Supplementary Information:

Title: Nucleophilicity at the boron atom in compounds R-B, (R =F, Cl, Br, I, CN, NC, CH_3, SiH_3, CF_3, H): the inductive effect of the groups R

Authors: Ibon Alkorta and Anthony Legon

Figure S1. Graph of D_e of the hydrogen-bonded complexes B···HBr and B···HI versus the nucleophilicities N_B of the Lewis bases B = N_2, CO, C_2H_2, C_2H_4, H_2S, PH_3, HCN, H_2O and NH_3. The N_B values are from Ref. 11. The D_e are from ref. 10 and were calculated at the CCSD(T)(F12c)/cc-pVDZ-F12 level. According to eq.(1), with the choice c'=1.0 kJ mol^{-1}, the gradient of each straight line is the electrophilicity E_{HX} of HBr or HI, as appropriate.

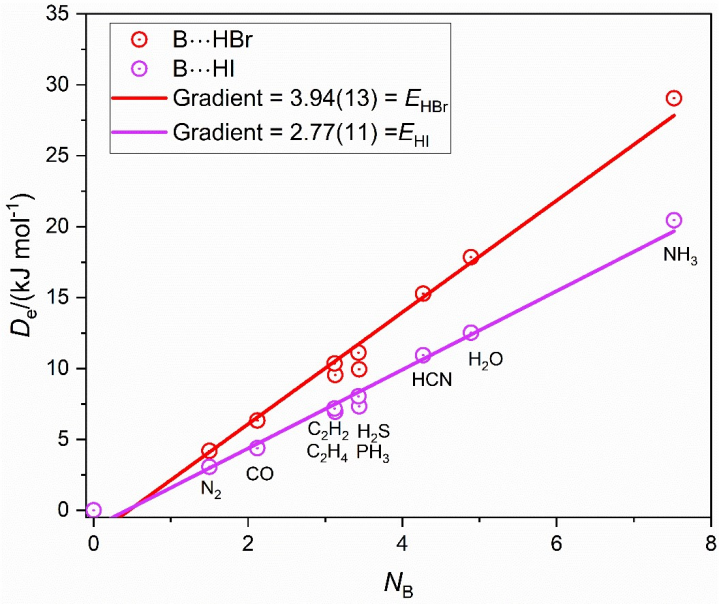


Figure.S2. Graphs of dissociation energy D_e of complexes R-B···HX versus the electrophilicity E_{HX} of the Lewis acids HX for R = H-, NC-, CN- and F_3C-.

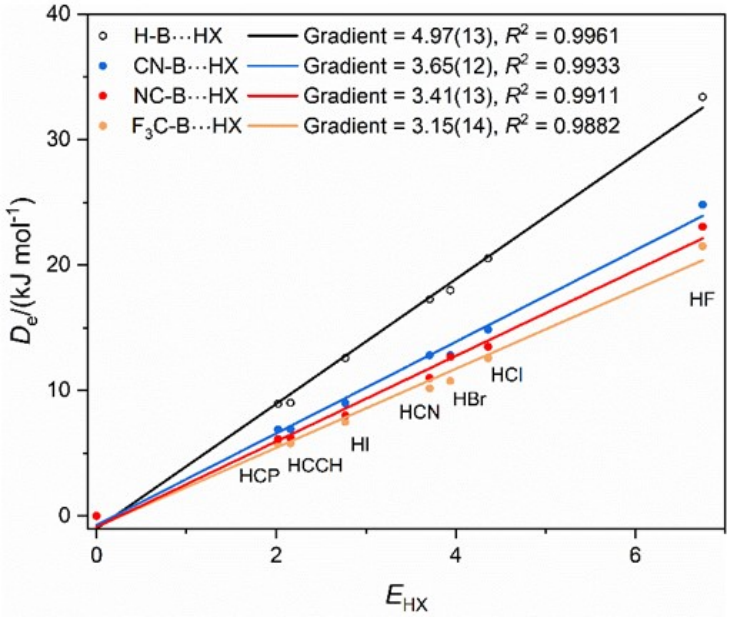


Table S1. Cartesian coordinates and energies of molecules R-B and complexes R-B□HX optimized at the CCSD(T)(F12c)/cc-pVDZ-F12 level.

R-B (R =F, Cl, Br, I, CN, NC, CH_3, SiH_3, CF_3, H)

