The Use of Electrostatic Potentials at Nuclei in the Analysis of Halogen Bonding

Supplementary Information

Vilakkathala U. Krishnapriya[a, b] and Cherumuttathu H. Suresh*[a, b]

[a]Chemical Science and Technology Division, CSIR-National Institute of Interdisciplinary Science and Technology, Thiruvananthapuram - 695019, Kerala, India

[b]Research Centre, University of Kerala, Thiruvananthapuram, 34, Kerala, India

Table S1: Change in MESP at the nuclei of donor and acceptor atoms of the remaining ammonia- halogen bonded complexes along with their BSSE corrected binding energy at M06-2X/aug-cc-pVTZ level of theory. All values are in kcal/mol.

Complex	ΔV_{n-D}	ΔV_{n-A}	$\Delta\Delta V_n$	E_{BSSE}	Complex	ΔV_{n-D}	ΔV_{n-A}	$\Delta\Delta V_n$	E_{BSSE}
$H_3N...BrCF_3$	12.1	-11.2	23.3	-3.6	$H_3N...ClCCH$	6.7	-12.3	18.9	-2.4
$H_3N...BrOCH_3$	17.7	-15.7	33.4	-6.2	$H_3N...ClCHCH_2$	-0.4	-9.4	9.0	-0.6
$H_3N...BrCCH$	10.6	-12.6	23.3	-3.8	$H_3N...Cl_2$	16.4	-15.4	31.8	-4.9
$H_3N...BrCHCH_2$	2.4	-10.0	12.4	-1.5	$H_3N...ClCN$	16.0	-14.7	30.7	-4.3
$H_3N...Br_2$	25.1	-14.2	39.3	-6.6	$H_3N...ClOCH_3$	9.1	-14.4	23.4	-3.7
$H_3N...BrF$	49.6	-29.3	78.9	-14.4	$H_3N...ClOF$	22.4	-19.8	42.2	-6.9
$H_3N...BrCN$	21.1	-15.2	36.3	-6.0	$H_3N...ClC_6H_5$	-0.2	-9.0	8.7	-0.6
$H_3N...BrOF$	37.4	-22.5	59.9	-10.3	$H_3N...ClC_6H_4F$	1.4	-9.0	10.4	-0.8
$H_3N...BrC_6H_4F$	4.4	-9.7	14.1	-1.8	$H_3N...ClC_6H_4Cl$	2.1	-9.1	11.2	-0.9
$H_3N...BrC_6H_4Cl$	5.0	-9.6	14.6	-1.9	$H_3N...ClCH_2CH_3$	-3.5	-8.4	4.9	0.1
$H_3N...BrCH_2CH_3$	-0.9	-9.0	8.1	-0.7	$H_3N...ClH$	0.4	-12.0	12.4	-0.8
$H_3N...BrH$	3.8	-12.2	16.0	-1.9	$H_3N...ClOCClH_2$	15.7	-14.8	30.5	-5.2
$H_3N...BrCH_2CH_2Br$	3.9	-9.2	13.1	-1.5	$H_3N...ClOCBr_3$	32.2	-14.6	46.8	-7.5
$H_3N...BrOCBr_3$	60.3	-14.7	75.0	-12.9	$H_3N...ClC_6H_4NO_2$	6.2	-9.2	15.4	-1.5
$H_3N...BrC_6H_4Br$	5.2	-9.5	14.7	-1.9	$H_3N...ClOCl$	21.2	-17.8	39.0	-6.4
$H_3N...BrC_6H_4NO_2$	9.4	-9.8	19.2	-2.5	$H_3N...ClOBr$	19.4	-16.6	36.0	-6.0
$H_3N...BrOCl$	38.8	-20.4	59.2	-10.0	$H_3N...ClOCHCl_2$	21.5	-15.6	37.1	-6.3
$H_3N...BrOCHCl_2$	41.2	-17.4	58.7	-10.3	$H_3N...ClOCHF_2$	19.0	-16.9	35.9	-6.2
$H_3N...BrOCHF_2$	37.9	-19.6	57.5	-9.9	$H_3N...ClOCClF_2$	29.7	-16.9	46.6	-7.6
$H_3N...BrOCClF_2$	53.6	-19.0	72.6	-12.5	$H_3N...ClOCCl_3$	29.0	-17.4	46.4	-7.4
$H_3N...BrOCCl_3$	56.1	-16.8	73.0	-12.5	$H_3N...ClNO_2BeCl_2$	47.0	-9.8	56.8	-10.2
$H_3N...BrOCF_3$	53.2	-21.4	74.6	-12.9	$H_3N...ClC_3N$	15.7	-15.7	31.4	-3.9
$H_3N...BrCH_3$	-0.1	-9.5	9.4	-1.0	$H_3N...ClC_5N$	15.5	-12.7	28.3	-3.8
$H_3N...BrCNBeCl_2$	39.2	-17.3	56.5	-9.6	$H_3N...FCN$	5.9	-11.8	17.7	-1.0
$H_3N...BrC_3N$	20.4	-13.5	33.9	-5.5	$H_3N...FNO_2BeCl_2$	11.2	-10.7	21.9	-1.8
$H_3N...BrC_5N$	20.2	-12.7	32.9	-5.4	$H_3N...FNCBeCl_2$	17.5	-6.1	23.6	-2.9
$H_3N...BrNO_2BeCl_2$	72.6	-18.5	91.2	-15.3	$H_3N...FC_3N$	6.0	-9.0	15.0	-0.9

Table S2: Change in MESP at the nuclei of donor and acceptor atoms of the remaining pyridine- halogen bonded complexes along with their BSSE corrected binding energy at M06-2X/aug-cc-pVTZ level of theory. All values are in kcal/mol.

Complex	ΔV_{n-D}	ΔV_{n-A}	$\Delta\Delta V_n$	E_{BSSE}	Complex	ΔV_{n-D}	ΔV_{n-A}	$\Delta\Delta V_n$	E_{BSSE}
$C_5H_5N...BrOCH_3$	15.6	-17.3	32.9	-6.8	$C_5H_5N...ClCCH$	4.9	-13.0	17.9	-2.6
$C_5H_5N...BrCCH$	8.0	-13.3	21.3	-4.1	$C_5H_5N...ClF$	37.4	-35.1	72.6	-11.8
$C_5H_5N...BrCHCH_2$	1.1	-8.4	9.5	-1.9	$C_5H_5N...ClOH$	8.4	-17.3	25.8	-4.7
$C_5H_5N...Br_2$	24.5	-16.5	41.0	-7.3	$C_5H_5N...ClOF$	19.1	-22.5	41.5	-7.5
$C_5H_5N...BrOF$	34.9	-26.6	61.5	-7.6	$C_5H_5N...ClC_6H_5$	-3.2	-2.5	0.7	-1.1
$C_5H_5N...BrC_6H_5$	-3.4	-1.3	2.1	-1.5	$C_5H_5N...ClC_6H_4F$	-3.3	-0.9	2.4	-1.2
$C_5H_5N...BrC_6H_4Cl$	0.5	-3.5	4.0	-11.7	$C_5H_5N...ClC_6H_4Cl$	-3.5	-0.4	3.1	-1.2
$C_5H_5N...BrH$	2.6	-12.1	14.7	-2.1	$C_5H_5N...ClH$	-12.1	-0.1	12.0	-0.9
$C_5H_5N...BrOCClH_2$	27.6	-19.3	46.9	-1.6	$C_5H_5N...ClCH_2CH_2Br$	-6.9	-0.1	6.8	-1.1
$C_5H_5N...BrCH_2CH_2Br$	2.6	-7.7	10.3	-2.2	$C_5H_5N...ClC_6H_4Br$	-3.5	-0.3	3.2	-1.2
$C_5H_5N...BrC_6H_4Br$	0.9	-3.8	4.7	-9.4	$C_5H_5N...ClC_6H_4NO_2$	3.0	-3.7	6.7	-1.4
$C_5H_5N...BrC_6H_4NO_2$	4.3	-4.1	8.4	-1.8	$C_5H_5N...ClOBr$	17.0	-18.6	35.6	-6.6
$C_5H_5N...BrOCl$	35.7	-23.7	59.3	-15.8	$C_5H_5N...ClOCHF_2$	17.3	-19.2	36.5	-6.7
$C_5H_5N...BrOBr$	34.7	-22.1	56.8	-1.7	$C_5H_5N...ClOCF_3$	33.7	-24.0	57.7	-9.0
$C_5H_5N...BrOCH_2F$	24.6	-20.0	44.5	-2.0	$C_5H_5N...ClCNBeCl_2$	25.4	-17.9	43.2	-7.9
$C_5H_5N...BrOCHF_2$	36.3	-23.1	59.4	-11.5	$C_5H_5N...ClC_3N$	12.4	-13.9	26.3	-4.2
$C_5H_5N...BrOCF_2Cl$	50.8	-22.3	73.2	-10.9	$C_5H_5N...ClC_5N$	12.3	-13.0	25.3	-4.1
$C_5H_5N...BrOCF_3$	50.0	-25.4	75.3	-9.0	$C_5H_5N...FCN$	4.6	-10.9	15.6	-1.1
$C_5H_5N...BrCNBeCl_2$	32.0	-20.0	52.0	-12.0	$C_5H_5N...FCNBeCl_2$	14.3	-12.7	27.0	-3.1
$C_5H_5N...BrC_3N$	16.1	-14.7	30.7	-11.4	$C_5H_5N...FC_3N$	5.0	-9.6	14.7	-1.0
$C_5H_5N...BrC_5N$	16.0	-13.8	29.8	-5.8	$C_5H_5N...FC_5N$	5.0	-9.0	14.0	-0.9

Table S3: BSSE values of halogen bonded NH_3 complexes at M06-2X/aug-cc-pVTZ level of theory. Values are in a.u.

Complex	BSSE value	Complex	BSSE value
$H_3N...BrCF_3$	0.00019	$H_3N...ClCF_3$	0.00011
$H_3N...BrOCH_3$	0.00010	$H_3N...ClCCH$	0.00013
$H_3N...BrCCH$	0.00020	$H_3N...ClCHCH_2$	0.00005
$H_3N...BrCHCH_2$	0.00007	$H_3N...Cl_2$	0.00018
$H_3N...Br_2$	0.00000	$H_3N...ClCN$	0.00018
$H_3N...BrF$	0.00036	$H_3N...ClOCH_3$	0.00010
$H_3N...BrCN$	0.00019	$H_3N...ClOF$	0.00019
$H_3N...BrOF$	0.00027	$H_3N...ClC_6H_5$	0.00007
$H_3N...BrC_6H_5$	0.00010	$H_3N...ClC_6H_4F$	0.00007
$H_3N...BrC_6H_4NH_2$	0.00010	$H_3N...ClC_6H_4Cl$	0.00008
$H_3N...BrC_6H_4F$	0.00011	$H_3N...ClCH_2CH_3$	0.00005
$H_3N...BrC_6H_4Cl$	0.00011	$H_3N...ClH$	0.00006
$H_3N...BrCH_2CH_3$	0.00009	$H_3N...ClOCClH_2$	0.00015
$H_3N...BrH$	0.00013	$H_3N...ClOCBr_3$	0.00017
$H_3N...BrOCH_2Cl$	0.00021	$H_3N...ClCCl_3$	0.00015
$H_3N...BrCH_2CH_2Br$	0.00010	$H_3N...ClPhBr$	0.00008
$H_3N...BrOCBr_3$	0.00025	$H_3N...ClC_6H_4NO_2$	0.00008
$H_3N...BrC_6H_4Br$	0.00011	$H_3N...ClOCl$	0.00013
$H_3N...BrC_6H_4NO_2$	0.00011	$H_3N...ClOBr$	0.00013
$H_3N...BrOCl$	0.00022	$H_3N...ClOCHCl_2$	0.00018
$H_3N...BrOBr$	0.00024	$H_3N...ClOCHF_2$	0.00008
$H_3N...BrOCHCl_2$	0.00027	$H_3N...ClOCClF_2$	0.00018
$H_3N...BrOCHF_2$	0.00023	$H_3N...ClOCCl_3$	0.00012
$H_3N...BrOCClF_2$	0.00022	$H_3N...ClOCF_3$	0.00012
$H_3N...BrOCCl_3$	0.00030	$H_3N...ClNO_2BeCl_2$	0.00021
$H_3N...BrOCF_3$	0.00024	$H_3N...ClC_3N$	0.00017
$H_3N...BrCH_3$	0.00013	$H_3N...ClC_5N$	0.00014
$H_3N...BrCNBeCl_2$	0.00017	$H_3N...FCN$	0.00010
$H_3N...BrC_3N$	0.00020	$H_3N...FNO_2BeCl_2$	0.00013
$H_3N...BrC_5N$	0.00016	$H_3N...FNCBeCl_2$	0.00018
$H_3N...BrNO_2BeCl_2$	0.00024	$H_3N...FC_3N$	0.00009
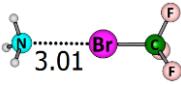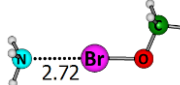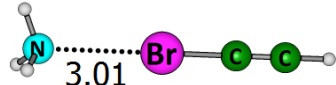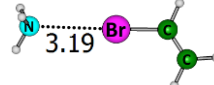
Table S4: BSSE values of halogen bonded pyridine complexes at M06-2X/aug-cc-pVTZ level of theory. Values are in a.u.
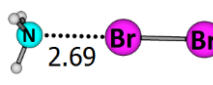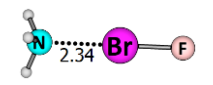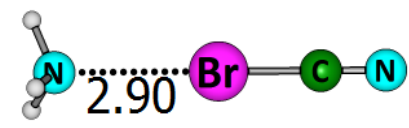
Complex	BSSE value	Complex	BSSE value
$C_5H_5N...BrCF_3$	0.00030	$C_5H_5N...ClCF_3$	0.00024
$C_5H_5N...BrOCH_3$	0.00023	$C_5H_5N...ClCCH$	0.00022
$C_5H_5N...BrCCH$	0.00031	$C_5H_5N...ClF$	0.00056
$C_5H_5N...BrCHCH_2$	0.00018	$C_5H_5N...ClCN$	0.00030
$C_5H_5N...Br_2$	0.00033	$C_5H_5N...ClOH$	0.00024
$C_5H_5N...BrCN$	0.00030	$C_5H_5N...ClOF$	0.00037
$C_5H_5N...BrOH$	0.00027	$C_5H_5N...ClC_6H_5$	0.00022
$C_5H_5N...BrOF$	0.00056	$C_5H_5N...ClC_6H_4F$	0.00023
$C_5H_5N...BrC_6H_5$	0.00026	$C_5H_5N...ClC_6H_4Cl$	0.00023
$C_5H_5N...BrC_6H_4Cl$	0.00022	$C_5H_5N...ClH$	0.00012
$C_5H_5N...BrH$	0.00019	$C_5H_5N...ClCH_2CH_2Br$	0.00016
$C_5H_5N...BrOCClH_2$	0.00039	$C_5H_5N...ClC_6H_4Br$	0.00024
$C_5H_5N...BrCH_2CH_2Br$	0.00020	$C_5H_5N...ClC_6H_4NO_2$	0.00026
$C_5H_5N...BrCCl_3$	0.00034	$C_5H_5N...ClOBr$	0.00034
$C_5H_5N...BrC_6H_4Br$	0.00026	$C_5H_5N...ClOCH_2F$	0.00026
$C_5H_5N...BrC_6H_4NO_2$	0.00025	$C_5H_5N...ClOCHF_2$	0.00032
$C_5H_5N...BrOCl$	0.00052	$C_5H_5N...ClOCF_2Cl$	0.00045
$C_5H_5N...BrOBr$	0.00059	$C_5H_5N...ClOCF_3$	0.00045
$C_5H_5N...BrOCH_2F$	0.00040	$C_5H_5N...ClCNBeCl_2$	0.00035
$C_5H_5N...BrOCHF_2$	0.00051	$C_5H_5N...ClC_3N$	0.00028
$C_5H_5N...BrOCF_2Cl$	0.00053	$C_5H_5N...ClC_5N$	0.00023
$C_5H_5N...BrOCF_3$	0.00059	$C_5H_5N...FCN$	0.00016
$C_5H_5N...BrCNBeCl_2$	0.00025	$C_5H_5N...FCNBeCl_2$	0.00030
$C_5H_5N...BrC_3N$	0.00032	$C_5H_5N...FC_3N$	0.00016
$C_5H_5N...BrC_5N$	0.00027	$C_5H_5N...FC_5N$	0.00013

Table S5: BSSE values of halogen bonded HCN, H_2O and $(CH_3)_2O$ complexes at M06-2X/aug-cc-pVTZ level of theory. Values are in a.u.

Complex	BSSE value	Complex	BSSE value
$HCN\ldots BrCHCH_2$	0.00018	$H_2O\ldots BrOCF_3$	0.00002
$HCN\ldots Br_2$	0.00023	$H_2O\ldots FOCl$	0.00015
$HCN\ldots BrF$	0.00024	$H_2O\ldots ClF$	0.00013
$HCN\ldots BrCH_2CH_2Br$	0.00020	$H_2O\ldots ClOCBr_3$	0.00016
$HCN\ldots BrCNBeCl_2$	0.00036	$(CH_3)_2O\ldots BrCCH$	0.00036
$HCN\ldots ClOCl$	0.00026	$(CH_3)_2O\ldots BrC_6H_4F$	0.00016
$HCN\ldots ClOCHCl_2$	0.00027	$(CH_3)_2O\ldots BrC_6H_4NO_2$	0.00017
$HCN\ldots ClCNBeCl_2$	0.00040	$(CH_3)_2O\ldots ClCCH$	0.00026
$H_2O\ldots BrOF$	0.00015	$(CH_3)_2O\ldots ClC_6H_4Cl$	0.00017
$H_2O\ldots BrC_6H_4Cl$	0.00011	$(CH_3)_2O\ldots ClC_6H_4NO_2$	0.00018
$H_2O\ldots BrOCl$	0.00012	$(CH_3)_2O\ldots ClOBr$	0.00038
$H_2O\ldots BrOCCl_3$	0.00009	$(CH_3)_2O\ldots ClC_3N$	0.00025

Table S6: Cartesian coordinates in (Å) and energy data (a.u.) of halogen bonded NH_3 complexes at M06-2X/aug-cc-pVTZ level of theory. All the optimized structures are corresponding to minima on the potential energy surface.

