Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for

Chemical Pressure-Chemical Knowledge: Squeezing Bonds and Lone Pairs within the Valence Shell Electron Pair Repulsion Model

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Computational details of studied molecules

Table S1: Calculation details and geometrical parameters of the molecules studied.

Molecule	ecut (ha)	k-points	nfft grid	Bond Length (Å)	Bond Angle (deg)
H_2O	270	1x1x1	288x288x288	d(O-H) = 0.97120	α(H-O-H) = 104.92
NH_3	220	1x1x1	256x256x256	d(N-H) = 1.0217	α(H-N-H) = 107.26
NF_3	300	1x1x1	300x300x300	d(N-F) =1.37301	α(F-N-F) = 101.70
AsH_3	280	1x1x1	288x288x288	d(As-H) =1.52132	α(H-As-H) =90.62
PH_3	240	1x1x1	270x270x270	d(P-H) =1.42719	α(H-P-H) = 91.83
PF_3	290	1x1x1	300x300x300	d(P-F) =1.56403	α(F-P-F) = 97.44
PCl_3	270	1x1x1	290x290x290	d(P-Cl) =2.03959	α(Cl-P-Cl) = 100.36
SO_2	260	1x1x1	288x288x288	d(S-O) = 1.4281	α(O-S-O) = 119.54
SF_4	280	1x1x1	290x290x290	$d(S\text{-}F)_{ax}$ =1.6482 $d(S\text{-}F)_{eq}$ =1.5541	$\alpha(F\text{-}S\text{-}F)_{ax}$ = 173.07 $\alpha(F\text{-}S\text{-}F)_{eq}$ = 100.61
ClF_3	360	1x1x1	324x324x324	$d(Cl\text{-}F)_{ax}$ =1.6921 $d(Cl\text{-}F)_{eq}$ =1.6026	$\alpha(F\text{-}Cl\text{-}F)_{ax}$ = 176.9 $\alpha(F\text{-}Cl\text{-}F)_{eq}$ = 88.19
XeF_2	380	1x1x1	340x340x340	d(Xe-F) = 2.0084	α(F-Xe-F) = 179.99
BeH_2	290	1x1x1	290x290x290	d(Be-H) = 1.3167	α(H-Be-H) = 179.99
BH_3	280	1x1x1	280x280x280	d(B-H) = 1.1983	α(H-B-H) = 120.00
BF_3	320	1x1x1	320x320x320	d(B-F) =1.3104	α(F-B-F) = 119.99
Ethylene	300	1x1x1	300x300x300	d(C-C) =1.3309 d(C-H) =1.0852	α(H-C-H) = 119.49

Chemical Pressure distribution in BH_3 Molecule

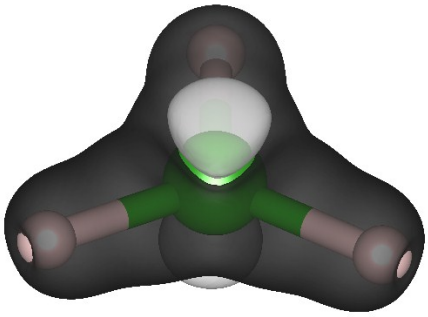

Figure S1. 3D isosurfaces of chemical pressure (CP) distributions within the BH_3 molecule. Isosurface values: CP=+0.013 (white) and –0.013 (black). Green and white spheres indicate boron and hydrogen atoms, respectively.

Chemical Pressure distribution in BF_3 Molecule

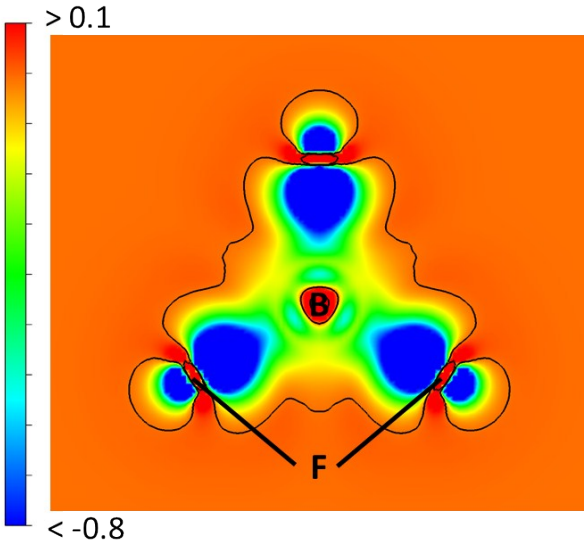

Figure S2. Chemical pressure heat-maps of the BF_3 molecule along the molecular plane. Black curves: CP = 0 contour.