NATURAL RESONANCE THEORY ANALYSIS:

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Maximum reference structures :    20
Maximum resonance structures :  1183
Memory requirements :    5942535 words of   5950426 available

  5 candidate reference structure(s) calculated by SR LEWIS
Initial loops searched    7 bonding pattern(s); all but  3 were discarded
Reference   1:  rho*=0.35546, f(w)=0.92492 converged after  33 iterations
Reference   2:  rho*=0.71432, f(w)=0.96753 converged after 156 iterations
Reference   3:  rho*=0.90720, ionic; deleted
Multi-ref( 2):  D(W)=0.06850, F(W)=0.09815 converged after 216 iterations
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		non-Lewis		fractional accuracy f(w)		
Ref	Wgt	density	d(0)	all NBOs	val+core	valence
1	0.72410	0.35546	0.05345	0.92492	0.95325	0.95337
2	0.27590	0.71432	0.13804	0.96753	0.97685	0.97689

TOPO matrix for the leading resonance structure:

	Atom	1	2	3	4	5	6
1.	H	0	0	1	0	0	0
2.	H	0	0	1	0	0	0
3.	N	1	1	1	1	0	0
4.	C	0	0	1	0	2	1
5.	O	0	0	0	2	2	0
6.	H	0	0	0	1	0	0

RS	Resonance Weight(%)	Added(Removed)
1*(2)	69.36	
2*	24.39	N 3- C 4, (C 4- O 5), (N 3), O 5
3	2.37	(N 3- C 4), C 4- O 5, N 3, (O 5)
4 (2)	1.99	C 4- O 5, (C 4- H 6), (O 5), H 6
5 (2)	0.76	N 3- C 4, (C 4- H 6), (N 3), H 6
6	0.36	(H 2- N 3), N 3- C 4, (C 4- H 6), H 2
7	0.16	(H 1- N 3), N 3- C 4, (C 4- O 5), O 5
8	0.15	(H 2- N 3), N 3- C 4, (C 4- O 5), O 5
9	0.14	(H 1- N 3), N 3- C 4, (C 4- O 5), H 1
10	0.14	(H 2- N 3), N 3- C 4, N 3- C 4, (C 4- O 5), (C 4- H 6), H 2, (N 3), O 5
11-15	0.17	
	100.00	* Total * [* = reference structure]

Natural Bond Order: (total/covalent/ionic)

Atom		1	2	3	4	5	6
1. H	t	0.0020	0.0000	0.9959	0.0000	0.0000	0.0000
	c	---	0.0000	0.5787	0.0000	0.0000	0.0000
	i	---	0.0000	0.4172	0.0000	0.0000	0.0000
2. H	t	0.0000	0.0050	0.9928	0.0000	0.0000	0.0000
	c	0.0000	---	0.5664	0.0000	0.0000	0.0000
	i	0.0000	---	0.4265	0.0000	0.0000	0.0000
3. N	t	0.9959	0.9928	0.7691	1.2422	0.0000	0.0000
	c	0.5787	0.5664	---	0.7519	0.0000	0.0000
	i	0.4172	0.4265	---	0.4903	0.0000	0.0000
4. C	t	0.0000	0.0000	1.2422	0.0000	1.7904	0.9674
	c	0.0000	0.0000	0.7519	---	1.0967	0.7956
	i	0.0000	0.0000	0.4903	---	0.6937	0.1719
5. O	t	0.0000	0.0000	0.0000	1.7904	2.2076	0.0000
	c	0.0000	0.0000	0.0000	1.0967	---	0.0000
	i	0.0000	0.0000	0.0000	0.6937	---	0.0000
6. H	t	0.0000	0.0000	0.0000	0.9674	0.0000	0.0275
	c	0.0000	0.0000	0.0000	0.7956	0.0000	---
	i	0.0000	0.0000	0.0000	0.1719	0.0000	---

Natural Atomic Valencies:

Atom	Valency	Co-Valency	Electro-Valency
1. H	0.9959	0.5787	0.4172
2. H	0.9928	0.5664	0.4265
3. N	3.2309	1.8969	1.3340
4. C	4.0000	2.6442	1.3558
5. O	1.7904	1.0967	0.6937
6. H	0.9674	0.7956	0.1719

```
$NRTSTR
  STR         ! Wgt = 69.36%
    LONE 3 1 5 2 END
    BOND S 1 3 S 2 3 S 3 4 D 4 5 S 4 6 END
  END
  STR         ! Wgt = 24.39%
    LONE 5 3 END
    BOND S 1 3 S 2 3 D 3 4 S 4 5 S 4 6 END
  END
$END
```