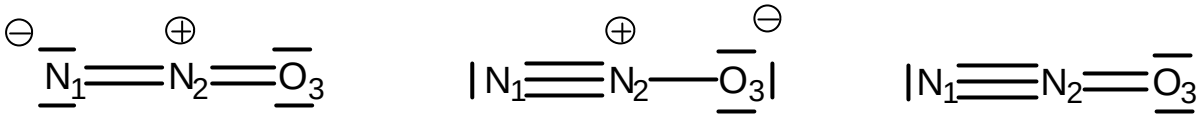
With the next example we want to learn how to use the NBO program to investigate different Lewis representations of one molecule such as dinitrogen oxide (laughing gas) , N_2O

The following three Lewis representations will be investigated (including a nitrogen atom with formal 5 bonds according to Lewis representation C)



A **B** **C**

INPUT for structure A

#hf/6-31G(d) scf=tight pop=nboread

N2O, NN and NO double bond at HF/6-31G(d)//HF/STO-3G, structure A

0,1
N
N, 1, B1
X, 2, 1.0, 1, 90.0
O, 2, B2, 3, 90.0, 1, 180.0

B1=1.1544
B2=1.2754

$NBO NLMO BNDIDX RESONANCE $END
$choose
lone 1 2
2 0
3 2 end
bond D 1 2
D 2 3 end
$end

THE $CHOOSE KEYLIST (DIRECTED NBO SEARCH)

A $CHOOSE keylist requests that the NBO search be directed to find a particular Lewis structure ('resonance structure') chosen by the user. (This is useful for testing the accuracy of alternative resonance structure representations of the wavefunction, relative to the optimal Lewis structure returned in a free NBO search.) In the $CHOOSE list, a resonance structure is specified by indicating where lone pairs and bonds (including multiple bonds) are to be found in the molecule. In some cases, the user may wish to specify only the location of bonds, letting the NBO algorithm seek the best location for lone pairs, but it is usually safest to completely specify the resonance structure, both lone pairs and bonds.

The format of the $CHOOSE list is:

first line: The keyword "$CHOOSE"

next line: The keyword "ALPHA" (only for open-shell wavefunction)

next lines: If one-center ('lone') NBOs are to be searched for, type the keyword "LONE" followed by a list of pairs of numbers, the first number of each pair being the atomic center and the second the number of valence lone pairs on that atom. Terminate the list with "END". (Note that only the occupied *valence* lone pairs should be entered, since the number of core orbitals on each center is presumed known.)

If two-center ('bond') NBOs are to be searched for, type the keyword "BOND", followed by the list of bond specifiers, and terminated by "END". Each bond specifier is one of the letters

"S" single bond
"D" double bond
"T" triple bond
"Q" quadruple bond

followed by the two atomic centers of the bond (e.g., "D 9 16" for a double bond between atoms 9 and 16).

If three-center NBOs are to be searched for, type the keyword "3CBOND", followed by the list of 3-c bond specifiers, and terminated by "END". Each 3-c bond specifier is again one of the letters "S" (single), "D" (double), "T" (triple), or "Q" (quadruple), followed by three integers for the three atomic centers (e.g., "S 4 8 10" for a single three-center bond 4-8-10). (Note that the 3CBOND keyword of the $NBO keylist is implicitly activated if 3-c bonds are included in a $CHOOSE list.)

next line: The word "END" to signal the end of the α spin list.

next line: The keyword "BETA" (for open-shell wavefunctions)

next lines: The input for β spin, same format as above. The overall $CHOOSE list should always end with the "$END" keyword.

Two examples will serve to illustrate the $CHOOSE format (each is rather artificial, inasmuch as the specified $CHOOSE structure corresponds to the 'normal' structure that would be found by the NBO program):

The closed-shell NNO, with atom numbering N(1)-N(2)-O(3), might be specified as

```
$CHOOSE
   LONE  1  2            2 lone pairs on N1
         2  0            0 lone paira on N2
         3  0     END    2 lone pairs on O1
   BOND  D  1  2         double bond between N1 N2
         D  2  3  END    double bond between N2 O2
$END
```

This would direct the NBO program to search for structure A

Open shell systems

The open-shell FH...O_2 complex, with atom numbering F(1)-H(2)...O(3)-O(4), and with the unpaired electrons on O_2 being of α spin, might be specified as

```
$CHOOSE
  ALPHA
    LONE  1  3
          3  3
          4  3     END
    BOND  S  1  2
          S  3  4  END
  END
  BETA
    LONE  1  3
          3  1
          4  1     END
    BOND  S  1  2
          T  3  4  END
  END
$END
```

Note that this example incorporates the idea of "different Lewis structures for different spins," with a distinct pattern of localized 1-c ('lone') and 2-c ('bond') functions for α and β spin.

As with other keylists, the $CHOOSE keylist can be condensed to a smaller number of lines, as long as no line is shared with another keylist. The order of keywords within the $CHOOSE keylist should be as shown above (i.e., ALPHA before BETA, LONE before BOND, etc.), but the order of entries within a LONE or BOND list is immaterial. A $CORE keylist (if present) must precede the $CHOOSE list.

OUTPUT for structure A

**********Gaussian NBO Version 3.1**********
N A T U R A L A T O M I C O R B I T A L A N D
N A T U R A L B O N D O R B I T A L A N A L Y S I S
**********Gaussian NBO Version 3.1**********

/RESON / : Allow strongly delocalized NBO set
/NLMO / : Form Natural Localized Molecular Orbitals
/BNDIDX / : Print bond indices based on the NAO density matrix

Analyzing the SCF density

Job title: N2O, NN and NO double bond at HF/6-31G(d)//HF/STO-3G

Storage needed: 6339 in NPA, 8259 in NBO, 6309 in NLMO (6291456 available)

NATURAL POPULATIONS: Natural atomic orbital occupancies

NAO	Atom	No	lang	Type(AO)	Occupancy	Energy
1	N	1		s	Cor(1s)	1.99958	-15.53265
2	N	1		s	Val(2s)	1.63423	-0.84630
3	N	1		s	**Ryd(3s)**	0.00576	1.41193
4	N	1		s	**Ryd(4s)**	0.00003	3.63535
5	N	1		px	Val(2p)	1.05940	-0.22750
6	N	1		px	Ryd(3p)	0.00172	0.91561
7	N	1		py	Val(2p)	1.05940	-0.22750
8	N	1		py	Ryd(3p)	0.00172	0.91561
9	N	1		pz	Val(2p)	1.21545	-0.22320
10	N	1		pz	Ryd(3p)	0.00167	0.85539
11	N	1		**dxy**	Ryd(3d)	0.00000	1.95665
12	N	1		**dxz**	Ryd(3d)	0.00710	2.30012
13	N	1		**dyz**	Ryd(3d)	0.00710	2.30012
14	N	1		**dx2y2**	Ryd(3d)	0.00000	1.95665
15	N	1		**dz2**	Ryd(3d)	0.00521	2.80226
16	N	2		s	Cor(1s)	1.99958	-15.71271
17	N	2		s	Val(2s)	1.12112	-0.64807
18	N	2		s	Ryd(3s)	0.00156	1.64629
19	N	2		s	Ryd(4s)	0.00041	3.05232
20	N	2		px	Val(2p)	1.13177	-0.31862
21	N	2		px	Ryd(3p)	0.00050	0.88364
22	N	2		py	Val(2p)	1.13177	-0.31862
23	N	2		py	Ryd(3p)	0.00050	0.88364
24	N	2		pz	Val(2p)	1.12104	-0.29552
25	N	2		pz	Ryd(3p)	0.01649	1.06226
26	N	2		dxy	Ryd(3d)	0.00000	1.88459
27	N	2		dxz	Ryd(3d)	0.00903	2.41657
28	N	2		dyz	Ryd(3d)	0.00903	2.41657

29	N	2		dx2y2	Ryd(3d)	0.00000	1.88459
30	N	2		dz2	Ryd(3d)	0.00318	3.46170
31	O	3	s	Cor(1s)	1.99983	-20.47495
32	O	3	s	Val(2s)	1.79593	-1.19624
33	O	3	s	Ryd(3s)	0.00209	1.92965
34	O	3	s	Ryd(4s)	0.00000	4.00924
35	O	3	px	Val(2p)	1.78447	-0.47472
36	O	3	px	Ryd(3p)	0.00239	1.22993
37	O	3	py	Val(2p)	1.78447	-0.47472
38	O	3	py	Ryd(3p)	0.00239	1.22993
39	O	3	pz	Val(2p)	1.07290	-0.23969
40	O	3	pz	Ryd(3p)	0.00023	1.30079
41	O	3	dxy	Ryd(3d)	0.00000	2.07202
42	O	3	dxz	Ryd(3d)	0.00360	2.37572
43	O	3	dyz	Ryd(3d)	0.00360	2.37572
44	O	3	dx2y2	Ryd(3d)	0.00000	2.07202
45	O	3	dz2	Ryd(3d)	0.00368	3.04979

Note that the occupancies of the Rydberg (Ryd) NAOs are typically much lower than those of the core (Cor) plus valence (Val) NAOs of the natural minimum basis set, reflecting the dominant role of the bond orbitals in describing molecular properties.

Summary of Natural Population Analysis:

		Natural Population			
	Natural	----------			
Atom No	Charge	Core	Valence	Rydberg	Total
N 1	0.00161	1.99958	4.96849	0.03032	6.99839
N 2	0.45401	1.99958	4.50571	0.04070	6.54599
O 3	-0.45562	1.99983	6.43779	0.01800	8.45562
* Total *	0.00000	5.99899	15.91199	0.08902	22.00000

N1 is almost neutral, N2 possesses a positive charge of 0.454e and O3 a egative charge of -0.4556e.

Natural Population

Core	**5.99899**	(99.9832% of 6)
Valence	**15.91199**	(99.4499% of 16)
Natural Minimal Basis	**21.91098**	(99.5954% of 22)
Natural Rydberg Basis	**0.08902**	(0.4046% of 22)

Atom No	Natural Electron Configuration
N 1	[core]2s(1.63)2p(3.33)3s(0.01)3p(0.01)3d(0.02)
N 2	[core]2s(1.12)2p(3.38)3p(0.02)3d(0.02)
O 3	[core]2s(1.80)2p(4.64)3p(0.01)3d(0.01)

NATURAL BOND ORBITAL ANALYSIS:

		Occupancies		Lewis Structure				Low	High	
	Occ.							occ	occ	
Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	(L)	(NL)	Dev
1(1)	1.90	20.79971	1.20029	3	4	0	4	2	2	0.61

Structure accepted: **NBOs selected via the $CHOOSE keylist**

Core	5.99899 (99.983% of 6)
Valence Lewis	14.80072 (92.505% of 16)
Total Lewis	20.79971 (94.544% of 22)
Valence non-Lewis	1.14334 (5.197% of 22)
Rydberg non-Lewis	0.05695 (0.259% of 22)
Total non-Lewis	**1.20029** (5.456% of 22)

1.20029 of 22 electrons are delocalized in this structure according to 5.456 %.

