

Natural NMR Chemical Shielding Tensor Analysis
 NCS Tensor analysis is using 8624 words
 Threshold for printing: 0.10 ppm

Summary of isotropic NMR chemical shielding
 Total Lewis (L) and non-Lewis (NL) contributions: (ppm)

| NBO | C(1) | N(2) | H(3) | H(4) | H(5) | H(6) | H(7) |
|---------------|--------|--------|-------|-------|-------|-------|-------|
| 1. C 1- N 2 L | -6.54 | 6.39 | 0.56 | 0.50 | 0.50 | 2.41 | 2.41 |
| NL | 0.17 | -0.35 | 0.03 | 0.08 | 0.08 | -0.09 | -0.09 |
| 2. C 1- H 3 L | -4.21 | 0.50 | 26.52 | 1.85 | 1.85 | 0.10 | 0.10 |
| NL | -0.61 | -0.39 | 0.07 | -0.05 | -0.05 | -0.01 | -0.01 |
| 3. C 1- H 4 L | -2.64 | 2.11 | 2.10 | 25.73 | 2.04 | 0.13 | 0.21 |
| NL | -0.21 | -1.42 | -0.01 | 0.05 | 0.04 | -0.04 | -0.08 |
| 4. C 1- H 5 L | -2.64 | 2.11 | 2.10 | 2.04 | 25.73 | 0.21 | 0.13 |
| NL | -0.21 | -1.42 | -0.01 | 0.04 | 0.05 | -0.08 | -0.04 |
| 5. N 2- H 6 L | 0.09 | 7.19 | 0.34 | 0.29 | 0.24 | 22.87 | 3.36 |
| NL | -0.01 | 0.17 | -0.02 | -0.12 | -0.01 | 0.03 | -0.04 |
| 6. N 2- H 7 L | 0.09 | 7.19 | 0.34 | 0.24 | 0.29 | 3.36 | 22.87 |
| NL | -0.01 | 0.17 | -0.02 | -0.01 | -0.12 | -0.04 | 0.03 |
| 7. C 1(cr) L | 202.40 | -0.07 | 0.16 | 0.13 | 0.13 | -0.03 | -0.03 |
| NL | 0.15 | 0.00 | 0.00 | -0.01 | -0.01 | 0.00 | 0.00 |
| 8. N 2(cr) L | 0.08 | 238.43 | 0.05 | 0.03 | 0.03 | 0.07 | 0.07 |
| NL | 0.00 | 0.10 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 9. N 2(lp) L | -0.11 | 6.52 | -0.46 | 0.18 | 0.18 | 5.43 | 5.43 |
| NL | -0.08 | 0.73 | -0.34 | -0.01 | -0.01 | 0.04 | 0.04 |
| Lewis | 186.52 | 270.38 | 31.70 | 31.01 | 31.01 | 34.56 | 34.56 |
| non-Lewis | -0.80 | -2.41 | -0.32 | -0.02 | -0.02 | -0.18 | -0.18 |
| Total | 185.72 | 267.97 | 31.39 | 30.99 | 30.99 | 34.38 | 34.38 |