CCSD(T)-F12C/USERDEF ENERGY=-124.53759263			
B	0.0000000000	0.0000000000	-0.8073638402
F	0.0000000000	0.0000000000	0.4593861449
CCSD(T)-F12C/USERDEF ENERGY=-484.48007620			
B	0.0000000000	0.0000000000	-1.3175494876
Cl	0.0000000000	0.0000000000	0.4017349720
CCSD(T)-F12C/USERDEF ENERGY=-440.42722520			
B	0.0000000000	0.0000000000	1.5884832075
Br	0.0000000000	0.0000000000	3.4831136908
CCSD(T)-F12C/USERDEF ENERGY=-319.54206443			
B	0.0000000000	0.0000000000	0.6477955214
I	0.0000000000	0.0000000000	2.7894687114
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-117.38824448			
B	0.0000000000	0.0000000000	0.5749622404
N	0.0000000000	0.0000000000	2.0008304502
C	0.0000000000	0.0000000000	3.1890740266
CCSD(T)-F12C/USERDEF Energy: -117.372797405136			
B	0.0000000000	0.0000000000	0.5620737379
C	0.0000000000	0.0000000000	2.1420098727
N	0.0000000000	0.0000000000	3.3068999663
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-64.51724847			
C	-0.0000000000	0.0000000000	-2.1424650822
H	0.5142574611	-0.8907200508	-2.5185671666
H	-1.0285149222	0.0000000000	-2.5185671666
H	0.5142574611	0.8907200508	-2.5185671666
B	-0.0000000000	0.0000000000	-0.5990079423
CCSD(T)-F12C/USERDEF ENERGY=-315.48874286			
B	-0.0000000000	0.0000000000	-1.6140175442
Si	0.0000000000	0.0000000000	0.5117340418
H	1.3963440209	0.0000000000	1.0169994316
H	-0.6981720105	1.2092693946	1.0169994316
H	-0.6981720105	-1.2092693946	1.0169994316
CCSD(T)-F12C/USERDEF ENERGY=-362.00381039			
B	-0.0000000000	0.0000000000	-1.7731725519
C	-0.0000000000	0.0000000000	-0.1182206285
F	1.2529016327	0.0000000000	0.3612223486
F	-0.6264508164	1.0850446424	0.3612223486
F	-0.6264508164	-1.0850446424	0.3612223486
CCSD(T)-F12C/USERDEF ENERGY=-25.23355377			
B	0.0000000000	0.0000000000	-0.1051330102
H	0.0000000000	0.0000000000	1.1275352108

HB□HX		
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-125.61996993		
F	0.6057032058	0.0000000000 -2.3255135253
H	0.4415996003	0.0000000000 -1.4033795896
B	0.0824534282	0.0000000000 0.6215287566
H	-0.1297562342	0.0000000000 1.8202949576
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-485.59805775		
Cl	0.0000000000	0.0000000000 -1.9728969272
H	0.0000000000	0.0000000000 -0.6779899909
B	0.0000000000	0.0000000000 1.5715067465
H	0.0000000000	0.0000000000 2.7936732651
CCSD(T)-F12C/USERDEF ENERGY=-441.55015868		
Br	0.0000000000	0.0000000000 -3.0760381092
H	0.0000000000	0.0000000000 -1.6368848855
B	0.0000000000	0.0000000000 0.6279907637
H	0.0000000000	0.0000000000 1.8512686605
CCSD(T)-F12C/USERDEF ENERGY=-320.67262861		
I	0.0000000000	0.0000000000 -3.4002869071
H	0.0000000000	0.0000000000 -1.7710805256
B	0.0000000000	0.0000000000 0.6557469451
H	0.0000000000	0.0000000000 1.8815180968
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-118.54038428		
N	0.0000000000	0.0000000000 -4.0740519667
C	0.0000000000	0.0000000000 -2.9181884654
H	0.0000000000	0.0000000000 -1.8430702749
B	0.0000000000	0.0000000000 0.7198849949
H	0.0000000000	0.0000000000 1.9434754661
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-102.44437073		
H	0.0000000000	0.0000000000 -5.3553391268
C	0.0000000000	0.0000000000 -4.2923743037
C	0.0000000000	0.0000000000 -3.0858915319
H	0.0000000000	0.0000000000 -2.0179386208
B	0.0000000000	0.0000000000 0.7260543070
H	0.0000000000	0.0000000000 1.9542754554
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-404.74033797		
P	0.0000000000	0.0000000000 -4.5442489655
C	0.0000000000	0.0000000000 -2.9995678981
H	0.0000000000	0.0000000000 -1.9235451863
B	0.0000000000	0.0000000000 0.8217156745
H	0.0000000000	0.0000000000 2.0500011142

FB□HX		
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-224.91940073		
F	0.0000000000	0.0000000000 -2.3419078412
H	0.0000000000	0.0000000000 -1.4137635638
B	0.0000000000	0.0000000000 0.7386020043
F	0.0000000000	0.0000000000 1.9966525679
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-584.89909207		
Cl	0.0000000000	0.0000000000 -2.0325327054

