# Structural Trends in Monoboronyl Compounds: Analysis of the Interaction of Second-row Elements with BO

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## Supporting Information

**Table S1.** T1 diagnostic values in the CCSD/aug-cc-pVTZ calculations for the different minima of [XBO] systems.

| Species | *T1* |
|---|---|
| NaBO($^1\Sigma^+$) | 0.019 |
| NaOB($^1$A') | 0.015 |
| NaOB($^1\Sigma^+$) | 0.018 |
| SiBO($^2\Pi$) | 0.023 |
| SiOB($^2\Pi$) | 0.020 |
| PBO($^3\Sigma^-$) | 0.023 |
| POB($^3$A") | 0.022 |
| SBO($^2\Pi$) | 0.022 |
| SOB($^2\Pi$) | 0.022 |
| SOB($^2$A") | 0.024 |
| SOB($^2$A') | 0.023 |
| ClBO($^1\Sigma^+$) | 0.016 |
| ClOB($^1$A') | 0.020 |

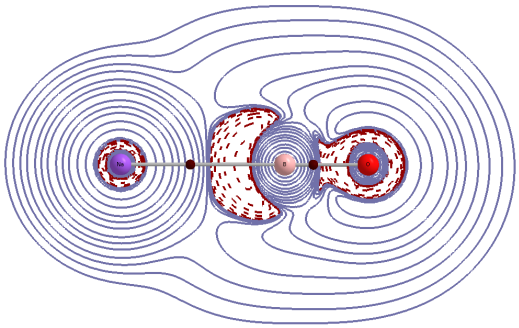
**Table S2.** Corre-valence and relativistic corrections for the geometrical parameters (in Å) and electronic energies (in a. u.) of the different linear XBO and XOB species. The contributions to the relative energies of the XOB species (relative to the XBO isomers) are given in kcal/mol.

| Species | | *r(X-B)* | *r(X-O)* | *r(B-O)* | *E* | *ΔE* |
|---|---|---|---|---|---|---|
| NaBO($^1\Sigma^+$) | Δx-core-valence | -0.0044 | | -0.0023 | -0.118056 | |
| | Δx-relativistic | -0.0012 | | -0.0004 | -0.267457 | |
| NaOB($^1\Sigma^+$) | Δx-core-valence | | -0.0024 | -0.0024 | -0.117792 | +0.17 |
| | Δx-relativistic | | -0.0011 | -0.0003 | -0.267398 | +0.04 |
| SiBO($^2\Pi$) | Δx-core-valence | -0.0053 | | -0.0023 | -0.420628 | |
| | Δx-relativistic | 0.0000 | | 0.0000 | -0.661513 | |
| SiOB($^2\Pi$) | Δx-core-valence | | -0.0031 | -0.0029 | -0.420280 | +0.22 |
| | Δx-relativistic | | 0.0010 | -0.0002 | -0.661421 | +0.06 |
| PBO($^3\Sigma^-$) | Δx-core-valence | -0.0050 | | -0.0023 | 0.425058 | |
| | Δx-relativistic | -0.0017 | | -0.0002 | -0.759979 | |
| POB($^3\Sigma^-$) | Δx-core-valence | | -0.0029 | -0.0031 | -0.424412 | +0.41 |
| | Δx-relativistic | | -0.0003 | -0.0005 | -0.759983 | +0.05 |
| SBO($^2\Pi$) | Δx-core-valence | -0.0042 | | -0.0023 | -0.430133 | |
| | Δx-relativistic | 0.0000 | | 0.0000 | -1.139888 | |
| SOB($^2\Pi$) | Δx-core-valence | | -0.0031 | -0.0031 | -0.429181 | +0.60 |
| | Δx-relativistic | | 0.0009 | -0.0003 | -1.139957 | -0.04 |
| ClBO($^1\Sigma^+$) | Δx-core-valence | -0.0060 | | -0.0029 | -0.444275 | |
| | Δx-relativistic | 0.0003 | | 0.0000 | -1.46723 | |
| ClOB($^1\Sigma^+$) | Δx-core-valence | | -0.0042 | -0.0030 | -0.435870 | +0.48 |
| | Δx-relativistic | | 0.0018 | -0.0004 | -1.467975 | -0.16 |