$H_3N…BrCF_3$

SCF E =-2968.4659
ZPE=-2968.4152
G=-2968.4519
H= -2968.4053

35	-0.5770800	0.0006620	0.0008540
7	-3.5891960	-0.0010400	-0.0006680
1	-3.9606050	-0.5888070	-0.7365780
1	-3.9642930	0.9287470	-0.1411290
1	-3.9613360	-0.3457330	0.8754190
6	1.3473140	-0.0003900	-0.0001720
9	1.8184330	-0.7565590	-0.9831850
9	1.8182630	1.2289460	-0.1643170
9	1.8215840	-0.4732470	1.1450690

$H_3N…BrOCH_3$

SCF E=-2745.8728
ZPE=-2745.7943
G=-2745.8290
H=-2745.7854

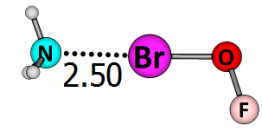|			
35	-0.1667590	-0.1667230	-0.0000190
7	-2.8392910	0.3249770	0.0000320
1	-3.1162330	0.8590650	-0.8136000
1	-3.1191190	0.8423150	0.8234150
1	-3.3532880	-0.5465510	-0.0097880
8	1.6263500	-0.5344780	0.0000480
6	2.4034690	0.6448090	0.0000050
1	2.2129520	1.2485230	0.8906950
1	3.4425270	0.3157800	0.0001650
1	2.2131610	1.2483170	-0.8908720

$H_3N…BrCCH$

SCF E= -2707.5211
ZPE=-2707.4660
G= -2707.4976
H= -2707.4576

35	-0.0278700	-0.0002350	0.0003090
7	-3.0385940	0.0000230	-0.0005200
1	-3.4148400	-0.6432270	-0.6858950
1	-3.4092690	0.9172030	-0.2161760
1	-3.4144230	-0.2698890	0.9000190
6	1.7725660	0.0003890	0.0000560
6	2.9695430	0.0002490	-0.0006910
1	4.0314830	0.0001570	-0.0012970

$H_3N…BrCHCH_2$

SCF E= -2708.7744
ZPE= -2708.6962
G= -2708.7306
H=-2708.6871

35	0.0547000	-0.1218240	0.0012250
7	3.2198640	0.2377060	-0.0008740
1	3.5625220	1.1830160	-0.1149580
1	3.6000020	-0.3144050	-0.7590660
1	3.6099010	-0.1231350	0.8605010
6	-1.8135150	-0.3878360	-0.0019470
6	-2.6872150	0.5995580	-0.0009500
1	-3.7463140	0.3783500	-0.0030050

1	-2.3804850	1.6360630	0.0019260
1	-2.0948020	-1.4303120	-0.0047910

H₃N...Br₂

SCF E= -5205.0351
ZPE=-5204.9979
G= -5205.0294
H= -5204.9906

35	-0.6668270	-0.0002270	-0.0011450
7	-3.3533260	0.0002430	0.0017600
1	-3.7108420	-0.0338700	-0.9441200
1	-3.7081520	0.8375720	0.4451420
1	-3.7103960	-0.8014990	0.5050930
35	1.6554750	0.0001150	0.0006190

H₃N...BrF

SCF E= -2730.6011
ZPE= -2730.5614
G= -2730.5890
H= -2730.5554

35	-0.1489780	-0.0001260	0.0001040
7	2.1860470	0.0000860	-0.0000780
1	2.5331790	0.4203110	0.8526330
1	2.5314140	0.5296390	-0.7903830
1	2.5336940	-0.9484030	-0.0635250
9	-1.9651550	0.0002520	-0.0002040

H₃N...BrCN

SCF E= -2723.6217
ZPE=-2723.5768
G=-2723.6076
H= -2723.5691

35	-0.0241570	0.0003050	0.0002100
7	-2.9196020	-0.0002620	-0.0001960
1	-3.2962880	0.0462980	0.9386470
1	-3.2918930	-0.8385380	-0.4294740
1	-3.2956110	0.7888640	-0.5116110
6	1.7790340	-0.0004310	-0.0001090
7	2.9274700	-0.0004140	-0.0004130

H₃N...BrOF

SCF E= -2805.7047
ZPE=-2805.6628
G= -2805.6949
H= -2805.6549

35	-0.1806910	-0.1505890	0.0000460
7	-2.6415960	0.2986830	0.0004320
1	-3.1634580	-0.4963120	-0.3461160
1	-2.8367310	1.0938150	-0.5944330
1	-2.9644320	0.5120270	0.9354590
8	1.6329750	-0.5337610	0.0001560
9	2.3017970	0.7044860	-0.0000880

H₃N...BrC₆H₅
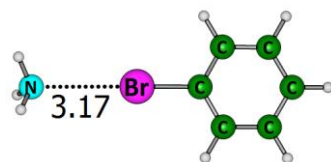
SCF E= -2862.4248
ZPE= -2862.2981
G= -2862.3364
H= -2862.2870

35	1.2081430	0.0053190	-0.0092580
7	4.3794640	-0.0067780	0.0135440
1	4.7907490	0.8531630	-0.3263530
1	4.7620630	-0.7636810	-0.5385770
1	4.6967420	-0.1375260	0.9656180
6	-0.6870240	0.0010520	-0.0017340
6	-1.3684780	-1.2066710	0.0005340
6	-1.3739680	1.2056920	0.0006650
6	-2.7562690	-1.2035390	0.0052380
1	-0.8173720	-2.1361690	-0.0015130
6	-2.7617320	1.1962370	0.0053740
1	-0.8270690	2.1376730	-0.0012820
6	-3.4558150	-0.0052310	0.0076000
1	-3.2900580	-2.1441520	0.0069430
1	-3.2997760	2.1344190	0.0071810
1	-4.5368330	-0.0076880	0.0111500

H₃N...BrC₆H₄NH₂
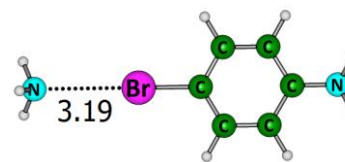
SCF E= -2917.7857
ZPE= -2917.6422
G= -2917.6819
H= -2917.6296

35	1.6386510	0.0000240	0.0162710
7	4.8255240	-0.0000480	-0.0215210
1	5.1575910	0.8153510	-0.5204810
1	5.1575300	-0.8155010	-0.5204340
1	5.2698460	-0.0000410	0.8876210
6	-0.2569790	0.0000080	0.0023130
6	-0.9512440	-1.1994910	-0.0020740
6	-0.9512660	1.1995020	-0.0020700
6	-2.3361270	-1.1983530	-0.0105720
1	-0.4103070	-2.1352380	0.0016640
6	-2.3361430	1.1983430	-0.0106060
1	-0.4103420	2.1352560	0.0016700
6	-3.0492510	-0.0000130	-0.0134230
1	-2.8729740	-2.1386910	-0.0197050
1	-2.8730110	2.1386680	-0.0197930
7	-4.4418020	-0.0000050	-0.0781380
1	-4.8855340	-0.8350150	0.2678250
1	-4.8855630	0.8347780	0.2683350

H₃N...BrC₆H₄F
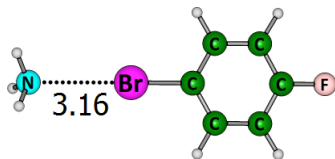
SCF E= -2961.6763
ZPE=-2961.557649
G=-2961.597064
H= -2961.545696

35	1.6171010	0.0042590	-0.0073990
7	4.7731820	-0.0067460	0.0128460

H₃N...BrC₆H₄Cl
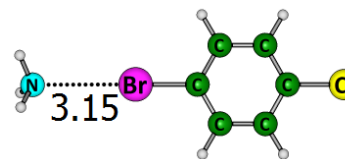
SCF E= -3322.0353
ZPE= -3321.9181
G= -3321.9584
H= -3321.9058

35	2.0280340	0.0033010	-0.0057410
7	5.1791680	-0.0060630	0.0107170

1	5.1781120	0.8544230	-0.3317230
1	5.1523430	-0.7622360	-0.5436560
1	5.1024300	-0.1364490	0.9610380
6	-0.2768020	0.0015380	-0.0025470
6	-0.9618470	-1.2044690	-0.0010770
6	-0.9653330	1.2055630	-0.0009660
6	-2.3489720	-1.2099350	0.0020940
1	-0.4143690	-2.1358500	-0.0024540
6	-2.3524830	1.2070180	0.0021930
1	-0.4205490	2.1385250	-0.0022650
6	-3.0175780	-0.0024160	0.0036540
1	-2.9111090	-2.1327090	0.0032820
1	-2.9172450	2.1281920	0.0034550
9	-4.3602600	-0.0043940	0.0068050

1	5.5783940	0.8565520	-0.3369850
1	5.5574670	-0.7601280	-0.5483460
1	5.5161370	-0.1342330	0.9564290
6	0.1357050	0.0015320	-0.0022530
6	-0.5509260	-1.2032650	-0.0012690
6	-0.5531690	1.2050440	-0.0011960
6	-1.9376240	-1.2060380	0.0007170
1	-0.0057880	-2.1361520	-0.0021600
6	-1.9398810	1.2052150	0.0007860
1	-0.0097810	2.1389510	-0.0020310
6	-2.6200050	-0.0010380	0.0016540
1	-2.4867730	-2.1364430	0.0014290
1	-2.4907440	2.1346090	0.0015530
17	-4.3587580	-0.0026440	0.0038470

H₃N...BrCH₂CH₃
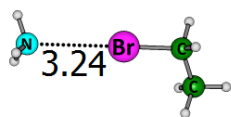
SCF E= -2710.0070
ZPE= -2709.9050
G= -2709.9412
H= -2709.8952

35	0.1223450	-0.2001130	0.0113830
7	3.3142160	0.3529030	-0.0050360
1	3.7989740	0.2924050	0.8810820
1	3.4781030	1.2793930	-0.3775320
1	3.7507280	-0.3077960	-0.6350610
6	-1.8078960	-0.4900780	-0.0254760
1	-2.0058470	-1.0580990	-0.9288290
1	-2.0322870	-1.1064730	0.8391270
6	-2.5602740	0.8211160	-0.0008230
1	-2.3026370	1.4316480	-0.8643530
1	-3.6348460	0.6304200	-0.0191630
1	-2.3247470	1.3859150	0.8993550
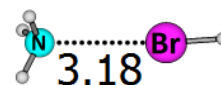
H₃N...BrH

SCF E= -2631.3958
ZPE= -2631.3524
G= -2631.3807
H= -2631.3459

35	-0.6835990	-0.0042790	0.0039790
7	2.4919690	-0.0029380	0.0036350
1	2.7493150	0.5884470	-0.7763760
1	2.9293100	-0.9033820	-0.1452060
1	2.9058410	0.3988480	0.8352050
1	-2.1022980	0.0864110	-0.0783350

H₃N...BrOCH₂Cl
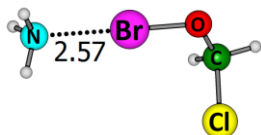
SCF E= -3205.4896
ZPE=-3205.4190
G= -3205.4541
H= -3205.4098

35	-0.8437900	-0.3027600	-0.0733240
7	-3.1178250	0.8774760	0.1525530
1	-2.9780080	1.8677840	-0.0024570
1	-3.5366330	0.7549700	1.0655360
1	-3.7684350	0.5371300	-0.5438530
8	0.7821830	-1.1624170	-0.2820460
6	1.7825480	-0.6460390	0.4965910
1	1.4812950	-0.4726670	1.5281080
1	2.6273740	-1.3258240	0.4292940
17	2.3870060	0.9569670	-0.1000780

H₃N...BrCH₂CH₂Br
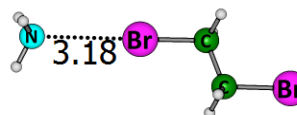
SCF E= -5283.6529
ZPE= -5283.5600
G= -5283.5987
H= -5283.5493

35	1.7303520	-0.2207640	0.0036970
7	4.8249040	0.5276140	-0.0052120
1	5.2368900	0.4521370	0.9161250
1	5.0401720	1.4516460	-0.3572790
1	5.2971480	-0.1396700	-0.6018390
6	-0.1587270	-0.7008390	-0.0048860
1	-0.3371000	-1.2873220	-0.8998110
1	-0.3405840	-1.3071730	0.8759970
6	-0.9807180	0.5601450	0.0075080
1	-0.8114560	1.1469090	0.9036250
1	-0.8071770	1.1672720	-0.8741040
35	-2.8793680	0.0969660	-0.0020390

H₃N...BrOCBr₃
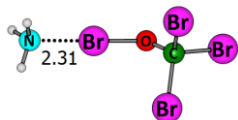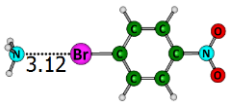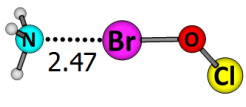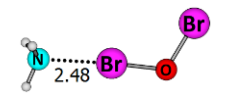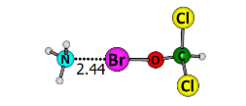
SCF E= -10466.7981
ZPE= -10466.7488
G= -10466.7902
H= -10466.7368
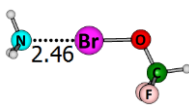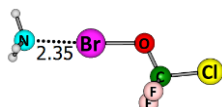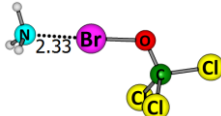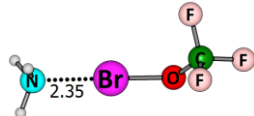
35	2.1419460	-0.0000440	-0.6258010
7	4.3873330	-0.0000280	-0.0846400
1	4.6018720	-0.8244920	0.4625360
1	4.6021450	0.8252960	0.4611280
1	4.9540500	-0.0008410	-0.9236520
8	0.2893380	-0.0000810	-1.1365470
6	-0.6132520	-0.0000100	-0.1811350
35	-2.3670430	-0.0001120	-1.0517070
35	-0.5089330	-1.5990410	0.9927700
35	-0.5089590	1.5992240	0.9925000

H₃N...BrC₆H₄Br
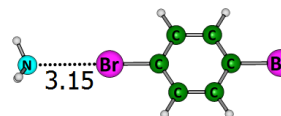
SCF E= -5436.0689
ZPE= -5435.9523
G= -5435.9397
H= -5435.9936

35	2.7272160	0.0033420	-0.0060810
7	5.8768990	-0.0069990	0.0129080
1	6.2770380	0.8557410	-0.3334430
1	6.2559450	-0.7607290	-0.5461120
1	6.2123090	-0.1360320	0.9590620
6	0.8351370	0.0018970	-0.0031610
6	0.1484000	-1.2026830	-0.0023300
6	0.1465390	1.2054180	-0.0022430
6	-1.2387500	-1.2055160	-0.0005440
1	0.6931440	-2.1358680	-0.0031390
6	-1.2406220	1.2060950	-0.0004540

1	0.6898390	2.1394450	-0.0029830
6	-1.9212300	-0.0002330	0.0003650
1	-1.7831450	-2.1386480	0.0000930
1	-1.7864540	2.1383870	0.0002550
35	-3.8150390	-0.0017180	0.0028270

H₃N...BrC₆H₄NO₂

SCF E= -3066.9383
ZPE= -3066.8083
G= -3066.8503
H= -3066.7948

35	2.2896390	0.0019090	-0.0019910
7	5.4097960	-0.0038030	0.0038080
1	5.7947870	0.8591860	-0.3591180
1	5.7836640	-0.7585870	-0.5575180
1	5.7700990	-0.1215910	0.9423900
6	0.4022230	0.0009890	-0.0008180
6	-0.2811180	-1.2085980	-0.0004860
6	-0.2823920	1.2098710	-0.0005070
6	-1.6653140	-1.2119750	0.0001490
1	0.2681610	-2.1385120	-0.0007190
6	-1.6665830	1.2117820	0.0000800
1	0.2659170	2.1403570	-0.0008040
6	-2.3323390	-0.0004450	0.0003730
1	-2.2281190	-2.1327380	0.0003690
1	-2.2303740	2.1319500	0.0002970
7	-3.8051680	-0.0011370	0.0009360
8	-4.3655050	1.0723860	0.0012640
8	-4.3645900	-1.0751420	0.0010910

H₃N...BrOCl

SCF E= -3166.1230
ZPE= -3166.0818
G=-3166.1146
H= -3166.0739

35	-0.5485740	-0.1919180	0.0006780
7	-2.9248310	0.4683030	-0.0005480
1	-3.0611900	1.2896550	-0.5756750
1	-3.2367540	0.6758880	0.9393910
1	-3.4913540	-0.2837150	-0.3712780
8	1.2263380	-0.7853200	-0.0014250
17	2.3325000	0.4729250	-0.0000550

H₃N...BrOBr

SCF E= -5280.1693
ZPE= -5280.1287
G= -5280.1627
H= -5280.1205

H₃N...BrOCHCl₂

SCF E= -3665.0989
ZPE= -3665.0379
G= -3665.0746
H= -3665.0278

35	1.0925820	0.2316110	-0.0001340
7	3.4279740	-0.6088360	0.0001370
1	3.5979880	-1.1779930	-0.8189910
1	3.5998160	-1.1690860	0.8250070
1	4.0787340	0.1660410	-0.0047980
8	-0.6214420	0.9597540	0.0002930
35	-1.9583200	-0.2669010	0.0000050

35	-1.1759280	0.0017330	0.3150690
7	-3.3277190	-0.0019280	-0.8384980
1	-4.0309670	-0.4748330	-0.2855120
1	-3.2326570	-0.4828360	-1.7238540
1	-3.6355990	0.9456130	-1.0157510
8	0.4425910	0.0018910	1.2671830
6	1.5720730	-0.0000520	0.5448590
1	2.4137100	-0.0001910	1.2291770
17	1.7622050	-1.4623340	-0.4915610
17	1.7650800	1.4594080	-0.4948280

H₃N...BrOCHF₂

SCF E= -2944.4055
ZPE= -2944.3407
G= -2944.3756
H= -2944.3314

35	-0.7449420	-0.2833090	-0.0001750
7	-3.0291880	0.6285030	0.0005480
1	-3.1572660	1.2090550	-0.8183130
1	-3.1617310	1.1997060	0.8252500
1	-3.7322670	-0.0992040	-0.0055120
8	0.9831260	-1.0178800	-0.0012880
6	1.9758360	-0.1158270	-0.0002760
1	2.9286410	-0.6456190	-0.0010740
9	1.9265670	0.7063860	-1.0791900
9	1.9267530	0.7036540	1.0807360