(Occupancy) Bond orbital/ Coefficients/ Hybrids

1. (1.99988) BD (1) N 1 - N 2
   (43.80%) 0.6618* N 1 s(31.43%)p 2.17(68.08%)d 0.02(0.49%)
   0.0000 0.5568 0.0654 -0.0023 0.0000
   0.0000 0.0000 0.0000 0.8245 0.0310
   0.0000 0.0000 0.0000 0.0000 0.0699
   (56.20%) 0.7497* N 2 s(52.29%)p 0.91(47.58%)d 0.00(0.13%)
   0.0000 0.7229 0.0162 0.0042 0.0000
   0.0000 0.0000 0.0000 -0.6891 -0.0308
   0.0000 0.0000 0.0000 0.0000 0.0367
2. (1.99754) **BD (2) N 1 - N 2**
   (48.14%) 0.6938* N 1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
   0.0000 0.0000 0.0000 0.0000 0.0000
   0.0000 0.9964 0.0070 0.0000 0.0000
   0.0000 0.0000 0.0839 0.0000 0.0000

(51.86%) 0.7202* N 2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9978 -0.0206 0.0000 0.0000
0.0000 0.0000 -0.0625 0.0000 0.0000

3. (1.99872) BD (1) N 2 - O 3
(55.51%) 0.7450* N 2 s(47.49%)p 1.10(52.37%)d 0.00(0.14%)
-0.0001 0.6889 -0.0182 -0.0023 0.0000
0.0000 0.0000 0.0000 0.7224 0.0424
0.0000 0.0000 0.0000 0.0000 0.0379
(44.49%) 0.6670* O 3 s(16.93%)p 4.89(82.71%)d 0.02(0.37%)
0.0000 0.4089 -0.0453 -0.0001 0.0000
0.0000 0.0000 0.0000 -0.9093 -0.0133
0.0000 0.0000 0.0000 0.0000 0.0605

4. (1.99825) **BD (2) N 2 - O 3**
(19.32%) 0.4396* N 2 s(0.00%)p 1.00(99.42%)d 0.01(0.58%)
0.0000 0.0000 0.0000 0.0000 0.9969
-0.0219 0.0000 0.0000 0.0000 0.0000
0.0000 0.0759 0.0000 0.0000 0.0000
(80.68%) 0.8982* O 3 s(0.00%)p 1.00(99.78%)d 0.00(0.22%)
0.0000 0.0000 0.0000 0.0000 0.9989
0.0086 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0466 0.0000 0.0000 0.0000

5. (1.99958) CR (1) N 1 s(100.00%)p 0.00(0.00%)
1.0000 0.0006 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 -0.0004 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000

6. (1.99958) CR (1) N 2 s(100.00%)
1.0000 0.0001 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0001 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000

7. (1.99983) CR (1) O 3 s(100.00%)p 0.00(0.00%)
1.0000 0.0004 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0002 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000

8. (1.97515) **LP (1) N 1** s(68.89%)p 0.45(31.08%)d 0.00(0.04%)
-0.0008 0.8297 -0.0201 0.0005 0.0000
0.0000 0.0000 0.0000 -0.5574 0.0092
0.0000 0.0000 0.0000 0.0000 -0.0196

9. (**1.06647**) **LP (2) N 1** s(0.00%)p 1.00(99.34%)d 0.01(0.66%)
0.0000 0.0000 0.0000 0.0000 0.9967
-0.0061 0.0000 0.0000 0.0000 0.0000
0.0000 0.0812 0.0000 0.0000 0.0000

10. (1.97671) **LP (1) O 3** s(83.26%)p 0.20(16.73%)d 0.00(0.02%)
-0.0004 0.9124 0.0091 0.0000 0.0000
0.0000 0.0000 0.0000 0.4090 0.0023
0.0000 0.0000 0.0000 0.0000 -0.0130

11. (**1.78801**) **LP (2) O 3** s(0.00%)p 1.00(99.80%)d 0.00(0.20%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9990 -0.0034 0.0000 0.0000
0.0000 0.0000 -0.0444 0.0000 0.0000

12. (0.00194) RY*(1) N 1 s(0.00%)p 1.00(95.85%)d 0.04(4.15%)

```
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000 -0.0240  0.9787  0.0000  0.0000
                                0.0000  0.0000  0.2037  0.0000  0.0000
13. (0.00175) RY*( 2) N   1          s(  0.00%)p 1.00( 95.81%)d 0.04(  4.19%)
                                0.0000  0.0000  0.0000  0.0000 -0.0107
                                0.9788  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.2048  0.0000  0.0000  0.0000
14. (0.00169) RY*( 3) N   1          s( 59.34%)p 0.59( 35.25%)d 0.09(  5.40%)
                                0.0000 -0.0353  0.7646  0.0869  0.0000
                                0.0000  0.0000  0.0000 -0.0784  0.5885
                                0.0000  0.0000  0.0000  0.0000  0.2325
15. (0.00007) RY*( 4) N   1          s( 47.41%)p 0.80( 38.04%)d 0.31( 14.56%)
16. (0.00001) RY*( 5) N   1          s( 90.01%)p 0.11(  9.98%)d 0.00(  0.01%)
17. (0.00000) RY*( 6) N   1          s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
18. (0.00000) RY*( 7) N   1          s(  0.00%)p 1.00(  4.85%)d19.61( 95.15%)
19. (0.00000) RY*( 8) N   1          s(  0.00%)p 1.00(  4.85%)d19.61( 95.15%)
20. (0.00000) RY*( 9) N   1          s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
21. (0.00000) RY*(10) N   1          s(  2.92%)p 6.01( 17.58%)d27.19( 79.50%)
22. (0.02188) RY*( 1) N   2          s(  0.00%)p 1.00(  0.58%)d99.99( 99.42%)
                                0.0000  0.0000  0.0000  0.0000 -0.0760
                               -0.0075  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.9971  0.0000  0.0000  0.0000
23. (0.01551) RY*( 2) N   2          s(  6.21%)p15.07( 93.59%)d 0.03(  0.20%)
                                0.0000  0.0046  0.2491 -0.0009  0.0000
                                0.0000  0.0000  0.0000  0.0562 -0.9658
                                0.0000  0.0000  0.0000  0.0000  0.0452
24. (0.00816) RY*( 3) N   2          s(  0.00%)p 1.00(  0.40%)d99.99( 99.60%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000  0.0623 -0.0105  0.0000  0.0000
                                0.0000  0.0000  0.9980  0.0000  0.0000
25. (0.00046) RY*( 4) N   2          s( 90.02%)p 0.00(  0.26%)d 0.11(  9.71%)
                                0.0000 -0.0176 -0.2523  0.9145  0.0000
                                0.0000  0.0000  0.0000  0.0000 -0.0514
                                0.0000  0.0000  0.0000  0.0000  0.3117
26. (0.00005) RY*( 5) N   2          s( 40.27%)p 0.10(  3.90%)d 1.39( 55.83%)
27. (0.00001) RY*( 6) N   2          s( 63.72%)p 0.04(  2.31%)d 0.53( 33.97%)
28. (0.00000) RY*( 7) N   2          s(  0.00%)p 1.00( 99.99%)d 0.00(  0.01%)
29. (0.00000) RY*( 8) N   2          s(  0.00%)p 1.00( 99.99%)d 0.00(  0.01%)
30. (0.00000) RY*( 9) N   2          s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
31. (0.00000) RY*(10) N   2          s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
32. (0.00273) RY*( 1) O   3          s(  0.00%)p 1.00( 96.51%)d 0.04(  3.49%)
                                0.0000  0.0000  0.0000  0.0000 -0.0172
                                0.9822  0.0000  0.0000  0.0000  0.0000
                                0.0000 -0.1869  0.0000  0.0000  0.0000
33. (0.00246) RY*( 2) O   3          s(  0.00%)p 1.00( 96.49%)d 0.04(  3.51%)
                                0.0000  0.0000  0.0000  0.0000  0.0000
                                0.0000 -0.0049  0.9823  0.0000  0.0000
                                0.0000  0.0000 -0.1875  0.0000  0.0000
34. (0.00019) RY*( 3) O   3          s( 62.56%)p 0.51( 31.87%)d 0.09(  5.58%)
                                0.0000  0.0131  0.7906 -0.0173  0.0000
                                0.0000  0.0000  0.0000 -0.0575  0.5616
```

0.0000 0.0000 0.0000 0.0000 -0.2362
35. (0.00002) RY*(4) O   3   s(29.86%)p 2.25(67.33%)d 0.09(2.81%)
36. (0.00003) RY*(5) O   3   s(9.06%)p 0.02(0.21%)d10.02(90.73%)
37. (0.00000) RY*(6) O   3   s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
38. (0.00000) RY*(7) O   3   s(0.00%)p 1.00(3.71%)d25.95(96.29%)
39. (0.00000) RY*(8) O   3   s(0.00%)p 1.00(3.71%)d25.95(96.29%)
40. (0.00000) RY*(9) O   3   s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
41. (0.00000) RY*(10) O   3   s(98.34%)p 0.01(1.16%)d 0.01(0.50%)
42. (0.01693) BD*(1) N   1 - N   2
(56.20%)   0.7497* N   1 s(31.43%)p 2.17(68.08%)d 0.02(0.49%)
0.0000 0.5568 0.0654 -0.0023 0.0000
0.0000 0.0000 0.0000 0.8245 0.0310
0.0000 0.0000 0.0000 0.0000 0.0699
(43.80%) -0.6618* N   2 s(52.29%)p 0.91(47.58%)d 0.00(0.13%)
0.0000 0.7229 0.0162 0.0042 0.0000
0.0000 0.0000 0.0000 -0.6891 -0.0308
0.0000 0.0000 0.0000 0.0000 0.0367
43. (0.20189) BD*(2) N   1 - N   2
(51.86%)   0.7202* N   1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9964 0.0070 0.0000 0.0000
0.0000 0.0000 0.0839 0.0000 0.0000
(48.14%) -0.6938* N   2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9978 -0.0206 0.0000 0.0000
0.0000 0.0000 -0.0625 0.0000 0.0000
44. (0.01560) BD*(1) N   2 - O   3
(44.49%)   0.6670* N   2 s(47.49%)p 1.10(52.37%)d 0.00(0.14%)
0.0001 -0.6889 0.0182 0.0023 0.0000
0.0000 0.0000 0.0000 -0.7224 -0.0424
0.0000 0.0000 0.0000 0.0000 -0.0379
(55.51%) -0.7450* O   3 s(16.93%)p 4.89(82.71%)d 0.02(0.37%)
0.0000 -0.4089 0.0453 0.0001 0.0000
0.0000 0.0000 0.0000 0.9093 0.0133
0.0000 0.0000 0.0000 0.0000 -0.0605
45. (0.90892) BD*(2) N   2 - O   3
(80.68%)   0.8982* N   2 s(0.00%)p 1.00(99.42%)d 0.01(0.58%)
0.0000 0.0000 0.0000 0.0000 0.9969
-0.0219 0.0000 0.0000 0.0000 0.0000
0.0000 0.0759 0.0000 0.0000 0.0000
(19.32%) -0.4396* O   3 s(0.00%)p 1.00(99.78%)d 0.00(0.22%)
0.0000 0.0000 0.0000 0.0000 0.9989
0.0086 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0466 0.0000 0.0000 0.0000

…..

