.93519900	-0.90607500
	F	-2.81346500	0.75033000	0.00000600	F	-2.81228500	0.82118100	-0.00001600
CH_2BrF	Cl	2.92621100	0.15739700	-0.00002900	Cl	3.12275000	0.17283500	-0.00015600
	C	0.99308000	1.00588500	0.00036300	C	1.10077500	1.01894500	0.00001200
	H	1.16447200	1.59133000	0.89605600	H	1.26426600	1.60024700	0.89838100
	H	1.16455400	1.59205500	-0.89484200	H	1.26430700	1.60027900	-0.89832800
	Br	-0.81622400	0.32785300	-0.00018300	Br	-0.72723800	0.39491800	-0.00000600
	Br	2.40439000	-0.36208100	0.00001200	Br	2.40952000	-0.41579300	0.00000000
CH_2Br_2	Cl	-3.75725500	-0.47180700	0.00015200	Cl	-4.00077000	-0.50491700	0.00000500
	C	0.00000000	0.00000000	3.35335057	C	0.00000000	0.00000000	3.34136900
	H	0.00000000	0.00000000	4.42335057	H	0.00000000	0.00000000	4.40659900
	C	0.00000000	0.00000000	2.15215057	C	0.00000000	0.00000000	2.13960200
	Br	0.00000000	0.00000000	0.24215057	Br	0.00000000	0.00000000	0.33394800
BrCCH	Cl	0.00000000	0.00000000	-2.70186043	Cl	0.00000000	0.00000000	-2.88121200
	C	1.36591000	-1.19152000	-0.00000100	C	1.39034600	-1.19177400	-0.00012700
	C	-0.01987400	-1.18398700	0.00001900	C	0.00539100	-1.18922500	-0.00013600
	C	-0.74768000	0.00001400	0.00003000	C	-0.71004800	0.00016200	0.00000200
	C	-0.01985500	1.18400600	0.00001900	C	0.00556700	1.18944800	0.00014900
	C	1.36593000	1.19151700	-0.00000200	C	1.39052200	1.19178700	0.00015700
	C	2.07665900	-0.00000600	-0.00001100	C	2.10064000	-0.00004900	0.00001900
	F	-0.64164900	2.36027200	0.00002900	F	-0.62756400	2.35801900	0.00028600
	F	2.01146900	2.35793300	-0.00001000	F	2.02927600	2.35721000	0.00030100
	F	2.01143000	-2.35794700	-0.00000900	F	2.02891800	-2.35729800	-0.00026100
	F	-0.64169100	-2.36024100	0.00003000	F	-0.62791300	-2.35770300	-0.00028000
$C_6Br_2F_4$	Br	-2.65292500	0.00003100	0.00006200	Br	-2.58900800	0.00026600	-0.00000900

	Br	3.95412300	-0.00001900	-0.0000380	Br	3.97241300	-0.00019600	0.00003200
	Cl	-5.54849900	-0.00004300	-0.0000900	Cl	-5.80812600	-0.00038900	-0.00009400
	C	0.18034900	0.67386200	-0.00419800	C	0.23768500	0.70030500	-0.00064300
	C	1.08415100	-0.57275600	-0.01317800	C	1.11302500	-0.57379400	0.00257900
	Br	-1.70662800	0.20479100	-0.0097680	Br	-1.64161800	0.25879900	0.00423900
	Br	2.98529200	-0.07632500	0.01588400	Br	2.99752100	-0.12445300	-0.00310200
	F	0.49657300	1.39810100	1.08867100	F	0.54315900	1.43008700	1.07922100
	F	0.50458500	1.41784700	-1.08143500	F	0.53894600	1.42172600	-1.08729900
	F	0.86786600	-1.29569000	-1.10811900	F	0.83502500	-1.30499500	-1.07571400
	F	0.84477500	-1.33052900	1.05284100	F	0.83953800	-1.29637100	1.08784700
$C_2Br_2F_4$	Cl	-4.51555400	-0.40061800	0.01897500	Cl	-4.72769700	-0.45383500	-0.00517100
	C	-0.64249100	-0.00000900	0.54390400	C	-0.71552500	-0.00000600	0.55955000