H₃N...BrOCClF₂

SCF E= -3404.0125
ZPE= -3403.9577
G= -3403.9946
H= -3403.9475

35	1.3507640	-0.2613260	0.0000990
7	3.6415390	0.2821360	-0.0001680
1	3.8699260	0.8233140	0.8242590
1	3.8678730	0.8254130	-0.8237820
1	4.1960240	-0.5647960	-0.0019500
8	-0.4852360	-0.7870580	-0.0001570
6	-1.3431650	0.2227990	0.0000190
9	-1.2107300	1.0259620	1.0728310
9	-1.2106740	1.0263510	-1.0725000
17	-2.9981080	-0.4366840	-0.0001560

H₃N...BrOCCl₃

SCF E= -4124.6982
ZPE= -4124.6474
G= -4124.6864
H= -4124.6362

H₃N...BrOCF₃

SCF E= -3043.6731
ZPE= -3043.6162
G= -3043.6524
H= -3043.6065

35	-1.5755960	0.0001080	-0.3749020		35	1.0469760	-0.2619560	-0.0000110
7	-3.8050680	-0.0001550	0.3134130		7	3.2832760	0.4663210	0.0000470
1	-3.9864440	0.8272340	0.8678830		1	3.7388990	0.2079970	0.8662880
1	-3.9825450	-0.8211820	0.8785020		1	3.3042280	1.4741710	-0.0928220
1	-4.4286860	-0.0068150	-0.4840530		1	3.7914020	0.0561100	-0.7734590
8	0.2303520	0.0002440	-0.9928770		8	-0.7414730	-0.8964920	0.0002280
6	1.1850610	0.0000090	-0.0734540		6	-1.6642620	0.0590320	0.0000100
17	1.1334340	1.4544520	0.9982810		9	-1.5952380	0.8636460	1.0735920
17	1.1335050	-1.4548540	0.9977390		9	-1.5950650	0.8633030	-1.0738200
17	2.7463460	0.0001710	-0.9343090		9	-2.8701720	-0.5065390	0.0000240

H₃N...BrCH₃
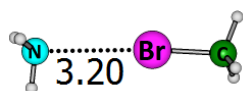
SCF E= -2670.6974
ZPE= -2670.6244
G= -2670.6581
H= -2670.6158

7	2.9306390	0.0166690	0.0007490
1	3.4679410	-0.4349110	-0.7280730
1	3.3587740	-0.2230390	0.8858240
1	3.0324610	1.0160020	-0.1231410
6	-2.2076100	0.0683040	0.0053460
1	-2.5169700	0.5626830	0.9186440
1	-2.5207790	0.6346630	-0.8637190
1	-2.5973980	-0.9417210	-0.0339800
35	-0.2712240	-0.0325770	-0.0026530

H₃N...BrCNBeCl₂
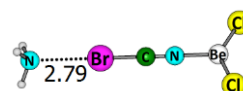
SCF E= -3658.9698
ZPE= -3658.9176
G= -3658.9056
H= -3658.9584

6	0.3278990	-0.0019850	-0.0000220
7	-0.8142850	-0.0014990	0.0000000
4	-2.5319500	0.0005360	-0.0000260
17	-3.2514970	1.7226980	-0.0000290
17	-3.2559600	-1.7197010	-0.0000250
35	2.1213450	-0.0019160	0.0001040
7	4.9109190	0.0031050	-0.0000940
1	5.2839380	0.9383220	0.1134660
1	5.2914700	-0.5605320	0.7509250
1	5.2882540	-0.3631540	-0.8662250

H₃N...BrC₃N

SCF E= -2799.7699
ZPE= -2799.7147
G= -2799.7490
H= -2799.7049

7	3.8266230	-0.0052210	0.0002180
1	4.2033130	-0.1604100	0.9273460

H₃N...BrC₅N
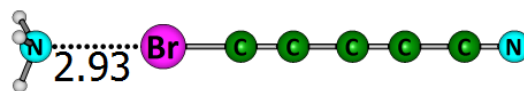
SCF E= -2875.9232
ZPE= -2875.8578
G= -2875.8955
H= -2875.8459

6	-1.0913670	0.0004990	-0.0006040
6	0.1137210	0.0002290	-0.0006780

1	4.2043080	0.8741840	-0.3307360
1	4.1992450	-0.7328490	-0.5975190
6	-0.8879620	0.0010030	0.0003730
6	-2.0892590	-0.0003040	0.0002940
6	-3.4652410	-0.0019270	0.0000050
7	-4.6152150	-0.0031290	-0.0001520
35	0.9019440	0.0024260	-0.0001030

7	4.8343940	0.0006870	0.0011610
1	5.2115030	-0.2395090	0.9098260
1	5.2031480	0.9119790	-0.2421940
1	5.2158120	-0.6615460	-0.6632620
6	-2.4549600	0.0006510	-0.0003230
6	-3.6602700	0.0006110	0.0000040
6	-5.0332750	0.0001050	0.0004410
7	-6.1839520	-0.0002370	0.0008050
35	1.9020960	-0.0007610	-0.0003190

H₃N...BrNO₂BeCl₂
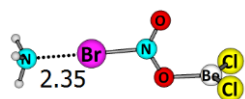
SCF E= -3771.2206
ZPE= -3771.1639
G= -3771.2057
H= -3771.1514

7	0.1229530	-0.0022640	0.4367240
8	-0.2485630	-0.0035100	1.5589390
8	-0.6272410	-0.0007090	-0.5481730
7	4.3594770	0.0027360	-0.4561670
1	4.7747550	0.8736100	-0.1468590
1	4.8138860	-0.7649130	0.0241700
1	4.5124190	-0.0974960	-1.4526560
4	-2.2967730	0.0008930	-0.2636230
17	-2.9864320	-1.7286860	-0.1736560
17	-2.9821570	1.7320790	-0.1711730
35	2.0623280	-0.0012000	0.0154830

H₃N...ClCF₃
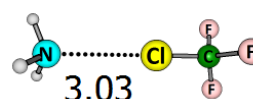
SCF E= -854.4331
ZPE= -854.3818
G= -854.4180
H= -854.3721

7	-3.6848880	0.0020340	0.0024770
1	-4.0665430	0.4934390	-0.7960320
1	-4.0408850	0.4588440	0.8326790
1	-4.0693630	-0.9343850	-0.0113540
6	1.1014990	0.0006380	0.0010650
9	1.5716090	-1.1426400	0.4795300
9	1.5783250	0.1633310	-1.2251830
9	1.5625260	0.9870150	0.7577790
17	-0.6500080	-0.0061950	-0.0093030

H₃N...ClCCH
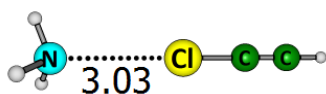
SCF E= -593.4838
ZPE= -593.4282
G= -593.4593
H= -593.4199
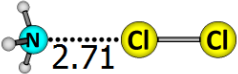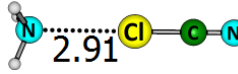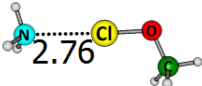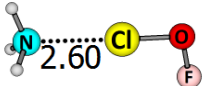
7	-3.0167920	-0.0008200	-0.0006020

H₃N...ClCHCH₂
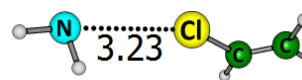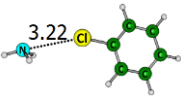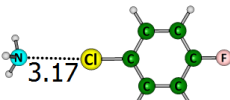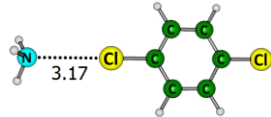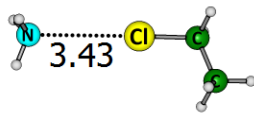
SCF E= -594.7396
ZPE= -594.6606
G= -594.6942
H= -594.6518

17	-0.0241960	-0.1178710	0.1785950

1	-3.3935150	0.9282860	-0.1405900
1	-3.3881330	-0.3450040	0.8759140
1	-3.3906680	-0.5888330	-0.7348110
6	1.6597650	-0.0001180	0.0000270
6	2.8554810	-0.0013230	-0.0005590
1	3.9168780	-0.0023310	-0.0011300
17	0.0165590	0.0013100	0.0004720

7	-3.2432070	-0.0786060	-0.0810400
1	-4.2401370	0.0167300	-0.2271160
1	-2.7994010	-0.0456440	-0.9903320
1	-2.9320210	0.7400630	0.4267050
6	1.5763450	0.5047760	-0.0533100
6	2.6397480	-0.2675830	-0.1459950
1	3.6125180	0.1814610	-0.2890650
1	2.5696980	-1.3439690	-0.0824550
1	1.6065620	1.5822520	-0.1107350

$H_3N...Cl_2$

SCF E= -976.9366
ZPE= -976.8990
G= -976.9286
H= -976.8918

7	-2.8517590	0.0001920	0.0001230
1	-3.2165830	0.5339390	-0.7782300
1	-3.2115080	0.4091250	0.8528200
1	-3.2158140	-0.9412080	-0.0707730
17	-0.1397980	-0.0004210	-0.0005610
17	1.8813400	0.0002330	0.0002850

$H_3N...ClCN$

SCF E= -609.5832
ZPE= -609.5381
G= -609.5687
H= -609.5302

7	-2.8874880	-0.0011910	-0.0012170
1	-3.2666960	-0.2108290	0.9139920
1	-3.2610020	-0.6915920	-0.6410260
1	-3.2660660	0.8957810	-0.2799020
6	1.6614790	-0.0004760	-0.0002390
7	2.8096230	-0.0019490	-0.0021220
17	0.0217620	0.0018510	0.0018680

$H_3N...ClOCH_3$

SCF E= -631.8231
ZPE= -631.7442
G= -631.7765
H= -631.7354

7	-2.8865760	0.2420210	0.0000040
1	-3.2047830	0.7494720	-0.8154550
1	-3.2046700	0.7434900	0.8191920
1	-3.3423050	-0.6613780	-0.0032670
8	1.4855510	-0.5930930	0.0000740
6	2.2498350	0.5974200	0.0000030
1	2.0475640	1.1931370	0.8921380
1	3.2892750	0.2727680	0.0000570

$H_3N...ClOF$

SCF E= -691.6532
ZPE= -691.6114
G= -691.6430
H= -691.6034

7	-2.7247830	-0.2247290	-0.0002360
1	-3.0126470	-0.6019830	0.8936260
1	-2.9470010	-0.9086700	-0.7123520
1	-3.2779260	0.6030530	-0.1813920
8	1.4851150	0.5714100	-0.0003870
9	2.1434420	-0.6700960	-0.0000390
17	-0.1682850	0.2317820	0.0003070

1	2.0476150	1.1930040	-0.8922330
17	-0.1652990	-0.2367300	-0.0000630

H₃N...ClC₆H₅

SCF E= -748.3901
ZPE= -748.2627
G= -748.3008
H= -748.2519

7	-4.5533860	0.2595820	0.0999550
1	-5.5172370	0.5537260	0.1930740
1	-4.1399550	0.8084040	-0.6434190
1	-4.0747760	0.5143700	0.9548470
6	0.2897790	-0.1504130	-0.0400330
6	0.7505100	1.1562290	-0.0475120
6	1.1663430	-1.2219010	0.0184410
6	2.1170960	1.3896300	0.0051420
1	0.0457820	1.9739150	-0.0945680
6	2.5304260	-0.9741550	0.0704500
1	0.7804500	-2.2310760	0.0230560
6	3.0090900	0.3283450	0.0641240
1	2.4829410	2.4071950	-0.0005010
1	3.2197390	-1.8060990	0.1161600
1	4.0728920	0.5153940	0.1048030
17	-1.4220940	-0.4540770	-0.1045180

H₃N...ClC₆H₄F

SCF E= -847.6410
ZPE= -847.5220
G= -847.5612
H= -847.5101

7	-5.0683140	0.0294860	0.0182090
1	-5.6148550	-0.7146060	-0.3962530
1	-5.3475590	0.8927380	-0.4301910
1	-5.3398140	0.0954900	0.9909640
6	-0.1588220	-0.0196580	-0.0101330
6	0.5105050	1.1945630	-0.0064370
6	0.5421240	-1.2160010	-0.0054730
6	1.8969950	1.2159450	0.0021530
1	-0.0528140	2.1163570	-0.0103680
6	1.9287570	-1.2009810	0.0031400
1	0.0029490	-2.1521160	-0.0087500
6	2.5797390	0.0161920	0.0068350
1	2.4485320	2.1449980	0.0051900
1	2.5042440	-2.1154270	0.0068680
9	3.9224550	0.0340270	0.0155790
17	-1.8953160	-0.0423790	-0.0215090

H₃N...ClC₆H₄Cl

SCF E= -1208.0000
ZPE= -1207.8827
G= -1207.9238
H= -1207.8703

7	5.5199960	-0.0034820	-0.0004570
1	5.8992870	0.8591680	-0.3696940

H₃N...ClCH₂CH₃

SCF E= -595.9705
ZPE= -595.8679
G= -595.9040
H= -595.8582

7	3.4519360	0.2536530	0.0006120
1	3.8646210	0.1466530	0.9183150

1	5.8870620	-0.7586830	-0.5654100
1	5.8923840	-0.1194770	0.9334530
6	0.6177180	0.0018120	0.0002210
6	-0.0674860	-1.2033250	0.0001530
6	-0.0695890	1.2057590	0.0001500
6	-1.4537000	-1.2057490	0.0000060
1	0.4828220	-2.1330820	0.0002300
6	-1.4558020	1.2057390	0.0000190
1	0.4791000	2.1364700	0.0002360
6	-2.1361200	-0.0006000	-0.0000560
1	-2.0030520	-2.1359540	-0.0000420
1	-2.0067930	2.1349760	-0.0000150
17	-3.8749430	-0.0020850	-0.0002070
17	2.3525360	0.0032110	0.0002940

1	3.6664380	1.1891890	-0.3195820
1	3.9231670	-0.3926090	-0.6191380
6	-1.7091970	-0.5517230	-0.0022080
1	-1.9344880	-1.1389090	-0.8879320
1	-1.9380930	-1.1436910	0.8793860
6	-2.4482630	0.7671870	-0.0000740
1	-2.1912280	1.3529840	-0.8808050
1	-3.5243860	0.5881760	-0.0024920
1	-2.1944070	1.3482830	0.8846810
17	0.0652690	-0.2952020	0.0021750
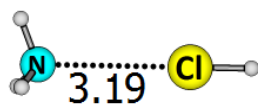
H₃N...ClH

SCF E= -517.3618
ZPE=-517.3177
G= -517.3454
H= -517.3112

7	-2.0541820	-0.0000160	0.0000790
1	-2.4278400	-0.5535890	0.7604600
1	-2.4262120	-0.3820850	-0.8600770
1	-2.4269360	0.9357370	0.0987020
17	1.1322080	0.0000200	0.0000290
1	2.4127240	-0.0002850	-0.0001370

H₃N...ClOCClH₂
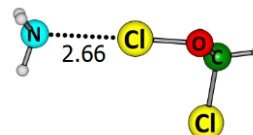
SCF E= -1091.4375
ZPE= -1091.3671
G= -1091.4023
H= -1091.3577

7	-3.3431150	0.7163320	0.1226910
1	-3.2371840	1.6228590	-0.3146430
1	-3.6345890	0.8666390	1.0798560
1	-4.0884750	0.2268830	-0.3556230
8	0.5268380	-1.2347600	-0.3071440
6	1.4939060	-0.6637350	0.4905330
1	1.1556900	-0.5140860	1.5131440
1	2.3595690	-1.3165510	0.4347780
17	2.0256520	0.9530610	-0.1016570
17	-0.9863190	-0.4848010	-0.1161310

H₃N...ClOCBr₃
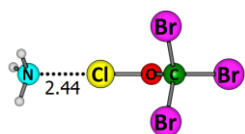
H₃N...ClCCl₃
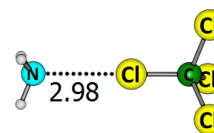
	SCF E= -8352.7411	
	ZPE= -8352.6923	
	G= -8352.7337	
	H= -8352.6801	

7	-4.5438370	0.0012070	0.5257300
1	-4.7549030	-0.6790440	-0.1929640
1	-4.8332640	0.9137890	0.1984400
1	-5.0787290	-0.2288580	1.3531460
8	-0.4389740	-0.0001110	1.2830240
6	0.3625620	-0.0000400	0.2025240
35	2.1684940	0.0041760	0.9185260
35	0.1204290	-1.5961190	-0.9227680
35	0.1153680	1.5921710	-0.9272120
17	-2.1376470	-0.0012470	0.9460470

	SCF E= -1935.4624	
	ZPE= -1935.4168	
	G= -1935.4552	
	H= -1935.4058	

7	4.1721520	0.0002490	-0.0000950
1	4.5460110	0.3527060	0.8720000
1	4.5480540	0.5764200	-0.7425750
1	4.5403530	-0.9338010	-0.1290920
6	-0.5695920	-0.0000220	-0.0000520
17	-1.1717610	1.6173360	-0.4074500
17	-1.1690200	-0.4553960	1.6048900
17	-1.1718700	-1.1625080	-1.1955530
17	1.1937130	0.0007480	-0.0018500

H₃N…ClC₆H₄Br
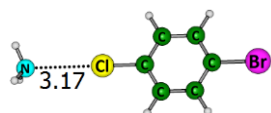
	SCF E= -3322.0337	
	ZPE= -3321.917	
	G= -3321.9589	
	H= -3321.9042	

7	6.2553100	-0.0046220	-0.0006030
1	6.6351260	0.8582620	-0.3687790
1	6.6219450	-0.7592970	-0.5665520
1	6.6278280	-0.1220160	0.9330880
6	1.3551720	0.0022840	0.0002840
6	0.6699780	-1.2027210	0.0002360
6	0.6680410	1.2061940	0.0002350
6	-0.7166620	-1.2053210	0.0001080
1	1.2199920	-2.1327200	0.0003040
6	-0.7186030	1.2065420	0.0001170
1	1.2165620	2.1370720	0.0003100
6	-1.3993050	0.0000610	0.0000350
1	-1.2611780	-2.1383040	0.0000550
1	-1.2646400	2.1386360	0.0000810
35	-3.2931080	-0.0014740	-0.0001710
17	3.0896620	0.0035340	0.0003310