H	0.0000000000	0.0000000000	-0.7486571194
B	0.0000000000	0.0000000000	1.6389829182
F	0.0000000000	0.0000000000	2.9000636589
CCSD(T)-F12C/USERDEF ENERGY=-540.85143196			
Br	0.0000000000	0.0000000000	-3.1552283884
H	0.0000000000	0.0000000000	-1.7293745211
B	0.0000000000	0.0000000000	0.7167393390
F	0.0000000000	0.0000000000	1.9784990017
CCSD(T)-F12C/USERDEF ENERGY=-419.97473944			
I	0.0000000000	0.0000000000	-3.4874568267
H	0.0000000000	0.0000000000	-1.8685716875
B	0.0000000000	0.0000000000	0.7522261234
F	0.0000000000	0.0000000000	2.0154378221
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-217.84213220			
N	0.0000000000	0.0000000000	-4.0987700695
C	0.0000000000	0.0000000000	-2.9431869928
H	0.0000000000	0.0000000000	-1.8716763296
B	0.0000000000	0.0000000000	0.7620831460
F	0.0000000000	0.0000000000	2.0234425040
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-201.74725777			
H	0.0000000000	0.0000000000	-5.3725963617
C	0.0000000000	0.0000000000	-4.3095855543
C	0.0000000000	0.0000000000	-3.1035453488
H	0.0000000000	0.0000000000	-2.0376481290
B	0.0000000000	0.0000000000	0.7642615729
F	0.0000000000	0.0000000000	2.0284060788
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-504.04323618			
P	0.0000000000	0.0000000000	-4.5663794175
C	0.0000000000	0.0000000000	-3.0224862528
H	0.0000000000	0.0000000000	-1.9483544177
B	0.0000000000	0.0000000000	0.8589748268
F	0.0000000000	0.0000000000	2.1231375192

ClB□HX			
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-584.86349819			
F	0.0000000000	0.0000000000	-2.3631711494
H	0.0000000000	0.0000000000	-1.4317682084
B	0.0000000000	0.0000000000	0.6802551178
Cl	0.0000000000	0.0000000000	2.3742148394
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-944.84272841			
Cl	0.0000000000	0.0000000000	-2.0036721116
H	0.0000000000	0.0000000000	-0.7155754194
B	0.0000000000	0.0000000000	1.6042968983
Cl	0.0000000000	0.0000000000	3.3056437261
CCSD(T)-F12C/USERDEF ENERGY=-900.79502225			
Br	0.0000000000	0.0000000000	-3.1183675929
H	0.0000000000	0.0000000000	-1.6875609307
B	0.0000000000	0.0000000000	0.6685962702
Cl	0.0000000000	0.0000000000	2.3720686829
CCSD(T)-F12C/USERDEF ENERGY=-779.91806618			
I	0.0000000000	0.0000000000	-3.4444223109
H	0.0000000000	0.0000000000	-1.8217505157
B	0.0000000000	0.0000000000	0.6963616228

Cl	0.0000000000	0.0000000000	2.4041088131
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-577.78559872			
N	0.0000000000	0.0000000000	-4.0866087142
C	0.0000000000	0.0000000000	-2.9308940033
H	0.0000000000	0.0000000000	-1.8578346003
B	0.0000000000	0.0000000000	0.7342911810
Cl	0.0000000000	0.0000000000	2.4374958909
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-561.69019632			
H	0.0000000000	0.0000000000	-5.3667274384
C	0.0000000000	0.0000000000	-4.3037458132
C	0.0000000000	0.0000000000	-3.0975335674
H	0.0000000000	0.0000000000	-2.0308325223
B	0.0000000000	0.0000000000	0.7392183080
Cl	0.0000000000	0.0000000000	2.4507072125
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-863.98621121			
P	0.0000000000	0.0000000000	-4.5543526109
C	0.0000000000	0.0000000000	-3.0100398938
H	0.0000000000	0.0000000000	-1.9351612815
B	0.0000000000	0.0000000000	0.8323389663
Cl	0.0000000000	0.0000000000	2.5438695587

BrB□HX			
CCSD(T)-F12C/USERDEF ENERGY=-540.81012832			
F	0.0000000000	0.0000000000	-2.3716593264
H	0.0000000000	0.0000000000	-1.4405628208
B	0.0000000000	0.0000000000	0.6796227885
Br	0.0000000000	0.0000000000	2.5421299581
CCSD(T)-F12C/USERDEF ENERGY=-900.78959699			
Cl	0.0000000000	0.0000000000	-2.1083794226
H	0.0000000000	0.0000000000	-0.8204059524
B	0.0000000000	0.0000000000	1.5044121741
Br	0.0000000000	0.0000000000	3.3767225683
CCSD(T)-F12C/USERDEF ENERGY=-856.74197728			
Br	0.0000000000	0.0000000000	-3.2154023280
H	0.0000000000	0.0000000000	-1.7844353714
B	0.0000000000	0.0000000000	0.5701066941
Br	0.0000000000	0.0000000000	2.4444674349
CCSD(T)-F12C/USERDEF ENERGY=-735.86511560			
I	0.0000000000	0.0000000000	-3.4887439796
H	0.0000000000	0.0000000000	-1.8661020675
B	0.0000000000	0.0000000000	0.6450137117
Br	0.0000000000	0.0000000000	2.5245687651
CCSD(T)-F12C/USERDEF ENERGY=-533.73244350			
N	0.0000000000	0.0000000000	-4.0260526064
C	0.0000000000	0.0000000000	-2.8703589925
H	0.0000000000	0.0000000000	-1.7975348852
B	0.0000000000	0.0000000000	0.8022140265
Br	0.0000000000	0.0000000000	2.6762067456
CCSD(T)-F12C/USERDEF ENERGY=-517.63719865			
H	0.0000000000	0.0000000000	-5.3664269629
C	0.0000000000	0.0000000000	-4.3034275924
C	0.0000000000	0.0000000000	-3.0972686034
H	0.0000000000	0.0000000000	-2.0307996480

