

ELECTRONIC SUPPLEMENTARY INFORMATION

Nature of Halogen Bonding Involving π -Systems, Nitroxide Radicals and Carbenes: A Highlight on the Importance of Charge Transfer

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Table S1 Magnitude of energy components for ClF (ClCF₃ for carbene acceptors) XB complexes partitioned using *Scheme B*. Values in parentheses correspond to attractive energy components expressed as a percentage of total *Scheme B* attractive energies. All energies reported are in kJ/mol.

XB acceptor	ClF (ClCF ₃ for carbene acceptors)					
	CLS_ELEC	CLS_PAULI	MOD_PAULI	POL	CT	DISP
H ₂ O	-48.94 (55)	53.13	66.09	-7.42 (8)	-20.38 (23)	-12.96 (14)
NH ₃	-139.58 (52)	193.54	215.64	-24.01 (9)	-80.32 (30)	-22.10 (8)
H ₂ CO	-53.68 (51)	63.06	79.15	-8.98 (9)	-26.14 (25)	-16.09 (15)
H ₂ NO·	-78.96 (51)	100.83	120.33	-14.18 (9)	-41.59 (27)	-19.51 (13)
Me ₂ CO	-73.52 (51)	88.68	109.92	-15.66 (11)	-34.02 (24)	-21.23 (15)
Me ₂ NO·	-76.05 (51)	93.29	114.68	-16.51 (11)	-36.33 (24)	-21.39 (14)
¹ Me ₂ C	-28.39 (57)	24.45	35.43	-3.57 (7)	-7.06 (14)	-10.97 (22)
³ Me ₂ C	-13.79 (43)	11.64	23.40	-1.49 (5)	-4.67 (15)	-11.76 (37)
¹ Ph ₂ C	-35.15 (54)	30.90	46.69	-4.79 (7)	-8.89 (14)	-15.79 (24)
³ Ph ₂ C	-11.74 (37)	8.57	22.81	-1.81 (6)	-3.62 (12)	-14.24 (45)
Ethyne	-36.07 (46)	45.56	61.17	-3.76 (5)	-23.20 (30)	-15.61 (20)
Ethene	-53.15 (46)	74.11	93.88	-6.79 (6)	-36.77 (32)	-19.76 (17)
Furan LP	-29.12 (50)	28.05	41.12	-5.32 (9)	-10.55 (18)	-13.07 (23)
Furan π	-42.36 (42)	56.80	78.78	-7.28 (7)	-29.72 (29)	-21.98 (22)
Benzene	-23.63 (38)	25.05	44.61	-4.68 (8)	-14.26 (23)	-19.56 (31)
Benzene Cen	-10.27 (38)	1.27	15.14	-1.84 (7)	-1.07 (4)	-13.87 (51)
Pyridine LP	-180.02 (50)	269.54	299.65	-40.56 (11)	-111.48 (31)	-30.11 (8)
Pyridine π	-19.64 (35)	22.51	40.91	-4.24 (8)	-13.15 (24)	-18.40 (33)
Naphthalene a	-34.02 (39)	42.49	65.76	-6.89 (8)	-23.19 (27)	-23.27 (27)
Naphthalene b	-17.12 (32)	12.08	35.12	-4.25 (8)	-9.01 (17)	-23.04 (43)

Table S2 Magnitude of energy components for BrF (BrCF₃ for carbene acceptors) XB complexes partitioned using *Scheme B*. Values in parentheses correspond to attractive energy components expressed as a percentage of total *Scheme B* attractive energies. All energies reported are in kJ/mol.

XB acceptor	BrF (BrCF ₃ for carbene acceptors)					
	CLS_ELEC	CLS_PAULI	MOD_PAULI	POL	CT	DISP
H ₂ O	-66.56 (56)	70.73	85.86	-12.51 (11)	-24.59 (21)	-15.13 (13)
NH ₃	-170.91 (56)	216.15	239.78	-34.35 (11)	-76.88 (25)	-23.63 (8)
H ₂ CO	-72.02 (53)	82.04	100.38	-14.99 (11)	-30.22 (22)	-18.34 (14)
H ₂ NO·	-100.64 (54)	121.41	142.80	-21.61 (12)	-44.24 (24)	-21.39 (11)
Me ₂ CO	-97.54 (53)	112.99	136.94	-25.39 (14)	-37.62 (20)	-23.95 (13)
Me ₂ NO·	-103.28 (52)	122.88	147.52	-27.38 (14)	-41.52 (21)	-24.63 (13)
¹ Me ₂ C:	-53.20 (58)	52.66	68.05	-7.41 (8)	-15.16 (17)	-15.39 (17)
³ Me ₂ C:	-25.40 (48)	25.81	41.22	-3.11 (6)	-9.50 (18)	-15.41 (29)
¹ Ph ₂ C:	-65.51 (56)	66.06	88.11	-10.37 (9)	-18.33 (16)	-22.05 (19)
³ Ph ₂ C:	-18.38 (40)	16.23	34.33	-3.30 (7)	-6.17 (13)	-18.10 (39)
Ethyne	-55.35 (47)	72.00	91.69	-7.80 (7)	-35.01 (30)	-19.69 (17)

Ethene	-82.07 (47)	115.12	139.86	-14.12 (8)	-53.45 (31)	-24.74 (14)
Furan LP	-43.12 (51)	43.98	60.37	-10.39 (12)	-14.48 (17)	-16.39 (19)
Furan π	-60.99 (44)	81.46	107.82	-13.86 (10)	-38.82 (28)	-26.36 (19)
Benzene	-35.14 (40)	39.66	63.76	-9.16 (10)	-20.17 (23)	-24.10 (27)
Benzene Cen	-14.40 (42)	2.42	18.94	-3.23 (9)	-0.50 (1)	-16.52 (48)
Pyridine LP	-29.02 (53)	35.17	57.89	-8.18 (14)	-18.41 (25)	-22.72 (8)
Pyridine π	-205.34 (37)	274.86	306.30	-53.28 (10)	-94.45 (24)	-31.45 (29)
Naphthalene a	-50.80 (41)	65.47	93.76	-13.47 (11)	-32.05 (26)	-28.29 (23)
Naphthalene b	-24.05 (34)	18.18	45.71	-7.59 (11)	-10.95 (16)	-27.53 (39)

Table S3 Magnitude of energy components for XF (XCF₃ for carbene acceptors) XB complexes partitioned using *Scheme C*. Values in parentheses correspond to attractive energy components expressed as a percentage of total *Scheme C* attractive energies. All energies reported are in kJ/mol.

Species	ClF (ClCF ₃ for carbene acceptors)				BrF (BrCF ₃ for carbene acceptors)			
	Elec	Exc	Ind	Disp	Elec	Exc	Ind	Disp
H ₂ O	-47.78 (57)	63.81	-20.78 (25)	-15.45 (18)	-65.47 (58)	84.49	-28.75 (25)	-19.17 (17)
NH ₃	-140.30 (55)	210.40	-83.56 (33)	-32.96 (13)	-172.89 (57)	238.37	-91.69 (30)	-37.03 (12)
H ₂ CO	-52.33 (53)	77.74	-27.40 (28)	-19.85 (20)	-70.91 (54)	100.58	-36.52 (28)	-24.00 (18)
Me ₂ CO	-71.25 (52)	107.70	-38.98 (28)	-26.98 (20)	-95.28 (53)	136.69	-51.09 (29)	-32.26 (18)
¹ Me ₂ C:	-30.25 (61)	35.77	-7.52 (15)	-11.53 (23)	-56.25 (62)	69.18	-16.94 (19)	-17.96 (20)
¹ Ph ₂ C:	-37.43 (59)	45.74	-8.52 (13)	-17.64 (28)	-	-	-	-
Ethyne	-33.52 (47)	58.64	-20.83 (29)	-17.23 (24)	-52.05 (48)	89.30	-33.88 (31)	-23.63 (22)
Ethene	-51.92 (46)	94.64	-37.79 (33)	-24.19 (21)	-80.97 (47)	142.40	-59.80 (34)	-32.93 (19)
Furan LP	-28.02 (49)	41.14	-13.10 (23)	-15.95 (28)	-42.08 (50)	61.59	-20.94 (25)	-21.05 (25)
Furan π	-40.64 (41)	78.98	-31.79 (32)	-26.25 (27)	-59.19 (43)	109.50	-46.23 (33)	-33.41 (24)
Benzene	-22.86 (38)	44.75	-15.91 (26)	-22.02 (36)	-34.30 (39)	64.86	-24.95 (28)	-28.59 (33)
Benzene Cen	-9.97 (36)	16.41	-3.45 (12)	-14.58 (52)	-13.90 (37)	22.04	-5.12 (14)	-18.05 (49)
Pyridine LP	-184.15 (52)	290.32	-121.47 (34)	-47.65 (13)	-210.63 (55)	301.55	-120.18 (31)	-51.14 (13)
Pyridine π	-18.13 (34)	40.77	-14.64 (27)	-20.77 (39)	-27.14 (35)	58.59	-22.64 (30)	-26.94 (35)
Naphthalene a	-32.27 (38)	65.44	-25.62 (30)	-27.35 (32)	-48.82 (39)	94.71	-39.65 (32)	-35.29 (29)
Naphthalene b	-15.66 (30)	34.86	-10.99 (21)	-24.99 (48)	-22.11 (32)	46.52	-15.72 (23)	-31.08 (45)

Fully Optimized Geometries

H₂O...ClF

O 2.2110316080 0.0007603041 0.0884027128
H 2.5109528907 0.7654575308 -0.4096062259
H 2.5095035880 -0.7633326912 -0.4114234430
Cl -0.3052955969 -0.0012854727 0.0257630589
F -1.9465204661 0.0015161960 -0.0360182261

H₂O...BrF

O 2.3474824903 0.0006249921 0.0781398191
H 2.6637050417 0.7660976291 -0.4093000129
H 2.6618121519 -0.7649743321 -0.4103547122
Br -0.1845655433 -0.0004533764 0.0176393911
F -1.9606203447 0.0010827710 -0.0469825020