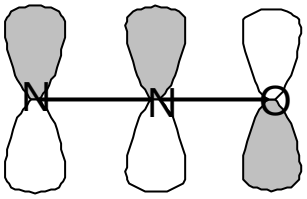
Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

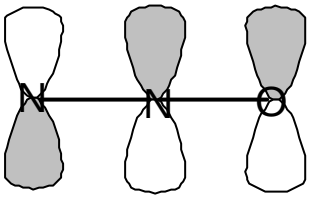
Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) N 1 - N 2	/ 23. RY*(2) N 2	0.53	2.72	0.034
2. BD (2) N 1 - N 2	/ 33. RY*(2) O 3	2.93	1.89	0.066
2. BD (2) N 1 - N 2	/ 43. BD*(2) N 1 - N 2	1.44	0.78	0.032
3. BD (1) N 2 - O 3	/ 14. RY*(3) N 1	2.26	2.52	0.067
3. BD (1) N 2 - O 3	/ 23. RY*(2) N 2	0.73	2.50	0.038
3. BD (1) N 2 - O 3	/ 42. BD*(1) N 1 - N 2	0.83	2.32	0.039
4. BD (2) N 2 - O 3	/ 9. LP (2) N 1	11.35	0.40	0.088
4. BD (2) N 2 - O 3	/ 13. RY*(2) N 1	1.73	1.57	0.046
4. BD (2) N 2 - O 3	/ 45. BD*(2) N 2 - O 3	8.20	0.47	0.075
5. CR (1) N 1	/ 23. RY*(2) N 2	5.25	16.70	0.265
5. CR (1) N 1	/ 44. BD*(1) N 2 - O 3	5.26	16.12	0.261
6. CR (1) N 2	/ 14. RY*(3) N 1	1.82	16.89	0.157
6. CR (1) N 2	/ 15. RY*(4) N 1	0.51	17.33	0.084
6. CR (1) N 2	/ 42. BD*(1) N 1 - N 2	0.80	16.69	0.103
7. CR (1) O 3	/ 23. RY*(2) N 2	2.41	21.64	0.205
7. CR (1) O 3	/ 42. BD*(1) N 1 - N 2	4.24	21.46	0.270
8. LP (1) N 1	/ 23. RY*(2) N 2	15.37	2.05	0.159
8. LP (1) N 1	/ 25. RY*(4) N 2	0.97	4.68	0.060
8. LP (1) N 1	/ 26. RY*(5) N 2	0.60	3.08	0.038
8. LP (1) N 1	/ 44. BD*(1) N 2 - O 3	17.45	1.48	0.144
9. LP (2) N 1	/ 13. RY*(2) N 1	8.15	1.16	0.119
9. LP (2) N 1	/ 18. RY*(7) N 1	2.88	2.50	0.104
9. LP (2) N 1	/ 22. RY*(1) N 2	10.85	2.62	0.204
9. LP (2) N 1	/ 29. RY*(8) N 2	2.99	1.11	0.070
9. LP (2) N 1	**/ 45. BD*(2) N 2 - O 3**	**2228.09**	**0.07**	**0.361**
10. LP (1) O 3	/ 14. RY*(3) N 1	0.75	2.34	0.038
10. LP (1) O 3	/ 23. RY*(2) N 2	8.00	2.32	0.122
10. LP (1) O 3	/ 42. BD*(1) N 1 - N 2	25.02	2.14	0.207
11. LP (2) O 3	/ 24. RY*(3) N 2	7.06	2.88	0.134
11. LP (2) O 3	/ 39. RY*(8) O 3	0.69	2.85	0.042
11. LP (2) O 3	**/ 43. BD*(2) N 1 - N 2**	**89.19**	**0.60**	**0.207**
43. BD*(2) N 1 - N 2	/ 12. RY*(1) N 1	5.65	0.81	0.190
43. BD*(2) N 1 - N 2	/ 19. RY*(8) N 1	1.23	2.15	0.144
43. BD*(2) N 1 - N 2	/ 24. RY*(3) N 2	2.72	2.29	0.217
43. BD*(2) N 1 - N 2	/ 28. RY*(7) N 2	1.69	0.76	0.101
45. BD*(2) N 2 - O 3	/ 13. RY*(2) N 1	4.79	1.09	0.096
45. BD*(2) N 2 - O 3	/ 22. RY*(1) N 2	14.16	2.55	0.249
45. BD*(2) N 2 - O 3	/ 29. RY*(8) N 2	3.63	1.04	0.081
45. BD*(2) N 2 - O 3	/ 32. RY*(1) O 3	4.72	1.39	0.107
45. BD*(2) N 2 - O 3	/ 38. RY*(7) O 3	2.03	2.53	0.095

There are two strong donor acceptor interactions describing the delocalization of two lone pairs: p-type LP(2) at N1 and p-type LP(2) at O3

The first interaction LP (2) N1 ® 45. BD*(2) N2 - O3 describes resonance with structure B



the second interaction LP (2) O3 ® 43. BD*(2) N1 - N2 is shown in the next figure



NATURAL LOCALIZED MOLECULAR ORBITAL (NLMO) ANALYSIS:

Maximum off-diagonal element of DM in NLMO basis: 0.55609E-10

Hybridization/Polarization Analysis of NLMOs in NAO Basis:
NLMO/Occupancy/Percent from Parent NBO/ Atomic Hybrid Contributions

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1. (2.00000) 99.9938% BD (1) N 1 N 2 0
   43.797% N 1 s(31.43%)p 2.17(68.08%)d 0.02(0.49%)
   56.197% N 2 s(52.29%)p 0.91(47.58%)d 0.00(0.13%)
2. (2.00000) 99.8771% BD (2) N 1 N 2 0
   48.079% N 1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
   51.798% N 2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
   0.123% O 3 s(0.00%)p 1.00(96.49%)d 0.04(3.51%)
3. (2.00000) 99.9358% BD (1) N 2 O 3 0
   0.064% N 1 s(62.06%)p 0.52(32.23%)d 0.09(5.71%)
   55.474% N 2 s(47.49%)p 1.10(52.36%)d 0.00(0.14%)
   44.462% O 3 s(16.93%)p 4.89(82.71%)d 0.02(0.37%)
4. (2.00000) 99.9124% BD (2) N 2 O 3 0
   0.088% N 1 s(0.00%)p 1.00(95.81%)d 0.04(4.19%)
   19.307% N 2 s(0.00%)p 1.00(99.42%)d 0.01(0.58%)
   80.605% O 3 s(0.00%)p 1.00(99.78%)d 0.00(0.22%)
5. (2.00000) 99.9789% CR (1) N 1 0 0
   99.980% N 1 s(100.00%)p 0.00(0.00%)d 0.00(0.00%)
   0.016% N 2 s(27.62%)p 2.52(69.64%)d 0.10(2.74%)
6. (2.00000) 99.9792% CR (1) N 2 0 0
   0.011% N 1 s(18.73%)p 3.88(72.70%)d 0.46(8.58%)
   99.984% N 2 s(100.00%)p 0.00(0.00%)d 0.00(0.00%)

7. (2.00000) 99.9913% CR (1) O 3 0 0
99.992% O 3 s(100.00%)p 0.00(0.00%)d 0.00(0.00%)
8. (2.00000) 98.7557% LP (1) N 1 0 0
98.756% N 1 s(68.86%)p 0.45(31.10%)d 0.00(0.04%)
0.815% N 2 s(25.33%)p 2.95(74.60%)d 0.00(0.07%)
0.429% O 3 s(16.58%)p 4.99(82.68%)d 0.04(0.75%)
9. (2.00000) **53.3236%** LP (2) N 1 0 0
53.324% N 1 s(0.00%)p 1.00(99.34%)d 0.01(0.66%)
37.758% N 2 s(0.00%)p 1.00(99.10%)d 0.01(0.90%)
8.918% O 3 s(0.00%)p 1.00(99.95%)d 0.00(0.05%)
10. (2.00000) 98.8352% LP (1) O 3 0 0
0.487% N 1 s(38.85%)p 1.56(60.43%)d 0.02(0.72%)
0.677% N 2 s(31.04%)p 2.21(68.75%)d 0.01(0.21%)
98.835% O 3 s(83.27%)p 0.20(16.72%)d 0.00(0.02%)
11. (2.00000) **89.4007%** LP (2) O 3 0 0
5.332% N 1 s(0.00%)p 1.00(99.69%)d 0.00(0.31%)
5.267% N 2 s(0.00%)p 1.00(95.26%)d 0.05(4.74%)
89.401% O 3 s(0.00%)p 1.00(99.80%)d 0.00(0.20%)

Individual LMO bond orders greater than 0.002 in magnitude,
with the overlap between the hybrids in the NLMO given:

Atom I	Atom J	NLMO	Bond Order	Hybrid Overlap
1	2	1	0.8759371	0.7981091
1	2	2	0.9615778	0.4555943
1	2	8	0.0163029	0.4595495
1	2	9	0.7551615	0.4674987
1	2	10	-0.0097464	-0.5269610
1	2	11	-0.1053408	-0.3947561
1	3	2	-0.0024583	-0.0433688
1	3	8	-0.0085820	-0.0307155
1	3	9	-0.1783670	-0.0411838
1	3	10	0.0097464	0.0036147
1	3	11	-0.1066459	-0.0418623
2	3	2	-0.0024583	-0.2462255
2	3	3	0.8892375	0.6755270
2	3	4	0.3861432	0.3384176
2	3	8	-0.0085820	-0.4656034
2	3	9	-0.1783670	-0.3256961
2	3	10	0.0135488	0.2973000
2	3	11	0.1053408	0.3684383

Atom-Atom Net Linear NLMO/NPA Bond Orders:

Atom	1	2	3
1. N	0.0000	**2.4939**	-0.2866
2. N	2.4939	0.0000	1.2051
3. O	-0.2866	**1.2051**	0.0000

The N1N2 and N2O3 bond orders indicate that Lewis structure B should be the primary (best) one.