B	0.0000000000	0.0000000000	0.7467637355
Br	0.0000000000	0.0000000000	2.6314089217
CCSD(T)-F12C/USERDEF ENERGY=-819.93323083			
P	0.0000000000	0.0000000000	-4.3511121940
C	0.0000000000	0.0000000000	-2.8068892848
H	0.0000000000	0.0000000000	-1.7321148889
B	0.0000000000	0.0000000000	1.0414233966
Br	0.0000000000	0.0000000000	2.9259779661

IB□HX			
CCSD(T)-F12C/USERDEF ENERGY=-419.92467321			
F	0.0000000000	0.0000000000	-2.3855745721
H	0.0000000000	0.0000000000	-1.4542890194
B	0.0000000000	0.0000000000	0.6683838494
I	0.0000000000	0.0000000000	2.7688803834
CCSD(T)-F12C/USERDEF ENERGY=-779.90432710			
Cl	0.0000000000	0.0000000000	-2.8386345613
H	0.0000000000	0.0000000000	-1.5501797409
B	0.0000000000	0.0000000000	0.7685238439
I	0.0000000000	0.0000000000	2.8812656717
CCSD(T)-F12C/USERDEF ENERGY=-735.85679435			
Br	0.0000000000	0.0000000000	-3.0017339794
H	0.0000000000	0.0000000000	-1.5698144570
B	0.0000000000	0.0000000000	0.7674716739
I	0.0000000000	0.0000000000	2.8830519759
CCSD(T)-F12C/USERDEF ENERGY=-614.97999499			
I	0.0000000000	0.0000000000	-3.2680602545
H	0.0000000000	0.0000000000	-1.6441138134
B	0.0000000000	0.0000000000	0.8443519881
I	0.0000000000	0.0000000000	2.9667972932
CCSD(T)-F12C/USERDEF ENERGY=-412.84709179			
N	0.0000000000	0.0000000000	-4.0375717302
C	0.0000000000	0.0000000000	-2.8818766741
H	0.0000000000	0.0000000000	-1.8089464790
B	0.0000000000	0.0000000000	0.7938532035
I	0.0000000000	0.0000000000	2.9090092221
CCSD(T)-F12C/USERDEF ENERGY=-396.75194228			
H	0.0000000000	0.0000000000	-5.3786669360
C	0.0000000000	0.0000000000	-4.3156586035
C	0.0000000000	0.0000000000	-3.1095295246
H	0.0000000000	0.0000000000	-2.0430944183
B	0.0000000000	0.0000000000	0.7412964284
I	0.0000000000	0.0000000000	2.8703029046
CCSD(T)-F12C/USERDEF ENERGY=-699.04800129			
P	0.0000000000	0.0000000000	-4.4988503945
C	0.0000000000	0.0000000000	-2.9546422214
H	0.0000000000	0.0000000000	-1.8798622847
B	0.0000000000	0.0000000000	0.8952546252
I	0.0000000000	0.0000000000	3.0241204242

NCB□HX			
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-217.75522672			
F	0.0000000000	0.0000000000	-2.4741998860
H	0.0000000000	0.0000000000	-1.5438530916
B	0.0000000000	0.0000000000	0.5782051282
C	0.0000000000	0.0000000000	2.1339205910
N	0.0000000000	0.0000000000	3.2988578577
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-577.73459528			
Cl	0.0000000000	0.0000000000	-3.0539950437
H	0.0000000000	0.0000000000	-1.7678859033
B	0.0000000000	0.0000000000	0.5880588122
C	0.0000000000	0.0000000000	2.1519792721
N	0.0000000000	0.0000000000	3.3169733480
CCSD(T)-F12C/USERDEF ENERGY=-533.68691918			
Br	0.0000000000	0.0000000000	-3.2181643186
H	0.0000000000	0.0000000000	-1.7901138057
B	0.0000000000	0.0000000000	0.6169753655
C	0.0000000000	0.0000000000	2.1827116167
N	0.0000000000	0.0000000000	3.3477216273
CCSD(T)-F12C/USERDEF ENERGY=-412.81011589			
I	0.0000000000	0.0000000000	-3.6004937288
H	0.0000000000	0.0000000000	-1.9802589309
B	0.0000000000	0.0000000000	0.6049968614
C	0.0000000000	0.0000000000	2.1749397407
N	0.0000000000	0.0000000000	3.3399465428
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-210.67719508			
N	0.0000000000	0.0000000000	-3.8392359868
C	0.0000000000	0.0000000000	-2.6835982041
H	0.0000000000	0.0000000000	-1.6115241457
B	0.0000000000	0.0000000000	1.0194004372
C	0.0000000000	0.0000000000	2.5842052502
N	0.0000000000	0.0000000000	3.7492526492
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-194.58252255			
H	0.0000000000	0.0000000000	-5.2185688035
C	0.0000000000	0.0000000000	-4.1555067135
C	0.0000000000	0.0000000000	-2.9494234694
H	0.0000000000	0.0000000000	-1.8833148064
B	0.0000000000	0.0000000000	0.9146028582
C	0.0000000000	0.0000000000	2.4873874100
N	0.0000000000	0.0000000000	3.6523235246
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-496.87849641			
P	0.0000000000	0.0000000000	-4.3151850494
C	0.0000000000	0.0000000000	-2.7710932019
H	0.0000000000	0.0000000000	-1.6967527262
B	0.0000000000	0.0000000000	1.1037428633
C	0.0000000000	0.0000000000	2.6767616760
N	0.0000000000	0.0000000000	3.8417264382