NH₃...ClF

N -2.1558302538 -0.0040343185 -0.0151216179
H -2.4957155206 -0.0726208370 -0.9648992789
H -2.5118402996 -0.7862618969 0.5172332312
H -2.4994559834 0.8539203192 0.3947021011
Cl 0.1419852477 -0.0231470256 0.0055767582
F 1.8256430798 -0.0376928679 0.0227895553

NH₃...BrF

N -2.2993739502 -0.0139426351 -0.0134183084
H -2.6394476166 -0.0575305444 -0.9650738013
H -2.6596770604 -0.8092671301 0.4969022367
H -2.6474378008 0.8323019164 0.4174711695
Br 0.0550035060 -0.0366132054 0.0059484094
F 1.8722398237 -0.0596387797 0.0221099414

H₂CO...ClF

O 1.8577657613 -0.6332564117 0.0395861286
C 2.5219927734 0.3691090468 0.0090792989
H 2.0558129426 1.3659220324 -0.0206433287
H 3.6206682374 0.3192925482 0.0098879307
Cl -0.5414711552 -0.1221188465 0.0105919020
F -2.1210796791 0.3362817946 -0.0137279054

H₂CO...BrF

O 1.9260316779 -0.4998242410 -0.0032590493
C 2.5929876526 0.5032022237 -0.0006869065
H 2.1287888939 1.5003228773 0.0023739484
H 3.6902057041 0.4460927979 -0.0012021090
Br -0.5166026353 -0.1065547190 -0.0003751864
F -2.2551696794 0.2787231560 0.0014644494

H₂NO···ClF

O 1.8053605465 -0.7401858012 0.0293795361
N 2.4161210527 0.3733259697 -0.0029457753
H 1.8780540910 1.2320335002 -0.0130176095
H 3.4262760644 0.3781487479 0.0192855154
Cl -0.4722139042 -0.1384431582 0.0082368232
F -2.0246376010 0.4296469176 -0.0083780786

H₂NO···BrF

O 2.1188267612 -0.7009795098 0.0405200238
N 2.7682132806 0.3910698794 0.0051985904
H 2.2614561815 1.2686247164 -0.0151173161
H 3.7779266438 0.3551695070 0.0078016602
Br -0.2055628407 -0.1334522710 0.0173770129
F -1.8996128246 0.4363523325 -0.0030933668

Me₂CO···ClF

O -0.6871613208 -0.8818467678 0.0044290584
C -1.5198703286 0.0039195897 0.0023940705
C -1.1115545445 1.4531984164 -0.0025268162
C -2.9820200340 -0.3637009170 0.0047572206
H -1.9613630392 2.1288024169 -0.0020855913
H -0.4911275213 1.6403310797 -0.8788704710
H -0.4862474169 1.6449934727 0.8692924799
H -3.6388344494 0.5009989684 0.0026510810
H -3.1841649090 -0.9763664744 0.8828845998
H -3.1856223477 -0.9817005885 -0.8692875240
Cl 1.6561282855 -0.4316151382 -0.0009722967
F 3.2858149038 -0.1412477169 -0.0050904602

Me₂CO···BrF

O 1.0911458114 -0.7277365185 -0.4545642881
C 1.9986239501 0.0146002988 -0.1268950990
C 1.7544700981 1.4477368494 0.2510779004
C 3.4086003299 -0.4942086511 -0.0694786801
H 2.6585243540 2.0463446919 0.1679241099
H 1.4201195789 1.4712108400 1.2908125543
H 0.9568319807 1.8660792276 -0.3576708268
H 4.0111411612 0.0355234529 -0.8091773964
H 3.4369280465 -1.5618560414 -0.2645398988
H 3.8397704736 -0.2720903384 0.9077013247
Br -1.2555043790 -0.1727297057 -0.3218057520
F -3.0036740433 0.2041311881 -0.2109460164

Me₂NO···ClF

N 1.6226550719 0.0075821902 0.1429505906
O 0.6718346517 0.8361182931 -0.0479844221
C 1.3671567011 -1.4105183617 -0.0282961350
H 1.3440572561 -1.6660999489 -1.0912733613
H 0.4051865248 -1.6462966580 0.4147844907
H 2.1544885590 -1.9778232555 0.4621219942
C 2.9734062517 0.5139338088 -0.0118352368
H 2.9879601619 1.5388388176 0.3447706414
H 3.2703829467 0.4925556081 -1.0641258089
H 3.6616525490 -0.0971382786 0.5679121353

Cl -1.6176759299 0.2032154619 -0.0102673450
F -3.2333197359 -0.1623570550 0.0182626941

Me₂NO···BrF

N -1.9952300000 -0.3498400000 0.3514700000
O -0.8865900000 -0.8265400000 -0.0658300000
C -2.1699400000 1.0886300000 0.4211400000
H -2.3278500000 1.4989300000 -0.5797900000
H -1.2751600000 1.5299400000 0.8486900000
H -3.0316900000 1.3117100000 1.0449000000
C -3.1546400000 -1.2136900000 0.2332200000
H -2.8302800000 -2.2333700000 0.4145300000
H -3.5812200000 -1.1421100000 -0.7708200000
H -3.9037400000 -0.9201300000 0.9648200000
Br 1.1664400000 0.3976400000 -0.0930800000
F 2.7457800000 1.2505100000 -0.1165900000

Ethyne···ClF

C 2.3174197714 -0.5988730423 0.0000012895
C 2.3174046039 0.5988870921 0.0000008083
H 2.3245414667 -1.6624826205 0.0000014264
H 2.3244967454 1.6624968719 0.0000007934
Cl -0.4738254977 -0.0000033895 -0.0000011045
F -2.1146745892 -0.0000000609 0.0000019489

Ethyne···BrF

C 2.5309482328 -0.5995479923 -0.0000040412
C 2.5309353252 0.5995605451 -0.0000043871
H 2.5511711994 -1.6632942358 -0.0000040742
H 2.5511348878 1.6633072539 -0.0000047561
Br -0.2382062889 -0.0000034357 0.0000006113
F -2.0169033558 -0.0000066041 -0.0000086405

Ethene···ClF

C 2.1925375957 -0.6648414917 -0.0000016331
C 2.1925549055 0.6648267012 0.0000051666
H 2.1991654631 -1.2299876968 0.9221794871
H 2.1991622997 -1.2299780497 -0.9221886976
H 2.1991994827 1.2299632907 0.9221920678
H 2.1991957594 1.2299724968 -0.9221761164
Cl -0.4909714914 0.0000061990 0.0000004642
F -2.1418940121 0.0000063214 0.0000038864

Ethene···BrF

C 2.4238921696 -0.6669611233 -0.0000008540
C 2.4239059067 0.6669428612 0.0000059833
H 2.4380574216 -1.2312870661 0.9223567092
H 2.4380551801 -1.2312774673 -0.9223643263
H 2.4380845472 1.2312590281 0.9223693118
H 2.4380819880 1.2312682642 -0.9223517377
Br -0.2359014958 0.0000050333 0.0000022401
F -2.0279217146 0.0000056129 0.0000070755

Furan···ClF (LP)

C 2.74384 -0.73379 0.00156

C	2.76618	0.70076	0.00165
C	1.44348	-1.09047	-0.00146
O	0.65140	0.01618	-0.00306
C	1.47748	1.09779	-0.00096
H	3.58659	-1.40216	0.00347
H	0.92991	-2.03444	-0.00270
H	0.99335	2.05726	-0.00220
H	3.62929	1.34266	0.00352
Cl	-1.93879	0.00878	0.00057
F	-3.57230	-0.00819	-0.00035

Furan...BrF (LP)

C	3.03375	-0.57283	-0.45585
C	2.97235	0.84776	-0.26181
C	1.77196	-1.02778	-0.32755
O	0.92475	0.00814	-0.06720
C	1.67813	1.14356	-0.03108
H	3.90516	-1.16828	-0.66313
H	1.31793	-2.00019	-0.38675
H	1.14339	2.05424	0.16712
H	3.78797	1.54823	-0.29181
Br	-1.61383	-0.18934	0.35196
F	-3.35744	-0.30160	0.64121

Furan...ClF (π)

C	-1.08027	-0.61350	0.98619
C	-1.67286	-1.13957	-0.20890
C	-1.08490	0.73662	0.84104
O	-1.63333	1.08471	-0.34581
C	-1.98148	-0.07004	-0.97107
H	-0.72797	-1.16169	1.84236
H	-0.77052	1.54569	1.47497
H	-2.42735	0.03967	-1.94273
H	-1.83236	-2.17293	-0.46077
Cl	1.53157	-0.01865	0.11841
F	3.07970	-0.00971	-0.44905

Furan...BrF (π)

C	-1.49185	-0.26903	1.11033
C	-2.04039	-1.20443	0.17144
C	-1.56544	0.94968	0.50860
O	-2.11885	0.83769	-0.72012
C	-2.39576	-0.47916	-0.90853
H	-1.13561	-0.46729	2.10618
H	-1.31831	1.94470	0.83217
H	-2.83081	-0.73494	-1.85733
H	-2.13875	-2.26875	0.29000
Br	1.12722	0.15588	0.14642
F	2.83428	0.05568	-0.37282

Benzene...ClF (Rim)

C	-1.0907986795	-0.6950905922	1.1535814418
C	-1.5049461518	-1.3896660300	0.0219499568
C	-1.9166304967	-0.6952790490	-1.1039750686
H	-1.5015226305	-2.4713057968	0.0215405725

C -1.0908236182 0.6952253402 1.1535042370
H -0.7750575249 -1.2360596984 2.0356040571
C -1.5049967383 1.3896600669 0.0217963527
H -0.7750987180 1.2363035921 2.0354656313
C -1.9166567224 0.6951330780 -1.1040514739
H -2.2361098515 -1.2354864412 -1.9848272993
H -1.5016135194 2.4712998844 0.0212663048
H -2.2361572552 1.2352312563 -1.9849630733
Cl 1.6755885647 0.0000090169 0.2389678651
F 3.2229521863 0.0000064740 -0.2976321663