	H	-0.79516900	-0.00004100	1.61522300	H	-0.86120100	0.00000600	1.63129300
	Br	-1.56747600	-1.60179500	-0.09870200	Br	-1.58055000	-1.59888700	-0.11729200
	Br	-1.56756700	1.60172300	-0.09871700	Br	-1.58039000	1.59897400	-0.11727500
	Br	1.25977100	0.00009700	0.15750700	Br	1.18322100	-0.00008200	0.20822600
$CHBr_3$	Cl	4.13439200	-0.00004600	-0.20480700	Cl	4.37497000	-0.00001000	-0.23921500
	C	0.55865600	0.00702400	0.17084400	C	0.60272300	0.01731700	0.17554100
	Br	-1.39389700	-0.12022800	-0.08492900	Br	-1.33607900	-0.06034400	-0.00121100
	Br	1.30734800	1.44276900	-0.95504100	Br	1.32668000	1.38470100	-1.02696400
	Br	1.43079600	-1.67135900	-0.28030300	Br	1.36348000	-1.70915400	-0.27001400
	C	0.96038200	0.40355000	1.62265300	C	1.08532700	0.43743800	1.60121900
	O	2.01602400	0.07129600	2.10557400	O	2.16173500	0.06294600	2.00844400
	N	0.06447200	1.20089400	2.24853000	N	0.26846100	1.27053900	2.26070300
	H	-0.87649100	1.30889600	1.89988900	H	-0.64664800	1.52490800	1.92425400
	H	0.27942000	1.46555800	3.19562100	H	0.57185000	1.61838800	3.15790700
CBr_3CONH_2	Cl	-4.24384100	-0.11799200	-0.13125100	Cl	-4.50702400	-0.10595600	-0.12932900
	C	-0.60292700	0.00002300	0.45584100	C	-0.66774900	0.00015000	0.45155200
	Br	-1.49911700	1.60004600	-0.26341000	Br	-1.51434200	1.59268900	-0.27768400
	Br	-1.49754000	-1.60091700	-0.26321300	Br	-1.49954900	-1.60130800	-0.27536400
	Br	1.32347700	0.00084900	0.11505300	Br	1.24438500	0.00856100	0.14774000
	F	-0.84476300	-0.00001900	1.77793200	F	-0.89323600	0.00010500	1.77394100
CBr_3F	Cl	4.10480800	0.00004700	-0.25479400	Cl	4.35166500	0.00001100	-0.26405800
	Br	0.67436100	-1.60136900	1.60592800	Br	0.97494400	-1.83618400	1.64972400
	Br	2.11495800	0.87543300	-0.05873200	Br	1.82841300	0.81420700	0.02843000
	C	0.96852500	-0.82912600	-0.15955200	C	0.97930800	-0.92774900	-0.08887600
	Br	1.89320900	-2.15983900	-1.2409220	Br	1.97973700	-2.01540200	-1.35713400
	C	-0.30331700	-0.41572000	-0.8882660	C	-0.52061400	-0.94268300	-0.51891700
	O	-0.43717500	-0.59226500	-2.0601750	O	-0.92794000	-1.83111300	-1.19561300
	C	-1.49593300	0.31254400	-0.14472500	C	-1.51984000	0.19063100	-0.09982000
	Br	-2.71388100	-1.14536300	0.3607380	Br	-3.32356300	-0.53631900	-0.16194500
	Br	-2.40228800	1.45393300	-1.4377310	Br	-1.32851500	1.54330500	-1.49649100
	Br	-1.07775400	1.39330600	1.40093300	Br	-1.25124200	0.97057900	1.65046600
CBr_3COCBr_3	Cl	3.61062400	3.04520000	0.09289200	Cl	3.11754600	3.63654200	0.16787200
	C	-1.07839400	-0.00012500	0.00009500	C	-1.13399800	0.00018900	0.00001000
$CBrCl_3$	Br	0.90689700	0.00033700	-0.00008700	Br	0.81621700	0.00012500	-0.00005300

	Cl	-1.71932100	0.40484300	-1.62405400	Cl	-1.74080500	-0.84109900	1.44509400
	Cl	-1.72041500	1.20383000	1.16275400	Cl	-1.74075200	-0.83131700	-1.45071300
	Cl	-1.71855000	-1.60946400	0.46119200	Cl	-1.74140300	1.67203100	0.00566100