CNB□HX			
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-217.77134431			
F	0.0000000000	0.0000000000	-2.4158339714
H	0.0000000000	0.0000000000	-1.4850897655

B	0.0000000000	0.0000000000	0.6299681807
N	0.0000000000	0.0000000000	2.0367545728
C	0.0000000000	0.0000000000	3.2271315828
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-577.75056949			
Cl	0.0000000000	0.0000000000	-2.9896030339
H	0.0000000000	0.0000000000	-1.7028808107
B	0.0000000000	0.0000000000	0.6374390049
N	0.0000000000	0.0000000000	2.0501894971
CCSD(T)-F12C/USERDEF ENERGY=-533.70284203			
Br	0.0000000000	0.0000000000	-3.1509354323
H	0.0000000000	0.0000000000	-1.7219560035
B	0.0000000000	0.0000000000	0.6647131689
N	0.0000000000	0.0000000000	2.0788057429
C	0.0000000000	0.0000000000	3.2685030093
CCSD(T)-F12C/USERDEF ENERGY=-412.82593683			
I	0.0000000000	0.0000000000	-3.5286876778
H	0.0000000000	0.0000000000	-1.9075860553
B	0.0000000000	0.0000000000	0.6504471346
N	0.0000000000	0.0000000000	2.0678048424
C	0.0000000000	0.0000000000	3.2571522414
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-210.69334013			
N	0.0000000000	0.0000000000	-3.7803527968
C	0.0000000000	0.0000000000	-2.6246721748
H	0.0000000000	0.0000000000	-1.5521278964
B	0.0000000000	0.0000000000	1.0528381320
N	0.0000000000	0.0000000000	2.4664802827
C	0.0000000000	0.0000000000	3.6563344534
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-194.59824241			
H	0.0000000000	0.0000000000	-5.1694953739
C	0.0000000000	0.0000000000	-4.1064751314
C	0.0000000000	0.0000000000	-2.9003117922
H	0.0000000000	0.0000000000	-1.8339191163
B	0.0000000000	0.0000000000	0.9428774208
N	0.0000000000	0.0000000000	2.3629347856
C	0.0000000000	0.0000000000	3.5518892074
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-496.89422993			
P	0.0000000000	0.0000000000	-4.2573253333
C	0.0000000000	0.0000000000	-2.7130992656
H	0.0000000000	0.0000000000	-1.6384972371
B	0.0000000000	0.0000000000	1.1396893455
N	0.0000000000	0.0000000000	2.5597302279
C	0.0000000000	0.0000000000	3.7487022626

H_3CB□HX			
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-164.90637732			
C	0.0000000000	0.0000000000	-2.1277187379
H	0.5142564297	-0.8907182644	-2.5031520460
H	-1.0285128595	0.0000000000	-2.5031520460
H	0.5142564297	0.8907182644	-2.5031520460
B	0.0000000000	0.0000000000	-0.5990038590
H	-0.0000000000	0.0000000000	1.4244044731

F	-0.0000000000	0.0000000000	2.3655997374
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-524.88400718			
C	-0.0000561882	0.0000000000	-1.9877346482
H	0.5142854898	-0.8908084615	-2.3632081957
H	-1.0286744329	0.0000000000	-2.3633311150
H	0.5142854898	0.8908084615	-2.3632081957
B	-0.0000439439	0.0000000000	-0.4557146592
H	0.0002388253	0.0000000000	1.7201639491
Cl	-0.0000352401	0.0000000000	3.0235583404
CCSD(T)-F12C/USERDEF ENERGY=-480.83614855			
C	-0.0000000001	0.0000000000	-1.8964752276
H	0.5143740300	-0.8909219540	-2.2717491065
H	-1.0287480600	0.0000000000	-2.2717491066
H	0.5143740300	0.8909219540	-2.2717491065
B	-0.0000000000	0.0000000000	-0.3645341400
H	0.0000000000	0.0000000000	1.7910011160
Br	-0.0000000000	0.0000000000	3.2431810469
CCSD(T)-F12C/USERDEF ENERGY=-359.95820994			
C	0.0000000000	0.0000000000	-1.9697264893
H	0.5143995647	-0.8909661815	-2.3453774175
H	-1.0287991295	0.0000000000	-2.3453774174
H	0.5143995647	0.8909661815	-2.3453774175
B	0.0000000001	0.0000000000	-0.4352665569
H	0.0000000001	0.0000000000	1.8495089219
I	-0.0000000001	0.0000000000	3.4910418524
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-157.82598898			
B	0.0082025774	0.0000000000	0.0021406062
C	1.5420933140	0.0000000000	0.0002281945
H	1.9197570345	0.0000000000	1.0281742804
H	1.9178388080	-0.8906026434	-0.5144221203
H	1.9178388080	0.8906026434	-0.5144221203
H	-2.5105171147	0.0000000000	-0.0020071487
C	-3.5881764073	0.0000000000	-0.0006005021
N	-4.7442630200	0.0000000000	0.0009088104
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-141.72896237			
C	0.0000000000	0.0000000000	-2.0878671089
H	0.5142431289	-0.8906952266	-2.4640345220
H	-1.0284862578	0.0000000000	-2.4640345219
H	0.5142431289	0.8906952266	-2.4640345220
B	0.0000000001	0.0000000000	-0.5490004453
H	0.0000000000	0.0000000000	2.1591300595
C	-0.0000000001	0.0000000000	3.2285275980
C	0.0000000000	0.0000000000	4.4353305856
H	0.0000000001	0.0000000000	5.4982386277
CCSD(T)-F12C/CC-PVDZ-F12 ENERGY=-444.02498998			
B	0.0155766041	0.0000000000	-0.0003094171
C	1.5542194629	0.0000000000	-0.0004274631
H	1.9305126584	0.0000000000	1.0280671431
H	1.9303954792	-0.8906965200	-0.5146917998
H	1.9303954792	0.8906965200	-0.5146917998
H	-2.6869005508	0.0000000000	0.0047253318
C	-3.7643501110	0.0000000000	0.0011953767
P	-5.3095520220	0.0000000000	-0.0038673719