Benzene···BrF (Rim)

C -1.4677443772 -0.6956796311 1.1342376069
C -1.9097983393 -1.3905455032 0.0114577832
C -2.3483234431 -0.6958694966 -1.1025243889
H -1.9056909693 -2.4720522618 0.0110995388
C -1.4677695569 0.6958270576 1.1341519745
H -1.1384390434 -1.2365766391 2.0113134558
C -1.9098493354 1.3905386666 0.0112877322
H -1.1384796991 1.2368437015 2.0111597052
C -2.3483499179 0.6957096372 -1.1026089836
H -2.6888049068 -1.2354498011 -1.9757409354
H -1.9057824072 2.4720454810 0.0107958918
H -2.6888526229 1.2351703670 -1.9758912181
Br 1.3012675970 0.0000076396 0.2309592649
F 2.9758754485 0.0000021186 -0.3544999735

Benzene···ClF (Cen)

C 1.3884565122 0.0000000000 1.4277915514
C 0.6942282561 -1.2024386116 1.4277915514
C -0.6942282561 -1.2024386116 1.4277915514
H 1.2350824316 -2.1392255231 1.4255607313
C 0.6942282561 1.2024386116 1.4277915514
H 2.4701648632 0.0000000000 1.4255607313
C -0.6942282561 1.2024386116 1.4277915514
H 1.2350824316 2.1392255231 1.4255607313
C -1.3884565122 0.0000000000 1.4277915514
H -1.2350824316 -2.1392255231 1.4255607313
H -1.2350824316 2.1392255231 1.4255607313
H -2.4701648632 0.0000000000 1.4255607313
Cl 0.0000000000 0.0000000000 -1.8405024419
F 0.0000000000 0.0000000000 -3.4701915334

Benzene···BrF (Cen)

C 1.3886655792 0.0000000000 1.7784754108
C 0.6943327896 -1.2026196690 1.7784754108
C -0.6943327896 -1.2026196690 1.7784754108
H 1.2351763793 -2.1393882453 1.7777457851
C 0.6943327896 1.2026196690 1.7784754108
H 2.4703527586 0.0000000000 1.7777457851
C -0.6943327896 1.2026196690 1.7784754108
H 1.2351763793 2.1393882453 1.7777457851
C -1.3886655792 0.0000000000 1.7784754108
H -1.2351763793 -2.1393882453 1.7777457851
H -1.2351763793 2.1393882453 1.7777457851

H -2.4703527586 0.0000000000 1.7777457851
Br 0.0000000000 0.0000000000 -1.5398153530
F 0.0000000000 0.0000000000 -3.3020677157

Pyridine...ClF (LP)

C 1.0853378723 -1.1491441174 0.0019280686
N 0.3777587039 -0.0247480417 0.0023449852
C 1.0021317606 1.1479244172 0.0002425058
C 2.4695142810 -1.1444570862 -0.0006933499
H 0.5147717717 -2.0686955479 0.0037347624
C 3.1280029182 0.0752225832 -0.0028954456
H 3.0136134677 -2.0774287645 -0.0010693572
C 2.3828892292 1.2440150242 -0.0024097308
H 0.3663272202 2.0235608101 0.0007223240
H 4.2087641622 0.1144928468 -0.0049629850
H 2.8576312909 2.2141589474 -0.0040677771
Cl -1.8024848405 -0.0953378581 0.0067956398
F -3.5034830508 -0.1555833046 0.0110995718

Pyridine...BrF (LP)

C 1.6177013512 -1.1550828475 0.0031384679
N 0.9046678458 -0.0323234755 0.0047488841
C 1.5278055958 1.1428870587 0.0023205145
C 3.0014471111 -1.1450108404 -0.0008540775
H 1.0520586448 -2.0774700340 0.0047959243
C 3.6565857135 0.0763440339 -0.0038407901
H 3.5478128297 -2.0765576422 -0.0010284486
C 2.9076211052 1.2425205703 -0.0022885489
H 0.8907026383 2.0172406044 0.0042204373
H 4.7371566379 0.1190010963 -0.0075496970
H 3.3784066853 2.2144971150 -0.0047348924
Br -1.3591123555 -0.0955294961 0.0077638775
F -3.1891369865 -0.1490147907 0.0102337155

Pyridine...ClF (π)

C -1.2800966989 -1.3104817701 0.1346952321
N -1.7307395345 -0.8816903153 -1.0414337999
C -1.9536513516 0.4233634985 -1.1686860551
C -1.0401361732 -0.4735202861 1.2183353196
H -1.1003616087 -2.3760687203 0.2185500055
C -1.2788008671 0.8863431842 1.0683206988
H -0.6871737265 -0.8829864963 2.1545760802
C -1.7439977012 1.3448429291 -0.1516260701
H -2.3198635681 0.7514065659 -2.1344478392
H -1.1016175115 1.5710072957 1.8866384913
H -1.9412557583 2.3939353170 -0.3200567411
Cl 1.6843399855 -0.1745614702 0.1713584322
F 3.2319514557 0.0099393213 -0.3246716829

Pyridine...BrF (π)

C -1.6704097113 -1.3080568288 0.0735930870
N -2.1473129738 -0.8388833406 -1.0767145605
C -2.3858496545 0.4671439332 -1.1494046666
C -1.4212378049 -0.5103648109 1.1862822771
H -1.4774029997 -2.3738826915 0.1131499498

C -1.6770578141 0.8533436150 1.0916250156
H -1.0605164223 -0.9531249061 2.1043963353
C -2.1668092363 1.3522897054 -0.1016497222
H -2.7732405862 0.8277425226 -2.0949967924
H -1.4937956167 1.5078418386 1.9329022009
H -2.3760290641 2.4049767377 -0.2270872330
Br 1.3015640074 -0.1856921954 0.1353499863
F 2.9759199101 0.0402290574 -0.3974014097

Naphthalene...ClF (a)

C -0.2825635033 2.3309848239 -0.4072611596
C -0.6620370486 1.8542091509 0.8707740889
C -0.0479826351 0.7548529324 1.4068652118
H -1.4326573393 2.3694887280 1.4278136107
C 0.9731299771 0.0733730278 0.6921055319
H -0.3228168868 0.3979874323 2.3915423724
C 0.6955281686 1.6956879738 -1.1111751337
H -0.7776516046 3.1984625033 -0.8211153256
C 1.3482132980 0.5500504666 -0.5839062509
H 0.9885825967 2.0554463714 -2.0895638830
C 1.6174411557 -1.0712164218 1.2176603357
C 2.3615569902 -0.1308957650 -1.3004377880
C 2.5918075216 -1.7090240950 0.5046443009
H 1.3215248760 -1.4356225086 2.1933679472
C 2.9688049481 -1.2326828600 -0.7697818022
H 2.6457895270 0.2369691198 -2.2783567095
H 3.0791226403 -2.5835420286 0.9137196109
H 3.7409307273 -1.7472239406 -1.3253323768
Cl -2.3651012080 -0.4106956598 0.2416625507
F -3.5507215599 -1.4068461101 -0.3142387068

Naphthalene...BrF (a)

C 0.2581917015 2.3857196175 -0.4175893475
C -0.1587688514 1.9135844042 0.8522787137
C 0.4039616934 0.7840502285 1.3877036565
H -0.9070774677 2.4611324142 1.4086801102
C 1.4105998419 0.0700950610 0.6812742540
H 0.1104683131 0.4384265690 2.3709301073
C 1.2209089455 1.7188070997 -1.11110036487
H -0.1978044108 3.2744514592 -0.8308313360
C 1.8226063831 0.5438811018 -0.5838186260
H 1.5419518585 2.0743312915 -2.0820620213
C 2.0055339559 -1.0991731805 1.2081949035
C 2.8207601382 -0.1667540594 -1.2908668563
C 2.9685077717 -1.7653351594 0.5047949028
H 1.6817488864 -1.4604914969 2.1760924701
C 3.3808135777 -1.2936713655 -0.7595810908
H 3.1323095435 0.1976662031 -2.2616216903
H 3.4186580079 -2.6591662478 0.9145732127
H 4.1423535568 -1.8311683647 -1.3078326945
Br -2.0202329578 -0.2044820605 0.2526574755
F -3.3990855391 -1.1881846879 -0.3076221874

Naphthalene...ClF (b)

C 2.4185792950 -0.7069590826 1.0447523686

C 2.4185792950 0.7069590826 1.0447523686
 C 1.2413861647 1.3951495405 1.0424531472
 H 3.3588465276 1.2412604071 1.0435926169
 C 0.0000000000 0.7083547484 1.0412057510
 H 1.2361672415 2.4779880708 1.0391435902
 C 1.2413861647 -1.3951495405 1.0424531472
 H 3.3588465276 -1.2412604071 1.0435926169
 C 0.0000000000 -0.7083547484 1.0412057510
 H 1.2361672415 -2.4779880708 1.0391435902
 C -1.2413861647 1.3951495405 1.0424531472
 C -1.2413861647 -1.3951495405 1.0424531472
 C -2.4185792950 0.7069590826 1.0447523686
 H -1.2361672415 2.4779880708 1.0391435902
 C -2.4185792950 -0.7069590826 1.0447523686
 H -1.2361672415 -2.4779880708 1.0391435902
 H -3.3588465276 1.2412604071 1.0435926169
 H -3.3588465276 -1.2412604071 1.0435926169
 Cl 0.0000000000 0.0000000000 -1.9503980988
 F 0.0000000000 0.0000000000 -3.5851204634

Naphthalene...BrF (b)