Linear NLMO/NPA Bond Orders, Totals by Atom:

Atom	1
1. N	**2.2073**
2. N	3.6990
3. O	**0.9185**

1\1\GINC-CUP181\SP\RHF\6-31G(d)\N2O1\LEX\23-Jan-2004\0\\#HF/6-31G(D) S
CF=TIGHT POP=NBOREAD\\N2O, NN and NO double bond at HF/6-31G(d)//HF/ST
O-3G\\0,1\N\N,1,1.1544\X,2,1.,1,90.\O,2,1.2754,3,90.,1,180.,0\\Version
=x86-Linux-G98RevA.11.3\State=1-SG\HF=-183.6570673\RMSD=8.290e-09\Dipo
le=0.,0.,-0.457351\PG=C*V [C*(N1N1O1)]\\@

INPUT for structure B

#hf/6-31G(d) scf=tight pop=nboread

N2O NN triple bond HF/6-31G(d)//HF/STO-3G

0,1
N
N, 1, B1
X, 2, 1.0, 1, 90.0
O, 2, B2, 3, 90.0, 1, 180.0

B1=1.1544
B2=1.2754

$NBO NLMO BNDIDX RESONANCE $END
$choose
lone 1 1
    2 0
    3 3 end
bond **T 1 2**
    S 2 3 end
$end

By the way, this fixed Lewis structure represents the structure the NBO program would find without the $choose keyword.

OUTPUT for structure B

```
*****************************Gaussian NBO Version 3.1**********************
         N A T U R A L   A T O M I C   O R B I T A L   A N D
       N A T U R A L   B O N D   O R B I T A L   A N A L Y S I S
*****************************Gaussian NBO Version 3.1**********************

     /RESON  / : Allow strongly delocalized NBO set
     /NLMO   / : Form Natural Localized Molecular Orbitals
     /BNDIDX / : Print bond indices based on the NAO density matrix

 Analyzing the SCF density

 Job title: N2O NN triple bond HF/6-31G(d)//HF/STO-3G

 Storage needed:      6339 in NPA,      8259 in NBO,      6309 in NLMO (    6291456 available)


 NATURAL POPULATIONS:  Natural atomic orbital occupancies

  NAO Atom No lang   Type(AO)    Occupancy      Energy
 --------------------------------------------------------
   1    N  1  s      Cor( 1s)     1.99958     -15.53265
   2    N  1  s      Val( 2s)     1.63423      -0.84630
   3    N  1  s      Ryd( 3s)     0.00576       1.41193
   4    N  1  s      Ryd( 4s)     0.00003       3.63535
   5    N  1  px     Val( 2p)     1.05940      -0.22750
   6    N  1  px     Ryd( 3p)     0.00172       0.91561
   7    N  1  py     Val( 2p)     1.05940      -0.22750
   8    N  1  py     Ryd( 3p)     0.00172       0.91561
   9    N  1  pz     Val( 2p)     1.21545      -0.22320
  10    N  1  pz     Ryd( 3p)     0.00167       0.85539
  11    N  1  dxy    Ryd( 3d)     0.00000       1.95665
  12    N  1  dxz    Ryd( 3d)     0.00710       2.30012
  13    N  1  dyz    Ryd( 3d)     0.00710       2.30012
  14    N  1  dx2y2  Ryd( 3d)     0.00000       1.95665
  15    N  1  dz2    Ryd( 3d)     0.00521       2.80226

  16    N  2  s      Cor( 1s)     1.99958     -15.71271
  17    N  2  s      Val( 2s)     1.12112      -0.64807
  18    N  2  s      Ryd( 3s)     0.00156       1.64629
  19    N  2  s      Ryd( 4s)     0.00041       3.05232
  20    N  2  px     Val( 2p)     1.13177      -0.31862
  21    N  2  px     Ryd( 3p)     0.00050       0.88364
  22    N  2  py     Val( 2p)     1.13177      -0.31862
  23    N  2  py     Ryd( 3p)     0.00050       0.88364
  24    N  2  pz     Val( 2p)     1.12104      -0.29552
  25    N  2  pz     Ryd( 3p)     0.01649       1.06226
  26    N  2  dxy    Ryd( 3d)     0.00000       1.88459
  27    N  2  dxz    Ryd( 3d)     0.00903       2.41657
  28    N  2  dyz    Ryd( 3d)     0.00903       2.41657
```

29	N	2	dx2y2	Ryd(3d)	0.00000	1.88459
30	N	2	dz2	Ryd(3d)	0.00318	3.46170
31	O	3	s	Cor(1s)	1.99983	-20.47495
32	O	3	s	Val(2s)	1.79593	-1.19624
33	O	3	s	Ryd(3s)	0.00209	1.92965
34	O	3	s	Ryd(4s)	0.00000	4.00924
35	O	3	px	Val(2p)	1.78447	-0.47472
36	O	3	px	Ryd(3p)	0.00239	1.22993
37	O	3	py	Val(2p)	1.78447	-0.47472
38	O	3	py	Ryd(3p)	0.00239	1.22993
39	O	3	pz	Val(2p)	1.07290	-0.23969
40	O	3	pz	Ryd(3p)	0.00023	1.30079
41	O	3	dxy	Ryd(3d)	0.00000	2.07202
42	O	3	dxz	Ryd(3d)	0.00360	2.37572
43	O	3	dyz	Ryd(3d)	0.00360	2.37572
44	O	3	dx2y2	Ryd(3d)	0.00000	2.07202
45	O	3	dz2	Ryd(3d)	0.00368	3.04979

Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	0.00161	1.99958	4.96849	0.03032	6.99839
N	2	0.45401	1.99958	4.50571	0.04070	6.54599
O	3	-0.45562	1.99983	6.43779	0.01800	8.45562
* Total *		0.00000	5.99899	15.91199	0.08902	22.00000

Natural Population

Core	5.99899 (99.9832% of 6)
Valence	15.91199 (99.4499% of 16)
Natural Minimal Basis	21.91098 (99.5954% of 22)
Natural Rydberg Basis	0.08902 (0.4046% of 22)

Atom	No	Natural Electron Configuration
N	1	[core]2s(1.63)2p(3.33)3s(0.01)3p(0.01)3d(0.02)
N	2	[core]2s(1.12)2p(3.38)3p(0.02)3d(0.02)
O	3	[core]2s(1.80)2p(4.64)3p(0.01)3d(0.01)

The NPA phase displays the same data as for structure A.

NATURAL BOND ORBITAL ANALYSIS:

		Occupancies		Lewis Structure				Low	High	
	Occ.							occ	occ	
Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	(L)	(NL)	Dev
1(1)	1.90	21.52054	0.47946	3	4	0	4	2	2	0.42

Structure accepted: NBOs selected via the $CHOOSE keylist

Core	5.99899 (99.983% of	6)
Valence Lewis	15.52156 (**97.010%** of	16)
Total Lewis	21.52054 (97.821% of	22)
Valence non-Lewis	**0.43631** (1.983% of	22)
Rydberg non-Lewis	**0.04315** (0.196% of	22)
Total non-Lewis	0.47946 (2.179% of	22)

0.47946 of 22 electrons are delocalized in structure B according to 2.179 %.

Remember for Structure A:

1.20029 of 22 electrons are delocalized in structure A according to 5.456 %

were found

(Occupancy) Bond orbital/ Coefficients/ Hybrids

1. (1.99988) BD (1) N 1 - N 2
   (43.80%) 0.6618* N 1 s(31.43%)p 2.17(68.08%)d 0.02(0.49%)
   0.0000 0.5568 0.0654 -0.0023 0.0000
   0.0000 0.0000 0.0000 0.8245 0.0310
   0.0000 0.0000 0.0000 0.0000 0.0699
   (56.20%) 0.7497* N 2 s(52.29%)p 0.91(47.58%)d 0.00(0.13%)
   0.0000 0.7229 0.0162 0.0042 0.0000
   0.0000 0.0000 0.0000 -0.6891 -0.0308
   0.0000 0.0000 0.0000 0.0000 0.0367
2. (1.99754) BD (2) N 1 - N 2
   (48.14%) 0.6938* N 1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
   0.0000 0.0000 0.0000 0.0000 0.9964
   0.0070 0.0000 0.0000 0.0000 0.0000
   0.0000 0.0839 0.0000 0.0000 0.0000