	Cl	3.67175400	0.00014200	0.00025300	Cl	3.94274800	0.00006000	0.00006200
	C	-0.46642300	0.00027700	0.00008300	C	-0.51753000	0.00011900	-0.00006900
	Br	-1.16739800	-1.03354700	-1.51600300	Br	-1.18177900	1.34775400	-1.24175600
	Br	-1.17143500	1.82856800	-0.13633700	Br	-1.18473200	0.40104500	1.78722000
	Br	1.52657600	0.00202100	0.00011400	Br	1.42801800	0.00020100	0.00152000
	Br	-1.16762900	-0.79740800	1.65230200	Br	-1.18268900	-1.74885500	-0.54711500
CBr_4	Cl	4.24085500	0.00065500	-0.00018500	Cl	4.54979500	-0.00034000	0.00029500
	C	0.61744900	-0.00003100	0.33422100	C	0.64895800	-0.00002800	0.32073300
	Br	1.42494400	-1.60145700	-0.4583300	Br	1.43979700	-1.59976800	-0.46345500
	Br	-1.39975200	0.00016400	0.09460100	Br	-1.29311000	0.00000900	0.10723100
	Br	1.42511300	1.60135400	-0.45833800	Br	1.43969100	1.59985500	-0.46333600
	C	0.95504500	-0.00004900	1.74259900	C	0.96546900	-0.00012000	1.73900400
	N	1.19157800	-0.00007100	2.86885600	N	1.20567100	-0.00020800	2.86237800
CBr_3CN	Cl	-4.03156900	-0.00006800	-0.2217980	Cl	-4.33232200	-0.00006100	-0.21826300
	C	0.57756300	0.00001300	0.15746800	C	0.60160000	-0.00002800	0.13691100
	Br	-1.45315600	0.00025000	0.00245000	Br	-1.34173800	-0.00019300	0.02660900
	Br	1.35938100	-1.58396500	-0.63192700	Br	1.36519900	-1.58335000	-0.64387300
	Br	1.36064600	1.58315900	-0.63270700	Br	1.36476700	1.58360700	-0.64374200
	N	0.88675400	0.00052200	1.66760200	N	0.91139700	-0.00002300	1.67738500
	O	0.94827200	1.07399800	2.21475500	O	0.98128800	1.07293100	2.21372300
	O	0.94962000	-1.07267300	2.21511200	O	0.98146700	-1.07302700	2.21367300
CBr_3NO_2	Cl	-4.07037000	0.00030200	-0.22826600	Cl	-4.36937700	-0.00006800	-0.22630100
	Br	1.27638700	0.00002900	0.00020600	Br	1.14729000	-0.00017600	0.00050400
	C	-0.81135500	0.00008700	-0.00006100	C	-0.76207100	-0.00010600	-0.00011600
	N	-1.37003100	0.89041400	1.08685700	N	-1.36198100	0.19211100	-1.40595500
	O	-2.22116500	1.69273000	0.77984000	O	-2.27561800	-0.53156700	-1.70218600
	O	-0.91373000	0.71481400	2.18453700	O	-0.87175700	1.06591600	-2.06117900
	N	-1.36928200	0.49615200	-1.3149080	N	-1.36229500	-1.31348800	0.53665500
	O	-0.91299600	1.53462500	-1.7114960	O	-0.87213000	-2.31806500	0.10808600
	O	-2.21961100	-0.17142300	-1.8568990	O	-2.27552600	-1.20775000	1.31195200
	N	-1.37050700	-1.38639000	0.2276280	N	-1.36298300	1.12134400	0.86868300
	O	-0.91249300	-2.25018100	-0.4709180	O	-0.87111100	1.25508600	1.95186100
	O	-2.22388600	-1.52044100	1.0739390	O	-2.27894900	1.73670400	0.39057200
$CBr(NO_2)_3$	Cl	3.77614000	-0.00022000	0.00023900	Cl	4.03463700	0.00026200	-0.00032200
	Br	1.11231500	-0.00006600	0.00009600	Br	0.94514800	-0.00022400	0.00010800
	N	-0.93524800	0.00005300	0.00008900	N	-0.93123100	-0.00000100	0.00004800
