NATURAL BOND ORBITAL ANALYSIS:

Cycle	Occ. Thresh.	Occupancies: Lewis	Occupancies: Non-Lewis	Lewis Structure: CR	BD	3C	LP	Low occ (L)	High occ (NL)	Dev
1(1)	1.90	23.26613	0.73387	3	7	0	2	3	2	0.15
2(2)	1.90	22.36333	1.63667	3	8	0	1	2	2	1.13
3(3)	1.90	22.90727	1.09273	3	7	0	2	3	2	0.15
4(4)	1.90	22.36333	1.63667	3	8	0	1	2	2	1.13
5(5)	1.90	22.90727	1.09273	3	7	0	2	3	2	0.15
6(6)	1.90	22.36333	1.63667	3	8	0	1	2	2	1.13
7(7)	1.90	22.90727	1.09273	3	7	0	2	3	2	0.15
8(8)	1.90	22.36333	1.63667	3	8	0	1	2	2	1.13
9(9)	1.90	22.90727	1.09273	3	7	0	2	3	2	0.15
10(1)	1.80	23.64454	0.35546	3	6	0	3	0	1	0.15
11(2)	1.80	23.64454	0.35546	3	6	0	3	0	1	0.15
12(1)	1.70	23.64454	0.35546	3	6	0	3	0	1	0.15
13(2)	1.70	23.64454	0.35546	3	6	0	3	0	1	0.15
14(1)	1.60	23.64454	0.35546	3	6	0	3	0	1	0.15
15(2)	1.60	23.64454	0.35546	3	6	0	3	0	1	0.15
16(1)	1.50	23.64454	0.35546	3	6	0	3	0	1	0.15
17(2)	1.50	23.64454	0.35546	3	6	0	3	0	1	0.15
18(1)	1.80	23.64454	0.35546	3	6	0	3	0	1	0.15

Strongly delocalized structure accepted

Core	5.99824 (99.971% of	6)
Valence Lewis	17.64630 (98.035% of	18)
Total Lewis	23.64454 (98.519% of	24)
Valence non-Lewis	0.32134 (1.339% of	24)
Rydberg non-Lewis	0.03413 (0.142% of	24)
Total non-Lewis	0.35546 (1.481% of	24)

(Occupancy) Bond orbital/ Coefficients/ Hybrids

1. (1.99309) BD (1) H 1- N 3
   (29.05%) 0.5390* H 1 s(100.00%)
   -1.0000 -0.0010
   (70.95%) 0.8423* N 3 s(30.92%)p 2.23(69.08%)
   0.0002 -0.5561 -0.0020 0.6879 0.0155
   -0.4660 0.0088 -0.0001 0.0000
2. (1.99322) BD (1) H 2- N 3
   (28.52%) 0.5341* H 2 s(100.00%)
   -1.0000 -0.0043
   (71.48%) 0.8454* N 3 s(30.20%)p 2.31(69.80%)
   0.0001 -0.5495 -0.0009 0.1158 0.0158
   0.8273 0.0052 0.0000 0.0000
3. (1.99828) BD (1) N 3- C 4
   (64.15%) 0.8009* N 3 s(38.85%)p 1.57(61.15%)
   0.0001 0.6233 0.0002 0.7163 0.0027
   0.3137 0.0030 -0.0002 0.0000
   (35.85%) 0.5988* C 4 s(31.97%)p 2.13(68.03%)
   0.0002 0.5648 0.0275 -0.7255 -0.0624
   -0.3862 -0.0294 0.0000 0.0000

