

Unusual substituent effects on the bonding of iminoboranes

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Supporting Information (A total of 4 pages)

Table S1. B3LYP/6-311++G(d,p) total energies in hartrees for substituted iminoboranes

| Compound | Energy |
|-----------------------------------|----------------|
| HBNH | -80.8347929226 |
| CH ₃ BNH | -120.181846417 |
| NH ₂ BNH | -136.248997011 |
| OHBNH | -156.131054493 |
| FBNH | -180.157165392 |
| HBNCH ₃ | -120.154999450 |
| HBNNH ₂ | -136.162587515 |
| HBNOH | -156.002828892 |
| HBNF | -179.995541014 |
| CH ₃ BNCH ₃ | -159.500510509 |
| NH ₂ BNNH ₂ | -191.574126475 |
| OHBNOH | -231.296844096 |
| FBNF | -279.312700960 |

Table S2. MP2(fc)/6-311++G(d,p) Optimized structures. Cartesian coordinates in Å

CH₃BNH

| | | | | |
|---|---|-----------|-----------|-----------|
| 5 | 0 | 0.000000 | 0.000000 | 0.185660 |
| 7 | 0 | 0.000000 | 0.000000 | 1.435883 |
| 1 | 0 | 0.000000 | 0.000000 | 2.431009 |
| 6 | 0 | 0.000000 | 0.000000 | -1.361305 |
| 1 | 0 | 0.842612 | -0.578859 | -1.747552 |
| 1 | 0 | -0.922613 | -0.440294 | -1.747552 |
| 1 | 0 | 0.080001 | 1.019153 | -1.747552 |

NH₂BNH

| | | | | |
|---|---|-----------|-----------|-----------|
| 5 | 0 | 0.042362 | 0.000000 | 0.117408 |
| 7 | 0 | 0.013235 | 0.000000 | 1.380904 |
| 1 | 0 | 0.459938 | 0.000000 | 2.272697 |
| 7 | 0 | -0.127170 | 0.000000 | -1.275857 |
| 1 | 0 | 0.062899 | 0.841241 | -1.797535 |
| 1 | 0 | 0.062899 | -0.841241 | -1.797535 |

OHBNH

| | | | | |
|---|---|-----------|-----------|-----------|
| 5 | 0 | -0.018135 | -0.005931 | 0.068959 |
| 7 | 0 | -0.033082 | -0.010820 | 1.319127 |
| 1 | 0 | -0.059782 | -0.019553 | 2.312063 |
| 8 | 0 | -0.050127 | -0.016395 | -1.277646 |
| 1 | 0 | 0.783043 | 0.256106 | -1.669573 |

FBNH

| | | | | |
|---|---|----------|----------|----------|
| 5 | 0 | 0.000000 | 0.000000 | 0.035808 |
|---|---|----------|----------|----------|

| | | | | |
|-----------------------------------|---|-----------|-----------|-----------|
| 7 | 0 | 0.000000 | 0.000000 | 1.280782 |
| 1 | 0 | 0.000000 | 0.000000 | 2.274318 |
| 9 | 0 | 0.000000 | 0.000000 | -1.268759 |
| HBNCH ₃ | | | | |
| 5 | 0 | 0.000000 | 0.000000 | -1.488343 |
| 7 | 0 | 0.000000 | 0.000000 | -0.238729 |
| 1 | 0 | 0.000000 | 0.000000 | -2.657130 |
| 6 | 0 | 0.000000 | 0.000000 | 1.180068 |
| 1 | 0 | 0.428123 | 0.930782 | 1.563180 |
| 1 | 0 | -1.020142 | -0.094625 | 1.563180 |
| 1 | 0 | 0.592019 | -0.836156 | 1.563180 |
| HBNNH ₂ | | | | |
| 5 | 0 | 0.052239 | -0.006082 | -1.443113 |
| 7 | 0 | -0.006925 | 0.000806 | -0.196758 |
| 1 | 0 | 0.085543 | -0.009959 | -2.610491 |
| 7 | 0 | 0.072337 | -0.008422 | 1.165700 |
| 1 | 0 | -0.307111 | 0.864558 | 1.521732 |
| 1 | 0 | -0.497512 | -0.770882 | 1.521732 |
| HBNOH | | | | |
| 5 | 0 | 0.014225 | -0.057527 | -1.410242 |
| 7 | 0 | -0.009650 | 0.039026 | -0.168570 |
| 1 | 0 | 0.022099 | -0.089373 | -2.576669 |
| 8 | 0 | 0.021285 | -0.086080 | 1.163663 |
| 1 | 0 | -0.195953 | 0.792469 | 1.498569 |
| HBNF | | | | |
| 5 | 0 | 0.000000 | 0.000000 | -1.385172 |
| 7 | 0 | 0.000000 | 0.000000 | -0.144582 |
| 1 | 0 | 0.000000 | 0.000000 | -2.551191 |
| 9 | 0 | 0.000000 | 0.000000 | 1.165458 |
| CH ₃ BNCH ₃ | | | | |
| 5 | | 0.000000 | 0.000026 | -0.627871 |
| 7 | | 0.000000 | 0.000001 | 0.623891 |
| 6 | | 0.000000 | -0.000026 | 2.042020 |
| 1 | | -0.886422 | 0.511741 | 2.429649 |
| 1 | | 0.000000 | -1.023586 | 2.429617 |
| 1 | | 0.886422 | 0.511741 | 2.429650 |
| 6 | | 0.000000 | 0.000023 | -2.178006 |
| 1 | | 0.884708 | 0.510794 | -2.567079 |
| 1 | | 0.000000 | -1.021605 | -2.566720 |
| 1 | | -0.884708 | 0.510794 | -2.567079 |
| NH ₂ BNNH ₂ | | | | |
| 5 | | -0.000001 | -0.000010 | -1.510183 |

| | | | |
|---|-----------|-----------|-----------|
| 7 | -0.000001 | -0.000010 | -0.124401 |
| 1 | 1.053894 | -0.000010 | -2.067675 |
| 1 | -1.053896 | -0.000010 | -2.067675 |
| 7 | -1.142172 | 0.000006 | 0.716064 |
| 1 | -1.952572 | -0.085576 | 0.105671 |
| 1 | -1.176419 | 0.915444 | 1.160420 |
| 7 | 1.142171 | 0.000006 | 0.716064 |
| 1 | 1.176445 | -0.915430 | 1.160422 |
| 1 | 1.952566 | 0.085611 | 0.105668 |

OHBNOH

| | | | |
|---|-----------|-----------|-----------|
| 5 | -0.053793 | 0.006282 | -0.636779 |
| 7 | -0.240657 | 0.047693 | 0.617010 |
| 8 | 0.381512 | -0.094199 | 1.827759 |
| 1 | -0.324010 | 0.069046 | 2.462221 |
| 8 | -0.109802 | -0.057696 | -1.977889 |
| 1 | 0.103900 | 0.780853 | -2.396355 |

FBNF

| | | | |
|---|-----------|----------|-----------|
| 5 | -0.134318 | 0.000000 | -0.628680 |
| 7 | -0.125634 | 0.000000 | 0.631779 |
| 9 | 0.598484 | 0.000000 | 1.753168 |
| 9 | -0.426148 | 0.000000 | -1.895285 |