C 2.4187848834 -0.7070279827 1.4046203389
 C 2.4187848834 0.7070279827 1.4046203389
 C 1.2420771837 1.3955857418 1.3947665642
 H 3.3590408112 1.2411834999 1.4084882521
 C 0.0000000000 0.7088938327 1.3887749044
 H 1.2368372733 2.4783465821 1.3906906571
 C 1.2420771837 -1.3955857418 1.3947665642
 H 3.3590408112 -1.2411834999 1.4084882521
 C 0.0000000000 -0.7088938327 1.3887749044
 H 1.2368372733 -2.4783465821 1.3906906571
 C -1.2420771837 1.3955857418 1.3947665642
 C -1.2420771837 -1.3955857418 1.3947665642
 C -2.4187848834 0.7070279827 1.4046203389
 H -1.2368372733 2.4783465821 1.3906906571
 C -2.4187848834 -0.7070279827 1.4046203389
 H -1.2368372733 -2.4783465821 1.3906906571
 H -3.3590408112 1.2411834999 1.4084882521
 H -3.3590408112 -1.2411834999 1.4084882521
 Br 0.0000000000 0.0000000000 -1.6438032366
 F 0.0000000000 0.0000000000 -3.4126607179

¹Me₂C:...ClCF₃

C 2.5072245985 0.0023783483 -0.1024523481
 C 3.3131272743 1.2247372065 -0.1941469681
 C 3.3068976734 -1.2240126974 -0.1954101387
 H 2.8371076445 2.0872373113 0.2700626936
 H 3.2535484412 1.4293482192 -1.2777738680
 H 4.3743672734 1.1516563555 0.0749310908
 H 2.8264433574 -2.0844291636 0.2681137964
 H 4.3684715176 -1.1566117523 0.0738357248
 H 3.2463332262 -1.4274811584 -1.2791726701
 Cl -0.6203770550 0.0008976909 -0.0227247348
 C -2.3674812915 -0.0008416183 0.0127064227
 F -2.8677111948 0.0002529761 -1.2221902070

F -2.8311940635 1.0764535608 0.6461902972
F -2.8291284335 -1.0806534831 0.6434326902

¹Me₂C:···BrCF₃

C 2.9235033735 0.0009971398 0.0563745551
C 3.7264602604 1.2255289543 0.0029734008
C 3.7189574545 -1.2284204100 0.0031205221
H 3.2259121217 2.0837979911 0.4491818946
H 3.7125418455 1.4350588022 -1.0813822999
H 4.7746605117 1.1548389025 0.3176206432
H 3.2131062127 -2.0835704223 0.4493455957
H 4.7675556766 -1.1641672339 0.3178232530
H 3.7037963442 -1.4379250466 -1.0812270180
Br -0.0891287716 0.0011874304 0.0181604036
C -2.0123110458 -0.0000982113 -0.0101835941
F -2.4729569755 0.0002194095 -1.2629646917
F -2.5015673373 1.0779757633 0.6058318172
F -2.5001469523 -1.0794406155 0.6047547708

³Me₂C:···ClCF₃

C 3.2452066417 -0.0022007469 0.5858836565
C 3.4295107464 1.3432229987 0.0363995624
C 3.4254179143 -1.3469972084 0.0334910184
H 3.1451375897 2.1122622019 0.7556368240
H 2.8200873117 1.4982290851 -0.8644213175
H 4.4754472747 1.5285777466 -0.2419593025
H 3.1416741916 -2.1167806740 0.7521768140
H 4.4702513267 -1.5337111750 -0.2480949512
H 2.8132649125 -1.4993801800 -0.8659220317
Cl 0.1258183365 0.0002543639 0.3173458080
C -1.5742244180 0.0011647592 -0.1139013693
F -1.7180250665 -0.0070548443 -1.4354127763
F -2.1756094404 1.0838270168 0.3674908504
F -2.1802861918 -1.0725509561 0.3814401062

³Me₂C:···BrCF₃

C 3.2700885325 -0.0018049915 0.5241464733
C 3.5378393626 1.3441437911 0.0119547906
C 3.5339378803 -1.3483369004 0.0114247497
H 3.1694783208 2.1121875662 0.6931174877
H 3.0542969300 1.5112258784 -0.9600383469
H 4.6137352814 1.5162439354 -0.1230953063
H 3.1637548442 -2.1155906675 0.6924916625
H 4.6093073013 -1.5233338230 -0.1240949297
H 3.0495801830 -1.5138133953 -0.9604350072
Br 0.2264019946 0.0002423700 0.2654870798
C -1.6659379161 0.0010544936 -0.0945925418
F -1.8905067283 -0.0005411465 -1.4054266480
F -2.2400568263 1.0804563918 0.4278003699
F -2.2415364417 -1.0761510488 0.4306894187

¹Ph₂C:···ClCF₃

C 3.3998183455 -2.5843132941 0.7689627233
C 2.7632699552 -1.3578307090 0.7073157684
C 1.5242619190 -1.2254100843 0.0502940279

C 0.9528186710 -2.3708804813 -0.5328238163
 C 1.6272978285 -3.5771532254 -0.5330702962
 C 2.8447383573 -3.6865970731 0.1299715318
 H 4.3342800090 -2.6837206129 1.3045408232
 H 3.1940416696 -0.4976130455 1.2014063133
 H -0.0206592677 -2.2739659475 -0.9944577392
 H 1.1938032167 -4.4420530106 -1.0160704499
 H 3.3552932311 -4.6399273749 0.1639352625
 C 0.7733818779 -0.0006565002 -0.0046010820
 C 1.5195765863 1.2271578139 -0.0547847932
 C 0.9403390622 2.3698726284 0.5260415653
 C 2.7616477952 1.3650092364 -0.7048849147
 C 1.6100328779 3.5787954774 0.5310237772
 H -0.0352618235 2.2687440813 0.9822639397
 C 3.3936061743 2.5940735452 -0.7620610172
 H 3.1985334784 0.5068891693 -1.1972573629
 C 2.8306587390 3.6936222049 -0.1252233672
 H 1.1704891545 4.4415365864 1.0124106027
 H 4.3305779210 2.6976451277 -1.2924489437
 H 3.3376465909 4.6489773507 -0.1555858727
 C -4.0518877689 -0.0035966803 0.0009322913
 F -4.5266678946 -1.1764265174 0.4205116648
 F -4.5245768308 0.9454215775 0.8092238846
 F -4.5311981121 0.2207223638 -1.2224910153
 Cl -2.3028831252 -0.0039724932 -0.0034632403

¹Ph₂C:···BrCF₃

C 3.6504545589 -2.5892574538 0.7666738036
 C 3.0176921309 -1.3613055034 0.7025354809
 C 1.7783869110 -1.2273451318 0.0459571005
 C 1.2020083457 -2.3724126996 -0.5336002452
 C 1.8723476950 -3.5808477475 -0.5296449945
 C 3.0902674857 -3.6917069434 0.1321592244
 H 4.5850278250 -2.6902541806 1.3015800762
 H 3.4505288103 -0.5013482222 1.1951189859
 H 0.2297189409 -2.2748108883 -0.9974264556
 H 1.4355483258 -4.4458348337 -1.0092838786
 H 3.5976755949 -4.6465850499 0.1686474592
 C 1.0340294708 -0.0002626489 -0.0094312836
 C 1.7759418464 1.2287166094 -0.0552086836
 C 1.1905015026 2.3714404092 0.5198614054
 C 3.0223027053 1.3666118153 -0.6974886613
 C 1.8582065660 3.5813258184 0.5258448733
 H 0.2133437127 2.2709800945 0.9726825049
 C 3.6530133634 2.5960722567 -0.7521151828
 H 3.4626280864 0.5084819747 -1.1866256121
 C 3.0832940155 3.6961150171 -0.1218853469
 H 1.4141246406 4.4443735159 1.0022785142
 H 4.5934057114 2.7001160981 -1.2761446210
 H 3.5890866009 4.6521117321 -0.1506892053
 C -3.8563905000 -0.0013101193 0.0039490734
 F -4.3357246941 -1.1694390377 0.4379497454
 F -4.3309457411 0.9573381355 0.8032995792
 F -4.3435986715 0.2098958279 -1.2209933494
 Br -1.9299032572 -0.0027592805 -0.0053685354

³Ph₂C:···ClCF₃

C 3.2806042220 -2.9212475192 0.6517193637
C 2.8135446892 -1.6229101759 0.6232395048
C 1.5719217926 -1.3173393950 0.0154741680
C 0.8250730852 -2.3798847166 -0.5391336146
C 1.3030592757 -3.6738263667 -0.4955424026
C 2.5313769475 -3.9539781809 0.0959151761
H 4.2329150597 -3.1358917550 1.1181483019
H 3.3887344567 -0.8238154503 1.0712510858
H -0.1265397089 -2.1635394636 -1.0050406563
H 0.7178410891 -4.4738194967 -0.9284989658
H 2.9011352412 -4.9695725653 0.1261929716
C 1.0961577502 0.0010393358 0.0010790532
C 1.5639223063 1.3222610182 -0.0141224081
C 0.8113063861 2.3803738527 0.5411922644
C 2.8028684948 1.6351886922 -0.6235895284
C 1.2814508469 3.6771625436 0.4967480531
H -0.1385017515 2.1582793086 1.0080736284
C 3.2619888047 2.9363341701 -0.6530490666
H 3.3822655891 0.8394637474 -1.0721756696
C 2.5072546458 3.9646106436 -0.0964386527
H 0.6920133228 4.4737053849 0.9303450450
H 4.2123088606 3.1566633863 -1.1208777120
H 2.8707759313 4.9824357692 -0.1274649662
C -3.8677000950 -0.0066244332 -0.0002273087
F -4.3307003276 -1.1977790280 0.3620457999
F -4.3296436725 0.9024294810 0.8514065165
F -4.3329671503 0.2757237694 -1.2118785971
Cl -2.1132470906 -0.0065887087 -0.0023410674