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 4. (1.99925) BD ( 1) C 4- O 5
              ( 30.54%)   0.5526* C 4 s(  0.00%)p 1.00(100.00%)
                                       0.0000 -0.0001  0.0000 -0.0001  0.0000
                                       0.0000  0.0000  0.9969 -0.0783
              ( 69.46%)   0.8334* O 5 s(  0.00%)p 1.00(100.00%)
                                       0.0000  0.0000  0.0000 -0.0001  0.0000
                                       0.0000  0.0000  1.0000 -0.0005
 5. (1.99802) BD ( 2) C 4- O 5
              ( 34.10%)   0.5840* C 4 s( 32.78%)p 2.05( 67.22%)
                                      -0.0001  0.5710  0.0420  0.6800  0.0792
                                      -0.4491 -0.0423  0.0002  0.0000
              ( 65.90%)   0.8118* O 5 s( 41.37%)p 1.42( 58.63%)
                                       0.0000  0.6431  0.0082 -0.6560  0.0051
                                       0.3949 -0.0026 -0.0001  0.0000
 6. (1.98929) BD ( 1) C 4- H 6
              ( 58.88%)   0.7673* C 4 s( 35.26%)p 1.84( 64.74%)
                                      -0.0001  0.5925 -0.0393  0.0311  0.0238
                                       0.8033 -0.0236  0.0001  0.0000
              ( 41.12%)   0.6412* H 6 s(100.00%)
                                       0.9999  0.0112
 7. (1.99922) CR ( 1) N 3             s(100.00%)p 0.00(  0.00%)
                                       1.0000  0.0001  0.0000 -0.0002  0.0000
                                       0.0000  0.0000  0.0000  0.0000
 8. (1.99939) CR ( 1) C 4             s(100.00%)p 0.00(  0.00%)
                                       1.0000  0.0000  0.0000  0.0002  0.0000
                                       0.0001  0.0000  0.0000  0.0000
 9. (1.99963) CR ( 1) O 5             s(100.00%)p 0.00(  0.00%)
                                       1.0000  0.0004  0.0000  0.0003  0.0000
                                      -0.0001  0.0000  0.0000  0.0000
10. (1.80683) LP ( 1) N 3             s(  0.00%)p 1.00(100.00%)
                                       0.0000  0.0001  0.0000  0.0002  0.0000
                                       0.0001  0.0000  0.9999 -0.0120
11. (1.98262) LP ( 1) O 5             s( 58.63%)p 0.71( 41.37%)
                                      -0.0005  0.7657 -0.0046  0.5447  0.0046
                                      -0.3420 -0.0027  0.0001  0.0000
12. (1.88568) LP ( 2) O 5             s(  0.01%)p 1.00( 99.99%)
                                      -0.0001  0.0092  0.0013  0.5224  0.0016
                                       0.8527  0.0015  0.0000  0.0000
13. (0.00054) RY*( 1) H 1             s(100.00%)
                                      -0.0010  1.0000
14. (0.00174) RY*( 1) H 2             s(100.00%)
                                      -0.0043  1.0000
15. (0.00111) RY*( 1) N 3             s( 31.01%)p 2.22( 68.99%)
                                       0.0000  0.0060  0.5569 -0.0084  0.1357
                                      -0.0020  0.8194  0.0000  0.0008
16. (0.00075) RY*( 2) N 3             s(  0.00%)p 1.00(100.00%)
                                       0.0000  0.0000  0.0005  0.0000 -0.0001
                                       0.0000  0.0006 -0.0120 -0.9999
17. (0.00028) RY*( 3) N 3             s(  9.01%)p10.10( 90.99%)
                                       0.0000  0.0113  0.2999 -0.0093  0.8870
                                      -0.0056 -0.3509  0.0000 -0.0001
18. (0.00004) RY*( 4) N 3             s( 60.01%)p 0.67( 39.99%)
19. (0.01600) RY*( 1) C 4             s(  5.85%)p16.08( 94.15%)
                                       0.0000 -0.0437  0.2380 -0.0966  0.9115
                                       0.0112 -0.3181  0.0000  0.0001
20. (0.00686) RY*( 2) C 4             s( 16.87%)p 4.93( 83.13%)
                                       0.0000 -0.0422  0.4085  0.0297 -0.3927