(51.86%) 0.7202* N 2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.0000 0.0000 0.0000 0.0000 0.9978
-0.0206 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0625 0.0000 0.0000 0.0000
3. (1.99754) BD (3) N 1 - N 2
(48.14%) 0.6938* N 1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9964 0.0070 0.0000 0.0000
0.0000 0.0000 0.0839 0.0000 0.0000
(51.86%) 0.7202* N 2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9978 -0.0206 0.0000 0.0000
0.0000 0.0000 -0.0625 0.0000 0.0000
4. (1.99872) BD (1) N 2 - O 3
(55.51%) 0.7450* N 2 s(47.49%)p 1.10(52.37%)d 0.00(0.14%)
-0.0001 0.6889 -0.0182 -0.0023 0.0000
0.0000 0.0000 0.0000 0.7224 0.0424
0.0000 0.0000 0.0000 0.0000 0.0379
(44.49%) 0.6670* O 3 s(16.93%)p 4.89(82.71%)d 0.02(0.37%)
0.0000 0.4089 -0.0453 -0.0001 0.0000
0.0000 0.0000 0.0000 -0.9093 -0.0133
0.0000 0.0000 0.0000 0.0000 0.0605
5. (1.99958) CR (1) N 1 s(100.00%)p 0.00(0.00%)
1.0000 0.0006 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 -0.0004 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
6. (1.99958) CR (1) N 2 s(100.00%)
1.0000 0.0001 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0001 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
7. (1.99983) CR (1) O 3 s(100.00%)p 0.00(0.00%)
1.0000 0.0004 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0002 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
8. (1.97515) LP (1) N 1 s(68.89%)p 0.45(31.08%)d 0.00(0.04%)
-0.0008 0.8297 -0.0201 0.0005 0.0000
0.0000 0.0000 0.0000 -0.5574 0.0092
0.0000 0.0000 0.0000 0.0000 -0.0196
9. (1.97671) LP (1) O 3 s(83.26%)p 0.20(16.73%)d 0.00(0.02%)
-0.0004 0.9124 0.0091 0.0000 0.0000
0.0000 0.0000 0.0000 0.4090 0.0023
0.0000 0.0000 0.0000 0.0000 -0.0130
10. (1.78801) LP (2) O 3 s(0.00%)p 1.00(99.80%)d 0.00(0.20%)
0.0000 0.0000 0.0000 0.0000 0.9990
-0.0034 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0444 0.0000 0.0000 0.0000
11. (1.78801) LP (3) O 3 s(0.00%)p 1.00(99.80%)d 0.00(0.20%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9990 -0.0034 0.0000 0.0000
0.0000 0.0000 -0.0444 0.0000 0.0000
12. (0.00194) RY*(1) N 1 s(0.00%)p 1.00(95.85%)d 0.04(4.15%)

```
                    0.0000  0.0000  0.0000  0.0000 -0.0240
                    0.9787  0.0000  0.0000  0.0000  0.0000
                    0.0000  0.2037  0.0000  0.0000  0.0000
13. (0.00194) RY*( 2) N   1          s(  0.00%)p 1.00( 95.85%)d 0.04(  4.15%)
                    0.0000  0.0000  0.0000  0.0000  0.0000
                    0.0000 -0.0240  0.9787  0.0000  0.0000
                    0.0000  0.0000  0.2037  0.0000  0.0000
14. (0.00169) RY*( 3) N   1          s( 59.34%)p 0.59( 35.25%)d 0.09(  5.40%)
                    0.0000 -0.0353  0.7646  0.0869  0.0000
                    0.0000  0.0000  0.0000 -0.0784  0.5885
                    0.0000  0.0000  0.0000  0.0000  0.2325
15. (0.00007) RY*( 4) N   1          s( 47.41%)p 0.80( 38.04%)d 0.31( 14.56%)
16. (0.00001) RY*( 5) N   1          s( 90.01%)p 0.11(  9.98%)d 0.00(  0.01%)
17. (0.00000) RY*( 6) N   1          s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
18. (0.00000) RY*( 7) N   1          s(  0.00%)p 1.00(  4.85%)d19.61( 95.15%)
19. (0.00000) RY*( 8) N   1          s(  0.00%)p 1.00(  4.85%)d19.61( 95.15%)
20. (0.00000) RY*( 9) N   1          s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
21. (0.00000) RY*(10) N   1          s(  2.92%)p 6.01( 17.58%)d27.19( 79.50%)
22. (0.01551) RY*( 1) N   2          s(  6.21%)p15.07( 93.59%)d 0.03(  0.20%)
                    0.0000  0.0046  0.2491 -0.0009  0.0000
                    0.0000  0.0000  0.0000  0.0562 -0.9658
                    0.0000  0.0000  0.0000  0.0000  0.0452
23. (0.00816) RY*( 2) N   2          s(  0.00%)p 1.00(  0.40%)d99.99( 99.60%)
                    0.0000  0.0000  0.0000  0.0000  0.0623
                   -0.0105  0.0000  0.0000  0.0000  0.0000
                    0.0000  0.9980  0.0000  0.0000  0.0000
24. (0.00816) RY*( 3) N   2          s(  0.00%)p 1.00(  0.40%)d99.99( 99.60%)
                    0.0000  0.0000  0.0000  0.0000  0.0000
                    0.0000  0.0623 -0.0105  0.0000  0.0000
                    0.0000  0.0000  0.9980  0.0000  0.0000
25. (0.00046) RY*( 4) N   2          s( 90.02%)p 0.00(  0.26%)d 0.11(  9.71%)
                    0.0000 -0.0176 -0.2523  0.9145  0.0000
                    0.0000  0.0000  0.0000  0.0000 -0.0514
                    0.0000  0.0000  0.0000  0.0000  0.3117
26. (0.00005) RY*( 5) N   2          s( 40.27%)p 0.10(  3.90%)d 1.39( 55.83%)
27. (0.00001) RY*( 6) N   2          s( 63.72%)p 0.04(  2.31%)d 0.53( 33.97%)
28. (0.00000) RY*( 7) N   2          s(  0.00%)p 1.00( 99.99%)d 0.00(  0.01%)
29. (0.00000) RY*( 8) N   2          s(  0.00%)p 1.00( 99.99%)d 0.00(  0.01%)
30. (0.00000) RY*( 9) N   2          s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
31. (0.00000) RY*(10) N   2          s(  0.00%)p 0.00(  0.00%)d 1.00(100.00%)
32. (0.00246) RY*( 1) O   3          s(  0.00%)p 1.00( 96.49%)d 0.04(  3.51%)
                    0.0000  0.0000  0.0000  0.0000 -0.0049
                    0.9823  0.0000  0.0000  0.0000  0.0000
                    0.0000 -0.1875  0.0000  0.0000  0.0000
33. (0.00246) RY*( 2) O   3          s(  0.00%)p 1.00( 96.49%)d 0.04(  3.51%)
                    0.0000  0.0000  0.0000  0.0000  0.0000
                    0.0000 -0.0049  0.9823  0.0000  0.0000
                    0.0000  0.0000 -0.1875  0.0000  0.0000
34. (0.00019) RY*( 3) O   3          s( 62.56%)p 0.51( 31.87%)d 0.09(  5.58%)
                    0.0000  0.0131  0.7906 -0.0173  0.0000
                    0.0000  0.0000  0.0000 -0.0575  0.5616
```

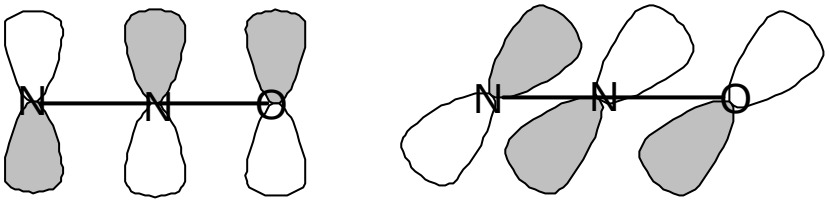
0.0000 0.0000 0.0000 0.0000 -0.2362
35. (0.00002) RY*(4) O   3   s(29.86%)p 2.25(67.33%)d 0.09(2.81%)
36. (0.00003) RY*(5) O   3   s(9.06%)p 0.02(0.21%)d10.02(90.73%)
37. (0.00000) RY*(6) O   3   s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
38. (0.00000) RY*(7) O   3   s(0.00%)p 1.00(3.71%)d25.95(96.29%)
39. (0.00000) RY*(8) O   3   s(0.00%)p 1.00(3.71%)d25.95(96.29%)
40. (0.00000) RY*(9) O   3   s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
41. (0.00000) RY*(10) O   3   s(98.34%)p 0.01(1.16%)d 0.01(0.50%)
42. (0.01693) BD*(1) N   1 - N   2
(56.20%)   0.7497* N   1 s(31.43%)p 2.17(68.08%)d 0.02(0.49%)
0.0000 0.5568 0.0654 -0.0023 0.0000
0.0000 0.0000 0.0000 0.8245 0.0310
0.0000 0.0000 0.0000 0.0000 0.0699
(43.80%) -0.6618* N   2 s(52.29%)p 0.91(47.58%)d 0.00(0.13%)
0.0000 0.7229 0.0162 0.0042 0.0000
0.0000 0.0000 0.0000 -0.6891 -0.0308
0.0000 0.0000 0.0000 0.0000 0.0367
43. (0.20189) BD*(2) N   1 - N   2
(51.86%)   0.7202* N   1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
0.0000 0.0000 0.0000 0.0000 0.9964
0.0070 0.0000 0.0000 0.0000 0.0000
0.0000 0.0839 0.0000 0.0000 0.0000
(48.14%) -0.6938* N   2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.0000 0.0000 0.0000 0.0000 0.9978
-0.0206 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0625 0.0000 0.0000 0.0000
44. (0.20189) BD*(3) N   1 - N   2
(51.86%)   0.7202* N   1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9964 0.0070 0.0000 0.0000
0.0000 0.0000 0.0839 0.0000 0.0000
(48.14%) -0.6938* N   2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9978 -0.0206 0.0000 0.0000
0.0000 0.0000 -0.0625 0.0000 0.0000
45. (0.01560) BD*(1) N   2 - O   3
(44.49%)   0.6670* N   2 s(47.49%)p 1.10(52.37%)d 0.00(0.14%)
0.0001 -0.6889 0.0182 0.0023 0.0000
0.0000 0.0000 0.0000 -0.7224 -0.0424
0.0000 0.0000 0.0000 0.0000 -0.0379
(55.51%) -0.7450* O   3 s(16.93%)p 4.89(82.71%)d 0.02(0.37%)
0.0000 -0.4089 0.0453 0.0001 0.0000
0.0000 0.0000 0.0000 0.9093 0.0133
0.0000 0.0000 0.0000 0.0000 -0.0605

