Supporting Information: Performance of PNOF3 for reactivity studies: X[BO]and X[CN] isomerization reactions (X=H,Li) as a case study

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Table S1: Potential surface scan for the for the BOH to HBO isomerization as a function of the H-B-O angle. Absolute energies in hartrees and relative energies, in parenthesis, with respect to B-O-H linear structure (angle of 0.0^o) in kcal/mol are shown. The cc-pVTZ basis set have been used for these calculations, considering 6d and 10f basis functions, and the geometries are partially optimized at the CCSD/cc-pVTZ level of theory with the H-B-O angle fixed at the values of column 1.

Angle	HF	PNOF3	CCSDT
0.0	-100.136080 (0.00)	-100.518226 (0.00)	-100.509785 (-0.00)
10.0	-100.138045 (-1.23)	-100.519130 (-0.57)	-100.510340 (-0.35)
20.0	-100.141682 (-3.52)	-100.521364 (-1.97)	-100.512567 (-1.75)
30.0	-100.139891 (-2.39)	-100.520455 (-1.40)	-100.511649 (-1.17)
40.0	-100.124527 (7.25)	-100.510844 (4.63)	-100.500742 (5.67)
50.0	-100.097200 (24.40)	-100.494805 (14.70)	-100.481430 (17.79)
60.0	-100.072517 (39.89)	-100.485610 (20.47)	-100.467932 (26.26)
70.0	-100.063665 (45.44)	-100.490714 (17.26)	-100.469601 (25.22)
80.0	-100.071564 (40.48)	-100.501707 (10.37)	-100.481708 (17.62)
90.0	-100.089393 (29.30)	-100.513992 (2.66)	-100.497684 (7.59)
100.0	-100.110724 (15.91)	-100.526352 (-5.10)	-100.514269 (-2.81)
110.0	-100.131782 (2.70)	-100.538616 (-12.79)	-100.530017 (-12.70)
120.0	-100.150857 (-9.27)	-100.550362 (-20.17)	-100.544309 (-21.66)
130.0	-100.167246 (-19.56)	-100.561250 (-27.00)	-100.556832 (-29.52)
140.0	-100.180701 (-28.00)	-100.570810 (-33.00)	-100.567411 (-36.16)
150.0	-100.191159 (-34.56)	-100.578759 (-37.99)	-100.575964 (-41.53)
160.0	-100.198626 (-39.25)	-100.584797 (-41.77)	-100.582444 (-45.59)
170.0	-100.203127 (-42.07)	-100.588782 (-44.27)	-100.586670 (-48.25)
180.0	-100.204605 (-43.00)	-100.590192 (-45.16)	-100.588181 (-49.19)

Table S2: Potential surface scan for the for the CNH to HCN isomerization as a function of the H-C-N angle. Absolute energies in hartrees and relative energies, in parenthesis, with respect to C-N-H linear structure (angle of 0.0^o) in kcal/mol are shown. The cc-pVTZ basis set have been used for these calculations, considering 6d and 10f basis functions, and the geometries are partially optimized at the CCSD/cc-pVTZ level of theory with the H-C-N angle fixed at the values of column 1.

Angle	HF	PNOF3	CCSDT
0.0	-92.892896 (0.00)	-93.298437 (0.00)	-93.285839 (-0.00)
10.0	-92.890910 (1.25)	-93.296457 (1.24)	-93.283564 (1.43)
20.0	-92.885233 (4.81)	-93.291395 (4.42)	-93.277705 (5.10)
30.0	-92.876519 (10.28)	-93.282372 (10.08)	-93.267888 (11.26)
40.0	-92.865546 (17.16)	-93.270856 (17.31)	-93.255842 (18.82)
50.0	-92.853934 (24.45)	-93.261064 (23.45)	-93.245436 (25.35)
60.0	-92.842595 (31.56)	-93.253688 (28.08)	-93.237201 (30.52)
70.0	-92.833971 (36.98)	-93.249816 (30.51)	-93.232742 (33.32)
80.0	-92.831372 (38.61)	-93.251769 (29.28)	-93.235106 (31.84)
90.0	-92.835235 (36.18)	-93.258675 (24.95)	-93.243417 (26.62)
100.0	-92.843771 (30.83)	-93.268177 (18.99)	-93.254714 (19.53)
110.0	-92.854909 (23.84)	-93.278237 (12.68)	-93.266548 (12.11)
120.0	-92.866865 (16.33)	-93.287733 (6.72)	-93.277587 (5.18)
130.0	-92.878405 (9.09)	-93.296049 (1.50)	-93.287311 (-0.92)
140.0	-92.888690 (2.64)	-93.303176 (-2.97)	-93.295542 (-6.09)
150.0	-92.897154 (-2.67)	-93.308925 (-6.58)	-93.302144 (-10.23)
160.0	-92.903419 (-6.60)	-93.313096 (-9.20)	-93.306977 (-13.26)
170.0	-92.907260 (-9.01)	-93.315660 (-10.81)	-93.309958 (-15.13)
180.0	-92.908551 (-9.82)	-93.316533 (-11.36)	-93.310979 (-15.78)

Table S3: Potential surface scan for the for the BOLiH to LiBO isomerization as a function of the Li-B-O angle. Absolute energies in hartrees and relative energies, in parenthesis, with respect to B-O-Li linear structure (angle of 0.0^o) in kcal/mol are shown. The cc-pVTZ basis set have been used for these calculations, considering 6d and 10f basis functions, and the geometries are partially optimized at the CCSD/cc-pVTZ level of theory with the Li-B-O angle fixed at the values of column 1.