	C	-1.69332100	-1.14748500	-0.00026000	C	-1.68748300	-1.16744500	-0.00004900
	O	-1.28817000	-2.28439500	0.00032600	O	-1.23609500	-2.28257100	0.00021100
	C	-1.69338900	1.14752200	0.00029000	C	-1.68725300	1.16759400	0.00000300
	O	-1.28830800	2.28446300	-0.00024800	O	-1.23564500	2.28263500	-0.00012300
	C	-3.17790500	0.76205900	0.00032000	C	-3.14994700	0.76516400	0.00024600
	H	-3.64458400	1.20594200	-0.88007100	H	-3.62326500	1.19895800	-0.88072600
BrSIM	H	-3.64392600	1.20476700	0.88165400	H	-3.62250300	1.19796900	0.88212800

	C	-3.17786000	-0.76211000	-0.00057600	C	-3.15009800	-0.76472500	-0.00048900
	H	-3.64470700	-1.20602000	0.87971100	H	-3.62362500	-1.19842700	0.88041600
	H	-3.64367200	-1.20483600	-0.88201200	H	-3.62261300	-1.19743600	-0.88243900
	Cl	3.60348600	0.00009500	-0.00015000	Cl	3.86782600	0.00016200	-0.00014400
	Br	-2.11275200	-0.00018500	0.00009300	Br	-1.93238600	-0.00007800	0.00007000
	N	-0.05317500	0.00005100	0.00068300	N	-0.05767800	-0.00004600	0.00046000
	C	0.72022800	1.14454500	0.00054500	C	0.71633900	1.16505400	0.00010600
	O	0.34712300	2.29190900	0.00043700	O	0.29719100	2.29123000	0.00005000
	C	0.72021300	-1.14447800	0.00037800	C	0.71640100	-1.16510100	0.00019300
	O	0.34706000	-2.29182000	0.00046900	O	0.29732400	-2.29130600	0.00003400
	C	2.16201000	0.69162700	0.00010300	C	2.13566100	0.69428100	0.00001100
	C	2.16200200	-0.69158500	0.00010500	C	2.13569800	-0.69424700	0.00001100
	C	3.33760600	1.41790600	-0.00024900	C	3.31018800	1.42114800	-0.00007600
	C	3.33760300	-1.41785900	-0.00020700	C	3.31026400	-1.42105100	-0.00009900
	C	4.53526500	0.69818300	-0.00057200	C	4.50596900	0.69775500	-0.00018500
	H	3.31902500	2.50151800	-0.00024000	H	3.30136100	2.50410700	-0.00006700
	C	4.53526200	-0.69813500	-0.00054800	C	4.50600800	-0.69759100	-0.00019700
	H	3.31903300	-2.50147100	-0.00021700	H	3.30149700	-2.50401000	-0.00008400
	H	5.48110200	1.22822900	-0.00084600	H	5.45049100	1.22786400	-0.00026400
	H	5.48109500	-1.22818700	-0.00082100	H	5.45056000	-1.22764500	-0.00027800
BrPIM	Cl	-4.58213700	0.00024000	-0.00061900	Cl	-4.83776000	0.00011000	-0.00024800
	Br	0.00000000	0.00000000	-0.55826700	Br	0.00000000	0.00000000	-0.53100900
	Br	0.00000000	0.00000000	2.01587600	Br	0.00000000	0.00000000	1.99336500
Br_2	Cl	0.00000000	0.00000000	-3.00096100	Cl	0.00000000	0.00000000	-3.01073400
	Br	-2.35759100	0.16266000	0.00010000	Br	-2.18524500	0.17093100	0.00009200
	N	-0.15906700	0.13874900	-0.0001130	N	-0.19730800	0.15611000	-0.00000800
	C	0.61439600	1.26213900	-0.00025500	C	0.58174300	1.29117000	-0.00029200
	O	0.23184800	2.41238500	-0.00027800	O	0.16642900	2.42582600	-0.00026500
	C	2.29308100	-0.46750500	-0.00041500	C	2.23058400	-0.46827200	-0.00056400
	C	2.08410100	0.89545000	-0.00032100	C	2.03060200	0.90138400	-0.00046200
