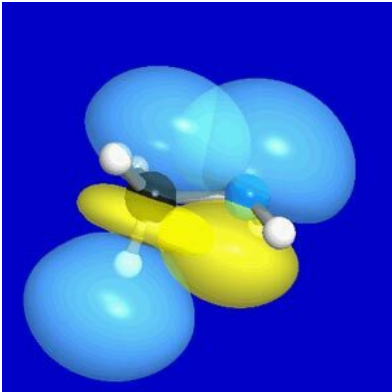




Natural Bond Orbital (NBO) 6.0 Win/macOS/Linux x64

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NBO Output: Natural Bond Orbitals

Gives: Occupancies, Bond-types, Atomic/Bonding-center, and their respective Natural Hybrid Orbitals (NHOs) composition (*i.e.* "covalent" or "ionic" character).

```
setiawan ~ setiawan@smuhpc4:~/projects/05-aromaticity-index/10-NBO6-analysis/02-AdvCC-Labs --- ssh
bash -- setiawan@smuhpc4:~/projects/05-aromaticity-index/10-NBO6-analysis/02-AdvCC-Labs --- ssh
----- Bond Orbital Coefficiental Hybrids -----
1. (1.99219) BB (1) C 1 1 C 2
   ( 16.026) 0.7672* C 1 1 ( 0.395)p 1.774 53.8953e 0.390 0.4358)
   F 0.461 ( 3.8261)
   C 0039 0.4000 3.8888 0.0023 0.7600
   C 0338 0.4031 3.3731 0.0172 0.4000
   C 0339 0.4000 3.8888 0.0159 0.4128
   C 0338 0.4000 3.8888 0.0188 0.4109
   C 0375 0.4100 3.9877 0.0388 0.4000
   C 0340 0.4000 3.8888 0.0025 0.4000
   ( 16.026) 0.7672* C 2 2 ( 0.395)p 1.774 53.8953e 0.390 0.4358)
   F 0.461 ( 3.8261)
   C 0338 0.4000 3.8888 0.0029 0.4792
   C 0339 0.4031 3.4295 0.0194 0.4016
   C 0339 0.4000 3.8888 0.0132 0.4120
   C 0339 0.4000 3.8888 0.0239 0.4129
   C 0375 0.4100 3.9877 0.0388 0.4070
   C 0369 0.4000 3.8888 0.0025 0.4080
2. (1.65388) BB (2) C 1 1 C 2
   ( 16.026) 0.7672* C 1 1 ( 0.395)p 1.004 89.3153e 0.390 0.4735)
   F 0.461 ( 3.8261)
   C 0039 0.4000 3.8888 0.0039 0.4000
   C 0039 0.4000 3.8888 0.0039 0.4000
   C 0037 0.4100 3.9888 0.0388 0.4000
   C 0021 0.4065 3.9892 0.0393 0.4000
   C 0338 0.4000 3.8888 0.0159 0.4000
   C 0339 0.4000 3.8888 0.0388 0.4000
   ( 16.026) 0.7672* C 2 2 ( 0.395)p 1.004 89.3153e 0.390 0.4735)
   F 0.461 ( 3.8261)
   C 0039 0.4000 3.8888 0.0039 0.4000
   C 0338 0.4000 3.8888 0.0388 0.4000
   C 0037 0.4100 3.9888 0.0388 0.4000
```



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