H₃N…ClC₆H₄NO₂
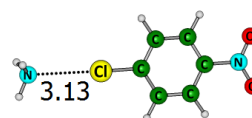
	SCF E= -952.9032	
	ZPE= -952.7728	
	G= -952.8143	
	H= -952.7595	

7	-5.7673110	-0.0185840	-0.0000160
1	-6.2013870	0.8957960	-0.0003090
1	-6.1111390	-0.5114450	0.8145100
1	-6.1108700	-0.5117830	-0.8144550
6	-0.9046460	0.0106500	0.0000230
6	-0.2277800	-1.2022150	0.0000700
6	-0.2168600	1.2173830	-0.0000570
6	1.1557500	-1.2107660	0.0000360
1	-0.7860380	-2.1266800	0.0001230
6	1.1667080	1.2133430	-0.0000480
1	-0.7667870	2.1468200	-0.0001040
6	1.8277040	-0.0017160	-0.0000030
1	1.7150590	-2.1335950	0.0000530
1	1.7343650	2.1310800	-0.0000930
7	3.3001970	-0.0082840	-0.0000070
8	3.8647840	1.0630260	0.0001300
8	3.8553160	-1.0845380	-0.0001430
17	-2.6334970	0.0182290	0.0000240

H₃N...ClOCl
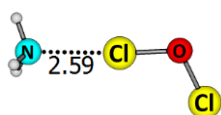
SCF E= -1052.0701
ZPE= -1052.0292
G= -1052.0618
H= -1052.0210

7	-3.1400380	-0.3682140	0.0001960
1	-3.4630650	-0.5757770	0.9362660
1	-3.2991590	-1.1852220	-0.5750210
1	-3.7041060	0.3875680	-0.3661540
8	0.9889250	0.8297370	-0.0002940
17	2.0748070	-0.4526020	-0.0000140
17	-0.6315600	0.2945450	0.0003610

H₃N...ClOBr
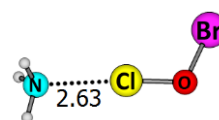
SCF E= -3166.1166
ZPE= -3166.0761
G= -3166.1098
H= -3166.0678

7	3.7461500	-0.4776470	0.0004950
1	3.9345450	-1.1557990	-0.7263210
1	3.9981140	-0.8917540	0.8885320
1	4.3484040	0.3206760	-0.1536960
8	-0.3169530	1.0066730	0.0016500
35	-1.6338690	-0.2529980	0.0000370
17	1.2480540	0.3454090	-0.0015580

H₃N...ClOCHCl₂
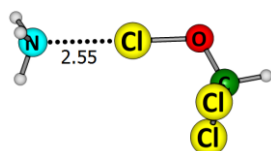
SCF E= -1551.0444
ZPE= -1550.9835
G= -1551.0207
H= -1550.9732

7	3.5736850	-0.0005980	-0.6708960
1	3.8730480	0.9432780	-0.8787570
1	3.4820500	-0.5007870	-1.5456620
1	4.2994400	-0.4488620	-0.1268220
8	-0.1842500	0.0012840	1.3396960
6	-1.2806580	-0.0000600	0.5382330
1	-2.1406250	-0.0003030	1.1982750
17	-1.4039330	1.4578470	-0.4900950
17	-1.4016920	-1.4598030	-0.4880010
17	1.3131690	0.0020120	0.5135230

H₃N...ClOCHF₂
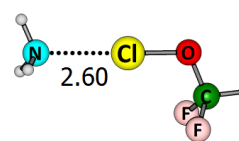
SCF E= -830.3510
ZPE= -830.2862
G= -830.3211
H= -830.2767

7	-3.2669000	-0.4737290	0.0006180
1	-3.4931300	-0.8590000	0.9084460
1	-3.3305520	-1.2196880	-0.6801210
1	-3.9666730	0.2200760	-0.2288130
8	0.7517560	1.0799010	-0.0016360
6	1.7058020	0.1151610	-0.0002980
1	2.6711120	0.6202630	-0.0011210
9	1.6112670	-0.6868170	1.0794990
9	1.6110540	-0.6899850	-1.0777450
17	-0.8389530	0.4479700	-0.0002130

H₃N...ClOCClF₂
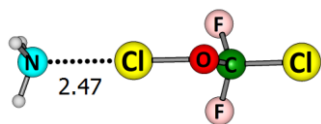
SCF E= -1289.9558
ZPE= -1289.9013
G= -1289.9377
H= -1289.8909

7	3.9335290	0.1362140	0.0009740
1	4.2575500	0.3187560	0.9419170
1	4.1101000	0.9580530	-0.5622180
1	4.4714130	-0.6320410	-0.3786510
8	-0.1510810	-0.8542100	-0.0009380
6	-0.9761520	0.2103720	-0.0001670
9	-0.8015970	0.9926110	1.0712340
9	-0.8029350	0.9929400	-1.0715850
17	-2.6306500	-0.4173040	0.0008010
17	1.5208020	-0.4001540	-0.0005780

H₃N...ClOCCl₃
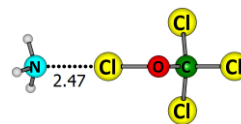
SCF E= -2010.6417
ZPE= -2010.5912
G= -2010.6293
H= -2010.5799

7	4.0838970	0.0008950	0.0737450
1	4.2487230	-0.7079510	0.7768010
1	4.3367680	0.9000860	0.4626060
1	4.6873470	-0.1867020	-0.7163790
8	0.0497120	-0.0007070	-1.0841960
6	-0.8555840	0.0001160	-0.0767020
17	-0.7241330	-1.4514160	0.9626000
17	-0.7201560	1.4499230	0.9643210
17	-2.4372530	0.0027490	-0.8750000
17	1.6977590	-0.0016520	-0.5757720

H₃N...ClOCF₃
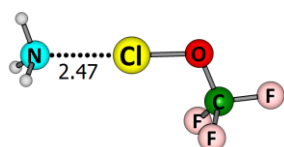
SCF E= -929.6163
ZPE= -929.5599
G= -929.5970
H= -929.5499

7	-3.5408290	0.3208310	-0.0000070
1	-3.7284490	0.8858230	-0.8182000
1	-3.7312290	0.8784860	0.8225670
1	-4.1753540	-0.4672940	-0.0046280
8	0.4470870	-0.9605070	-0.0001400
6	1.3359320	0.0541430	-0.0000330
9	1.2239970	0.8391790	-1.0726210
9	1.2241680	0.8388120	1.0728420
9	2.5469910	-0.4843830	-0.0002320
17	-1.1839910	-0.4074180	0.0001010

H₃N...ClNO₂BeCl₂
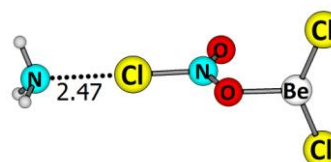
SCF E= -1657.1693
ZPE= -1657.1130
G= -1657.1555
H= -1657.1003

7	0.5804450	-0.0007540	0.4194680
8	0.2324960	-0.0011240	1.5450670
8	-0.1566030	-0.0002570	-0.5657820
7	4.7353390	0.0006500	-0.4577220
1	5.1617080	0.8736530	-0.1722530
1	5.2062550	-0.7522720	0.0289590
1	4.8972210	-0.1177280	-1.4503100
4	-1.8497070	0.0003010	-0.2736730
17	-2.5011040	-1.7359320	-0.1652650
17	-2.4996740	1.7370220	-0.1645040
17	2.3134850	-0.0006830	0.0428160

H₃N...ClC₃N
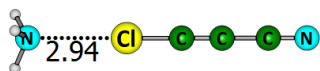
SCF E= -685.7321
ZPE= -685.6766
G= -685.7106
H= -685.6668

7	4.0754350	0.0025280	-0.0003030
1	4.4483750	0.6991390	0.6330450
1	4.4538050	0.2047540	-0.9175410
1	4.4561060	-0.8911330	0.2858220
6	-0.4970980	-0.0017980	-0.0000770
6	-1.6968960	-0.0008000	0.0000480
6	-3.0725270	0.0007420	0.0000600
7	-4.2223420	0.0026950	-0.0001650
17	1.1334820	-0.0022460	0.0001040

H₃N...ClC₅N
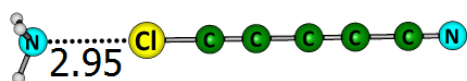
SCF E= -761.8854
ZPE= -761.8194
G= -761.8566
H= -761.8076

6	0.4915690	0.0011090	-0.0001770
6	-0.7119150	0.0018790	0.0008470
7	-5.2914230	-0.0034030	-0.0022910
1	-5.6681680	-0.7154160	-0.6159060
1	-5.6709450	0.8833410	-0.3106100
1	-5.6668860	-0.1806160	0.9212480
6	1.8550880	-0.0002090	0.0001170
6	3.0601390	-0.0012100	-0.0000480
6	4.4332540	-0.0010440	-0.0005520
7	5.5838520	-0.0010830	-0.0009210
17	-2.3417540	0.0024080	0.0015660

H₃N...FCN
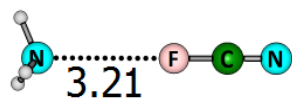
SCF E= -249.2042
ZPE= -249.1583
G= -249.1907
H= -249.1501

7	-2.9327000	-0.0008650	-0.0014130
1	-3.3124350	0.6110610	0.7101250
1	-3.3074500	-0.9248210	0.1740370
1	-3.3117410	0.3075830	-0.8879780
9	0.2755350	0.0030160	0.0035010
6	1.5355110	0.0001910	0.0004180
7	2.6810920	-0.0022940	-0.0029010

H₃N...FNO₂BeCl₂
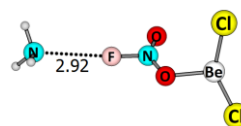
SCF E= -1296.7746
ZPE= -1296.7180
G= -1296.7621
H= -1296.7046

7	0.8451030	0.0236650	0.5795790
8	0.6681120	0.6459480	1.5417740
8	0.0807710	-0.5082980	-0.1927810
9	2.1394230	-0.1769900	0.2231480
7	4.9211150	-0.3682150	-0.6476450
1	5.3891750	0.5249870	-0.5562160
1	5.4975120	-1.0515530	-0.1724240
1	4.9344400	-0.6072380	-1.6315470
4	-1.6309020	-0.0486320	-0.2420340
17	-2.6934320	-1.5421580	-0.0886540
17	-1.7128570	1.7910920	-0.4404930

	H₃N...FCNBeCl₂				H₃N...FC₃N		

	H₃N...FCNBeCl₂	
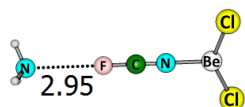
SCF E= -1184.5457
ZPE= -1184.4923
G= -1184.5347
H= -1184.4799

6	-1.2370720	0.0000960	0.0124200
7	-0.0999870	0.0001500	0.0074720
4	1.6417190	0.0000470	-0.0005780
17	2.3330040	1.7272750	-0.0039030
17	2.3323620	-1.7274910	-0.0039020
9	-2.4782500	0.0000310	0.0174970
7	-5.4304620	0.0001840	-0.0119380
1	-5.8003450	0.8065030	-0.5005490
1	-5.8003950	-0.8178900	-0.4805310
1	-5.8375330	0.0116750	0.9153580
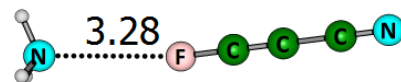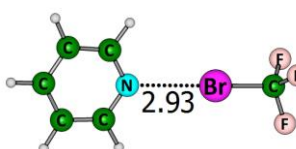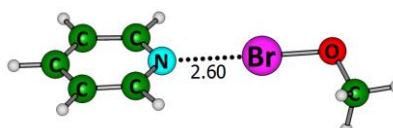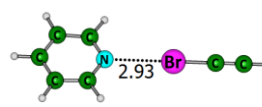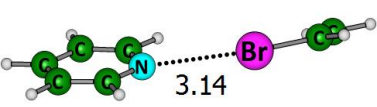
SCF E= -325.3520
ZPE= -325.2954
G= -325.3309
H= -325.2855

7	4.2930400	0.1993430	0.0004190
1	4.6284310	0.7124790	0.8060110
1	4.6227230	0.6910410	-0.8207250
1	4.7561870	-0.7007070	0.0106620
9	1.0482870	-0.2991760	-0.0005510
6	-0.2057550	-0.1721110	0.0014930
6	-1.3916690	-0.0518620	-0.0002320
6	-2.7621640	0.0869110	-0.0000890
7	-3.9050960	0.2023920	-0.0001370

Table S7: Cartesian coordinates in (Å) and energy data (a.u.) of halogen bonded pyridine complexes at M06-2X/aug-cc-pVTZ level of theory. All the optimized structures are corresponding to minima on the potential energy surface.

C₅H₅N... BrCF₃				C₅H₅N...BrOCH₃			

C₅H₅N... BrCF₃

SCF E= -3160.1787
ZPE= -3160.0738
G= -3160.1159
H= -3160.0619

C₅H₅N...BrOCH₃

SCF E= -2937.5861
ZPE= -2937.4536
G= -2937.4937
H= -2937.4426

	C₅H₅N... BrCF₃				C₅H₅N...BrOCH₃		
35	0.9620840	0.0089920	-0.0001060	35	1.3823450	-0.2281170	-0.0824870
6	2.8867770	-0.0038520	0.0000040	8	3.2080270	-0.3949230	-0.1652470
9	3.3546740	-0.6265570	1.0745810	6	3.8603760	0.7648180	0.3049750
9	3.3548910	-0.6285090	-1.0733240	1	3.6240080	0.9604370	1.3541310
9	3.3684600	1.2327130	-0.0010390	1	4.9282670	0.5696720	0.2055760
6	-4.7471700	-0.0184030	-0.0000970	1	3.5963260	1.6424170	-0.2906780
6	-4.0273360	-1.2025100	-0.0000180	6	-3.9706100	0.1878080	0.0418350
6	-2.6418750	-1.1330960	0.0001170	6	-3.3606640	-1.0539570	0.1208100
7	-1.9696440	0.0144480	0.0001790	6	-1.9753900	-1.1122790	0.1020230
6	-2.6688790	1.1458130	0.0001110	7	-1.2107670	-0.0286790	0.0111000
6	-4.0556830	1.1824040	-0.0000350	6	-1.7990840	1.1607730	-0.0647910
1	-5.8287090	-0.0312920	-0.0002050	6	-3.1763220	1.3194940	-0.0529520
1	-4.5238960	-2.1621920	-0.0000550	1	-5.0488260	0.2726250	0.0529440
1	-2.0433060	-2.0367970	0.0001810	1	-3.9409190	-1.9624170	0.1938950
1	-2.0919470	2.0634130	0.0001730	1	-1.4536770	-2.0603010	0.1609640
1	-4.5748280	2.1300370	-0.0000990	1	-1.1361280	2.0148990	-0.1381630
				1	-3.6098290	2.3069680	-0.1187450

C₅H₅N...BrCCH	C₅H₅N...BrCHCH₂

C₅H₅N...BrCCH

SCF E= -2899.2340
ZPE= -2899.1245
G= -2899.1624

C₅H₅N...BrCHCH₂

SCF E= -2900.4874
ZPE= -2900.3546
G= -2900.3948

H= -2899.1142			
35	-1.6576960	0.0001560	-0.0000020
6	-3.4590000	-0.0001310	0.0000220
6	-4.6560420	-0.0003240	0.0000410
1	-5.7181120	-0.0004920	0.0000610
6	4.0505320	-0.0004200	0.0000710
6	3.3444340	-1.1927260	0.0000280
6	1.9581960	-1.1392640	-0.0000510
7	1.2723980	0.0003220	-0.0000910
6	1.9588070	1.1395420	-0.0000510
6	3.3450760	1.1922630	0.0000310
1	5.1321580	-0.0007110	0.0001360
1	3.8520490	-2.1466050	0.0000590
1	1.3700810	-2.0497640	-0.0000800
1	1.3711810	2.0503560	-0.0000920
1	3.8532000	2.1458700	0.0000610

H= -2900.3438			
35	1.6670050	-0.3980730	0.0333030
6	3.5194680	-0.0401450	0.0795390
6	4.0367160	1.1438370	-0.1822950
1	5.1088100	1.2819460	-0.1368320
1	3.4222720	1.9932600	-0.4455130
1	4.1112970	-0.9035950	0.3438030
6	-4.0361430	0.6534570	0.0077750
6	-2.9211730	1.4728300	0.0760120
6	-1.6650530	0.8831860	0.0571000
7	-1.4736290	-0.4304000	-0.0229380
6	-2.5511150	-1.2077270	-0.0877240
6	-3.8491060	-0.7168810	-0.0758600
1	-5.0325430	1.0744870	0.0198030
1	-3.0167910	2.5473050	0.1423140
1	-0.7685060	1.4911370	0.1071770
1	-2.3683100	-2.2739760	-0.1522220
1	-4.6875480	-1.3965350	-0.1308350

$C_5H_5N...Br_2$			
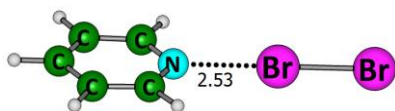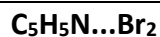
SCF E= -5396.7488
ZPE= -5396.6575
G= -5396.6950
H= -5396.6480

35	-0.7403550	0.0001780	0.0001550
35	-3.0787620	-0.0001090	-0.0001140
6	4.5518220	-0.0004460	-0.0001500
6	3.8490220	1.1941730	-0.0000780
6	2.4636140	1.1456820	0.0000170
7	1.7903540	0.0003310	0.0000700
6	2.4629660	-1.1453840	0.0000180

$C_5H_5N...BrCN$			
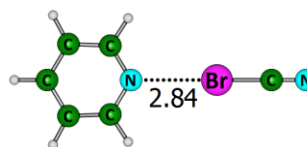
SCF E= -2915.3348
ZPE= -2915.2359
G= -2915.2732
H= -2915.2260

35	-1.629760	-0.000165	0.000044
6	-3.433875	0.000167	0.000069
7	-4.582367	0.000360	-0.000076
6	3.985250	0.000380	0.000116
6	3.280247	-1.192595	0.000032
6	1.894492	-1.140682	-0.000104
7	1.209168	-0.000271	-0.000179