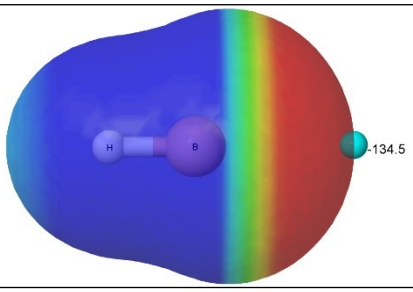
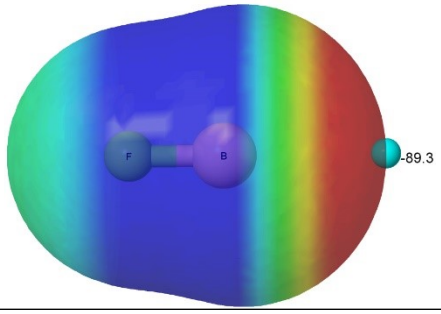
F_3CB:HX			
CCSD(T)-F12C/USERDEF ENERGY=-362.00381039			
B	-0.0000000000	0.0000000000	-1.7731725519
C	-0.0000000000	0.0000000000	-0.1182206285
F	1.2529016327	0.0000000000	0.3612223486
F	-0.6264508164	1.0850446424	0.3612223486
F	-0.6264508164	-1.0850446424	0.3612223486
CCSD(T)-F12C/USERDEF ENERGY=-462.38566749			
B	-0.0000000000	0.0000000000	-0.7971726208
C	-0.0000000000	0.0000000000	0.8438076596
F	1.2531012682	0.0000000000	1.3148074529
F	-0.6265506341	1.0852175317	1.3148074529
F	-0.6265506341	-1.0852175317	1.3148074529
H	-0.0000000000	0.0000000000	-2.9388950130
F	0.0000000000	0.0000000000	-3.8683795424
CCSD(T)-F12C/USERDEF ENERGY=-822.36528087			
B	-0.0000000000	0.0000000000	-0.0715560742
C	-0.0000000000	0.0000000000	1.5744057954
F	1.2530452086	0.0000000000	2.0481144803
F	-0.6265226043	1.0851689827	2.0481144803
F	-0.6265226043	-1.0851689827	2.0481144803
H	-0.0000000000	0.0000000000	-2.4493759334
Cl	-0.0000000000	0.0000000000	-3.7345374363
CCSD(T)-F12C/USERDEF ENERGY=-778.31765465			
B	-0.0000000000	0.0000000000	1.0568940772
C	-0.0000000000	0.0000000000	2.7040694544
F	1.2530215756	0.0000000000	3.1783229463
F	-0.6265107878	1.0851485160	3.1783229463
F	-0.6265107878	-1.0851485160	3.1783229463
H	-0.0000000000	0.0000000000	-1.3719829216
Br	0.0000000000	0.0000000000	-2.7992329210
CCSD(T)-F12C/USERDEF ENERGY=-657.44095158			
B	-0.0000000000	0.0000000000	1.9155709250
C	-0.0000000000	0.0000000000	3.5651633065
F	1.2530202562	0.0000000000	4.0408907738
F	-0.6265101281	1.0851473734	4.0408907738
F	-0.6265101281	-1.0851473734	4.0408907738
H	-0.0000000000	0.0000000000	-0.6900551154
I	0.0000000000	0.0000000000	-2.3099440861
CCSD(T)-F12C/USERDEF ENERGY=-455.30791155			
B	-0.0000000000	0.0000000000	-0.2318929686
C	-0.0000000000	0.0000000000	1.4142158920
F	1.2531649705	0.0000000000	1.8880820355
F	-0.6265824853	1.0852726996	1.8880820355
F	-0.6265824853	-1.0852726996	1.8880820355
H	-0.0000000000	0.0000000000	-2.8869859986
C	0.0000000000	0.0000000000	-3.9586700286
N	0.0000000000	0.0000000000	-5.1142324693
CCSD(T)-F12C/USERDEF ENERGY=-439.21338712			
B	-0.0000000000	0.0000000000	-0.2291328403
C	-0.0000000000	0.0000000000	1.4216186428
F	1.2529804116	0.0000000000	1.8985981179
F	-0.6264902058	1.0851128669	1.8985981179
F	-0.6264902058	-1.0851128669	1.8985981179