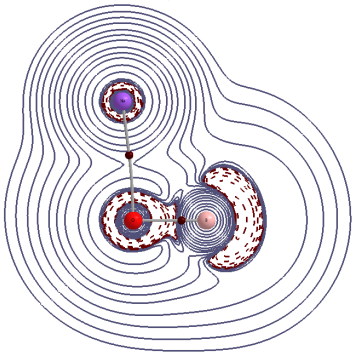
**Table S3.** Electronic spin-orbit corrections for different minima of the [XBO] systems computed at the CASSCF(N,10)/aug-cc-pVTZ level of theory (N=9,10,11 for Si, P, and S systems, respectively).

| Species | $\Delta E_{SO}(cm^{-1})$ | States |
|---|---|---|
| SiBO($^2\Pi$) | 68 | $^2\Pi$ |
| SiOB($^2\Pi$) | 69 | $^2\Pi$ |
| PBO($^3\Sigma^-$) | 0.0 | $^3\Sigma^- {}^1\Delta$ |
| POB($^3\Sigma^-$) | 0.0 | $^3\Sigma^- {}^1\Delta$ |
| SBO($^2\Pi$) | 170 | $^2\Pi$ |
| SOB($^2\Pi$) | 182 | $^2\Pi$ |

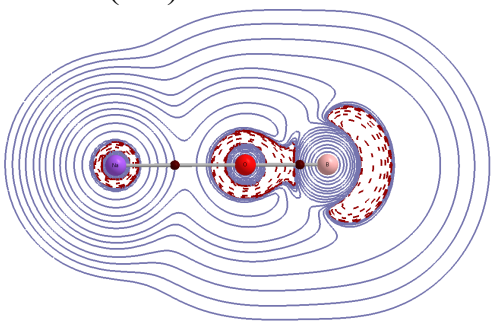
NaBO ($^1\Sigma^+$)



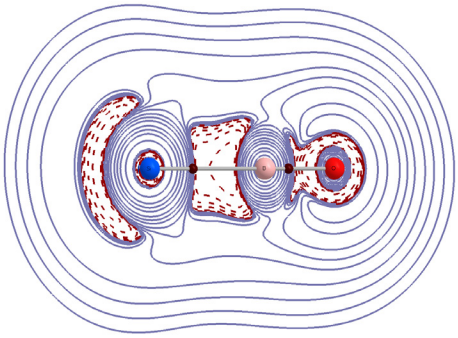
NaOB ($^1A'$)



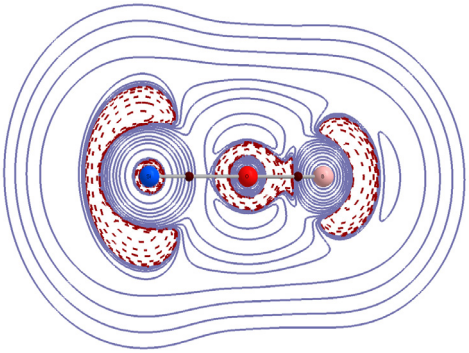
NaOB ($^1\Sigma^+$)



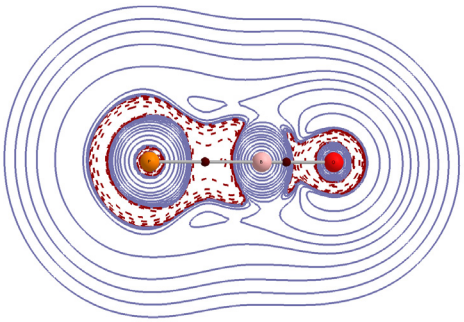
SiBO ($^2\Pi$)



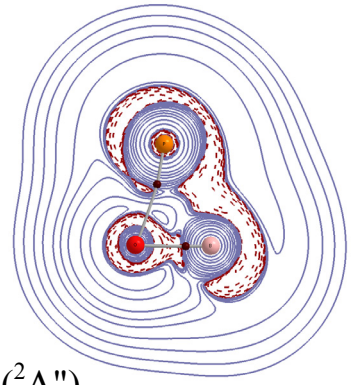
SiOB ($^2\Pi$)