³Ph₂C:···BrCF₃

C 3.5497607464 -2.9086751304 0.6738608218
C 3.0725365399 -1.6142143974 0.6430230143
C 1.8383456843 -1.3162971407 0.0163507676
C 1.1095058074 -2.3822962992 -0.5548063063
C 1.5971667428 -3.6725365400 -0.5082250537
C 2.8177698885 -3.9451306431 0.1021592680
H 4.4961379902 -3.1174002865 1.1547571411
H 3.6339152965 -0.8120122146 1.1028209921
H 0.1645712379 -2.1723376731 -1.0365210725
H 1.0256684816 -4.4752522361 -0.9541921458
H 3.1951467443 -4.9578428241 0.1346491352
C 1.3575758566 0.0009029270 0.0000800226
C 1.8330610907 1.3200600044 -0.0159368764
C 1.1001885148 2.3829982759 0.5557551337
C 3.0658400379 1.6230190646 -0.6429371703
C 1.5828247272 3.6751499540 0.5094792495
H 0.1562379594 2.1692289243 1.0377030783
C 3.5379971069 2.9193504276 -0.6735252888
H 3.6302101454 0.8231473531 -1.1031316545
C 2.8021361067 3.9527278891 -0.1012357173
H 1.0083577220 4.4754680508 0.9559444978
H 4.4833918447 3.1319420762 -1.1546543651
H 3.1755228958 4.9669284950 -0.1334984461

C -3.7536280144 -0.0031067948 0.0010610632
F -4.2185037292 -1.1952106591 0.3595817761
F -4.2152422263 0.9033790927 0.8563619271
F -4.2207338018 0.2839453659 -1.2093057253
Br -1.8304630519 -0.0044945710 -0.0026459677

Optimized Geometries on Frozen PESes

Ethyne...ClF (Frozen)

C 2.5664351159 -0.5979121901 0.0000012256
C 2.5664238930 0.5979304285 0.0000008887
H 2.5761844428 -1.6610778649 0.0000014598
H 2.5761532689 1.6610963261 0.0000007757
Cl -0.9819962904 -0.0000061204 -0.0000007666
F -2.6078379298 -0.0000057284 0.0000015788

Ethyne...BrF (Frozen)

C 2.5942330638 -0.5980116620 0.0000011914
C 2.5942230775 0.5980307260 0.0000008575
H 2.6061856355 -1.6612912299 0.0000015107
H 2.6061577618 1.6613105563 0.0000008254
Br -0.9743119641 -0.0000068696 -0.0000009755
F -2.7311250741 -0.0000066700 0.0000017525

Ethene...ClF (Frozen)

C 2.8331197255 0.6617603203 0.0000678262
C 2.8331335779 -0.6617447202 0.0000718262
H 2.8383986823 1.2284817594 -0.9218843818
H 2.8383988689 1.2284873881 0.9220164989
H 2.8384243129 -1.2284715664 -0.9218769602
H 2.8384244639 -1.2284660578 0.9220239346
Cl -0.6594813294 -0.0000137381 -0.0000148569
F -2.2853083021 -0.0000133854 -0.0000738869

Ethene...BrF (Frozen)

C 2.6426444767 -0.6620233454 -0.0000010728
C 2.6426535920 0.6620010544 0.0000056983
H 2.6492655876 -1.2283817297 0.9221873164
H 2.6492638262 -1.2283722463 -0.9221953074
H 2.6492823562 1.2283498809 0.9221998987
H 2.6492804689 1.2283592461 -0.9221827624
Br -0.8944904542 0.0000075644 0.0000034296
F -2.6516458505 0.0000147186 0.0000072014

H₂CO...ClF (Frozen)

O 2.1736321283 -0.5774591768 0.0369936961
C 2.8672211794 0.4008757709 0.0093813511
H 2.4363632410 1.4161493541 -0.0222534658
H 3.9675288289 0.3290346002 0.0150313020
Cl -0.7877749586 -0.2384873753 0.0120762359
F -2.3767304190 0.1162348269 -0.0057331192

H₂CO...BrF (Frozen)

O 2.1899000894 -0.5518783183 0.0318591211
C 2.9067455811 0.4102749246 0.0094339715
H 2.5003427515 1.4350023660 -0.0269228625
H 4.0042897952 0.3103083400 0.0233619421
Br -0.8005187453 -0.2661677293 0.0090759566
F -2.5205194720 0.1088084171 -0.0013121287

H₂NO⁺...ClF(Frozen)

O 2.0502130322 -0.7779386577 0.0238430309
N 2.6035434433 0.3631504083 -0.0453045050
H 2.0296885300 1.1970361355 -0.0524170020
H 3.6034576014 0.4380379652 0.0877665055
Cl -0.8840374820 -0.1715306056 0.0092977448
F -2.3739048755 0.4857709303 0.0093746371

H₂NO⁺...BrF(Frozen)

O 2.0470401261 -0.7313569298 0.0231466747
N 2.6546859368 0.3820670710 -0.0366577432
H 2.1240421194 1.2439890985 -0.0223340647
H 3.6610005399 0.4028416858 0.0620675347
Br -0.9075111289 -0.1969511435 0.0034971829
F -2.5502973439 0.4339363940 0.0028408269

Me₂CO...ClF (Frozen)

O -0.6853791486 -0.7825033043 -0.1088391030
C -1.5733335464 0.0355976239 -0.0449241152
C -1.2889539329 1.5031820404 0.1569660738
C -3.0232532974 -0.3617981447 -0.1630131201
H -1.8055126382 1.8649237858 1.0470847431
H -1.6755292030 2.0735426239 -0.6890377208
H -0.2203411252 1.6705375020 0.2554227712
H -3.4928668057 0.1776372269 -0.9866818339
H -3.5590106780 -0.0838303846 0.7458786320
H -3.1046679690 -1.4321832121 -0.3266001267
Cl 2.2512074985 -0.6135908607 0.0214115514
F 3.8716181238 -0.4557485556 0.0999075991

Me₂CO...BrF (Frozen)

O -0.2545156828 0.2692839687 0.0476084942
C -1.4309593410 0.5474396316 0.0287735799
C -1.9048563587 1.9718194507 0.1693705501
C -2.4926860793 -0.5088389862 -0.1415985996
H -2.7043056406 2.0406260660 0.9073936192
H -2.3190750700 2.3069558048 -0.7833744284
H -1.0745878045 2.6142287482 0.4467795566
H -3.1760204205 -0.2345203447 -0.9457069588
H -3.0859851920 -0.5743001356 0.7719860403
H -2.0340281902 -1.4707509489 -0.3497016653
Br 2.3214279880 -1.2438801552 -0.0595583492
F 3.8495690697 -2.1222967584 -0.0843964882

Me₂NO⁺...ClF (Frozen)

N -1.7992055126 -0.4033255937 0.2192787342
O -0.6587290342 -0.7927913863 -0.1868883161

C -2.0257391088 1.0237099293 0.3522779221
 H -2.2439863815 1.4702669036 -0.6224421868
 H -1.1237414115 1.4735447751 0.7557310890
 H -2.8632876813 1.2032495115 1.0233298083
 C -2.9341861112 -1.2786840783 -0.0062725324
 H -2.5954566052 -2.3021464816 0.1204417209
 H -3.3228329155 -1.1511855038 -1.0212040890
 H -3.7229104092 -1.0531218324 0.7088059376
 Cl 1.9614534262 0.6154915855 -0.1701714040
 F 3.3987717448 1.3849221713 -0.1578366838

Me₂NO···BrF (Frozen)

N -1.8170853944 -0.4022493818 0.2248774039
 O -0.6721280599 -0.7896447439 -0.1707412887
 C -2.0487961921 1.0238680092 0.3583937575
 H -2.2476324071 1.4730994241 -0.6190784187
 H -1.1571306898 1.4752908585 0.7826503661
 H -2.9003588115 1.1986390121 1.0126185027
 C -2.9466551341 -1.2829053160 -0.0068301099
 H -2.6036616483 -2.3047076851 0.1214261981
 H -3.3303578487 -1.1566515008 -1.0236655898
 H -3.7398861516 -1.0610036070 0.7042667928
 Br 1.9854477886 0.6004551214 -0.1850038956
 F 3.5483945490 1.4157398092 -0.1838637183

Furan···ClF (LP) (Frozen)

C	3.11739	-0.56304	-0.46294
C	3.02910	0.85416	-0.26477
C	1.85866	-1.03592	-0.34864
O	0.99015	-0.02181	-0.09381
C	1.72442	1.12105	-0.04734
H	4.00039	-1.14321	-0.66416
H	1.42628	-2.01745	-0.42029
H	1.17537	2.02499	0.14444
H	3.83087	1.57073	-0.28262
Cl	-1.99551	-0.18423	0.40893
F	-3.59302	-0.26336	0.70631

Furan···BrF (LP) (Frozen)

C	3.1261461450	-0.5619107156	-0.4648624209
C	3.0403280148	0.8558572520	-0.2672413873
C	1.8671709920	-1.0328203653	-0.3514137852
O	0.9996994228	-0.0163904103	-0.0975812084
C	1.7365790819	1.1257638319	-0.0498396888
H	4.0082394640	-1.1444326754	-0.6639209640
H	1.4342332426	-2.0142465779	-0.4196977411
H	1.1893039333	2.0298716980	0.1456847417
H	3.8441382954	1.5703852065	-0.2854822674
Br	-1.9768216759	-0.2199850207	0.4041814948
F	-3.7048969159	-0.2501822233	0.7252832264

Furan···ClF (π) (Frozen)

C	-1.25741	-0.57444	1.08703
C	-1.63273	-1.11543	-0.18678
C	-1.35947	0.76805	0.96710

O	-1.76910	1.10512	-0.28172
C	-1.92980	-0.05464	-0.96802
H	-0.95833	-1.11432	1.96845
H	-1.18880	1.58529	1.64427
H	-2.25484	0.04356	-1.98772
H	-1.67169	-2.15131	-0.47460
Cl	1.93811	-0.13968	-0.18985
F	3.48429	-0.13162	-0.69353

Furan...BrF (π) (Frozen)

C	-1.68555	-0.21507	1.19238
C	-2.04118	-1.17830	0.19076
C	-1.81464	0.99670	0.60666
O	-2.22221	0.86322	-0.67984
C	-2.35426	-0.46711	-0.91379
H	-1.38654	-0.40403	2.20878
H	-1.66628	2.00356	0.95302
H	-2.67330	-0.74174	-1.90267
H	-2.05820	-2.24973	0.28705
Br	1.58083	-0.03851	-0.04003
F	3.24706	-0.04896	-0.59596