6	3.8483600	-1.1946600	-0.0000790	6	1.893952	1.140443	-0.000117
1	5.6332860	-0.0007400	-0.0002190	6	3.279691	1.193015	0.000040
1	4.3585160	2.1467770	-0.0001060	1	5.066782	0.000623	0.000222
1	1.8669760	2.0500020	0.0000660	1	3.788357	-2.146067	0.000072
1	1.8658350	-2.0493830	0.0000670	1	1.306956	-2.051430	-0.000167
1	4.3573040	-2.1475600	-0.0001070	1	1.306005	2.050931	-0.000188
				1	3.787342	2.146733	0.000105

C₅H₅N… BrOH
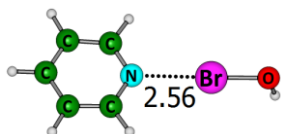
SCF E= -2898.2928
ZPE= -2898.1886
G= -2898.2244
H= -2898.1790

35	-1.7380310	0.0012490	-0.0107020
8	-3.5799690	0.0110120	-0.0807120
1	-3.8618190	-0.1128130	0.8304280
6	3.5928340	0.0007110	-0.0002630
6	2.8878810	1.1939540	0.0044810
6	1.5022910	1.1426300	0.0094500
7	0.8262780	-0.0016420	0.0100240
6	1.5042650	-1.1447220	0.0047560
6	2.8899110	-1.1937520	-0.0001870
1	4.6743650	0.0016260	-0.0045740
1	3.3960680	2.1473290	0.0037180
1	0.9059680	2.0473150	0.0122470
1	0.9095090	-2.0504420	0.0036100
1	3.3997020	-2.1462630	-0.0047360

C₅H₅N…BrOF
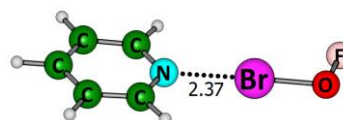
SCF E= -2997.4195
ZPE= -2997.3237
G= -2997.3605
H= -2997.3137

35	-1.2837340	-0.2212790	0.0000380
8	-3.1420460	-0.4297150	0.0001930
9	-3.6890730	0.8683790	-0.0000930
6	3.8210950	0.1994500	0.0001940
6	3.2257810	-1.0522300	0.0000360
6	1.8427220	-1.1266200	-0.0001700
7	1.0759440	-0.0407770	-0.0003120
6	1.6421010	1.1614390	-0.0001660
6	3.0171250	1.3285880	0.0001120
1	4.8983440	0.2942270	0.0003830
1	3.8163600	-1.9566110	0.0000540
1	1.3237360	-2.0773620	-0.0003180
1	0.9645190	2.0065390	-0.0002470
1	3.4412160	2.3219520	0.0002290

	C5H5N...BrC6H5		
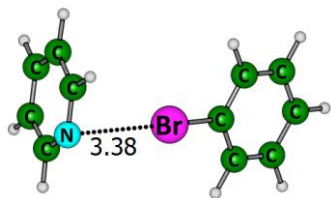
SCF E= -3054.1373
ZPE= -3053.9562
G= -3054.0004
H= -3053.9431

35	-0.0606680	-0.2626970	-0.5603620
6	-1.8934420	-0.0444420	-0.1326530
6	-2.4570650	1.2213510	-0.1635820
6	-2.6470750	-1.1572460	0.2070470
6	-3.8001190	1.3702680	0.1529070
1	-1.8532100	2.0758740	-0.4329680
6	-3.9887270	-0.9940130	0.5215260
1	-2.1889650	-2.1356300	0.2245040
6	-4.5680100	0.2665240	0.4958210
1	-4.2448570	2.3557790	0.1286330
1	-4.5805610	-1.8591890	0.7877080
1	-5.6136960	0.3888050	0.7411840
6	3.2339710	0.9036800	1.3977170
6	3.1789310	-0.4755820	1.5123420
6	3.2034610	-1.2370320	0.3523620
7	3.2775960	-0.7141750	-0.8691680
6	3.3316570	0.6120310	-0.9650420
6	3.3132430	1.4616120	0.1322320
1	3.2127510	1.5321000	2.2779540
1	3.1107760	-0.9568790	2.4775590
1	3.1545620	-2.3183730	0.4067460
1	3.3881170	1.0160330	-1.9692350
1	3.3543420	2.5321880	-0.0092990

	C5H5N...BrC6H4Cl		
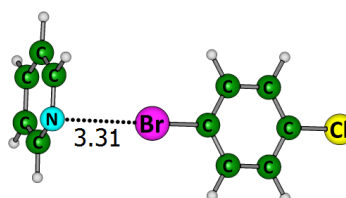
SCF E= -3513.7474
ZPE= -3513.5758
G= -3513.6225
H= -3513.5615

6	-1.1522330	-0.1906570	-0.2125590
6	-1.9348800	-1.2749950	0.1525260
6	-1.7171380	1.0606640	-0.4030850
6	-3.2994380	-1.1061680	0.3305320
1	-1.4830080	-2.2456430	0.2975220
6	-3.0819800	1.2301470	-0.2268860
1	-1.0974650	1.8976410	-0.6905000
6	-3.8617440	0.1451370	0.1383250
1	-3.9236430	-1.9403180	0.6167040
1	-3.5393470	2.1980260	-0.3738010
17	-5.5715560	0.3573830	0.3577490
35	0.7081030	-0.4283810	-0.4639160
6	4.1190220	1.1905730	1.2636720
6	4.1180090	1.5520340	-0.0742880
6	4.0512480	0.5494310	-1.0310050
7	3.9877390	-0.7467840	-0.7336260
6	3.9895930	-1.0798820	0.5548830
6	4.0536790	-0.1542400	1.5871450
1	4.1679410	1.9436760	2.0387290
1	4.1653150	2.5884060	-0.3770060
1	4.0440730	0.7971770	-2.0859560
1	3.9314540	-2.1399150	0.7736910
1	4.0485220	-0.4860120	2.6157940

C₅H₅N...BrH

	C₅H₅N...BrH		

C₅H₅N...BrH
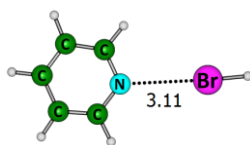
SCF E= -2823.1085
ZPE= -2823.0103
G= -2823.0455
H= -2823.0022

35	2.4045850	-0.0056570	-0.01542
1	3.8183400	0.1275810	-0.12546
6	-3.4588510	0.1480800	-0.07286
6	-2.6311200	1.2579180	-0.01866
6	-1.2609300	1.0568700	0.070071
7	-0.6992200	-0.1481030	0.106831
6	-1.5030610	-1.2065120	0.05419
6	-2.8843490	-1.1121870	-0.03592
1	-4.5322100	0.2636070	-0.14276
1	-3.0330510	2.2606750	-0.04494
1	-0.5813800	1.9007030	0.112658
1	-1.0188660	-2.1757260	0.085941
1	-3.4888980	-2.0071470	-0.07451

C₅H₅N...BrOCH₂Cl

C₅H₅N...BrOCH₂Cl
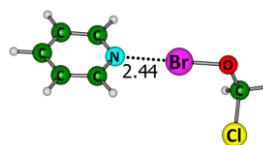
SCF E= -3397.2037
ZPE= -3397.0794
G= -3397.1209
H= -3397.0678

35	0.6594750	-0.5507730	-0.3476040
8	2.4706350	-0.9327500	-0.5559520
6	3.2465680	-0.4870530	0.4743620
1	2.8271650	-0.6983270	1.4568190
1	4.2368390	-0.9179710	0.3544160
17	3.4944060	1.3158570	0.4504100
6	-4.3907370	0.5028050	0.2904430
6	-3.8622230	-0.6943890	0.7470670
6	-2.5163770	-0.9463610	0.5342100
7	-1.7207090	-0.0834540	-0.0888100
6	-2.2253470	1.0653340	-0.5274050
6	-3.5594410	1.4008760	-0.3600790
1	-5.4367820	0.7327930	0.4406460
1	-4.4753410	-1.4211380	1.2596090
1	-2.0516300	-1.8651510	0.8711540
1	-1.5304580	1.7312780	-1.0246520
1	-3.9310780	2.3449130	-0.7311100

C₅H₅N...BrCH₂CH₂Br

C₅H₅N...BrCH₂CH₂Br
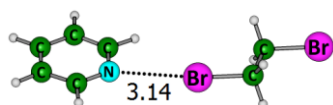
SCF E= -5475.3659
ZPE= -5475.2184
G= -5475.2628
H= -5475.2058

C₅H₅N...BrCCl₃

C₅H₅N...BrCCl₃
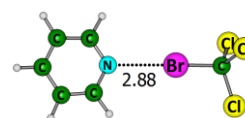
SCF E= -4241.2108
ZPE= -4241.1114
G= -4241.1560
H= -4241.0982

35	0.0762900	-0.9078280	-0.0000430
6	-1.8736220	-0.9186220	-0.0000440
1	-2.1890700	-1.4555430	-0.8881230
1	-2.1890680	-1.4556120	0.8879940
6	-2.3684490	0.5026020	0.0000110
1	-2.0596470	1.0413070	0.8889960
1	-2.0596700	1.0413630	-0.8889490
35	-4.3229150	0.5103600	0.0000350
6	5.4987640	1.1623860	0.0000330
6	5.5580860	-0.2219670	0.0001070
6	4.3674680	-0.9350460	0.0000830
7	3.1687980	-0.3588400	-0.0000060
6	3.1238320	0.9702560	-0.0000780
6	4.2556360	1.7736520	-0.0000630
1	6.4047270	1.7535290	0.0000480
1	6.5041560	-0.7442540	0.0001850
1	4.3772150	-2.0186600	0.0001410
1	2.1331660	1.4116150	-0.0001510
1	4.1581770	2.8499280	-0.0001240

35	-0.2859360	-0.0280990	-0.0064490
6	-2.2276520	0.0044240	0.0017340
17	-2.8310560	-0.4295750	1.6103330
17	-2.8529830	-1.1541010	-1.1849150
17	-2.8041780	1.6282470	-0.4134140
6	5.3646810	0.0462950	0.0068810
6	4.6958010	-1.1672370	0.0048940
6	3.3086080	-1.1566780	-0.0018860
7	2.5899970	-0.0376760	-0.0066300
6	3.2395590	1.1226040	-0.0045150
6	4.6233560	1.2171330	0.0021070
1	6.4457920	0.0792400	0.0122080
1	5.2325080	-2.1049960	0.0086060
1	2.7475960	-2.0839960	-0.0035290
1	2.6232040	2.0142740	-0.0081310
1	5.1022450	2.1857460	0.0036190

C₅H₅N...BrC₆H₄Br

SCF E= -5627.7801
ZPE= -5627.6098
G= -5627.6564
H= -5627.5953

35	1.4334790	-0.4029610	-0.4494790
6	-0.4395450	-0.2211940	-0.2491800
6	-1.2002470	-1.3311010	0.0834230
6	-1.0342520	1.0158340	-0.4417860
6	-2.5739470	-1.2028390	0.2243350
1	-0.7258270	-2.2907480	0.2297930

C₅H₅N...BrC₆H₄NO₂
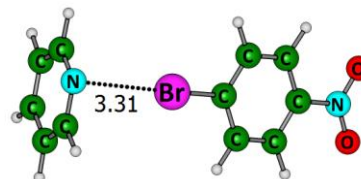
SCF E= -3258.6499
ZPE= -3258.4655
G= -3258.5134
H= -3258.4500

6	0.8708530	-0.1750370	-0.3329160
6	1.4694030	1.0709360	-0.4660580
6	1.6103840	-1.2969360	0.0179210
6	2.8295070	1.1994170	-0.2428150
1	0.8758670	1.9298300	-0.7419930
6	2.9706900	-1.1718020	0.2415380

6	-2.4080770	1.1456300	-0.3008450
1	-0.4309820	1.8733530	-0.7024940
6	-3.1662190	0.0343490	0.0301650
1	-3.1779250	-2.0604710	0.4824910
1	-2.8829520	2.1048000	-0.4488190
35	-5.0430360	0.2072640	0.2172960
6	4.7086210	1.2373790	1.2572920
6	4.7417250	1.5619370	-0.0891210
6	4.7572260	0.5309630	-1.0179400
7	4.7429640	-0.7578170	-0.6861180
6	4.7137960	-1.0558510	0.6107570
6	4.6955550	-0.1003500	1.6168920
1	4.6903760	2.0124080	2.0117540
1	4.7507800	2.5908190	-0.4197310
1	4.7768930	0.7497290	-2.0792680
1	4.6987940	-2.1110820	0.8576210
1	4.6667990	-0.4032640	2.6539200

1	1.1255530	-2.2570780	0.1150710
6	3.5542890	0.0749500	0.1076960
1	3.3294480	2.1513080	-0.3374260
1	3.5780860	-2.0206790	0.5162340
35	-0.9834960	-0.3494230	-0.6331630
6	-4.2038120	1.0027260	1.5284270
6	-4.1587280	-0.3770890	1.6432360
6	-4.1989110	-1.1387500	0.4837690
7	-4.2775580	-0.6153020	-0.7375100
6	-4.3242830	0.7114440	-0.8335230
6	-4.2902770	1.5610210	0.2633550
1	-4.1724210	1.6312420	2.4082900
1	-4.0890940	-0.8584780	2.6083050
1	-4.1593510	-2.2204880	0.5379420
1	-4.3878390	1.1153510	-1.8373260
1	-4.3279350	2.6317870	0.1222900
7	5.0015010	0.2106200	0.3480010
8	5.4862840	1.3139430	0.2325650
8	5.6146850	-0.7896290	0.6464450

C₅H₅N...BrOCl

SCF E= -3357.8380
ZPE= -3357.7431
G= -3357.7821
H= -3357.7327

35	-0.9194260	-0.2328070	-0.2774390
8	-2.7784040	-0.4437780	-0.5019380
17	-3.6677320	0.4642840	0.5879750
6	4.1320780	0.2159030	0.2469870
6	3.3563050	1.3215990	-0.0645380
6	1.9903620	1.1496440	-0.2155430
7	1.4083340	-0.0364490	-0.0715890

C₅H₅N...BrOBr

SCF E= -5471.8844
ZPE= -5471.7898
G= -5471.8283
H= -5471.7795

35	-0.3092020	-0.5537600	-0.0002180
8	-2.1457890	-0.9686020	-0.0000360
35	-3.2131240	0.4917790	0.0001630
6	4.6732090	0.5560220	0.0002240
6	4.2702750	-0.7701460	0.0003640
6	2.9129790	-1.0492280	0.0001330
7	1.9956530	-0.0883310	-0.0001080

6	2.1469830	-1.1003120	0.2264450
6	3.5192770	-1.0185710	0.3953060
1	5.2015150	0.3156320	0.3736230
1	3.7953540	2.3007190	-0.1885020
1	1.3325070	1.9753550	-0.4570770
1	1.6129430	-2.0366130	0.3320690
1	4.0878950	-1.9038770	0.6393850

6	2.3763670	1.1848820	-0.0002070
6	3.7111460	1.5537640	-0.0001140
1	5.7247000	0.8089840	0.0003690
1	4.9885200	-1.5768430	0.0006660
1	2.5380990	-2.0651910	0.0003200
1	1.5794130	1.9187000	-0.0005070
1	3.9835560	2.5990730	-0.0002630

C$_5$H$_5$N...BrOCH$_2$F
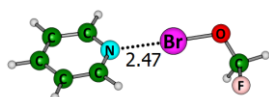
SCF E= -3036.8490
ZPE= -3036.7228
G= -3036.7628
H= -3036.7116

35	0.9950420	-0.3907070	-0.1981250
8	2.8292010	-0.6585790	-0.3464930
6	3.5530570	0.0775700	0.5497910
1	3.1543620	0.0147600	1.5654340
1	4.5828650	-0.2775420	0.4900260
9	3.5552750	1.4170370	0.2107490
6	-4.1731570	0.3474690	0.1388710
6	-3.3141400	1.4087000	-0.0995640
6	-1.9536350	1.1540600	-0.1730460
7	-1.4476560	-0.0658710	-0.0237620
6	-2.2704240	-1.0839930	0.2051460
6	-3.6440200	-0.9241610	0.2949870
1	-5.2405910	0.5093250	0.2029270
1	-3.6855490	2.4150860	-0.2266080
1	-1.2371450	1.9457520	-0.3563840
1	-1.8058760	-2.0560530	0.3193180
1	-4.2781340	-1.7780760	0.4841010

C$_5$H$_5$N...BrOCHF$_2$
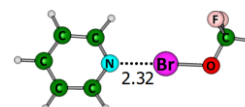
SCF E= -3136.1205
ZPE= -3136.0020
G= -3136.0422
H= -3135.9903

35	0.6741600	-0.4964670	-0.1553410
8	2.5296950	-0.8888200	-0.2454250
6	3.3353700	0.1281970	0.0697380
1	4.3734240	-0.1953090	-0.0115930
9	3.1515080	1.2083030	-0.7392130
9	3.1198300	0.5900210	1.3318110
6	-4.3048980	0.4527010	0.1358620
6	-3.3914660	1.4831380	-0.0226300
6	-2.0464680	1.1663300	-0.1162500
7	-1.6126050	-0.0883930	-0.0584460
6	-2.4828970	-1.0810770	0.0936710
6	-3.8454390	-0.8538250	0.1946210
1	-5.3624110	0.6648690	0.2138180
1	-3.7089000	2.5143560	-0.0719710
1	-1.2853780	1.9268560	-0.2390770
1	-2.0638020	-2.0787410	0.1367670
1	-4.5251220	-1.6840680	0.3180410

C₅H₅N...BrOCF₂Cl

35	-0.0040670	0.3132750	-0.3109880
8	1.8979870	0.5807260	-0.5473020
6	2.6621210	-0.1845900	0.2003210
9	2.4671170	-0.0059020	1.5243210
9	2.4688240	-1.5044480	-0.0126530
17	4.3797700	0.1762090	-0.1499450
6	-4.9140900	-0.2520880	0.2397290
6	-4.3399510	1.0063580	0.3326300
6	-2.9727260	1.1252950	0.1556320
7	-2.2076610	0.0681130	-0.0989590
6	-2.7475750	-1.1436640	-0.1902230
6	-4.1067800	-1.3470180	-0.0269290
1	-5.9794490	-0.3788950	0.3751690
1	-4.9344460	1.8832100	0.5423350
1	-2.4626300	2.0780300	0.2190750
1	-2.0607830	-1.9546240	-0.3965100
1	-4.5161810	-2.3431120	-0.1072640