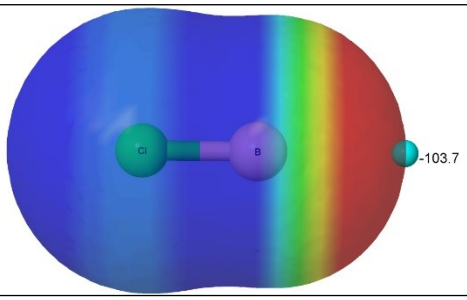
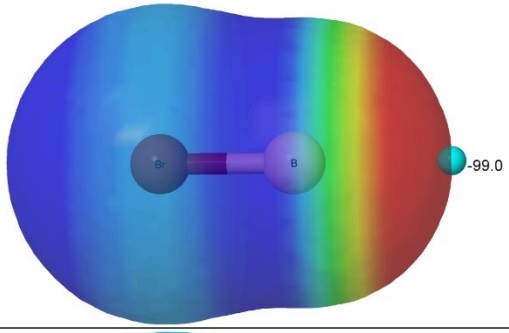
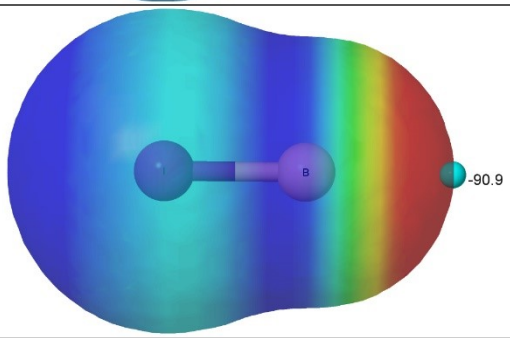
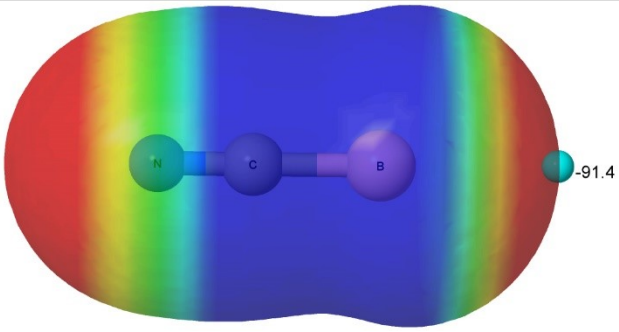
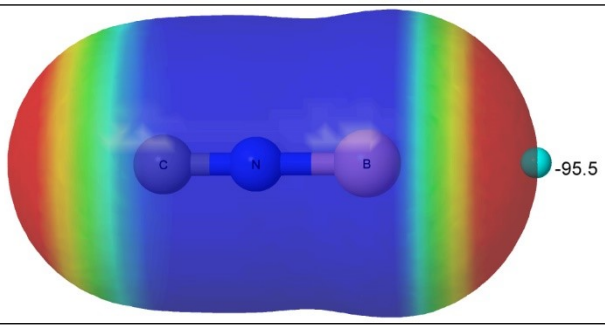
H	-0.0000000000	0.0000000000	-3.0477830476
C	0.0000000000	0.0000000000	-4.1136661946
C	0.0000000000	0.0000000000	-5.3196634043
H	0.0000000000	0.0000000000	-6.3827487723
CCSD(T)-F12C/USERDEF ENERGY=-741.50936811			
B	-0.0000000000	0.0000000000	0.6215957501
C	-0.0000000000	0.0000000000	2.2724263722
F	1.2529834248	0.0000000000	2.7493831127
F	-0.6264917124	1.0851154764	2.7493831127
F	-0.6264917124	-1.0851154764	2.7493831127
H	-0.0000000000	0.0000000000	-2.1985531210
C	0.0000000000	0.0000000000	-3.2727189338
P	0.0000000000	0.0000000000	-4.8166768128