Benzene...ClF (Frozen)

C	-1.3865365257	-0.6941163664	1.3210320583
C	-1.5448704450	-1.3882737047	0.1291844641
C	-1.7040838083	-0.6943180244	-1.0629154310
H	-1.5423175517	-2.4701227829	0.1286533121
C	-1.3865952394	0.6942873612	1.3209600163
H	-1.2605235305	-1.2352179584	2.2491477686
C	-1.5449852028	1.3883018870	0.1290367555
H	-1.2606307579	1.2354989449	2.2490184436
C	-1.7041411201	0.6942021439	-1.0629889486
H	-1.8256264676	-1.2357348997	-1.9915236697
H	-1.5425226109	2.4701513200	0.1283844870
H	-1.8257282924	1.2355101420	-1.9916549724
Cl	1.8817415855	-0.0000613702	-0.5517433866
F	3.4949488116	-0.0001255911	-0.7663635597

Benzene...BrF (Frozen)

C	-1.4232811028	-0.6941099907	1.3360028387
C	-1.5641210255	-1.3885289721	0.1418694006
C	-1.7048206428	-0.6945014875	-1.0525973719
H	-1.5622222959	-2.4703431587	0.1416475911
C	-1.4233285093	0.6942765219	1.3359272850
H	-1.3113049376	-1.2352601654	2.2658463623
C	-1.5642170124	1.3885516315	0.1417179604
H	-1.3113898897	1.2355371707	2.2657111067
C	-1.7048689066	0.6943795240	-1.0526736631
H	-1.8115290382	-1.2356230983	-1.9831787340
H	-1.5623934165	2.4703659234	0.1413759122
H	-1.8116164031	1.2353907931	-1.9833149407
Br	1.9332967505	-0.0000697150	-0.5975145108
F	3.6699252748	-0.0000838759	-0.8725918989

Naphthalene...ClF (a) (Frozen)

C -0.2593326996 2.3935289155 -0.3123349754
C -0.5152918520 2.0071709482 1.0235219659
C 0.1135415521 0.9192791621 1.5575022504
H -1.2124168269 2.5789125490 1.6210588494
C 1.0294348694 0.1596805741 0.7861170182
H -0.0796550364 0.6198522851 2.5803345519
C 0.6179960150 1.6811972973 -1.0769194285
H -0.7645150239 3.2560163947 -0.7252411985
C 1.2841266924 0.5460482144 -0.5505575924
H 0.8165089734 1.9725872835 -2.1008684805
C 1.6896970846 -0.9794377280 1.3107900163
C 2.1936246061 -0.2172511905 -1.3244340832
C 2.5607666661 -1.6949211004 0.5424193496
H 1.4882863536 -1.2735765538 2.3334266150
C 2.8160090069 -1.3087197755 -0.7930588030
H 2.3851611565 0.0816068896 -2.3475250055
H 3.0598003880 -2.5625507487 0.9522464493
H 3.5074526688 -1.8850072841 -1.3926075598
Cl -2.3764095581 -0.7581116557 -0.2634403120
F -3.4638843948 -1.7465413361 -0.9614432023

Naphthalene...BrF (a) (Frozen)

C -0.2509686993 2.3967450849 -0.3074900727
C -0.5010256502 2.0141341790 1.0308300895
C 0.1328659196 0.9295120519 1.5663436162
H -1.1967457858 2.5866594506 1.6292935920
C 1.0465357448 0.1682944905 0.7934373965
H -0.0550736875 0.6336974261 2.5912460724
C 0.6248213576 1.6833362738 -1.0728815100
H -0.7606114600 3.2559253947 -0.7216108722
C 1.2948191582 0.5508198057 -0.5456491408
H 0.8183516469 1.9712746482 -2.0987262811
C 1.7076663316 -0.9704276436 1.3179417335
C 2.1994729286 -0.2156435410 -1.3220535532
C 2.5731901084 -1.6894371752 0.5466964003
H 1.5105176219 -1.2620220301 2.3421257690
C 2.8223951446 -1.3069158700 -0.7910038477
H 2.3859117096 0.0799098665 -2.3470049989
H 3.0718917619 -2.5576131591 0.9557025717
H 3.5091148449 -1.8864573802 -1.3927878450
Br -2.4292376331 -0.7698235250 -0.2764306827
F -3.6129907214 -1.8222052070 -1.0389920118

Naphthalene...ClF (b) (Frozen)

C 2.4184698982 -0.7066975159 1.4218728243
C 2.4184703097 0.7066975455 1.4218728109
C 1.2403183876 1.3946278121 1.4300485703
H 3.3587042640 1.2411848982 1.4134259777
C 0.0000001643 0.7076548118 1.4362849602
H 1.2353516934 2.4775882839 1.4276093186
C 1.2403181746 -1.3946278950 1.4300486038
H 3.3587037790 -1.2411849778 1.4134260434
C 0.0000000000 -0.7076545621 1.4362849861

H 1.2353515528 -2.4775883468 1.4276094063
 C -1.2403184421 1.3946284484 1.4300486198
 C -1.2403184187 -1.3946284193 1.4300487902
 C -2.4184698833 0.7066975204 1.4218728401
 H -1.2353520981 2.4775889068 1.4276093660
 C -2.4184699702 -0.7066976622 1.4218729714
 H -1.2353518360 -2.4775888781 1.4276096233
 H -3.3587040402 1.2411845420 1.4134260375
 H -3.3587040031 -1.2411848696 1.4134262395
 Cl 0.0000001997 0.0000001776 -1.9513419912
 F 0.0000002679 0.0000001839 -3.5777068943

Naphthalene...BrF (b) (Frozen)

C 2.4185867808 -0.7067069589 1.4356600241
 C 2.4185866068 0.7067067027 1.4356600222
 C 1.2405272773 1.3948055789 1.4444602202
 H 3.3587956933 1.2411338761 1.4262654408
 C -0.0000003799 0.7077990433 1.4513306303
 H 1.2355946500 2.4777346446 1.4417134339
 C 1.2405274042 -1.3948057040 1.4444603703
 H 3.3587960165 -1.2411338416 1.4262654638
 C -0.0000000962 -0.7077989374 1.4513307650
 H 1.2355945758 -2.4777346911 1.4417136538
 C -1.2405268980 1.3948056923 1.4444602796
 C -1.2405271206 -1.3948057185 1.4444604325
 C -2.4185870529 0.7067069196 1.4356598940
 H -1.2355939742 2.4777347157 1.4417135370
 C -2.4185868670 -0.7067068551 1.4356598867
 H -1.2355941141 -2.4777347442 1.4417137363
 H -3.3587962725 1.2411338811 1.4262652929
 H -3.3587959792 -1.2411339573 1.4262653102
 Br -0.0000001544 0.0000001592 -2.0107141623
 F -0.0000000923 0.0000001974 -3.7689951274

¹Me₂C:...ClCF₃ (Frozen)

C 3.0746780342 0.0012571435 0.0480816989
 C 3.8906468680 1.2210038218 0.0001026675
 C 3.8825875595 -1.2238388789 0.0003756688
 H 3.3925754617 2.0868378257 0.4337636163
 H 3.8957898005 1.4222430315 -1.0855971028
 H 4.9344103749 1.1447120723 0.3312538741
 H 3.3787134504 -2.0864227712 0.4337966454
 H 4.9267318479 -1.1544321124 0.3318452141
 H 3.8867881606 -1.4249606357 -1.0853596585
 Cl -0.5354770215 0.0013152712 0.0129909192
 C -2.2815756018 -0.0001362689 -0.0043383707
 F -2.7394318562 0.0002104550 -1.2539662629
 F -2.7589290480 1.0771556788 0.6138742464
 F -2.7571253120 -1.0789621791 0.6126060965

¹Me₂C:...BrCF₃ (Frozen)

C 3.1187129659 0.0013172797 0.0489051517

C 3.9334880019 1.2214806448 0.0003301067
 C 3.9252245842 -1.2243050410 0.0002411067
 H 3.4352893596 2.0864117952 0.4357587811
 H 3.9358842900 1.4239511398 -1.0851962861
 H 4.9778848521 1.1456579819 0.3291447898
 H 3.4210831570 -2.0860267379 0.4351840032
 H 4.9700163238 -1.1556472119 0.3293797472
 H 3.9266144600 -1.4263316058 -1.0853798402
 Br -0.4772443873 0.0015401140 0.0135325682
 C -2.3907939542 -0.0001950413 -0.0047830204
 F -2.8503986009 -0.0007371752 -1.2540628155
 F -2.8686617038 1.0774585136 0.6130792079
 F -2.8667166302 -1.0785922024 0.6132957522

³Me₂C:···ClCF₃ (Frozen)

C 3.4982320097 -0.0025222782 0.6162441863
 C 3.6172947887 1.3427236565 0.0481539041
 C 3.6148434309 -1.3474938803 0.0469978971
 H 3.4502164499 2.1121982655 0.8027517722
 H 2.8879683069 1.5113771434 -0.7559290500
 H 4.6142687934 1.5169439103 -0.3784799971
 H 3.4459513765 -2.1173110378 0.8008431821
 H 4.6116251590 -1.5233246231 -0.3794245440
 H 2.8854787171 -1.5139684148 -0.7575041705
 Cl -0.0536161996 0.0005099484 0.2617401236
 C -1.7581785707 0.0015126877 -0.1478602305
 F -1.9175995659 -0.0021006734 -1.4665463041
 F -2.3516701065 1.0817834385 0.3460943975
 F -2.3544318711 -1.0743456893 0.3523480856

³Me₂C:···BrCF₃ (Frozen)