	C	3.55584700	-1.03157100	0.00018500	C	3.48430400	-1.04954500	0.00009100
	H	3.69102500	-2.10631400	0.00026900	H	3.61544900	-2.12410800	0.00023100
	C	3.16084900	1.76856500	-0.00008300	C	3.11696000	1.76137000	-0.00009200
	H	2.98222300	2.83741800	-0.00021000	H	2.96245600	2.83330100	-0.00004600
	C	4.64017300	-0.15573700	0.00050500	C	4.57539900	-0.18057000	0.00045200
	H	5.64863800	-0.55313300	0.00089600	H	5.57820100	-0.58913400	0.00094800
	C	4.44452300	1.22777300	0.00027600	C	4.39398300	1.20340500	0.00035500
	H	5.30615000	1.88551800	0.00048100	H	5.26108400	1.85205000	0.00067000
	O	0.51843100	-2.01253600	1.24072700	O	0.42453700	-2.01085700	1.23893400
	S	0.69348800	-1.27664100	-0.00017100	S	0.65246400	-1.28882100	-0.00019300
	O	0.51792500	-2.01264800	-1.2409350	O	0.42335300	-2.01094000	-1.23902900
BrSAC	Cl	-4.70577300	0.21212600	0.00018400	Cl	-4.74046400	0.21104600	0.00023900
	Br	0.00000000	0.00000000	0.00000000	Br	0.00000000	0.00000000	0.00000000
	Cl	0.00000000	0.00000000	2.43634300	Cl	0.00000000	0.00000000	2.42695600
BrCl	Cl	0.00000000	0.00000000	-2.43634300	Cl	0.00000000	0.00000000	-2.42695600
BrF	Br	0.00000000	0.39355600	0.00000000	Br	0.00000000	0.38196000	0.00000000

	F	0.00210600	2.35490000	0.00000000	F	0.00251200	2.35571700	0.00000000
	Cl	-0.00111500	-2.05697500	0.00000000	Cl	-0.00133000	-2.03353100	0.00000000
	C	3.26315200	1.13128000	0.00022600	C	3.12708900	1.13484000	-0.00006600
	C	1.87081400	1.13780500	-0.00024400	C	1.73559600	1.14700800	0.00005200
	C	1.87081100	-1.13778000	-0.00024200	C	1.73545600	-1.14695900	0.00005200
	C	3.26314700	-1.13127100	0.00021700	C	3.12691000	-1.13501600	-0.00006900
	H	3.82131800	2.06095900	0.00041000	H	3.68206400	2.06536100	-0.00011200
	H	1.30240000	2.06139400	-0.00043500	H	1.16333200	2.06667600	0.00010500
	H	1.30239100	-2.06136500	-0.00042300	H	1.16300900	-2.06652300	0.00010500
	H	3.82131100	-2.06095200	0.00042000	H	3.68179800	-2.06558400	-0.00010000
	Br	-1.35309900	-0.00002800	-0.00016500	Br	-1.21752500	0.00007800	0.00007300
	N	3.96260100	0.00000400	0.00045800	N	3.82160100	-0.00011600	-0.00012900
	N	1.18340400	0.00001600	-0.00047000	N	1.06281800	0.00008200	0.00010700
pyrazine-Br^+	Cl	-3.55991400	0.00003600	0.00036200	Cl	-3.50694500	-0.00009800	-0.00013000
	Br	2.46367400	-0.00113700	-0.04210400	Br	2.42085900	-0.00137000	0.00082100
	C	-1.05024700	-1.12899600	0.01306500	C	-1.02654000	-1.12817600	0.00106400
	C	-1.04805700	1.12766100	0.01327700	C	-1.02441500	1.12695200	0.00106600
	C	-2.43440500	-1.19741200	-0.00108000	C	-2.40885600	-1.19646100	-0.00022800
	C	-2.43208000	1.19876600	-0.00085800	C	-2.40659400	1.19784300	-0.00022500
	N	-0.38187000	-0.00131800	0.02015400	N	-0.35685400	-0.00124700	0.00172300
	F	-3.07635000	-2.35253000	-0.00783100	F	-3.04941400	-2.35330500	-0.00084200