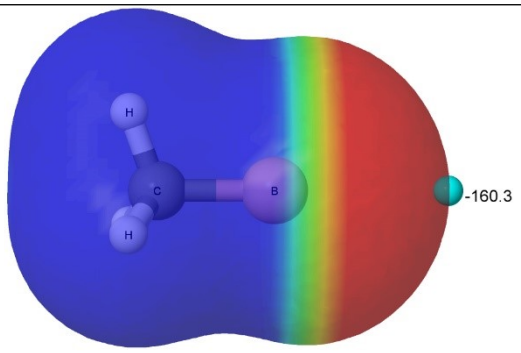
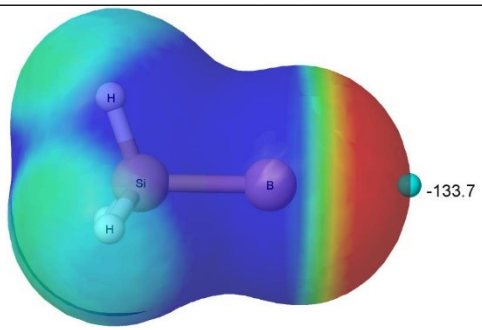
H_3SiB:HX			
CCSD(T)-F12C/USERDEF ENERGY=-315.48874286			
B	-0.0000000000	0.0000000000	-1.6140175442
Si	0.0000000000	0.0000000000	0.5117340418
H	1.3963440209	0.0000000000	1.0169994316
H	-0.6981720105	1.2092693946	1.0169994316
H	-0.6981720105	-1.2092693946	1.0169994316
CCSD(T)-F12C/USERDEF ENERGY=-415.87624775			
B	-0.0000000000	0.0000000000	-0.1299370405
Si	-0.0000000000	0.0000000000	1.9669305408
H	1.4024226565	0.0000000000	2.4462515381
H	-0.7012113283	1.2145336474	2.4462515381
H	-0.7012113283	-1.2145336474	2.4462515381
H	-0.0000000000	0.0000000000	-2.1678676972
F	0.0000000000	0.0000000000	-3.1081324075
CCSD(T)-F12C/USERDEF ENERGY=-775.85431182			
B	-0.0000000000	0.0000000000	0.7542513846
Si	-0.0000000000	0.0000000000	2.8590118460
H	1.4012255318	0.0000000000	3.3435077081
H	-0.7006127659	1.2134969070	3.3435077081
H	-0.7006127659	-1.2134969070	3.3435077081
H	-0.0000000000	0.0000000000	-1.4369116167
Cl	0.0000000000	0.0000000000	-2.7391780512
CCSD(T)-F12C/USERDEF ENERGY=-731.80662028			
B	-0.0000000000	0.0000000000	1.8241939301
Si	-0.0000000000	0.0000000000	3.9291492249
H	1.4015142208	0.0000000000	4.4128862511
H	-0.7007571104	1.2137469190	4.4128862511
H	-0.7007571104	-1.2137469190	4.4128862511
H	-0.0000000000	0.0000000000	-0.3391037780
Br	0.0000000000	0.0000000000	-1.7905691127
CCSD(T)-F12C/USERDEF ENERGY=-610.92894650			
B	-0.0000000000	0.0000000000	2.5569879778
Si	-0.0000000000	0.0000000000	4.6670244413
H	1.4006988681	0.0000000000	5.1546511667
H	-0.7003494340	1.2130408028	5.1546511667
H	-0.7003494340	-1.2130408028	5.1546511667
H	-0.0000000000	0.0000000000	0.2658313653
I	0.0000000000	0.0000000000	-1.3756028849

CCSD(T)-F12C/USERDEF ENERGY=-408.79607194			
B	-0.0000000000	0.0000000000	0.6684038773
Si	-0.0000000000	0.0000000000	2.7772424962
H	1.4003847971	0.0000000000	3.2657663976
H	-0.7001923986	1.2127688094	3.2657663976
H	-0.7001923986	-1.2127688094	3.2657663976
H	-0.0000000000	0.0000000000	-1.8832882077
C	0.0000000000	0.0000000000	-2.9599571125
N	0.0000000000	0.0000000000	-4.1159226223
CCSD(T)-F12C/USERDEF ENERGY=-392.69982562			
B	-0.0000000000	0.0000000000	0.6989260588
Si	-0.0000000000	0.0000000000	2.8167212149
H	1.3980919131	0.0000000000	3.3144650373
H	-0.6990459565	1.2107831136	3.3144650373
H	-0.6990459565	-1.2107831136	3.3144650373
H	-0.0000000000	0.0000000000	-2.0416145173
C	0.0000000000	0.0000000000	-3.1102419336
C	0.0000000000	0.0000000000	-4.3168170195
H	0.0000000000	0.0000000000	-5.3798142962
CCSD(T)-F12C/USERDEF ENERGY=-694.99584337			
B	-0.0000000000	0.0000000000	1.7115069596
Si	-0.0000000000	0.0000000000	3.8290922981
H	1.3981956893	0.0000000000	4.3265215991
H	-0.6990978446	1.2108729864	4.3265215991
H	-0.6990978446	-1.2108729864	4.3265215991
H	-0.0000000000	0.0000000000	-1.0227186622
C	0.0000000000	0.0000000000	-2.0994699744
P	0.0000000000	0.0000000000	-3.6443238277

Table S2. Molecular electrostatic potential on the 0.001 au electron density isosurface (MESP) at MP2/aug-cc-pVTZ computational level. The minimum associated to the boron atom (σ_{min}) is indicated with a small sphere in cyan colour and its value is given in kJ mol^{-1}.

	σ_{min}	MESP
BH	-134.5	
BF	-89.3	

BCl	-103.7	
BBr	-99.0	
BI	-90.9	
BCN	-91.4	
BNC	-95.5	

BCH3	-160.3	
BSiH3	-133.7	
BCF3	-83.3