C 3.5225426224 -0.0022853843 0.5905360023
 C 3.6956585443 1.3430340859 0.0365387273
 C 3.6930770453 -1.3479374991 0.0365390051
 H 3.4565440899 2.1126416269 0.7714164618
 H 3.0474277647 1.5117200834 -0.8342860371
 H 4.7294062179 1.5171226723 -0.2911693162
 H 3.4522320317 -2.1170857163 0.7713331545
 H 4.7265444239 -1.5241168015 -0.2909343425
 H 3.0447063514 -1.5152777497 -0.8344409237
 Br -0.0626632646 0.0008808279 0.2718720035
 C -1.9395818117 0.0016764714 -0.1358769092
 F -2.1282823269 0.0010825791 -1.4506555602
 F -2.5230332012 1.0802746957 0.3737061244
 F -2.5241957689 -1.0757474382 0.3748508621

Optimized Geometries on Polarized PESes

Ethyne...ClF (Polarization)

C 2.5327707971 -0.5979715797 0.0000011990
C 2.5327584847 0.5979889183 0.0000008639
H 2.5406918312 -1.6612198669 0.0000014753
H 2.5406572915 1.6612374219 0.0000007904
Cl -0.9125101029 -0.0000055784 -0.0000007664
F -2.5390058011 -0.0000044643 0.0000015998

Ethyne...BrF (Polarization)

C 3.0165187921 -0.5980207833 -0.0000032929
C 3.0165133398 0.5980438469 -0.0000036487
H 3.0295298701 -1.6611954106 -0.0000032475
H 3.0295157255 1.6612185997 -0.0000041212
Br -0.4432311204 -0.0000080287 -0.0000052037
F -2.2014746071 -0.0000202261 -0.0000064814

Ethene...ClF (Polarization)

C 2.5416740888 -0.6618752576 -0.0000027725
C 2.5416832422 0.6618509287 0.0000041609
H 2.5464589426 -1.2283970698 0.9220830918
H 2.5464604025 -1.2283874131 -0.9220945698
H 2.5464756819 1.2283629949 0.9220959643
H 2.5464771581 1.2283726534 -0.9220816908
Cl -0.8632825186 0.0000171960 0.0000035444
F -2.4899749973 0.0000369676 0.0000052717

Ethene...BrF (Polarization)

C 2.6084497678 -0.6622135966 -0.0000010683
C 2.6084594793 0.6621917192 0.0000057135
H 2.6150042205 -1.2284229368 0.9223228518
H 2.6150024919 -1.2284135065 -0.9223308025
H 2.6150219396 1.2283915383 0.9223354159
H 2.6150201848 1.2284009432 -0.9223182311
Br -0.7911046617 0.0000078562 0.0000033654
F -2.5495994193 0.0000131259 0.0000071571

H₂CO...ClF (Polarization)

O 2.1330459953 -0.5803302710 0.0371198350
C 2.8283136956 0.3973640266 0.0093344674
H 2.3986095175 1.4128362524 -0.0222538656
H 3.9280497695 0.3226235352 0.0146581348
Cl -0.7078618321 -0.2268962767 0.0121481848
F -2.2999171458 0.1207507335 -0.0055107563

H₂CO...BrF (Polarization)

O 2.1329848587 -0.5499983111 0.0337042851
C 2.8581749071 0.4067954381 0.0090432434
H 2.4595160168 1.4341637855 -0.0252731773
H 3.9540764718 0.2959921160 0.0206127660
Br -0.6977122069 -0.2424187584 0.0093209197
F -2.4268000475 0.1018137299 -0.0019120369

H₂NO···ClF (Polarization)

O 2.0036204719 -0.7746084061 0.0242759315
N 2.5620425954 0.3642423616 -0.0400859572
H 1.9919748634 1.2009681045 -0.0411108177
H 3.5646275259 0.4316544790 0.0745521073
Cl -0.7969472838 -0.1630435588 0.0092856150
F -2.2963579233 0.4753131958 0.0056435324

H₂NO···BrF (Polarization)

O 1.9506268370 -0.6913914223 0.0302119388
N 2.6198057927 0.3867433025 -0.0026546601
H 2.1397731057 1.2778333466 -0.0123380728
H 3.6296387116 0.3448216876 0.0192914367
Br -0.8160834232 -0.1596571531 0.0069353453
F -2.4948007744 0.3761764148 -0.0088855767

Me₂CO···ClF (Polarization)

O -0.6631816097 -0.7848637843 -0.1171945755
C -1.5515749382 0.0333876584 -0.0477472753
C -1.2674897337 1.5001601634 0.1550640105
C -3.0003180478 -0.3668539540 -0.1611415268
H -1.7822601865 1.8597410088 1.0470514084
H -1.6578136855 2.0707380627 -0.6890640444
H -0.1989968669 1.6700840840 0.2505369762
H -3.4749740677 0.1753738001 -0.9800107449
H -3.5320640448 -0.0937135133 0.7515534367
H -3.0802279688 -1.4367026527 -0.3287425686
Cl 2.1401099719 -0.5922652660 0.0215127327
F 3.7627684556 -0.4393192662 0.1057575218

Me₂CO···BrF (Polarization)

O -0.6698118465 -0.7806433731 -0.0891935829
C -1.5602600448 0.0381990842 -0.0322352999
C -1.2798624966 1.5069460623 0.1505791534
C -3.0057367978 -0.3685801127 -0.1458196914
H -1.8919803977 1.9145202373 0.9554077848
H -1.5563680974 2.0394203263 -0.7613653328
H -0.2270127252 1.6721789561 0.3597204018
H -3.5080786732 0.2254718021 -0.9099204514
H -3.5134258292 -0.1669256985 0.7990448796
H -3.0805164078 -1.4257176982 -0.3820342607
Br 2.1140883226 -0.6015690482 0.0056280029
F 3.8729422715 -0.4575341967 0.0577637474

Me₂NO···ClF (Polarization)

N -1.7763600905 -0.3957699408 0.2167525631
O -0.6349875765 -0.7864425105 -0.1861612080
C -2.0029972189 1.0310731310 0.3512804171
H -2.2110232473 1.4796946156 -0.6245873636
H -1.1054951619 1.4805454518 0.7651886423
H -2.8473284170 1.2085309804 1.0141365321
C -2.9094453060 -1.2736860891 -0.0074570420
H -2.5675798912 -2.2962972040 0.1172382267

H -3.3004310327 -1.1455443790 -1.0213118691
H -3.6970209870 -1.0508290656 0.7096338103
Cl 1.8425248232 0.5826413146 -0.1647728530
F 3.2802941058 1.3560136956 -0.1548898557

Me₂NO···BrF (Polarization)

N -1.7828709959 -0.3902307816 0.2229394690
O -0.6360098091 -0.7799604621 -0.1657706406
C -2.0161413971 1.0354492092 0.3587330401
H -2.2008995746 1.4873448108 -0.6200687617
H -1.1319684666 1.4873995460 0.7979138328
H -2.8773835241 1.2059434614 1.0009774055
C -2.9083490002 -1.2754137452 -0.0102545542
H -2.5614318782 -2.2956913960 0.1191269616
H -3.2901548817 -1.1503871977 -1.0277786706
H -3.7032782378 -1.0556359631 0.6993664917
Br 1.8070247956 0.5503105547 -0.1770571216
F 3.3716129697 1.3708019636 -0.1830774520

Furan···ClF (LP) (Polarization)

C 2.7958058435 -0.7335647323 0.0014574691
C 2.8186635961 0.7002557573 0.0016155290
C 1.4938962312 -1.0874093251 -0.0012225291
O 0.7006341945 0.0169611769 -0.0027535785
C 1.5286722635 1.0954552093 -0.0009966343
H 3.6376209835 -1.4031984793 0.0031165302
H 0.9825332866 -2.0327727453 -0.0023598082
H 1.0478377940 2.0566916774 -0.0019189042
H 3.6813963189 1.3427245538 0.0034167141
Cl -2.1744891917 0.0091857691 -0.0001128666
F -3.8021413202 -0.0099488616 -0.0002019213

Furan···BrF (LP) (Polarization)

C 3.0830780997 -0.5680215937 -0.4651289486
C 3.0177981869 0.8517208531 -0.2714249333
C 1.8209598713 -1.0238555045 -0.3324607076
O 0.9704324880 0.0053193628 -0.0673894168
C 1.7217500431 1.1397868424 -0.0353624812
H 3.9549766365 -1.1617222420 -0.6755474485
H 1.3737944783 -1.9994562548 -0.3918153137
H 1.1878968594 2.0508822959 0.1647283155
H 3.8301555215 1.5559284599 -0.3046269493
Br -1.8303714065 -0.2083344273 0.3859673682
F -3.5663507784 -0.3003377918 0.6681705152

Furan···ClF (π) (Polarization)

C -1.22481 -0.58078 1.07009
C -1.64382 -1.12028 -0.19085
C -1.30614 0.76294 0.94580
O -1.74292 1.10204 -0.29282
C -1.94281 -0.05767 -0.96887
H -0.91138 -1.12281 1.94529
H -1.10318 1.58000 1.61409
H -2.29288 0.04187 -1.98009
H -1.70937 -2.15644 -0.47262

Cl	1.86860	-0.12052	-0.13020
F	3.40895	-0.10775	-0.65517

Furan...BrF (π) (Polarization)

C	-1.64396	-0.21715	1.17918
C	-2.01749	-1.17953	0.18295
C	-1.77946	0.99533	0.59515
O	-2.20686	0.86260	-0.68454
C	-2.34597	-0.46740	-0.91637
H	-1.33210	-0.40691	2.19172
H	-1.62537	2.00199	0.93942
H	-2.67974	-0.74120	-1.90052
H	-2.03432	-2.25086	0.27946
Br	1.46223	-0.02416	0.00060
F	3.12877	-0.05268	-0.56071

Benzene...ClF (Polarization)