	F	-0.35930800	-2.25106600	0.01983900	F	-0.33153500	-2.25102700	0.00166100
	F	-0.35498000	2.24840200	0.02026600	F	-0.32734000	2.24851600	0.00166400
	F	-3.07177700	2.35513100	-0.00740200	F	-3.04497500	2.35589000	-0.00083600
	C	-3.13276900	0.00135900	-0.00831800	C	-3.10725700	0.00135100	-0.00086000
	F	-4.44784000	0.00264000	-0.02198500	F	-4.42232100	0.00260700	-0.00206200
F_5Pyr-Br^+	Cl	4.63360300	0.00143500	-0.11898000	Cl	4.59941900	0.00138300	-0.00246800
	Br	0.00000000	0.00000000	0.70560600	Br	0.00000000	0.00000000	0.70620900
Br^+	Cl	0.00000000	0.00000000	-1.45271800	Cl	0.00000000	0.00000000	-1.45396000
	C	0.91080700	0.87748300	0.60233100	C	1.75618100	0.39991800	0.09349500
	C	0.14234400	-0.27830800	1.24014600	C	0.62312800	0.94163700	0.96092100
	C	-1.13385700	0.43457300	1.69231700	C	0.65414400	2.40965400	0.56855100
	N	-1.36566000	1.49438800	0.67004800	N	0.79125100	2.33974200	-0.93612100
	C	-0.16267900	1.61387700	-0.19023800	C	1.54564900	1.06266900	-1.27123900
	Br	2.47274000	0.42590000	-0.44166200	Br	1.90019500	-1.52156500	-0.04902200
	Br	-0.28098500	-1.69610000	-0.0307470	Br	-1.12184100	0.19601000	0.48272900
$C_4H_8Br_2N^+$	H	1.28333300	1.50755400	1.41269200	H	2.69886600	0.71991300	0.53524200
	H	0.68029100	-0.75451400	2.05436500	H	0.77523500	0.78233600	2.02354200
	H	-1.99585400	-0.23140800	1.73455600	H	-0.23457100	2.97584000	0.83015700
	H	-0.97362800	0.88087100	2.67721200	H	1.54554900	2.90034500	0.95929900
	H	-2.46168500	1.08117900	-0.1208190	H	-0.14103400	2.30390500	-1.35713900
	H	-1.60391500	2.37764200	1.10763200	H	1.25390900	3.16955700	-1.31077300
	H	0.08756400	2.65569600	-0.38057200	H	2.47569400	1.31503300	-1.77174600
	H	-0.35606400	1.10976100	-1.1403410	H	0.91597000	0.46426200	-1.92426000
	Cl	-3.55008900	0.55786800	-0.91576900	Cl	-4.09090400	-0.79401400	-0.51303500
3-BrPYR^+	Br	-1.05802600	0.01564800	-0.00102900	Br	-0.91796000	0.01454000	-0.00005400

	N	2.94514300	-1.14264100	0.00056800	N	2.99961400	-1.13887900	0.00009400
	H	3.42755600	-2.03534400	0.00076700	H	3.48940600	-2.02998800	0.00004500
	C	3.02942200	1.19861800	0.00069700	C	3.07157900	1.20415500	0.00011800
	H	3.61042100	2.11127600	0.00103300	H	3.64648500	2.11913900	0.00003200
	C	1.63712800	1.22518300	-0.00015800	C	1.68195200	1.22942300	0.00003400
	H	1.11179500	2.17474300	-0.00049400	H	1.15306500	2.17453400	0.00008700
	C	0.88886700	0.04313500	-0.00058900	C	0.96397200	0.03408000	-0.00018400
	C	3.68220000	-0.01585300	0.00103300	C	3.72572500	-0.01028500	-0.00000700
	H	4.75626100	-0.13245600	0.00177900	H	4.79992100	-0.12145100	-0.00019500
	C	1.59829600	-1.14771400	-0.00022600	C	1.65745800	-1.16161100	0.00003200
	H	1.11420400	-2.11687900	-0.00056400	H	1.18190700	-2.13225500	0.00010700
	Cl	-3.68357700	-0.02180900	0.00147000	Cl	-4.10256400	-0.01889900	0.00007000