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) N 1 - N 2	/ 22. RY*(1) N 2	0.53	2.72	0.034
2. BD (2) N 1 - N 2	/ 32. RY*(1) O 3	2.93	1.89	0.066
2. BD (2) N 1 - N 2	/ 43. BD*(2) N 1 - N 2	1.44	0.78	0.032
3. BD (3) N 1 - N 2	/ 33. RY*(2) O 3	2.93	1.89	0.066
3. BD (3) N 1 - N 2	/ 44. BD*(3) N 1 - N 2	1.44	0.78	0.032
4. BD (1) N 2 - O 3	/ 14. RY*(3) N 1	2.26	2.52	0.067
4. BD (1) N 2 - O 3	/ 22. RY*(1) N 2	0.73	2.50	0.038
4. BD (1) N 2 - O 3	/ 42. BD*(1) N 1 - N 2	0.83	2.32	0.039
5. CR (1) N 1	/ 22. RY*(1) N 2	5.25	16.70	0.265
5. CR (1) N 1	/ 45. BD*(1) N 2 - O 3	5.26	16.12	0.261
6. CR (1) N 2	/ 14. RY*(3) N 1	1.82	16.89	0.157
6. CR (1) N 2	/ 15. RY*(4) N 1	0.51	17.33	0.084
6. CR (1) N 2	/ 42. BD*(1) N 1 - N 2	0.80	16.69	0.103
6. CR (1) N 2	/ 45. BD*(1) N 2 - O 3	0.95	16.30	0.111
7. CR (1) O 3	/ 22. RY*(1) N 2	2.41	21.64	0.205
7. CR (1) O 3	/ 42. BD*(1) N 1 - N 2	4.24	21.46	0.270
8. LP (1) N 1	/ 22. RY*(1) N 2	15.37	2.05	0.159
8. LP (1) N 1	/ 25. RY*(4) N 2	0.97	4.68	0.060
8. LP (1) N 1	/ 26. RY*(5) N 2	0.60	3.08	0.038
8. LP (1) N 1	/ 45. BD*(1) N 2 - O 3	17.45	1.48	0.144
9. LP (1) O 3	/ 14. RY*(3) N 1	0.75	2.34	0.038
9. LP (1) O 3	/ 22. RY*(1) N 2	8.00	2.32	0.122
9. LP (1) O 3	/ 42. BD*(1) N 1 - N 2	25.02	2.14	0.207
10. LP (2) O 3	/ 23. RY*(2) N 2	7.06	2.88	0.134
10. LP (2) O 3	/ 29. RY*(8) N 2	0.90	1.36	0.033
10. LP (2) O 3	/ 38. RY*(7) O 3	0.69	2.85	0.042
10. LP (2) O 3	**/ 43. BD*(2) N 1 - N 2**	**89.19**	**0.60**	**0.207**
11. LP (3) O 3	/ 24. RY*(3) N 2	7.06	2.88	0.134
11. LP (3) O 3	/ 28. RY*(7) N 2	0.90	1.36	0.033
11. LP (3) O 3	/ 39. RY*(8) O 3	0.69	2.85	0.042
11. LP (3) O 3	**/ 44. BD*(3) N 1 - N 2**	**89.19**	0.60	0.207
43. BD*(2) N 1 - N 2	/ 12. RY*(1) N 1	5.65	0.81	0.190
43. BD*(2) N 1 - N 2	/ 18. RY*(7) N 1	1.23	2.15	0.144
43. BD*(2) N 1 - N 2	/ 23. RY*(2) N 2	2.72	2.29	0.217
43. BD*(2) N 1 - N 2	/ 29. RY*(8) N 2	1.69	0.76	0.101
44. BD*(3) N 1 - N 2	/ 13. RY*(2) N 1	5.65	0.81	0.190
44. BD*(3) N 1 - N 2	/ 19. RY*(8) N 1	1.23	2.15	0.144
44. BD*(3) N 1 - N 2	/ 24. RY*(3) N 2	2.72	2.29	0.217
44. BD*(3) N 1 - N 2	/ 28. RY*(7) N 2	1.69	0.76	0.101

Theses two interactions correspond to the delocalization of the two p-type LPs of oxygen into the p* NBOs along the NN unit.



The energies for these interactions are not as large as the analogue interaction energies of structure A.

NATURAL LOCALIZED MOLECULAR ORBITAL (NLMO) ANALYSIS:

Maximum off-diagonal element of DM in NLMO basis: 0.55609E-10

Hybridization/Polarization Analysis of NLMOs in NAO Basis:
NLMO/Occupancy/Percent from Parent NBO/ Atomic Hybrid Contributions

---

1. (2.00000) 99.9938% BD (1) N 1 N 2 0
43.797% N 1 s(31.43%)p 2.17(68.08%)d 0.02(0.49%)
56.197% N 2 s(52.29%)p 0.91(47.58%)d 0.00(0.13%)
2. (2.00000) 99.8771% BD (2) N 1 N 2 0
48.079% N 1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
51.798% N 2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.123% O 3 s(0.00%)p 1.00(96.49%)d 0.04(3.51%)
3. (2.00000) 99.8771% BD (3) N 1 N 2 0
48.079% N 1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
51.798% N 2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.123% O 3 s(0.00%)p 1.00(96.49%)d 0.04(3.51%)
4. (2.00000) 99.9358% BD (1) N 2 O 3 0
0.064% N 1 s(62.06%)p 0.52(32.23%)d 0.09(5.71%)
55.474% N 2 s(47.49%)p 1.10(52.36%)d 0.00(0.14%)
44.462% O 3 s(16.93%)p 4.89(82.71%)d 0.02(0.37%)
5. (2.00000) 99.9789% CR (1) N 1 0 0
99.980% N 1 s(100.00%)p 0.00(0.00%)d 0.00(0.00%)
0.016% N 2 s(27.62%)p 2.52(69.64%)d 0.10(2.74%)
6. (2.00000) 99.9792% CR (1) N 2 0 0
0.011% N 1 s(18.73%)p 3.88(72.70%)d 0.46(8.58%)
99.984% N 2 s(100.00%)p 0.00(0.00%)d 0.00(0.00%)
7. (2.00000) 99.9913% CR (1) O 3 0 0
99.992% O 3 s(100.00%)p 0.00(0.00%)d 0.00(0.00%)
8. (2.00000) 98.7557% LP (1) N 1 0 0
98.756% N 1 s(68.86%)p 0.45(31.10%)d 0.00(0.04%)
0.815% N 2 s(25.33%)p 2.95(74.60%)d 0.00(0.07%)
0.429% O 3 s(16.58%)p 4.99(82.68%)d 0.04(0.75%)
9. (2.00000) 98.8352% LP (1) O 3 0 0
0.487% N 1 s(38.85%)p 1.56(60.43%)d 0.02(0.72%)
0.677% N 2 s(31.04%)p 2.21(68.75%)d 0.01(0.21%)
98.835% O 3 s(83.27%)p 0.20(16.72%)d 0.00(0.02%)
10. (2.00000) 89.4007% LP (2) O 3 0 0
5.332% N 1 s(0.00%)p 1.00(99.69%)d 0.00(0.31%)
5.267% N 2 s(0.00%)p 1.00(95.26%)d 0.05(4.74%)
89.401% O 3 s(0.00%)p 1.00(99.80%)d 0.00(0.20%)
11. (2.00000) 89.4007% LP (3) O 3 0 0
5.332% N 1 s(0.00%)p 1.00(99.69%)d 0.00(0.31%)
5.267% N 2 s(0.00%)p 1.00(95.26%)d 0.05(4.74%)
89.401% O 3 s(0.00%)p 1.00(99.80%)d 0.00(0.20%)

Individual LMO bond orders greater than 0.002 in magnitude,
with the overlap between the hybrids in the NLMO given:

Atom I	Atom J	NLMO	Bond Order	Hybrid Overlap
1	2	1	0.8759371	0.7981091
1	2	2	0.9615778	0.4555943
1	2	3	0.9615778	0.4555943
1	2	8	0.0163029	0.4595495
1	2	9	-0.0097464	-0.5269610
1	2	10	-0.1053408	-0.3947561
1	2	11	-0.1053408	-0.3947561
1	3	2	-0.0024583	-0.0433688
1	3	3	-0.0024583	-0.0433688
1	3	8	-0.0085820	-0.0307155
1	3	9	0.0097464	0.0036147
1	3	10	-0.1066459	-0.0418623
1	3	11	-0.1066459	-0.0418623
2	3	2	-0.0024583	-0.2462255
2	3	3	-0.0024583	-0.2462255
2	3	4	0.8892375	0.6755270
2	3	8	-0.0085820	-0.4656034
2	3	9	0.0135488	0.2973000
2	3	10	0.1053408	0.3684383
2	3	11	0.1053408	0.3684383

Atom-Atom Net Linear NLMO/NPA Bond Orders:

Atom	1	2	3
1. N	0.0000	**2.5968**	-0.2156
2. N	2.5968	0.0000	1.1002
3. O	-0.2156	**1.1002**	0.0000

The bond orders dpend on the reference Lewis structure, hence different bonders are found for strucutre A and B

cf. Structure A

Atom	1	2	3
1. N	0.0000	**2.4939**	-0.2866
2. N	2.4939	0.0000	1.2051
3. O	-0.2866	**1.2051**	0.0000

Linear NLMO/NPA Bond Orders, Totals by Atom:

Atom		1
1.	N	**2.3812**
2.	N	3.6970
3.	O	**0.8846**

1\1\GINC-CUP181\SP\RHF\6-31G(d)\N2O1\LEX\23-Jan-2004\0\\#HF/6-31G(D) S
CF=TIGHT POP=NBOREAD\\N2O NN triple bond HF/6-31G(d)//HF/STO-3G\\0,1\N
\N,1,1.1544\X,2,1.,1,90.\O,2,1.2754,3,90.,1,180.,0\\Version=x86-Linux-
G98RevA.11.3\State=1-SG\HF=-183.6570673\RMSD=8.290e-09\Dipole=0.,0.,-0
.457351\PG=C*V [C*(N1N1O1)]\\@

INPUT for structure C

```
#hf/6-31G(d) scf=tight pop=nboread

N2O NN triple bond + NO double bond  HF/6-31G(d)//HF/STO-3G

0,1
N
N, 1, B1
X, 2, 1.0, 1, 90.0
O, 2, B2,  3, 90.0, 1, 180.0

B1=1.1544
B2=1.2754

$NBO NLMO BNDIDX RESONANCE $END
$choose
lone 1 1
    2 0
    3 2 end
bond T 1 2
    D 2 3 end
$end
```

OUTPUT for structure C

NATURAL BOND ORBITAL ANALYSIS:

	Occupancies		Lewis Structure					Low	High	
	Occ.							occ	occ	
Cycle	Thresh.	Lewis	Non-Lewis	CR	BD	3C	LP	(L)	(NL)	Dev
1(1)	1.90	19.71896	2.28104	3	5	0	3	**4**	**3**	**0.42**

Structure accepted: NBOs selected via the $CHOOSE keylist

WARNING: 1 low occupancy (<1.9990e) core orbital found on N 1
1 low occupancy (<1.9990e) core orbital found on N 2

Core	5.78541 (96.424% of 6)
Valence Lewis	13.93355 (87.085% of 16)
Total Lewis	19.71896 (89.632% of 22)
Valence non-Lewis	1.17421 (5.337% of 22)
Rydberg non-Lewis	1.10683 (5.031% of 22)
Total non-Lewis	**2.28104** (**10.368%** of 22)

C 2.28 of 22 electrons are delocalized in structure B according to 10.3 %.

Remember for structures:

B 0.47946 of 22 electrons are delocalized in structure B according to 2.179 %.