C	-1.3968225292	-0.6940590539	1.3317397325
C	-1.5334409695	-1.3882994451	0.1371602740
C	-1.6714189515	-0.6943852928	-1.0576612551
H	-1.5297768626	-2.4701233211	0.1367178670
C	-1.3968746281	0.6942250258	1.3316632370
H	-1.2874305567	-1.2352750734	2.2618756784
C	-1.5335453493	1.3883235902	0.1370075157
H	-1.2875229889	1.2355514742	2.2617396338
C	-1.6714712458	0.6942677293	-1.0577375927
H	-1.7764281954	-1.2356713617	-1.9883252290
H	-1.5299628278	2.4701476636	0.1364459202
H	-1.7765210374	1.2354435745	-1.9884610895
Cl	1.8145383102	-0.0000802785	-0.5844974751
F	3.4248066768	-0.0000841298	-0.8294398797

Benzene...BrF (Polarization)

C	-1.4121331631	-0.6940767269	1.3352682349
C	-1.5492081708	-1.3886424237	0.1406913842
C	-1.6848209487	-0.6945690421	-1.0544271107
H	-1.5464418087	-2.4704260249	0.1405776873
C	-1.4121810811	0.6942411731	1.3351910254
H	-1.3037976052	-1.2352419562	2.2654779367
C	-1.5493042660	1.3886646510	0.1405370837
H	-1.3038832306	1.2355168887	2.2653407838
C	-1.6848684516	0.6944494547	-1.0545040860
H	-1.7877069198	-1.2355261418	-1.9855095415
H	-1.5466104629	2.4704483429	0.1403024737
H	-1.7877927973	1.2352962278	-1.9856462996
Br	1.8387275442	-0.0000803859	-0.5927500898
F	3.5781502064	-0.0000729354	-0.8623221446

Naphthalene...ClF (a) (Polarization)

C	-0.2661360396	2.3910561113	-0.3170681941
C	-0.5276974513	2.0010410634	1.0167815333
C	0.0998842074	0.9122944336	1.5510136102
H	-1.2287288708	2.5698376839	1.6125403916
C	1.0190224972	0.1547337269	0.7812319057
H	-0.0994976020	0.6092068045	2.5716767909

C 0.6147571383 1.6809963229 -1.0795587974
 H -0.7715947008 3.2531214852 -0.7304472875
 C 1.2791467668 0.5447840080 -0.5532849973
 H 0.8168473641 1.9745234883 -2.1021884673
 C 1.6765470229 -0.9860079347 1.3055232773
 C 2.1911307958 -0.2168917965 -1.3257486373
 C 2.5499490608 -1.7000241580 0.5384399319
 H 1.4709192326 -1.2828269366 2.3265274276
 C 2.8105930440 -1.3103161155 -0.7949664181
 H 2.3868200219 0.0846340360 -2.3472569253
 H 3.0467613058 -2.5691700940 0.9477346721
 H 3.5038537866 -1.8855187514 -1.3934426822
 Cl -2.2993256019 -0.7181841486 -0.2282007481
 F -3.3823513368 -1.7175260880 -0.9203199608

Naphthalene...BrF (a) (Polarization)

C -0.2562969551 2.3838971141 -0.3300088703
 C -0.5366547602 1.9775209903 0.9954767105
 C 0.0904790077 0.8871215264 1.5284599600
 H -1.2496672060 2.5364262827 1.5865396297
 C 1.0282850113 0.1444616956 0.7658369375
 H -0.1198887423 0.5739661305 2.5439130484
 C 0.6425584179 1.6883793343 -1.0846105347
 H -0.7618325659 3.2462137715 -0.7424927312
 C 1.3068255953 0.5512188195 -0.5597864525
 H 0.8592776773 1.9942599485 -2.1005490121
 C 1.6853005172 -0.9968511529 1.2888277047
 C 2.2370254058 -0.1949225498 -1.3254912932
 C 2.5762666196 -1.6959405275 0.5281676812
 H 1.4646428177 -1.3069263043 2.3026886541
 C 2.8557907363 -1.2895670483 -0.7963165429
 H 2.4469981058 0.1191061269 -2.3403130495
 H 3.0724008575 -2.5662351837 0.9357583432
 H 3.5627948834 -1.8533104502 -1.3895399563
 Br -2.4144834464 -0.6779092886 -0.0907127358
 F -3.5989213358 -1.7311460941 -0.8568610657

Naphthalene...ClF (b) (Polarization)

C 2.4185073062 -0.7066698657 1.0759176218
 C 2.4185073062 0.7066698657 1.0759176218
 C 1.2404129974 1.3946043355 1.0806836678
 H 3.3586517095 1.2412884061 1.0708561413
 C 0.0000000000 0.7076773543 1.0844631218
 H 1.2354445203 2.4775699569 1.0793859608
 C 1.2404129974 -1.3946043355 1.0806836678
 H 3.3586517095 -1.2412884061 1.0708561413
 C 0.0000000000 -0.7076773543 1.0844631218
 H 1.2354445203 -2.4775699569 1.0793859608
 C -1.2404129974 1.3946043355 1.0806836678
 C -1.2404129974 -1.3946043355 1.0806836678
 C -2.4185073062 0.7066698657 1.0759176218
 H -1.2354445203 2.4775699569 1.0793859608
 C -2.4185073062 -0.7066698657 1.0759176218
 H -1.2354445203 -2.4775699569 1.0793859608
 H -3.3586517095 1.2412884061 1.0708561413

H -3.3586517095 -1.2412884061 1.0708561413
Cl 0.0000000000 0.0000000000 -2.2709422340
F 0.0000000000 0.0000000000 -3.8986977446

Naphthalene...BrF (b) (Polarization)

C 2.4186302839 -0.7067475900 1.0763453661
C 2.4186302839 0.7067475899 1.0763453657
C 1.2407769948 1.3949902801 1.0852444523
H 3.3588490518 1.2410890866 1.0664154988
C 0.0000000000 0.7079744082 1.0918608407
H 1.2357690295 2.4778751434 1.0817421630
C 1.2407769949 -1.3949902802 1.0852444529
H 3.3588490519 -1.2410890865 1.0664154992
C 0.0000000000 -0.7079744084 1.0918608410
H 1.2357690296 -2.4778751435 1.0817421638
C -1.2407769956 1.3949902798 1.0852444519
C -1.2407769957 -1.3949902799 1.0852444520
C -2.4186302849 0.7067475901 1.0763453671
H -1.2357690303 2.4778751431 1.0817421651
C -2.4186302849 -0.7067475901 1.0763453670
H -1.2357690305 -2.4778751432 1.0817421650
H -3.3588490528 1.2410890869 1.0664155019
H -3.3588490529 -1.2410890869 1.0664155015
Br 0.0000000000 0.0000000000 -2.2176842565
F 0.0000000000 0.0000000000 -3.9783675265

¹Me₂C:...ClCF₃ (Polarization)

C 3.0275003902 0.0011804588 0.0509112195
C 3.8423385784 1.2213072428 0.0009961568
C 3.8344649890 -1.2241691684 0.0012508897
H 3.3454636590 2.0865035464 0.4373535094
H 3.8430926326 1.4239011989 -1.0845261329
H 4.8872998593 1.1452101183 0.3278420094
H 3.3319373426 -2.0861755530 0.4374385156
H 4.8798137001 -1.1548041679 0.3283602192
H 3.8342281244 -1.4266766460 -1.0842952629
Cl -0.4480761267 0.0012773863 0.0138956173
C -2.1931829908 -0.0001082941 -0.0058317680
F -2.6507155228 0.0002593234 -1.2561920140
F -2.6727532340 1.0772607069 0.6117502763
F -2.6710286829 -1.0789836988 0.6104760170

¹Me₂C:...BrCF₃ (Polarization)

C 3.0583706385 0.0011785209 0.0502140736
C 3.8714099300 1.2220383009 0.0010881526
C 3.8634898195 -1.2249137100 0.0011501183
H 3.3736746388 2.0855443267 0.4400193876
H 3.8693587354 1.4273624264 -1.0839791782
H 4.9168226073 1.1465644052 0.3257870366
H 3.3600816219 -2.0852637010 0.4398048446
H 4.9092965979 -1.1562668973 0.3260981717
H 3.8603843788 -1.4299937809 -1.0839682234
Br -0.3641107976 0.0014234581 0.0143956990
C -2.2770680861 -0.0001331872 -0.0064368739
F -2.7371690676 -0.0002112766 -1.2565049528

F -2.7579525799 1.0774621474 0.6111370424
F -2.7562057187 -1.0788085792 0.6106239544

³Me₂C:···ClCF₃ (Polarization)

C 3.4623784233 -0.0023960370 0.6144900995
C 3.5833195058 1.3428281548 0.0465969489
C 3.5807101384 -1.3474970757 0.0457546653
H 3.4058852985 2.1123438897 0.7988154849
H 2.8618852682 1.5084223167 -0.7652871805
H 4.5841357983 1.5199100557 -0.3696600708
H 3.4012124560 -2.1171382122 0.7973564227
H 4.5813531942 -1.5264809648 -0.3701054753
H 2.8593407755 -1.5109649754 -0.7666155614
Cl 0.0101794612 0.0004349979 0.2527174985
C -1.6966493906 0.0014313168 -0.1447669889
F -1.8659920249 -0.0013817898 -1.4625558253
F -2.2874888447 1.0813407253 0.3538848859
F -2.2898873409 -1.0748699488 0.3588043488

³Me₂C:···BrCF₃ (Polarization)

C 3.4760162392 -0.0022040093 0.5871707660
C 3.6550098210 1.3430888768 0.0346462730
C 3.6522610472 -1.3478600871 0.0346378422
H 3.4057837753 2.1130072689 0.7658464487
H 3.0178709888 1.5104358745 -0.8446095798
H 4.6928191050 1.5174507034 -0.2796249780
H 3.4011444509 -2.1172757694 0.7657214736
H 4.6897793686 -1.5244702845 -0.2793356450
H 3.0150213816 -1.5137778338 -0.8448145191
Br 0.0119032185 0.0007360262 0.2664533218
C -1.8665490782 0.0015619367 -0.1320245819
F -2.0625627169 0.0009592293 -1.4461249990
F -2.4484594511 1.0801787478 0.3801577456
F -2.4496554313 -1.0758482262 0.3813296842