

PROPERty Analysis for P = KINETIC (all values in a.u.)

| | Lewis(L) | | Non-Lewis(NL) | | | L + NL | |
|----------------------|----------|--------|---------------|-----------------|--------|---------|--------|
| | NBO | P(NBO) | NL | P(NL) | (%-NL) | P(NLMO) | e-corr |
| 1. CR (1) N 3 | 22.8091 | | 26 | 0.0214 (0.1) | | 22.8453 | 0.0000 |
| | | | 15 | 0.0208 (0.1) | | | |
| | | | 24 | 0.0156 (0.1) | | | |
| | | | rem | -0.0216 (-0.1) | | | |
| 2. CR (1) C 4 | 16.4799 | | 17 | -0.0105 (-0.1) | | 16.4997 | 0.0000 |
| | | | 27 | -0.0103 (-0.1) | | | |
| | | | 15 | 0.0084 (0.1) | | | |
| | | | rem | 0.0322 (0.2) | | | |
| 3. CR (1) O 5 | 30.4278 | | 25 | 0.0432 (0.1) | | 30.4976 | 0.0000 |
| | | | 31 | 0.0181 (0.1) | | | |
| | | | 17 | -0.0166 (-0.1) | | | |
| | | | rem | 0.0250 (0.1) | | | |
| 4. LP (1) N 3 | 1.7329 | | 16 | -0.1434 (-8.3) | | 1.5892 | 0.0000 |
| | | | 30 | -0.0049 (-0.3) | | | |
| | | | 28 | 0.0046 (0.3) | | | |
| | | | rem | 0.0000 (0.0) | | | |
| 5. LP (1) O 5 | 1.9631 | | 25 | -0.0549 (-2.8) | | 1.8970 | 0.0000 |
| | | | 26 | -0.0050 (-0.3) | | | |
| | | | 14 | -0.0025 (-0.1) | | | |
| | | | rem | -0.0037 (-0.2) | | | |
| 6. LP (2) O 5 | 2.5600 | | 15 | -0.1009 (-3.9) | | 2.2837 | 0.0000 |
| | | | 18 | -0.0999 (-3.9) | | | |
| | | | 26 | -0.0474 (-1.9) | | | |
| | | | rem | -0.0282 (-1.1) | | | |
| 7. BD (1) H 1- N 3 | 1.2267 | | 17 | -0.0102 (-0.8) | | 1.2125 | 0.0000 |
| | | | 15 | -0.0034 (-0.3) | | | |
| | | | 26 | 0.0028 (0.2) | | | |
| | | | rem | -0.0034 (-0.3) | | | |
| 8. BD (1) H 2- N 3 | 1.2331 | | 18 | -0.0081 (-0.7) | | 1.2179 | 0.0000 |
| | | | 17 | -0.0072 (-0.6) | | | |
| | | | 15 | -0.0041 (-0.3) | | | |
| | | | rem | 0.0042 (0.3) | | | |
| 9. BD (1) N 3- C 4 | 1.3642 | | 29 | -0.0018 (-0.1) | | 1.3588 | 0.0000 |
| | | | 18 | -0.0013 (-0.1) | | | |
| | | | 14 | -0.0010 (-0.1) | | | |
| | | | rem | -0.0014 (-0.1) | | | |
| 10. BD (1) C 4- O 5 | 1.7983 | | 22 | -0.0047 (-0.3) | | 1.7936 | 0.0000 |
| | | | rem | 0.0000 (0.0) | | | |
| 11. BD (2) C 4- O 5 | 1.6619 | | 13 | -0.0031 (-0.2) | | 1.6585 | 0.0000 |
| | | | rem | -0.0003 (0.0) | | | |
| 12. BD (1) C 4- H 6 | 0.9525 | | 14 | -0.0075 (-0.8) | | 0.9381 | 0.0000 |
| | | | 29 | -0.0042 (-0.4) | | | |
| | | | 21 | -0.0035 (-0.4) | | | |
| | | | rem | 0.0008 (0.1) | | | |
| * Sum * | 84.2096 | | | -0.4218 (-0.5) | | 83.7917 | 0.0000 |
| | | | | * Total * | | 83.7917 | |