A 1.20029 of 22 electrons are delocalized in structure A according to 5.456 %

(Occupancy) Bond orbital/ Coefficients/ Hybrids

---

1. (1.99954) BD (1) N 1 - N 2
(43.80%) 0.6618* N 1 s(31.46%)p 2.16(68.00%)d 0.02(0.55%)
-0.0006 0.5559 0.0743 -0.0020 0.0000
0.0000 0.0000 0.0000 0.8236 0.0400
0.0000 0.0000 0.0000 0.0000 0.0738
(56.20%) 0.7497* N 2 s(52.51%)p 0.90(47.37%)d 0.00(0.12%)
0.0021 0.7245 0.0127 0.0048 0.0000
0.0000 0.0000 0.0000 -0.6880 -0.0190
0.0000 0.0000 0.0000 0.0000 0.0340
2. (1.99754) BD (2) N 1 - N 2
(48.14%) 0.6938* N 1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9964 0.0070 0.0000 0.0000
0.0000 0.0000 0.0839 0.0000 0.0000
(51.86%) 0.7202* N 2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9978 -0.0206 0.0000 0.0000
0.0000 0.0000 -0.0625 0.0000 0.0000
3. (0.33969) BD (3) N 1 - N 2
(**0.63%**) 0.0791* N 1 s(46.37%)p 0.97(45.12%)d 0.18(8.51%)
0.0903 0.0927 -0.6681 -0.0231 0.0000
0.0000 0.0000 0.0000 0.0564 -0.6694
0.0000 0.0000 0.0000 0.0000 -0.2917
(**99.37%**) 0.9969* N 2 s(21.84%)p 3.42(74.73%)d 0.16(3.43%)
0.3120 0.2347 -0.2528 0.0452 0.0000
0.0000 0.0000 0.0000 0.2114 0.8382
0.0000 0.0000 0.0000 0.0000 -0.1853
4. (1.86536) BD (1) N 2 - O 3
(52.52%) 0.7247* N 2 s(42.57%)p 1.32(56.14%)d 0.03(1.28%)
-0.0576 0.6447 0.0798 -0.0202 0.0000
0.0000 0.0000 0.0000 0.6935 -0.2837
0.0000 0.0000 0.0000 0.0000 0.1133
(47.48%) 0.6891* O 3 s(16.93%)p 4.89(82.71%)d 0.02(0.37%)
0.0000 0.4089 -0.0453 -0.0001 0.0000
0.0000 0.0000 0.0000 -0.9093 -0.0133
0.0000 0.0000 0.0000 0.0000 0.0605
5. (1.99825) BD (2) N 2 - O 3
(19.32%) 0.4396* N 2 s(0.00%)p 1.00(99.42%)d 0.01(0.58%)
0.0000 0.0000 0.0000 0.0000 0.9969
-0.0219 0.0000 0.0000 0.0000 0.0000
0.0000 0.0759 0.0000 0.0000 0.0000
(80.68%) 0.8982* O 3 s(0.00%)p 1.00(99.78%)d 0.00(0.22%)
0.0000 0.0000 0.0000 0.0000 0.9989
0.0086 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0466 0.0000 0.0000 0.0000
6. (1.98301) CR (1) N 1 s(99.56%)p 0.00(0.37%)d 0.00(0.07%)
0.9959 -0.0052 0.0607 0.0021 0.0000
0.0000 0.0000 0.0000 -0.0065 0.0609

0.0000 0.0000 0.0000 0.0000 0.0265
7. **(1.80258) CR (1) N 2** s(90.89%)p 0.10(8.65%)d 0.01(0.46%)
0.9483 -0.0396 0.0880 -0.0161 0.0000
0.0000 0.0000 0.0000 -0.0259 -0.2929
0.0000 0.0000 0.0000 0.0000 0.0678
8. (1.99983) CR (1) O 3 s(100.00%)p 0.00(0.00%)
1.0000 0.0004 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0002 0.0000
0.0000 0.0000 0.0000 0.0000 0.0000
9. (1.96844) LP (1) N 1 s(68.26%)p 0.47(31.74%)d 0.00(0.00%)
-0.0034 0.8259 0.0191 0.0019 0.0000
0.0000 0.0000 0.0000 -0.5613 0.0485
0.0000 0.0000 0.0000 0.0000 -0.0025
10. (1.97671) LP (1) O 3 s(83.26%)p 0.20(16.73%)d 0.00(0.02%)
-0.0004 0.9124 0.0091 0.0000 0.0000
0.0000 0.0000 0.0000 0.4090 0.0023
0.0000 0.0000 0.0000 0.0000 -0.0130
11. (**1.78801) LP (2) O 3** s(0.00%)p 1.00(99.80%)d 0.00(0.20%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.9990 -0.0034 0.0000 0.0000
0.0000 0.0000 -0.0444 0.0000 0.0000
12. **(1.06647) RY*(1) N 1** s(0.00%)p 1.00(99.34%)d 0.01(0.66%)
0.0000 0.0000 0.0000 0.0000 0.9967
-0.0061 0.0000 0.0000 0.0000 0.0000
0.0000 0.0812 0.0000 0.0000 0.0000
13. (0.00194) RY*(2) N 1 s(0.00%)p 1.00(95.85%)d 0.04(4.15%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0240 0.9787 0.0000 0.0000
0.0000 0.0000 0.2037 0.0000 0.0000
14. (0.00175) RY*(3) N 1 s(0.00%)p 1.00(95.81%)d 0.04(4.19%)
0.0000 0.0000 0.0000 0.0000 -0.0107
0.9788 0.0000 0.0000 0.0000 0.0000
0.0000 0.2048 0.0000 0.0000 0.0000
15. (0.00011) RY*(4) N 1 s(61.05%)p 0.43(26.47%)d 0.20(12.48%)
0.0000 0.0082 0.6554 0.4253 0.0000
0.0000 0.0000 0.0000 -0.0071 -0.5144
0.0000 0.0000 0.0000 0.0000 -0.3533
16. (0.00001) RY*(5) N 1 s(48.85%)p 0.51(25.11%)d 0.53(26.04%)
17. (0.00000) RY*(6) N 1 s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
18. (0.00000) RY*(7) N 1 s(0.00%)p 1.00(4.85%)d19.61(95.15%)
19. (0.00000) RY*(8) N 1 s(0.00%)p 1.00(4.85%)d19.61(95.15%)
20. (0.00000) RY*(9) N 1 s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
21. (0.00000) RY*(10) N 1 s(44.46%)p 0.07(3.19%)d 1.18(52.35%)
22. (0.02188) RY*(1) N 2 s(0.00%)p 1.00(0.58%)d99.99(99.42%)
0.0000 0.0000 0.0000 0.0000 -0.0760
-0.0075 0.0000 0.0000 0.0000 0.0000
0.0000 0.9971 0.0000 0.0000 0.0000
23. (0.00816) RY*(2) N 2 s(0.00%)p 1.00(0.40%)d99.99(99.60%)
0.0000 0.0000 0.0000 0.0000 0.0000
0.0000 0.0623 -0.0105 0.0000 0.0000
0.0000 0.0000 0.9980 0.0000 0.0000

24. (0.00060) RY*(3) N   2   s(9.11%)p 0.85(7.78%)d 9.12(83.10%)
                0.0000 0.0496 -0.1524 0.2558 0.0000
                0.0000 0.0000 0.0000 0.0139 -0.2787
                0.0000 0.0000 0.0000 0.0000 -0.9116
25. (0.00046) RY*(4) N   2   s(89.93%)p 0.00(0.26%)d 0.11(9.81%)
                0.0000 -0.0177 -0.2520 0.9140 0.0000
                0.0000 0.0000 0.0000 0.0000 -0.0510
                0.0000 0.0000 0.0000 0.0000 0.3132
26. (0.00002) RY*(5) N   2   s(93.15%)p 0.05(5.06%)d 0.02(1.79%)
27. (0.00000) RY*(6) N   2   s(0.00%)p 1.00(99.99%)d 0.00(0.01%)
28. (0.00000) RY*(7) N   2   s(0.00%)p 1.00(99.99%)d 0.00(0.01%)
29. (0.00000) RY*(8) N   2   s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
30. (0.00000) RY*(9) N   2   s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
31. (0.00273) RY*(1) O   3   s(0.00%)p 1.00(96.51%)d 0.04(3.49%)
                0.0000 0.0000 0.0000 0.0000 -0.0172
                0.9822 0.0000 0.0000 0.0000 0.0000
                0.0000 -0.1869 0.0000 0.0000 0.0000
32. (0.00246) RY*(2) O   3   s(0.00%)p 1.00(96.49%)d 0.04(3.51%)
                0.0000 0.0000 0.0000 0.0000 0.0000
                0.0000 -0.0049 0.9823 0.0000 0.0000
                0.0000 0.0000 -0.1875 0.0000 0.0000
33. (0.00019) RY*(3) O   3   s(62.56%)p 0.51(31.87%)d 0.09(5.58%)
                0.0000 0.0131 0.7906 -0.0173 0.0000
                0.0000 0.0000 0.0000 -0.0575 0.5616
                0.0000 0.0000 0.0000 0.0000 -0.2362
34. (0.00002) RY*(4) O   3   s(29.86%)p 2.25(67.33%)d 0.09(2.81%)
35. (0.00003) RY*(5) O   3   s(9.06%)p 0.02(0.21%)d10.02(90.73%)
36. (0.00000) RY*(6) O   3   s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
37. (0.00000) RY*(7) O   3   s(0.00%)p 1.00(3.71%)d25.95(96.29%)
38. (0.00000) RY*(8) O   3   s(0.00%)p 1.00(3.71%)d25.95(96.29%)
39. (0.00000) RY*(9) O   3   s(0.00%)p 0.00(0.00%)d 1.00(100.00%)
40. (0.00000) RY*(10) O   3   s(98.34%)p 0.01(1.16%)d 0.01(0.50%)
41. (0.01710) BD*(1) N   1 - N   2
      (56.20%)   0.7497* N   1 s(31.46%)p 2.16(68.00%)d 0.02(0.55%)
                -0.0006 0.5559 0.0743 -0.0020 0.0000
                0.0000 0.0000 0.0000 0.8236 0.0400
                0.0000 0.0000 0.0000 0.0000 0.0738
      (43.80%) -0.6618* N   2 s(52.51%)p 0.90(47.37%)d 0.00(0.12%)
                0.0021 0.7245 0.0127 0.0048 0.0000
                0.0000 0.0000 0.0000 -0.6880 -0.0190
                0.0000 0.0000 0.0000 0.0000 0.0340
42. (**0.20189**) BD*(2) N   1 - N   2
      (51.86%)   0.7202* N   1 s(0.00%)p 1.00(99.30%)d 0.01(0.70%)
                0.0000 0.0000 0.0000 0.0000 0.0000
                0.0000 0.9964 0.0070 0.0000 0.0000
                0.0000 0.0000 0.0839 0.0000 0.0000
      (48.14%) -0.6938* N   2 s(0.00%)p 1.00(99.61%)d 0.00(0.39%)
                0.0000 0.0000 0.0000 0.0000 0.0000
                0.0000 0.9978 -0.0206 0.0000 0.0000
                0.0000 0.0000 -0.0625 0.0000 0.0000
43. (0.02307) BD*(3) N   1 - N   2