                                       0.0375 -0.8215  0.0000  0.0001
21. (0.00097) RY*( 3) C 4             s( 77.26%)p 0.29( 22.74%)
                                       0.0000  0.0130  0.8789  0.0039 -0.0650
                                       0.0490  0.4698  0.0000  0.0005
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22. (0.00024) RY*( 4) C 4            s(  0.00%)p 1.00(100.00%)
                                      0.0000  0.0000  0.0005  0.0000  0.0000
                                      0.0000  0.0001 -0.0783 -0.9969
23. (0.00129) RY*( 1) O 5            s(  0.42%)p99.99( 99.58%)
                                      0.0000  0.0003  0.0646  0.0013 -0.5176
                                      0.0016 -0.8532  0.0000 -0.0003
24. (0.00031) RY*( 2) O 5            s(  0.00%)p 1.00(100.00%)
                                      0.0000  0.0000  0.0003  0.0000 -0.0004
                                      0.0000 -0.0001  0.0005  1.0000
25. (0.00013) RY*( 3) O 5            s(  0.79%)p99.99( 99.21%)
                                      0.0000  0.0076  0.0887  0.0001 -0.8486
                                      0.0004  0.5215  0.0000 -0.0004
26. (0.00001) RY*( 4) O 5            s( 98.79%)p 0.01(  1.21%)
27. (0.00385) RY*( 1) H 6            s(100.00%)
                                     -0.0112  0.9999
28. (0.00611) BD*( 1) H 1- N 3
              ( 70.95%)   0.8423* H 1 s(100.00%)
                                     -1.0000 -0.0010
              ( 29.05%)  -0.5390* N 3 s( 30.92%)p 2.23( 69.08%)
                                      0.0002 -0.5561 -0.0020  0.6879  0.0155
                                     -0.4660  0.0088 -0.0001  0.0000
29. (0.00964) BD*( 1) H 2- N 3
              ( 71.48%)   0.8454* H 2 s(100.00%)
                                     -1.0000 -0.0043
              ( 28.52%)  -0.5341* N 3 s( 30.20%)p 2.31( 69.80%)
                                      0.0001 -0.5495 -0.0009  0.1158  0.0158
                                      0.8273  0.0052  0.0000  0.0000
30. (0.05837) BD*( 1) N 3- C 4
              ( 35.85%)   0.5988* N 3 s( 38.85%)p 1.57( 61.15%)
                                     -0.0001 -0.6233 -0.0002 -0.7163 -0.0027
                                     -0.3137 -0.0030  0.0002  0.0000
              ( 64.15%)  -0.8009* C 4 s( 31.97%)p 2.13( 68.03%)
                                     -0.0002 -0.5648 -0.0275  0.7255  0.0624
                                      0.3862  0.0294  0.0000  0.0000
31. (0.19262) BD*( 1) C 4- O 5
              ( 69.46%)   0.8334* C 4 s(  0.00%)p 1.00(100.00%)
                                      0.0000 -0.0001  0.0000 -0.0001  0.0000
                                      0.0000  0.0000  0.9969 -0.0783
              ( 30.54%)  -0.5526* O 5 s(  0.00%)p 1.00(100.00%)
                                      0.0000  0.0000  0.0000 -0.0001  0.0000
                                      0.0000  0.0000  1.0000 -0.0005
32. (0.00600) BD*( 2) C 4- O 5
              ( 65.90%)   0.8118* C 4 s( 32.78%)p 2.05( 67.22%)
                                     -0.0001  0.5710  0.0420  0.6800  0.0792
                                     -0.4491 -0.0423  0.0002  0.0000
              ( 34.10%)  -0.5840* O 5 s( 41.37%)p 1.42( 58.63%)
                                      0.0000  0.6431  0.0082 -0.6560  0.0051
                                      0.3949 -0.0026 -0.0001  0.0000
33. (0.04859) BD*( 1) C 4- H 6
              ( 41.12%)   0.6412* C 4 s( 35.26%)p 1.84( 64.74%)
                                      0.0001 -0.5925  0.0393 -0.0311 -0.0238
                                     -0.8033  0.0236 -0.0001  0.0000
              ( 58.88%)  -0.7673* H 6 s(100.00%)
                                     -0.9999 -0.0112
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