SCF E= -3595.7287
ZPE= -3595.6206
G= -3595.6626
H= -3595.6079

C₅H₅N...BrOCF₃

35	-0.318196	-0.476881	-0.000040
8	-2.200788	-0.884359	0.000046
6	-2.990063	0.173265	-0.000035
9	-2.820510	0.969224	1.074471
9	-2.820515	0.969058	-1.074664
9	-4.266363	-0.219084	-0.000001
6	4.576491	0.424396	0.000251
6	4.107774	-0.880330	0.000312
6	2.740064	-1.092615	0.000131
7	1.876466	-0.081987	-0.000104
6	2.314976	1.173049	-0.000178
6	3.666832	1.470383	0.000000
1	5.639251	0.623555	0.000401
1	4.783614	-1.722621	0.000493
1	2.309485	-2.085891	0.000176
1	1.553451	1.942721	-0.000396
1	3.992171	2.500177	-0.000056

SCF E= -3235.3894
ZPE= -3235.2792
G= -3235.3199
H= -3235.2670

C₅H₅N...BrCNBeCl₂
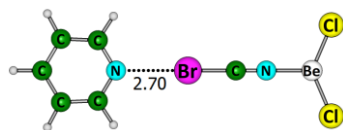
SCF E= -3850.6836
ZPE= -3850.5778
G= -3850.6247
H= -3850.5633

C₅H₅N...BrC₃N
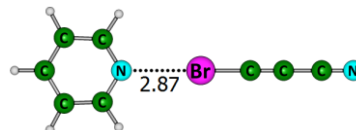
SCF E= -2991.4830
ZPE= -2991.3736
G= -2991.4145
H= -2991.3617

6	1.3226900	0.0000050	-0.0000020
7	2.4650800	0.0000050	0.0000090
4	4.1800310	0.0000120	0.0000150
17	4.9063500	-1.7202640	0.0002250
17	4.9064390	1.7202380	-0.0001830
35	-0.4755530	0.0000060	-0.0000320
6	-5.9447190	-0.0000220	0.0000840
6	-5.2403300	-1.1934540	-0.0002320
6	-3.8554390	-1.1428110	-0.0003050
7	-3.1726690	0.0000290	-0.0000810
6	-3.8554810	1.1428430	0.0002300
6	-5.2403750	1.1934360	0.0003370
1	-7.0261090	-0.0000420	0.0001500
1	-5.7482900	-2.1467940	-0.0004320
1	-3.2676500	-2.0532300	-0.0005480
1	-3.2677250	2.0532840	0.0003940
1	-5.7483690	2.1467570	0.0006130

6	-2.6315460	-0.0001570	0.0001110
6	-3.8329510	0.0001400	0.0003650
6	-5.2089090	0.0003510	0.0000200
7	-6.3589260	0.0007840	-0.0003670
35	-0.8408020	-0.0004890	0.0000460
6	4.8011830	0.0009280	0.0000510
6	4.0963740	-1.1921610	-0.0000220
6	2.7105190	-1.1403590	-0.0000810
7	2.0242930	-0.0004780	-0.0001220
6	2.7093600	1.1400820	-0.0000920
6	4.0951690	1.1932940	-0.0000170
1	5.8827280	0.0014690	0.0000880
1	4.6048040	-2.1454890	-0.0000200
1	2.1236080	-2.0515570	-0.0001340
1	2.1215350	2.0506950	-0.0001240
1	4.6026290	2.1471410	-0.0000090

$C_5H_5N...BrC_5N$

2.87

SCF E= -3067.6363
ZPE= -3067.5164
G= -3067.5606
H= -3067.5026

6	-2.9335440	0.0000900	0.0002430
6	-1.7283070	0.0001590	-0.0001620
6	-4.2970210	-0.0000360	-0.0003340
6	-5.5024130	-0.0001690	-0.0001700
6	-6.8753660	-0.0002740	-0.0001450
7	-8.0260950	-0.0003180	0.0008170
35	0.0608200	0.0003230	-0.0001870
6	5.7082890	-0.0008020	0.0004030
6	5.0022450	-1.1931390	0.0002440
6	3.6164380	-1.1399630	-0.0000550
7	2.9310730	0.0004430	-0.0002100

$C_5H_5N...ClCF_3$

2.93
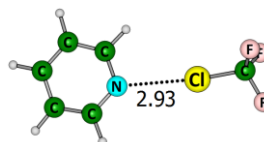
SCF E= -1046.1459
ZPE= -1046.0405
G= -1046.0832
H= -1046.0288

6	-2.9369320	-0.0307510	0.0000120
9	-3.3204330	-0.7075410	-1.0735290
9	-3.3201330	-0.7074730	1.0736790
9	-3.5669250	1.1358600	0.0000410
17	-1.2011720	0.2054810	-0.0002600
6	4.4269010	-0.3511080	-0.0002280
6	4.0292670	0.9761040	-0.0001250
6	2.6708570	1.2592890	0.0001790
7	1.7280950	0.3208120	0.0003520
6	2.1213830	-0.9500550	0.0002510
6	3.4537060	-1.3369820	-0.0000370

6	3.6174290	1.1402470	-0.0000370	1	5.4767250	-0.6120990	-0.0004330
6	5.0032940	1.1921650	0.0002250	1	4.7516940	1.7797450	-0.0002770
1	6.7898230	-0.0012410	0.0006260	1	2.3239590	2.2859160	0.0003270
1	5.5095370	-2.1470760	0.0003830	1	1.3317690	-1.6935430	0.0004180
1	3.0287670	-2.0506790	-0.0001920	1	3.7154230	-2.3854900	-0.0000920
1	3.0306030	2.0515020	-0.0001070				
1	5.5114660	2.1456320	0.0003110				

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C₅H₅N...ClCCH
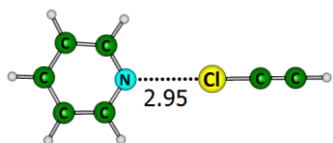
SCF E= -785.1964
ZPE= -785.0866
G= -785.1256
H= -785.0763

C₅H₅N...ClF

SCF E= -808.2557
ZPE= -808.1622
G= -808.1952
H= -808.1539

6	-3.7574100	-0.0040570	0.0000170	9	-3.6726170	-0.0002680	-0.0002430
6	-4.9530870	-0.0182730	-0.0000150	17	-1.9710200	0.0002240	0.0000370
1	-6.0144160	-0.0305880	-0.0000450	6	2.9508970	-0.0005630	-0.0002170
17	-2.1140330	0.0165330	0.0000650	6	2.2498690	1.1954390	-0.0000900
6	3.6173150	-0.0388250	0.0001050	6	0.8654430	1.1504350	0.0001790
6	2.9425820	1.1713300	0.0000330	7	0.2020220	0.0005100	0.0002940
6	1.5550800	1.1540360	-0.0000850	6	0.8645530	-1.1499480	0.0001790
7	0.8373790	0.0340840	-0.0001550	6	2.2489310	-1.1960270	-0.0000870
6	1.4952720	-1.1218440	-0.0000940	1	4.0322200	-0.0009800	-0.0004600
6	2.8797870	-1.2119120	0.0000310	1	2.7603510	2.1472510	-0.0002040
1	4.6986020	-0.0673870	0.0001970	1	0.2594700	2.0477340	0.0002920
1	3.4748820	2.1117120	0.0000760	1	0.2578660	-2.0467640	0.0002810
1	0.9931920	2.0809150	-0.0001400	1	2.7586800	-2.1482330	-0.0002000
1	0.8854500	-2.0180290	-0.0001450				
1	3.3619560	-2.1789990	0.0000740				

C₅H₅N...ClCN
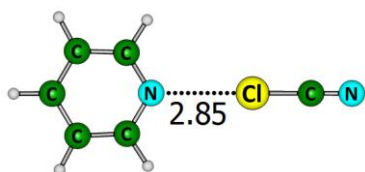
SCF E= -801.2960
ZPE= -801.1967
G= -801.2350
H= -801.1868

6	3.7131880	-0.0011860	0.0000440
7	4.8613500	-0.0049040	0.0001150
17	2.0731030	0.0040280	-0.0000630
6	-3.5537070	-0.0078790	0.0000730
6	-2.8414100	-1.1964180	0.0000370
6	-1.4556730	-1.1359680	-0.0000450
7	-0.7740780	0.0067500	-0.0000770
6	-1.4676770	1.1422660	-0.0000340
6	-2.8540140	1.1880930	0.0000340
1	-4.6352610	-0.0136120	0.0001390
1	-3.3438040	-2.1530110	0.0000770
1	-0.8653680	-2.0450280	-0.0000600
1	-0.8869970	2.0574730	-0.0000610
1	-3.3664690	2.1393250	0.0000660

C₅H₅N...ClOH
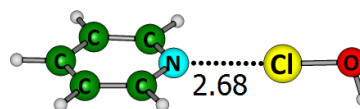
SCF E= -784.2407
ZPE= -784.1362
G= -784.1728
H= -784.1266

8	-3.9833940	0.0286080	-0.0756550
17	-2.2899440	0.0011620	-0.0197070
1	-4.2531360	-0.2347020	0.8104300
6	3.1595580	0.0114560	0.0043830
6	2.4647310	-1.1875370	-0.0012040
6	1.0780040	-1.1470290	-0.0023300
7	0.3857790	-0.0123680	0.0024130
6	1.0582740	1.1340980	0.0072520
6	2.4440800	1.1982870	0.0084090
1	4.2411570	0.0208220	0.0052140
1	2.9814590	-2.1364890	-0.0052370
1	0.4948420	-2.0604470	-0.0078950
1	0.4591280	2.0371350	0.0096900
1	2.9444150	2.1559940	0.0121030

C₅H₅N...ClOF
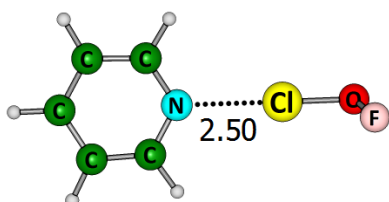
SCF E= -883.3666
ZPE= -883.2709
G= -883.3088
H= -883.2608

C₅H₅N...ClC₆H₅
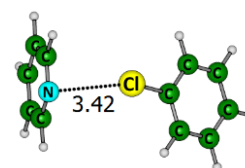
SCF E= -940.1030
ZPE= -939.9215
G= -939.9658
H= -939.9085

8	-3.3768560	-0.1252570	-0.4859190
9	-3.9551330	0.2044900	0.7523130
17	-1.7001580	-0.0857200	-0.2587180
6	3.5464210	0.0635300	0.1148630
6	2.8046280	1.2302190	0.0183000
6	1.4240140	1.1306640	-0.0591000
7	0.7856660	-0.0349480	-0.0446200
6	1.4993110	-1.1523210	0.0486080
6	2.8835040	-1.1533440	0.1309240
1	4.6255550	0.1022840	0.1766630
1	3.2810070	2.1997510	0.0020810
1	0.8013600	2.0142790	-0.1350420
1	0.9368140	-2.0782990	0.0567320
1	3.4220760	-2.0869690	0.2050790

|			
6	1.7581860	-0.0974760	-0.2931750
6	2.3283110	1.1635050	-0.2220250
6	2.4931420	-1.2357410	-0.0024920
6	3.6598480	1.2819230	0.1488070
1	1.7340140	2.0345320	-0.4578630
6	3.8239050	-1.1030390	0.3668030
1	2.0253910	-2.2074830	-0.0688850
6	4.4101930	0.1522950	0.4434490
1	4.1101480	2.2634560	0.2066670
1	4.4022820	-1.9877550	0.5954410
1	5.4474340	0.2498920	0.7315930
17	0.0902690	-0.2507630	-0.7589250
6	-2.9669090	-0.2913100	1.5413180
6	-3.1859620	-1.2485540	0.5644830
6	-3.3115930	-0.8322200	-0.7534000
7	-3.2332270	0.4405540	-1.1332580
6	-3.0204810	1.3494850	-0.1852790
6	-2.8821400	1.0375770	1.1599950
1	-2.8607270	-0.5760200	2.5794930
1	-3.2543250	-2.2985020	0.8112610
1	-3.4801280	-1.5567760	-1.5417480
1	-2.9555940	2.3791060	-0.5176380
1	-2.7094780	1.8199660	1.8853040

C₅H₅N...ClC₆H₄F
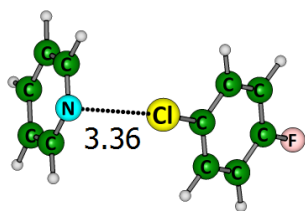
SCF E= -1039.3541
ZPE= -1039.1805
G= -1039.2247
H= -1039.16680

6	1.3099560	-0.1226780	-0.4233630
6	1.9101470	1.1259630	-0.3866750

C₅H₅N...ClC₆H₄Cl
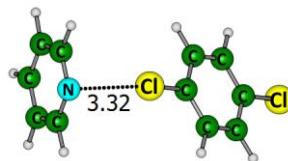
SCF E= -1399.7130
ZPE= -1399.5411
G= -1399.5870
H= -1399.5269

6	-0.8864660	-0.1908110	-0.4482310
6	-1.6250410	-1.3163210	-0.1185800

6	2.0273940	-1.2686180	-0.1176020	6	-1.4827740	1.0586100	-0.5076480
6	3.2479650	1.2335090	-0.0384900	6	-2.9777100	-1.1906780	0.1567470
1	1.3337250	2.0061210	-0.6317010	1	-1.1438460	-2.2827800	-0.0779950
6	3.3655410	-1.1661280	0.2312100	6	-2.8355200	1.1852040	-0.2326520
1	1.5411210	-2.2325220	-0.1551880	1	-0.8924990	1.9248350	-0.7692750
6	3.9502520	0.0839550	0.2639710	6	-3.5716460	0.0593630	0.0982890
1	3.7470360	2.1910060	0.0000310	1	-3.5688620	-2.0570540	0.4159730
1	3.9538360	-2.0387760	0.4758040	1	-3.3175100	2.1510700	-0.2761800
9	5.2454150	0.1850050	0.6009240	17	-5.2665610	0.2177790	0.4452470
17	-0.3659670	-0.2510990	-0.8608090	17	0.8069860	-0.3505230	-0.7899620
6	-3.2624680	0.2101130	1.6456540	6	3.7579760	0.9195380	1.4106530
6	-3.4335460	-1.0400490	1.0744080	6	3.9428180	1.4736550	0.1544770
6	-3.6557500	-1.1172170	-0.2933400	6	4.1101730	0.6200300	-0.9268530
7	-3.7155810	-0.0533320	-1.0902570	7	4.1032690	-0.7065570	-0.8244610
6	-3.5515460	1.1417060	-0.5283600	6	3.9268990	-1.2256120	0.3880060
6	-3.3232260	1.3266630	0.8278580	6	3.7506530	-0.4603160	1.5320960
1	-3.0837120	0.3126660	2.7076120	1	3.6204890	1.5512900	2.2779740
1	-3.3938070	-1.9409810	1.6700060	1	3.9545990	2.5443480	0.0081500
1	-3.7893690	-2.0804500	-0.7721470	1	4.2520940	1.0216100	-1.9235430
1	-3.6008390	1.9939640	-1.1961620	1	3.9217060	-2.3077430	0.4479880
1	-3.1945470	2.3226190	1.2273600	1	3.6075560	-0.9390070	2.4904510

C₅H₅N...ClH
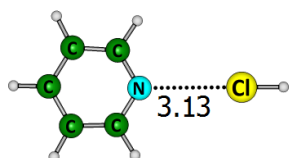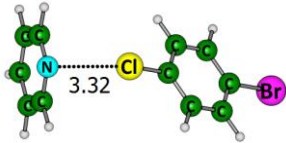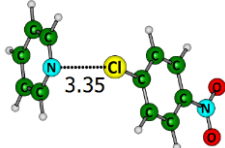
SCF E= -709.0743
ZPE= -708.9757
G= -709.0104
H= -708.9674
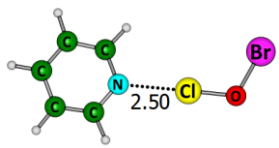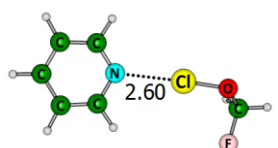
17	3.1565420	-0.0007510	0.0000190
1	4.4370750	0.0055860	0.0000560
6	-2.7582090	0.0251690	0.0000390
6	-2.0733790	-1.1793280	0.0000170
6	-0.6856680	-1.1502260	-0.0000340
7	0.0235460	-0.0253940	-0.0000600
6	-0.6441880	1.1244310	-0.0000360

C₅H₅N...ClCH₂CH₂Br
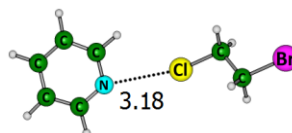
SCF E= -3361.3290
ZPE= -3361.1808
G= -3361.2247
H= -3361.1683

6	1.6530830	-0.4747260	0.3872300
1	1.8892830	-0.6994230	1.4226880
1	1.6954850	-1.3853250	-0.2021010
6	2.5695560	0.5845170	-0.1701230
1	2.3414740	0.8094370	-1.2061210
1	2.5441010	1.4917930	0.4232860

6	-2.0298120	1.2039430	0.0000160
1	-3.8397550	0.0449780	0.0000810
1	-2.5981410	-2.1240610	0.0000370
1	-0.1162700	-2.0725810	-0.0000540
1	-0.0415520	2.0254890	-0.0000570
1	-2.5198480	2.1671780	0.0000360

35	4.4081040	-0.0632590	-0.1277940
17	-0.0298460	0.1327500	0.3303340
6	-5.7284420	-0.5476740	-0.2221560
6	-5.5366540	0.8228830	-0.1545030
6	-4.2434900	1.3025120	0.0015820
7	-3.1742210	0.5161140	0.0886500
6	-3.3707870	-0.7975380	0.0215830
6	-4.6226980	-1.3773060	-0.1318760
1	-6.7206580	-0.9614800	-0.3431500
1	-6.3673170	1.5111190	-0.2204580
1	-4.0585420	2.3689460	0.0586960
1	-2.4819060	-1.4140770	0.0926620
1	-4.7220240	-2.4524730	-0.1793840