4-BrPYR$^+$	Br	1.03764500	0.00003700	0.00001600	Br	0.91721600	-0.00000200	0.00001100
	C	-0.86687300	0.00002100	0.00001100	C	-0.95644800	-0.00004800	0.00010600
	N	-3.61744100	-0.00004400	-0.00002800	N	-3.67244800	0.00004100	-0.00020200
	H	-4.62900100	-0.00006600	0.00007700	H	-4.68850600	0.00006400	-0.00049200
	C	-1.59357100	1.20711800	-0.00000100	C	-1.65429500	1.20964200	0.00015900
	H	-1.07106700	2.15532900	-0.00001200	H	-1.13772400	2.15880400	0.00037600
	C	-2.96151700	1.18408400	-0.00000400	C	-3.02923200	1.18040800	-0.00003500
	H	-3.57657900	2.07396200	-0.00003200	H	-3.64359400	2.06912200	-0.00007200
	C	-1.59351800	-1.20710900	-0.00000200	C	-1.65436800	-1.20968900	0.00016000
	H	-1.07097100	-2.15529600	-0.00000700	H	-1.13786000	-2.15888300	0.00038100
	C	-2.96146600	-1.18414000	-0.00000500	C	-3.02929900	-1.18036600	-0.00003300
	H	-3.57648500	-2.07404800	-0.00003100	H	-3.64372300	-2.06903900	-0.00008900
	Cl	3.69354600	-0.00004300	-0.00002100	Cl	4.10575600	0.00000100	-0.00007200
	Cl	2.46766400	2.83388000	0.02660200	Cl	2.77101700	2.80155300	0.02296600
	Br	0.16452100	1.48229300	0.00650800	Br	0.08040200	1.41677200	0.00046200
	C	1.22634600	-0.14801800	0.06109100	C	1.19925500	-0.15658800	0.03142700
	F	3.41386900	-3.54285000	0.14437900	F	3.51041900	-3.45978500	0.06597500
	C	2.31987900	-0.23358200	-0.78011100	C	1.83820400	-0.50850600	-1.14403200
	H	2.60670700	0.60444700	-1.40158600	H	1.73938200	0.08696400	-2.04147900
	C	3.06406200	-1.40680800	-0.75111300	C	2.63202400	-1.64802500	-1.12724800
	H	3.93268000	-1.53471400	-1.38365500	H	3.16196200	-1.97635100	-2.01159300
	C	2.69059700	-2.41797100	0.11810500	C	2.74373400	-2.36167600	0.05475900
	C	1.60014200	-2.31353600	0.96493200	C	2.10418200	-1.99320600	1.22660400
$C_{12}H_8BrF_2^+$	H	1.35715600	-3.12816200	1.63430200	H	2.23451300	-2.58270100	2.12445900
	C	0.84360800	-1.14781400	0.93620900	C	1.30830100	-0.85403800	1.22085100
	H	-0.01918000	-1.03712600	1.58013400	H	0.80394900	-0.52994200	2.12164200
	C	-1.54298900	0.49879800	-0.04888800	C	-1.63248900	0.51948700	-0.03092700
	F	-5.15449100	-1.35724600	-0.19241900	F	-5.22297900	-1.33758400	-0.08554900
	C	-2.43516300	0.68669400	0.99507100	C	-2.34668300	0.43890700	1.15447600
	H	-2.17616100	1.31528300	1.83918700	H	-1.96270800	0.86003500	2.07455100
	C	-3.67435800	0.05339300	0.94783400	C	-3.58105800	-0.19955700	1.13267000
	H	-4.40353300	0.16780900	1.73954500	H	-4.18296400	-0.29293000	2.02700800
	C	-3.96741900	-0.74260200	-0.14493900	C	-4.03491000	-0.72083300	-0.06690400
	C	-3.08154900	-0.93028900	-1.19562300	C	-3.32028100	-0.63218000	-1.25114900

	H	-3.36552800	-1.56074100	-2.02851000	H	-3.72665100	-1.05286100	-2.16153200
	C	-1.84968100	-0.29200800	-1.14811000	C	-2.08837000	0.00791300	-1.23686300
	H	-1.13592700	-0.41969000	-1.95381600	H	-1.50724900	0.10049000	-2.14546100