Angle	HF	PNOF3	CCSDT
0.0	-107.086539 (0.00)	-107.491868 (0.00)	-107.482026 (0.00)
10.0	-107.086329 (0.13)	-107.491888 (-0.01)	-107.482073 (-0.03)
20.0	-107.085730 (0.51)	-107.491753 (0.07)	-107.481757 (0.17)
30.0	-107.084822 (1.08)	-107.491529 (0.21)	-107.481108 (0.58)
40.0	-107.083589 (1.85)	-107.491738 (0.08)	-107.480733 (0.81)
50.0	-107.081662 (3.06)	-107.492400 (-0.33)	-107.480619 (0.88)
60.0	-107.078101 (5.29)	-107.491631 (0.15)	-107.479281 (1.72)
70.0	-107.072583 (8.76)	-107.488398 (2.18)	-107.475601 (4.03)
80.0	-107.066685 (12.46)	-107.484212 (4.80)	-107.470974 (6.94)
90.0	-107.062271 (15.23)	-107.480947 (6.85)	-107.467312 (9.23)
100.0	-107.060288 (16.47)	-107.479340 (7.86)	-107.465549 (10.34)
110.0	-107.060605 (16.27)	-107.479256 (7.91)	-107.465661 (10.27)
120.0	-107.062588 (15.03)	-107.480663 (7.03)	-107.467201 (9.30)
130.0	-107.065510 (13.20)	-107.482626 (5.80)	-107.469641 (7.77)
140.0	-107.068726 (11.18)	-107.485023 (4.30)	-107.472478 (5.99)
150.0	-107.071725 (9.30)	-107.487331 (2.85)	-107.475210 (4.28)
160.0	-107.074124 (7.79)	-107.489098 (1.74)	-107.477369 (2.92)
170.0	-107.075673 (6.82)	-107.490207 (1.04)	-107.478686 (2.10)
180.0	-107.076192 (6.49)	-107.490507 (0.85)	-107.479121 (1.82)

Table S4: Potential surface scan for the for the CNLi to LiCN isomerization as a function of the Li-C-N angle. Absolute energies in hartrees and relative energies, in parenthesis, with respect to C-N-Li linear structure (angle of 0.0^o) in kcal/mol are shown. The cc-pVTZ basis set have been used for these calculations, considering 6d and 10f basis functions, and the geometries are partially optimized at the CCSD/cc-pVTZ level of theory with the Li-C-N angle fixed at the values of column 1.

Angle	HF	PNOF3	CCSDT
0.0	-99.820431 (0.00)	-100.245809 (0.00)	-100.231249 (-0.00)
10.0	-99.820100 (0.21)	-100.245323 (0.30)	-100.230879 (0.23)
20.0	-99.819261 (0.73)	-100.244297 (0.95)	-100.229950 (0.81)
30.0	-99.818296 (1.34)	-100.243313 (1.57)	-100.229069 (1.37)
40.0	-99.817543 (1.81)	-100.243444 (1.48)	-100.228872 (1.49)
50.0	-99.816970 (2.17)	-100.243814 (1.25)	-100.229398 (1.16)
60.0	-99.816012 (2.77)	-100.244598 (0.76)	-100.229937 (0.82)
70.0	-99.814153 (3.94)	-100.244337 (0.92)	-100.229339 (1.20)
80.0	-99.811405 (5.66)	-100.242320 (2.19)	-100.227369 (2.43)
90.0	-99.808501 (7.49)	-100.239959 (3.67)	-100.224972 (3.94)
100.0	-99.806157 (8.96)	-100.238124 (4.82)	-100.223064 (5.14)
110.0	-99.804832 (9.79)	-100.236965 (5.55)	-100.222063 (5.76)
120.0	-99.804553 (9.96)	-100.237013 (5.52)	-100.221975 (5.82)
130.0	-99.805119 (9.61)	-100.237448 (5.25)	-100.222595 (5.43)
140.0	-99.806211 (8.92)	-100.238582 (4.54)	-100.223664 (4.76)
150.0	-99.807488 (8.12)	-100.239769 (3.79)	-100.224923 (3.97)
160.0	-99.808648 (7.39)	-100.240843 (3.12)	-100.226091 (3.24)
170.0	-99.809445 (6.89)	-100.241532 (2.68)	-100.226910 (2.72)
180.0	-99.809750 (6.70)	-100.241477 (2.72)	-100.227204 (2.54)