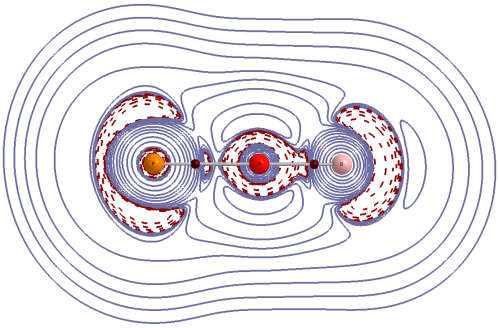
PBO ($^3\Sigma^-$)



POB ($^3A''$)

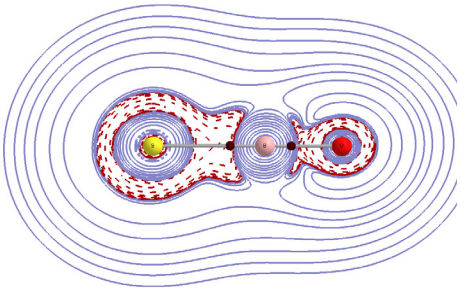


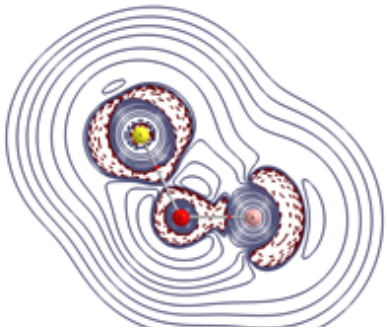
POB ($^3\Sigma^-$)



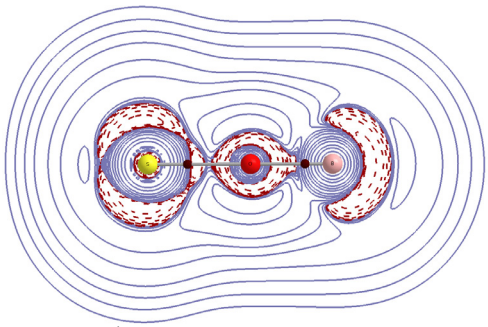
SOB ($^2A''$)

SBO ($^2\Pi$)

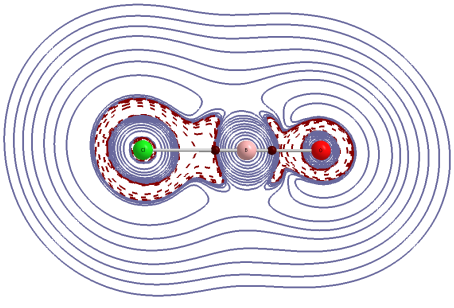




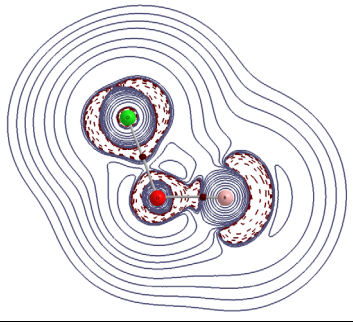
SOB ($^2\Pi$)



ClBO ($^1\Sigma^+$)



ClOB ($^1A'$)



ClOB ($^1\Sigma^+$)

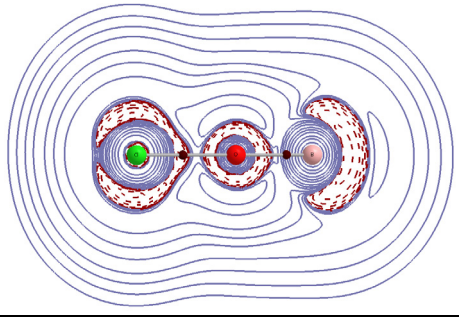


**Figure S1** Molecular graphs and contour maps of the Laplacian of the electronic charge density, $\nabla^2\rho$, for MBO/MOB species. Dark brown dots represent bond critical points. Red lines correspond to negative values of the Laplacian and blue lines to positive ones. The contour maps were calculated at the CCSD/aug-cc-pVTZ