(99.37%) 0.9969* N 1 s(46.37%)p 0.97(45.12%)d 0.18(8.51%)
0.0903 0.0927 -0.6681 -0.0231 0.0000
0.0000 0.0000 0.0000 0.0564 -0.6694
0.0000 0.0000 0.0000 0.0000 -0.2917
(0.63%) -0.0791* N 2 s(21.84%)p 3.42(74.73%)d 0.16(3.43%)
0.3120 0.2347 -0.2528 0.0452 0.0000
0.0000 0.0000 0.0000 0.2114 0.8382
0.0000 0.0000 0.0000 0.0000 -0.1853

44. (0.02324) BD*(1) N 2 - O 3
(47.48%) 0.6891* N 2 s(42.57%)p 1.32(56.14%)d 0.03(1.28%)
0.0576 -0.6447 -0.0798 0.0202 0.0000
0.0000 0.0000 0.0000 -0.6935 0.2837
0.0000 0.0000 0.0000 0.0000 -0.1133
(52.52%) -0.7247* O 3 s(16.93%)p 4.89(82.71%)d 0.02(0.37%)
0.0000 -0.4089 0.0453 0.0001 0.0000
0.0000 0.0000 0.0000 0.9093 0.0133
0.0000 0.0000 0.0000 0.0000 -0.0605

45. (**0.90892**) BD*(2) N 2 - O 3
(80.68%) 0.8982* N 2 s(0.00%)p 1.00(99.42%)d 0.01(0.58%)
0.0000 0.0000 0.0000 0.0000 0.9969
-0.0219 0.0000 0.0000 0.0000 0.0000
0.0000 0.0759 0.0000 0.0000 0.0000
(19.32%) -0.4396* O 3 s(0.00%)p 1.00(99.78%)d 0.00(0.22%)
0.0000 0.0000 0.0000 0.0000 0.9989
0.0086 0.0000 0.0000 0.0000 0.0000
0.0000 -0.0466 0.0000 0.0000 0.0000

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) N 1 - N 2	/ 3. BD (3) N 1 - N 2	206.07	0.78	0.392
1. BD (1) N 1 - N 2	/ 43. BD*(3) N 1 - N 2	7.29	2.64	0.124
1. BD (1) N 1 - N 2	/ 44. BD*(1) N 2 - O 3	3.10	2.20	0.074
2. BD (2) N 1 - N 2	/ 32. RY*(2) O 3	2.93	1.89	0.066
2. BD (2) N 1 - N 2	/ 42. BD*(2) N 1 - N 2	1.44	0.78	0.032
3. BD (3) N 1 - N 2	/ 16. RY*(5) N 1	1.04	3.36	0.128
3. BD (3) N 1 - N 2	/ 21. RY*(10) N 1	0.72	4.08	0.117
3. BD (3) N 1 - N 2	/ 24. RY*(3) N 2	6.77	3.69	0.342
3. BD (3) N 1 - N 2	/ 25. RY*(4) N 2	3.15	4.57	0.260
3. BD (3) N 1 - N 2	/ 34. RY*(4) O 3	4.78	1.97	0.210
3. BD (3) N 1 - N 2	/ 40. RY*(10) O 3	2.67	4.85	0.246
3. BD (3) N 1 - N 2	/ 41. BD*(1) N 1 - N 2	1.31	1.77	0.102
3. BD (3) N 1 - N 2	/ 43. BD*(3) N 1 - N 2	8.15	1.86	0.258
4. BD (1) N 2 - O 3	/ 3. BD (3) N 1 - N 2	**1382**.41	0.35	0.653
4. BD (1) N 2 - O 3	/ 24. RY*(3) N 2	3.63	4.04	0.112
4. BD (1) N 2 - O 3	/ 25. RY*(4) N 2	1.29	4.92	0.074

4. BD (1) N 2 - O 3	/ 34. RY*(4) O 3	1.66	2.31	0.057
4. BD (1) N 2 - O 3	/ 40. RY*(10) O 3	1.07	5.20	0.069
4. BD (1) N 2 - O 3	/ 41. BD*(1) N 1 - N 2	3.16	2.12	0.075
4. BD (1) N 2 - O 3	/ 43. BD*(3) N 1 - N 2	5.89	2.21	0.105
4. BD (1) N 2 - O 3	/ 44. BD*(1) N 2 - O 3	2.30	1.77	0.059
5. BD (2) N 2 - O 3	/ 12. RY*(1) N 1	11.35	0.40	0.088
5. BD (2) N 2 - O 3	/ 14. RY*(3) N 1	1.73	1.57	0.046
5. BD (2) N 2 - O 3	/ 45. BD*(2) N 2 - O 3	8.20	0.47	0.075
6. CR (1) N 1	/ 3. BD (3) N 1 - N 2	2.60	14.60	0.190
6. CR (1) N 1	/ 43. BD*(3) N 1 - N 2	190.24	16.46	1.582
6. CR (1) N 1	/ 44. BD*(1) N 2 - O 3	7.69	16.02	0.314
7. CR (1) N 2	/ 3. BD (3) N 1 - N 2	**2404.48**	13.15	5.207
7. CR (1) N 2	/ 24. RY*(3) N 2	2.78	16.83	0.203
7. CR (1) N 2	/ 40. RY*(10) O 3	0.52	18.00	0.091
7. CR (1) N 2	/ 41. BD*(1) N 1 - N 2	1.06	14.92	0.118
7. CR (1) N 2	/ 43. BD*(3) N 1 - N 2	10.46	15.01	0.370
7. CR (1) N 2	/ 44. BD*(1) N 2 - O 3	26.08	14.57	0.576
8. CR (1) O 3	/ 24. RY*(3) N 2	0.50	23.38	0.097
8. CR (1) O 3	/ 41. BD*(1) N 1 - N 2	4.25	21.46	0.271
9. LP (1) N 1	/ 3. BD (3) N 1 - N 2	66.23	0.09	0.076
9. LP (1) N 1	/ 41. BD*(1) N 1 - N 2	0.77	1.86	0.034
9. LP (1) N 1	/ 43. BD*(3) N 1 - N 2	30.31	1.95	0.218
9. LP (1) N 1	/ 44. BD*(1) N 2 - O 3	25.67	1.51	0.176
10. LP (1) O 3	/ 24. RY*(3) N 2	0.57	4.06	0.043
10. LP (1) O 3	/ 41. BD*(1) N 1 - N 2	25.18	2.14	0.208
10. LP (1) O 3	/ 44. BD*(1) N 2 - O 3	1.54	1.79	0.047
11. LP (2) O 3	/ 23. RY*(2) N 2	7.06	2.88	0.134
11. LP (2) O 3	/ 28. RY*(7) N 2	0.90	1.36	0.033
11. LP (2) O 3	/ 38. RY*(8) O 3	0.69	2.85	0.042
11. LP (2) O 3	/ 42. BD*(2) N 1 - N 2	89.19	0.60	0.207
12. RY*(1) N 1	/ 14. RY*(3) N 1	8.15	1.16	0.119
12. RY*(1) N 1	/ 18. RY*(7) N 1	2.88	2.50	0.104
12. RY*(1) N 1	/ 22. RY*(1) N 2	10.85	2.62	0.204
12. RY*(1) N 1	/ 27. RY*(6) N 2	2.99	1.11	0.070
12. RY*(1) N 1	/ 45. BD*(2) N 2 - O 3	**2228**.09	0.07	0.361
42. BD*(2) N 1 - N 2	/ 13. RY*(2) N 1	5.65	0.81	0.190
42. BD*(2) N 1 - N 2	/ 19. RY*(8) N 1	1.23	2.15	0.144
42. BD*(2) N 1 - N 2	/ 23. RY*(2) N 2	2.72	2.29	0.217
42. BD*(2) N 1 - N 2	/ 28. RY*(7) N 2	1.69	0.76	0.101
45. BD*(2) N 2 - O 3	/ 14. RY*(3) N 1	4.79	1.09	0.096
45. BD*(2) N 2 - O 3	/ 22. RY*(1) N 2	14.16	2.55	0.249
45. BD*(2) N 2 - O 3	/ 27. RY*(6) N 2	3.63	1.04	0.081
45. BD*(2) N 2 - O 3	/ 31. RY*(1) O 3	4.72	1.39	0.107
45. BD*(2) N 2 - O 3	/ 37. RY*(7) O 3	2.03	2.53	0.095

Such large interaction energies clearly indicate that this Lewis structure is far away from any sense

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NATURAL LOCALIZED MOLECULAR ORBITAL (NLMO) ANALYSIS:

Highest occupied NBOs are not at the beginning of the NBO list;
The NLMO program is not currently set up to handle this.
1\1\GINC-CUP181\SP\RHF\6-31G(d)\N2O1\LEX\23-Jan-2004\0\\#HF/6-31G(D) S
CF=TIGHT POP=NBOREAD\\N2O NN triple bond + NO double bond HF/6-31G(d)/
/HF/STO-3G\\0,1\N\N,1,1.1544\X,2,1.,1,90.\O,2,1.2754,3,90.,1,180.,0\\V
ersion=x86-Linux-G98RevA.11.3\State=1-SG\HF=-183.6570673\RMSD=8.290e-0
9\Dipole=0.,0.,-0.457351\PG=C*V [C*(N1N1O1)]\\@

WHERE THERE IS MUCH DESIRE TO LEARN, THERE OF NECESSITY WILL BE
MUCH ARGUING, MUCH WRITING, MANY OPINIONS; FOR OPINION IN GOOD
MEN
IS BUT KNOWLEDGE IN THE MAKING. -- JOHN MILTON.
Job cpu time: 0 days 0 hours 0 minutes 6.9 seconds.
File lengths (MBytes): RWF= 10 Int= 0 D2E= 0 Chk= 6 Scr= 1
Normal termination of Gaussian 98.