$C_5H_5N...ClC_6H_4Br$

3.32

SCF E= -3513.7466
ZPE= -3513.5751
G= -3513.6225
H= -3513.5607

6	-0.1242020	-0.2300980	-0.5098570
6	-0.8535070	-1.3566710	-0.1641950
6	-0.7371640	1.0076960	-0.6205400
6	-2.2145930	-1.2441980	0.0742050
1	-0.3594550	-2.3141010	-0.0827630
6	-2.0986500	1.1217450	-0.3824010
1	-0.1532980	1.8750480	-0.8928750
6	-2.8260180	-0.0058170	-0.0369790
1	-2.7949770	-2.1143280	0.3442110
1	-2.5881990	2.0811460	-0.4670470
35	-4.6849030	0.1442860	0.2871510
17	1.5787190	-0.3754710	-0.8075250
6	4.4680880	0.9759610	1.4251240

$C_5H_5N...ClC_6H_4NO_2$

3.35

SCF E= -1144.6156
ZPE= -1144.4312
G= -1144.4791
H= -1144.4158

6	0.5925360	-0.1544750	-0.5223070
6	1.2075900	1.0898810	-0.5023630
6	1.3056480	-1.3180500	-0.2671520
6	2.5595600	1.1743940	-0.2205070
1	0.6294130	1.9782870	-0.7089080
6	2.6579720	-1.2366500	0.0147070
1	0.8019030	-2.2729320	-0.2918350
6	3.2593770	0.0085820	0.0335410
1	3.0730670	2.1233090	-0.1955950
1	3.2462830	-2.1180210	0.2193770
17	-1.0979980	-0.2520970	-0.8721780
6	-3.9974030	-0.2791940	1.6665100

6	4.6805790	1.4967270	0.1590400
6	4.8786460	0.6149190	-0.8942080
7	4.8765940	-0.7083890	-0.7556040
6	4.6741820	-1.1951490	0.4659830
6	4.4656200	-0.4001630	1.5840600
1	4.3056280	1.6306750	2.2707710
1	4.6902810	2.5630910	-0.0161270
1	5.0425400	0.9897480	-1.8979360
1	4.6739070	-2.2752550	0.5558830
1	4.3029030	-0.8539910	2.5513680

6	-4.2876680	-1.2146410	0.6870200
6	-4.4584830	-0.7744890	-0.6181840
7	-4.3580980	0.5012400	-0.9830060
6	-4.0796570	1.3895390	-0.0323820
6	-3.8912550	1.0528570	1.3007390
1	-3.8558980	-0.5826940	2.6951230
1	-4.3792320	-2.2654870	0.9221390
1	-4.6840360	-1.4808140	-1.4089040
1	-4.0019840	2.4222620	-0.3521950
1	-3.6677400	1.8192620	2.0292910
7	4.6983990	0.0956690	0.3357260
8	5.2016560	1.1966710	0.3477990
8	5.2874410	-0.9394720	0.5536740

C5H5N...ClOBr

SCF E= -3357.8299
ZPE= -3357.7355
G= -3357.7745
H= -3357.7251

8	-2.1724380	-1.0808930	0.0000040
35	-3.2103620	0.4109260	-0.0000110
17	-0.5011290	-0.7245020	0.0000660
6	4.6084580	0.5385060	0.0000390
6	4.2644830	-0.8039500	-0.0000140
6	2.9195000	-1.1416670	-0.0000480
7	1.9506750	-0.2322610	-0.0000820
6	2.2834330	1.0544570	-0.0000470
6	3.6000530	1.4889320	0.0000380
1	5.6472970	0.8399640	0.0000870
1	5.0187050	-1.5775480	-0.0000410
1	2.6028800	-2.1778270	-0.0000420
1	1.4595010	1.7586900	-0.0001050
1	3.8227030	2.5461450	0.0001040

C5H5N...ClOCH2F

SCF E= -922.7965
ZPE= -922.6702
G= -922.7110
H= -922.6589

8	3.0128520	-0.7445680	-0.4186620
6	3.6733230	0.0171870	0.5178050
1	3.2499020	-0.1043730	1.5159110
1	4.7177430	-0.2893420	0.4639890
9	3.6027850	1.3528180	0.2052500
17	1.3229790	-0.5918850	-0.2785380
6	-3.9179310	0.4491390	0.1351330
6	-3.5233370	-0.8696100	0.2946660
6	-2.1754710	-1.1747880	0.1764640
7	-1.2468120	-0.2591870	-0.0822190
6	-1.6311590	1.0043850	-0.2344420
6	-2.9544580	1.4073480	-0.1352940
1	-4.9603380	0.7254170	0.2195540
1	-4.2410100	-1.6495790	0.5047650

C₅H₅N...ClOCHF₂
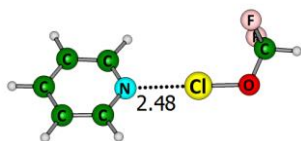
SCF E= -1022.0643
ZPE= -1021.9456
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H= -1021.9339

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6	3.4045680	0.0527950	0.0411400
1	4.4426820	-0.2644150	-0.0513030
9	3.1902570	1.1334110	-0.7403600
9	3.1640500	0.4541840	1.3074870
17	0.9454830	-0.6629940	-0.2150680
6	-4.1658400	0.4421550	0.1093300
6	-3.2058060	1.4326110	-0.0237850
6	-1.8745570	1.0553100	-0.1098950
7	-1.4843450	-0.2144490	-0.0688720
6	-2.4064060	-1.1629260	0.0600160
6	-3.7612950	-0.8825800	0.1526440
1	-5.2143140	0.6986690	0.1787100
1	-3.4771390	2.4777560	-0.0608850
1	-1.0873140	1.7923790	-0.2158150
1	-2.0414650	-2.1826410	0.0898620
1	-4.4766010	-1.6855490	0.2564740

C₅H₅N...ClOCF₂Cl
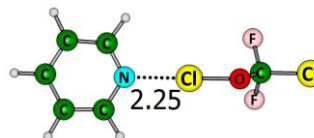
SCF E= -1481.6699
ZPE= -1481.5619
G= -1481.6049
H= -1481.5492

8	-1.8293980	-0.2951670	-0.8346320
6	-2.5731710	0.0619310	0.2132310
9	-2.3690310	-0.7159210	1.2882880
9	-2.3344400	1.3198760	0.6184960
17	-4.2809400	-0.0653820	-0.2623390
17	-0.0933210	-0.1997070	-0.5029550
6	4.8421240	0.1264790	0.2315360
6	4.0739220	1.2644210	0.0414310
6	2.7116150	1.1157430	-0.1602460
7	2.1285710	-0.0772800	-0.1753650
6	2.8580090	-1.1718240	0.0067940
6	4.2266560	-1.1153270	0.2146830
1	5.9087070	0.2067350	0.3914070
1	4.5160350	2.2498840	0.0483660
1	2.0583590	1.9658370	-0.3144470
1	2.3211580	-2.1121560	-0.0160300
1	4.7896770	-2.0256200	0.3596830

C₅H₅N...ClOCF₃

C₅H₅N...ClOCF₃
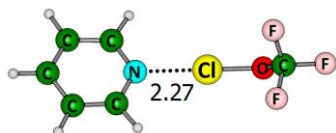
SCF E= -1121.3306
ZPE= -1121.2203
G= -1121.2613
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8	-2.1922990	-0.5265300	-0.8092810
6	-2.9473310	0.0589060	0.1272410
9	-2.7195110	-0.4144290	1.3583260
9	-2.7714360	1.3849750	0.1892710
9	-4.2223670	-0.1703300	-0.1701670
17	-0.4746470	-0.3219800	-0.5190240
6	4.4504340	0.1944160	0.2893520
6	3.6567390	1.3055150	0.0513000
6	2.3051810	1.1137640	-0.1855270
7	1.7550770	-0.0950810	-0.1916040
6	2.5103960	-1.1634710	0.0359210
6	3.8700970	-1.0642570	0.2822700
1	5.5089700	0.3086790	0.4792630
1	4.0707360	2.3031240	0.0489450
1	1.6342180	1.9425540	-0.3756270
1	2.0013230	-2.1194320	0.0199690
1	4.4533390	-1.9546300	0.4661140

C₅H₅N...ClCNBeCl₂

C₅H₅N...ClCNBeCl₂
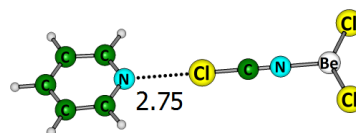
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ZPE= -1736.5367
G= -1736.5833
H= -1736.5224

6	-1.1724550	-0.0034550	-0.0000010
7	-2.3142610	-0.0016520	-0.0001010
4	-4.0344370	0.0011340	-0.0000280
17	-4.7542400	-1.7199830	-0.0001570
17	-4.7487170	1.7245820	0.0001600
17	0.4514660	-0.0058920	0.0000300
6	5.9740290	0.0072640	-0.0000970
6	5.2739240	-1.1884930	0.0001720
6	3.8883400	-1.1425730	0.0002740
7	3.1964910	-0.0050290	0.0001010
6	3.8782460	1.1385580	-0.0001650
6	5.2633300	1.1967810	-0.0002500
1	7.0554570	0.0120820	-0.0001450
1	5.7855680	-2.1399730	0.0003040
1	3.3077920	-2.0577480	0.0005170
1	3.2896350	2.0485990	-0.0002990
1	5.7665290	2.1527650	-0.0004190

C₅H₅N...ClC₃N
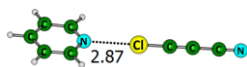
C₅H₅N...ClC₃N

SCF E= -877.4449
ZPE= -877.3352
G= -877.3763
H= -877.3233

6	2.7030080	0.0147270	-0.0001470
6	3.9028170	0.0005450	-0.0001790

C₅H₅N...ClC₅N

C₅H₅N...ClC₅N
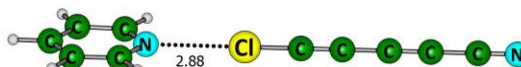
SCF E= -953.5982
ZPE= -953.4779
G= -953.5219
H= -953.4641

6	-2.8265470	-0.0051120	-0.0000320

6	5.2782870	-0.0171320	-0.0001780
7	6.4280500	-0.0324820	0.0001300
17	1.0723500	0.0352740	-0.0000040
6	-4.5764640	-0.0548090	-0.0003190
6	-3.8305150	-1.2225690	-0.0001220
6	-2.4471310	-1.1226770	0.0002570
7	-1.7977120	0.0386450	0.0004390
6	-2.5237620	1.1539060	0.0002410
6	-3.9109440	1.1604280	-0.0001430
1	-5.6574400	-0.0914040	-0.0006220
1	-4.3053910	-2.1931550	-0.0002660
1	-1.8315410	-2.0149240	0.0004210
1	-1.9695950	2.0853870	0.0003990
1	-4.4501250	2.0967670	-0.0003090

6	-1.6229360	-0.0095500	0.0000360
6	-4.1899570	-0.0004590	-0.0000890
6	-5.3950990	0.0035320	-0.0001430
6	-6.7681830	0.0079320	-0.0001780
7	-7.9188100	0.0117780	0.0000810
17	0.0071710	-0.0161980	0.0001370
6	5.6626840	0.0255780	-0.0003100
6	4.9744720	-1.1769910	-0.0001620
6	3.5876600	-1.1443390	0.0001390
7	2.8827140	-0.0158110	0.0003000
6	3.5536990	1.1331300	0.0001520
6	4.9388140	1.2071230	-0.0001540
1	6.7441400	0.0417990	-0.0005490
1	5.4960800	-2.1232440	-0.0002780
1	3.0160240	-2.0652370	0.0002670
1	2.9548940	2.0366700	0.0002800
1	5.4319720	2.1685370	-0.0002650

C₅H₅N...FCN
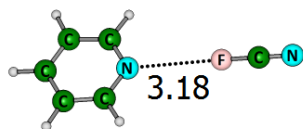
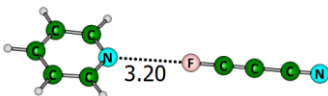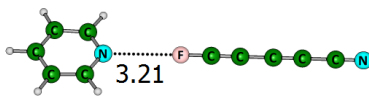SCF E= -440.9166
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9	2.6296370	-0.0108330	-0.0011060
6	3.8895990	0.0001290	-0.0003340
7	5.0350810	0.0100960	0.0002940
6	-3.3329980	-0.0564140	-0.0009730
6	-2.5767260	-1.2173440	-0.0003010
6	-1.1936340	-1.1053750	0.0009110
7	-0.5499630	0.0590320	0.0014740
6	-1.2880110	1.1662770	0.0008190
6	-2.6758870	1.1631670	-0.0003970
1	-4.4137330	-0.1015820	-0.0019180

C₅H₅N...FCNBeCl₂
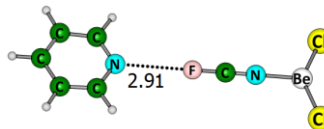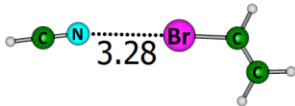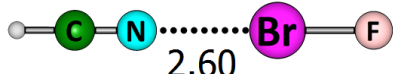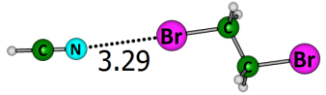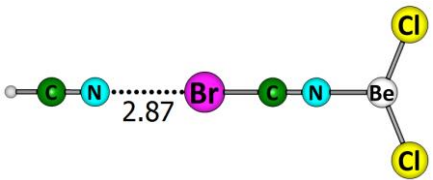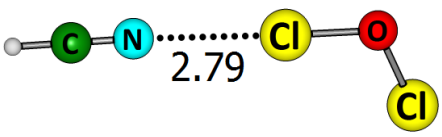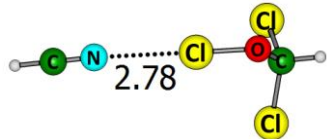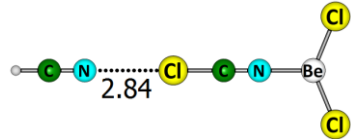
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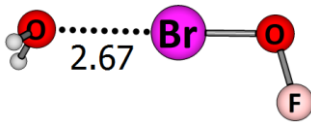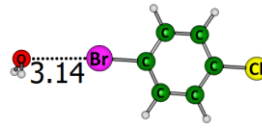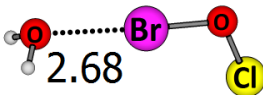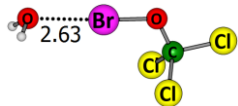
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7	-2.1533000	-0.0003160	0.0000940
4	-3.8944170	0.0001300	-0.0000420
17	-4.5861680	1.7273930	-0.0000770
17	-4.5867270	-1.7269530	-0.0001510
9	0.2248150	-0.0006610	0.0003850
6	5.9150590	0.0000240	-0.0002890
6	5.2080150	1.1914650	-0.0002090
6	3.8218110	1.1374220	0.0000450
7	3.1298610	0.0001070	0.0002150
6	3.8217380	-1.1372210	0.0001340
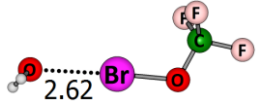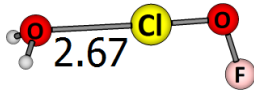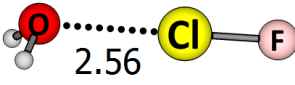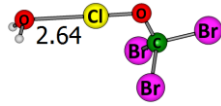
1	-3.0432920	-2.1921310	-0.0007250		6	5.2079630	-1.1913600	-0.0001080
1	-0.5739620	-1.9946700	0.0014500		1	6.9965940	0.0000110	-0.0004730
1	-0.7438190	2.1035760	0.0013060		1	5.7146230	2.1458830	-0.0003360
1	-3.2218090	2.0957730	-0.0008720		1	3.2409170	2.0524260	0.0000800
					1	3.2408040	-2.0522030	0.0003140
					1	5.7144850	-2.1458230	-0.0001680

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SCF E= -517.0644
ZPE= -516.9535
G= -516.9962
H= -516.9417

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6	3.9463000	0.0040410	-0.0000330	6	-1.5719990	-0.0106990	0.0100470
6	5.3237800	-0.0089630	0.0000170	9	-0.3101890	-0.0145450	0.0135610
7	6.4724690	-0.0199850	0.0001400	6	-4.1342760	-0.0026380	0.0025940
9	1.4939640	0.0261360	0.0000140	6	-5.3376290	0.0015150	-0.0011610
6	-4.4923650	0.0181920	0.0002440	6	-6.7117140	0.0063940	-0.0056360
6	-3.7661200	1.1981040	0.0001030	7	-7.8619460	0.0107180	-0.0095370
6	-2.3804870	1.1214540	-0.0001690	6	5.6845220	-0.0010660	-0.0008390
7	-1.7072830	-0.0260550	-0.0003020	6	4.9808410	1.1923940	-0.0018920
6	-2.4166790	-1.1516820	-0.0001620	6	3.5939050	1.1419960	-0.0041930
6	-3.8041680	-1.1842110	0.0001100	7	2.8990760	0.0074240	-0.0054460
1	-5.5738760	0.0355070	0.0004580	6	3.5869700	-1.1313440	-0.0043890
1	-4.2576540	2.1605340	0.0002030	6	4.9735480	-1.1902150	-0.0021000
1	-1.7835990	2.0261780	-0.0002830	1	6.7661610	-0.0043900	0.0009440
1	-1.8487260	-2.0747860	-0.0002740	1	5.4905680	2.1453030	-0.0009510
1	-4.3261020	-2.1304660	0.0002130	1	3.0141370	2.0577500	-0.0050990
				1	3.0016420	-2.0435720	-0.0054450
				1	5.4774530	-2.1462220	-0.0013290

SCF E= -593.2169
ZPE= -593.0957
G= -593.1422
H= -593.0818
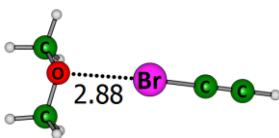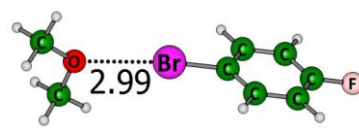
Table S8: Cartesian coordinates in (Å) and energy data (a.u.) of halogen bonded HCN, H₂O and (CH₃)₂O complexes at M06-2X/aug-cc-pVTZ level of theory. All the optimized structures are corresponding to minima on the potential energy surface.

HCN…BrCHCH₂	HCN…Br₂

SCF E= -2745.6441
ZPE= -2745.5843
G= -2745.6192
H= -2745.5755

SCF E= -5241.9007
ZPE= -5241.8826
G= -5241.9100
H= -5241.8752

	HCN…BrCHCH₂				HCN…Br₂		
35	-0.2988110	-0.1943310	-0.0000160	35	1.9337420	0.0002770	0.0000260
6	-2.1820170	-0.2923540	0.0002250	35	-0.3605720	-0.0004230	-0.0000650
6	-2.9628880	0.7695960	-0.0000010	1	-5.4939080	0.0010620	-0.0003980
1	-4.0372150	0.6418660	0.0001490	6	-4.4271670	0.0007290	-0.0001510
1	-2.5655820	1.7746450	-0.0003440	7	-3.2862920	-0.0000480	0.0003810
1	-2.5523710	-1.3062170	0.0005520				
1	5.1307810	0.5375390	0.0016320				
6	4.0890920	0.3082740	0.0005590				
7	2.9739490	0.0629500	-0.0008750				

HCN…BrF	HCN…BrCH₂CH₂Br

SCF E= -2767.4602
ZPE= -2767.4407
G= -2767.4654
H= -2767.4340

SCF E= -5320.5227
ZPE= -5320.4482
G= -5320.4378
H= -5320.4879

	HCN…BrF				HCN…BrCH₂CH₂Br		
35	-0.5074360	-0.0002480	0.0000000	35	1.4346670	0.3000500	-0.0060920
9	-2.2795570	0.0009320	-0.0000010	6	-0.4666570	0.7225570	0.0098280
1	4.2947210	0.0033570	0.0000140	1	-0.6586980	1.2944160	0.9111590
6	3.2274940	0.0009760	-0.0000040	1	-0.6661870	1.3317270	-0.8650280
7	2.0880840	-0.0012740	0.0000010	6	-1.2497860	-0.5627110	-0.0138150
				1	-1.0650920	-1.1345900	-0.9163750
				1	-1.0559050	-1.1729490	0.8612470
				35	-3.1600540	-0.1523830	0.0042630
				1	6.8480880	-0.6189440	0.0403610

6	5.7872510	-0.5107180	0.0174820
7	4.6516430	-0.3946840	-0.0069030

HCN...BrCNBeCl$_2$

SCF E= -3695.8367
ZPE= -3695.8037
G= -3695.8457
H= -3695.7916

6	0.0474070	-0.0000890	0.0000240
7	-1.0945770	0.0000410	-0.0001250
4	-2.8155320	0.0000350	-0.0003680
17	-3.5324370	1.7222330	-0.0005540
17	-3.5324550	-1.7221530	-0.0003950
35	1.8269990	-0.0000890	0.0002410
1	6.9043270	0.0003130	0.0019920
6	5.8365570	0.0001840	0.0003800
7	4.6963240	0.0000630	0.0008010

HCN...ClOCl

SCF E= -1088.93601655
ZPE= -1088.914193
G= -1088.948152
H= -1088.905921

8	-1.4571230	0.8057760	-0.0018740
17	-2.4237180	-0.5718820	0.0000270
17	0.1878860	0.4236020	0.0006950
1	5.0627990	-0.6566880	-0.0073440
6	4.0272720	-0.3994880	-0.0022810
7	2.9199560	-0.1245470	0.0033930

HCN...ClOCHCl$_2$

SCF E= -1587.9101
ZPE= -1587.8683
G= -1587.9067
H= -1587.8580

8	0.6668310	0.0001450	1.3726270
6	1.6436870	0.0000010	0.4158310
1	2.5799920	0.0000060	0.9620430
17	1.6165070	-1.4589070	-0.6070390
17	1.6166550	1.4586940	-0.6073390

HCN...ClCNBeCl$_2$

SCF E= -1581.7982
ZPE= -1581.7647
G= -1581.8060
H= -1581.7527

6	-0.5142910	-0.0000560	-0.0002200
7	0.6272230	-0.0000240	0.0002430
4	2.3516630	-0.0000550	0.0001470
17	3.0623150	-1.7237670	0.0002270
17	3.0625410	1.7234850	0.0002280
17	-2.1313040	0.0006640	-0.0012000

17	-0.9127440	0.0001800	0.7757630
1	-5.4363730	-0.0004750	-1.2843680
6	-4.5147020	-0.0001810	-0.7470080
7	-3.5284690	0.0001340	-0.1735960

1	-7.1760780	-0.0004080	0.0034880
6	-6.1084670	-0.0004400	0.0006670
7	-4.9678530	-0.0003900	0.0006000

H$_2$O...BrOF

SCF E= -2825.5752
ZPE= -2825.5467
G= -2825.5786
H= -2825.5387

35	0.1492100	-0.1802190	0.0016050
8	-1.6456350	-0.4955010	-0.0002370
9	-2.2785310	0.7598320	-0.0035200
8	2.7866200	0.2435640	0.0023510
1	3.0726390	0.7811160	0.7453110
1	3.0839150	0.7035600	-0.7867150

H$_2$O...BrC$_6$H$_4$Cl

SCF E= -2825.5786
ZPE= -3341.8072
G= -3341.8472
H= -3341.7950

35	-2.0357950	-0.0794010	-0.0012530
6	-0.1443250	-0.0342900	-0.0005070
6	0.5669600	-1.2242380	0.0001240
6	0.5142690	1.1852840	-0.0008290
6	1.9531830	-1.1946490	0.0003920
1	0.0426290	-2.1688790	0.0003710
6	1.9005260	1.2164770	-0.0005510
1	-0.0502760	2.1063980	-0.0013430
6	2.6079930	0.0257350	0.0000280
1	2.5231420	-2.1124570	0.0008410
1	2.4302330	2.1580540	-0.0008220
17	4.3454400	0.0632600	0.0002680
8	-5.1729560	0.0733810	0.0049780
1	-5.2980680	0.6405010	-0.7590480
1	-5.2752820	0.6470490	0.7675560

H$_2$O...BrOCl

SCF E= -3185.9931
ZPE= -3185.9658
G= -3185.9997
H= -3185.9658

H$_2$O...BrOCCl$_3$

SCF E= -4144.5657
ZPE= -4144.5288
G= -4144.5676
H= -4144.5172

35	0.5117450	0.2296880	0.0017210
8	-1.2445040	0.7658880	-0.0008130
17	-2.3248190	-0.5195980	-0.0016340
8	3.1120900	-0.4266350	0.0021110
1	3.3265110	-0.9973180	0.7444870
1	3.3436360	-0.9226040	-0.7873450

35	-1.5086040	-0.0047550	-0.4204510
8	0.2407040	-0.0006680	-0.9931080
6	1.1966410	0.0010260	-0.0327800
17	1.1159470	1.4513600	1.0135110
17	1.1223730	-1.4507120	1.0119340
17	2.7353890	0.0048930	-0.9115380
8	-4.0429080	-0.0027660	0.2851190
1	-4.2376460	-0.7162430	0.8984330
1	-4.2764920	0.8098080	0.7415190

H₂O...BrOCF₃

SCF E= -3063.5405
ZPE= -3063.4974
G= -3063.5335
H= -3063.4873

35	0.9909290	-0.2620150	-0.0039120
8	-0.7372760	-0.8853760	-0.0250950
6	-1.6764530	0.0834960	0.0011180
9	-1.5982930	0.8488830	1.0901520
9	-1.6093500	0.8947450	-1.0550760
9	-2.8584130	-0.5153750	-0.0059250
8	3.4876970	0.5279990	0.0166290
1	3.9583200	0.3217710	-0.7951210
1	4.0090410	0.1525270	0.7306970

H₂O...FOCl

SCF E= -711.5264
ZPE= -711.4976
G= -711.5290
H= -711.4896

17	-0.1508650	-0.2589730	-0.0042590
8	1.4946990	-0.5544220	0.0002820
9	2.1250710	0.7010530	0.0045780
8	-2.7938370	0.1527770	-0.0038220
1	-3.0814860	0.7058600	-0.7341290
1	-3.0863430	0.6003680	0.7936470

H₂O...ClF

SCF E= -636.4104
ZPE= -636.3846
G= -636.4122
H= -636.3780

H₂O...ClOCBr₃

SCF E= -8372.6131
ZPE= -8372.5775
G= -8372.5653
H= -8372.6184

9	-1.9566040	0.0000100	0.0247810
17	-0.3195280	-0.0000100	-0.0156210
8	2.2368020	0.0000000	-0.0898600
1	2.5734420	0.7666330	0.3806880
1	2.5735550	-0.7665540	0.3807330

8	-0.4084490	-0.0015510	1.2989400
6	0.3776850	-0.0001830	0.1854050
35	2.1799500	-0.0252400	0.8917440
35	0.0895140	-1.5807320	-0.9346370
35	0.1203020	1.6039350	-0.9073930
17	-2.0782360	0.0106450	1.0038240
8	-4.6846270	0.0047740	0.5743940
1	-4.9070000	0.6907070	-0.0598710
1	-4.9262980	-0.8250420	0.1557980

$(CH_3)_2O...BrCCH$

SCF E= -2805.9811
ZPE= -2805.8801
G= -2805.9158
H= -2805.8701

35	-0.6587840	-0.0000430	-0.1934260
6	-2.4230220	-0.0000400	0.1508520
6	-3.5974660	0.0000390	0.3797650
1	-4.6401740	0.0001040	0.5825980
8	2.2071840	0.0000010	-0.4213270
6	2.5373020	-1.1665470	0.2936590
1	2.0013820	-1.2045120	1.2488350
1	2.2446210	-2.0194440	-0.3138900
1	3.6132800	-1.2133250	0.4905770
6	2.5369760	1.1666900	0.2935870
1	2.0001650	1.2051370	1.2482400
1	3.6127810	1.2131980	0.4915290
1	2.2451580	2.0194720	-0.3145320

$(CH_3)_2O...BrC_6H_4F$

SCF E= -3060.1364
ZPE= -3059.9719
G= -3060.0157
H= -3059.9582

35	0.8418260	-0.0862600	-0.2255540
6	-1.0463820	-0.0372460	-0.0993910
6	-1.7518510	-1.2094980	0.1269730
6	-1.7081710	1.1744300	-0.2296330
6	-3.1349180	-1.1721890	0.2267890
1	-1.2246970	-2.1472570	0.2261530
6	-3.0909030	1.2179000	-0.1305190
1	-1.1473290	2.0804340	-0.4076340
6	-3.7779080	0.0423750	0.0968720
1	-3.7122060	-2.0680160	0.4049940
1	-3.6351260	2.1464050	-0.2262560
9	-5.1158380	0.0820340	0.1961680
8	3.8222940	0.0449850	0.0015240
6	4.0674350	0.4037750	1.3379910
1	4.6664590	1.3192870	1.3954930
1	3.1041680	0.5738720	1.8137100
1	4.5963810	-0.3953670	1.8688250
6	5.0088180	-0.2107870	-0.7054090
1	5.6532950	0.6749790	-0.7255990
1	5.5658780	-1.0378280	-0.2514680
1	4.7367520	-0.4781590	-1.7235840

| | **(CH₃)₂O…BrC₆H₄NO₂** | | | | **(CH₃)₂O…ClCCH** | | |

(CH₃)₂O…BrC₆H₄NO₂
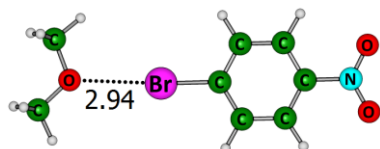
SCF E= -3165.3980
ZPE= -3165.2223
G= -3165.2689
H= -3165.2069

35	-1.5193260	-0.1087210	-0.0296230
6	0.3660620	-0.0573480	-0.0139010
6	1.0165560	1.1697780	-0.0037990
6	1.0809470	-1.2485140	-0.0137110
6	2.4001770	1.2089070	0.0067280
1	0.4434500	2.0851290	-0.0043740
6	2.4646260	-1.2141040	-0.0030620
1	0.5568380	-2.1927870	-0.0222200
6	3.0982750	0.0150500	0.0069840
1	2.9389890	2.1438960	0.0147270
1	3.0522800	-2.1193320	-0.0026840
7	4.5707610	0.0535720	0.0186230
8	5.1578580	-1.0054260	0.0200690
8	5.1022890	1.1414880	0.0260220
8	-4.4536030	-0.0088130	-0.0817720
6	-5.4632640	-0.9713920	0.0902080
1	-6.2456820	-0.8581090	-0.6677850
1	-5.0056880	-1.9524270	-0.0118090
1	-5.9210730	-0.8870590	1.0816780
6	-4.9452630	1.3030680	0.0334760
1	-5.7038750	1.5058620	-0.7300620
1	-5.3878690	1.4713960	1.0211810
1	-4.1073420	1.9829790	-0.1043110

(CH₃)₂O…ClCCH
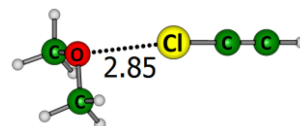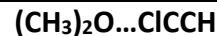
SCF E= -691.9442
ZPE= -691.8426
G= -691.8776
H= -691.8327

17	-0.8781550	-0.0000950	-0.2847180
6	-2.4844990	-0.0001110	0.0571410
6	-3.6539030	0.0000560	0.3049370
1	-4.6927090	0.0002380	0.5241170
8	1.9641020	0.0000070	-0.4713770
6	2.2404640	-1.1651550	0.2659490
1	1.6414730	-1.1996370	1.1831310
1	1.9867240	-2.0188070	-0.3578850
1	3.3004110	-1.2162850	0.5368510
6	2.2400720	1.1653240	0.2658550
1	1.6412050	1.1996010	1.1831230
1	3.3000400	1.2169230	0.5365880
1	1.9858750	2.0188390	-0.3579800

(CH₃)₂O...ClC₆H₄Cl
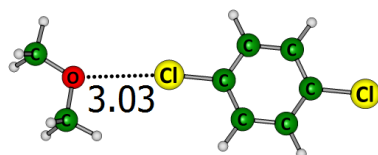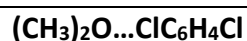
SCF E= -1306.4604
ZPE= -1306.2970
G= -1306.3409
H= -1306.2830

6	-0.3577190	-0.1496300	-0.0000730
6	-1.1198630	-1.3076160	0.0001450
6	-0.9629680	1.0971430	-0.0002650
6	-2.5030200	-1.2180890	0.0001700
1	-0.6319440	-2.2715590	0.0002560
6	-2.3460280	1.1884030	-0.0002000
1	-0.3548390	1.9901860	-0.0004330
6	-3.1047150	0.0294170	0.0000240
1	-3.1120560	-2.1104790	0.0002660
1	-2.8342910	2.1520730	-0.0003020
17	-4.8387460	0.1420880	0.0000410
17	1.3728420	-0.2640180	-0.0000640
8	4.3989950	-0.0796270	0.0002220
6	4.6101060	1.3086710	0.0003920
1	5.1672500	1.6228710	-0.8894000
1	3.6343400	1.7891970	0.0004270
1	5.1672290	1.6226860	0.8902560
6	5.6055260	-0.7977170	-0.0003590
1	6.2016100	-0.5657850	-0.8901430
1	6.2024540	-0.5657650	0.8888690
1	5.3607230	-1.8570770	-0.0001950

(CH₃)₂O...ClC₆H₄NO₂
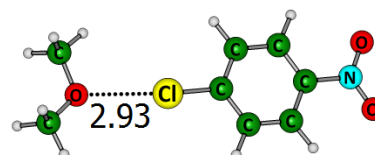
SCF E= -1051.3632
ZPE= -1051.1873
G= -1051.2339
H= 1051.1720

17	-1.6854060	-0.1630270	-0.0390060
6	0.0416420	-0.0971600	-0.0223400
6	0.6775250	1.1372280	-0.0064510
6	0.7679340	-1.2811210	-0.0254220
6	2.0599950	1.1908810	0.0068190
1	0.0898320	2.0432640	-0.0046140
6	2.1504750	-1.2316330	-0.0119810
1	0.2486140	-2.2279030	-0.0386460
6	2.7710350	0.0043920	0.0039960
1	2.5890660	2.1313310	0.0195170
1	2.7481700	-2.1302520	-0.0138330
7	4.2425540	0.0585000	0.0190010
8	4.8408020	-0.9942640	0.0190510
8	4.7626060	1.1519480	0.0303950
8	-4.6137000	-0.0560020	-0.0841050
6	-5.6850260	-0.9467930	0.0949300
1	-6.4564300	-0.7934790	-0.6677000
1	-5.2922440	-1.9568810	0.0075570
1	-6.1409900	-0.8211980	1.0831420
6	-5.0175990	1.2859140	0.0125320
1	-5.7589210	1.5302620	-0.7563660
1	-5.4512770	1.4970540	0.9963310
1	-4.1353490	1.9060570	-0.1305020

(CH₃)₂O...ClOBr
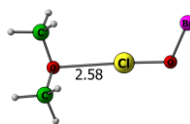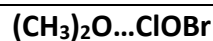
SCF E= -3264.5753
ZPE= -3264.4895

(CH₃)₂O...ClC₃N
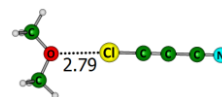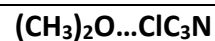
SCF E= -784.1916
ZPE= -784.0905

	G= -3264.5271				G= -784.1308		
	H= -3264.4791				H= -784.0786		
8	1.1843370	-1.0427280	-0.3506000	6	-1.6001990	0.0465540	-0.0207430
35	2.2768890	0.3171410	0.1776160	6	-2.7992460	0.0175160	-0.0005580
17	-0.4473520	-0.6060190	-0.4014490	6	-4.1742810	-0.0163820	0.0236760
8	-2.9615740	-0.0171220	-0.3401130	7	-5.3234910	-0.0456740	0.0444990
6	-3.4056550	-0.6053690	0.8610410	17	0.0274790	0.0868470	-0.0455490
1	-4.4440780	-0.3286960	1.0675860	8	2.8180720	0.0308310	-0.0763530
1	-3.3342770	-1.6836860	0.7429820	6	3.4132380	-1.2387740	0.0401190
1	-2.7782980	-0.2927180	1.7023780	1	3.8822360	-1.3635220	1.0216170
6	-2.9857760	1.3904420	-0.2846750	1	2.6302390	-1.9840850	-0.0799660
1	-4.0042180	1.7546410	-0.1179100	1	4.1728290	-1.3874010	-0.7341240
1	-2.3392220	1.7592360	0.5189120	6	3.7563480	1.0708260	0.0566790
1	-2.6195570	1.7619890	-1.2383760	1	4.2447900	1.0341090	1.0360550
				1	4.5237560	1.0056790	-0.7215330
				1	3.2237030	2.0134430	-0.0434260