NATURAL BOND ORBITALS (Summary):

NBO	Occupancy	Energy	Principal Delocalizations (geminal,vicinal,remote)
Molecular unit 1 (CH3NO)			
1. BD (1) H 1- N 3	1.99309	-0.89250	32(v),20(v)
2. BD (1) H 2- N 3	1.99322	-0.87920	33(v),19(v),32(v),21(v)
3. BD (1) N 3- C 4	1.99828	-1.10527	29(g),28(g)
4. BD (1) C 4- O 5	1.99925	-0.50592	31(g),16(v)
5. BD (2) C 4- O 5	1.99802	-1.40674	19(g),28(v)
6. BD (1) C 4- H 6	1.98929	-0.75792	29(v),23(v),15(v)
7. CR (1) N 3	1.99922	-15.31924	20(v),19(v),13(v),14(v)
8. CR (1) C 4	1.99939	-11.16963	27(v),29(v),28(v)
9. CR (1) O 5	1.99963	-20.09206	19(v),25(g),20(v)
10. LP (1) N 3	1.80683	-0.39458	31(v),22(v)
11. LP (1) O 5	1.98262	-0.93620	19(v),20(v),33(v),30(v) 29(r)
12. LP (2) O 5	1.88568	-0.40982	30(v),33(v),20(v)
13. RY*(1) H 1	0.00054	0.92402	
14. RY*(1) H 2	0.00174	0.95071	
15. RY*(1) N 3	0.00111	2.04745	
16. RY*(2) N 3	0.00075	1.39282	
17. RY*(3) N 3	0.00028	1.80642	
18. RY*(4) N 3	0.00004	2.12398	
19. RY*(1) C 4	0.01600	0.88161	
20. RY*(2) C 4	0.00686	1.00133	
21. RY*(3) C 4	0.00097	1.44455	
22. RY*(4) C 4	0.00024	0.94578	
23. RY*(1) O 5	0.00129	2.03359	
24. RY*(2) O 5	0.00031	1.91310	
25. RY*(3) O 5	0.00013	1.95762	
26. RY*(4) O 5	0.00001	3.41208	
27. RY*(1) H 6	0.00385	0.88794	
28. BD*(1) H 1- N 3	0.00611	0.65748	
29. BD*(1) H 2- N 3	0.00964	0.65791	
30. BD*(1) N 3- C 4	0.05837	0.69936	
31. BD*(1) C 4- O 5	0.19262	0.16326	24(g),22(g)
32. BD*(2) C 4- O 5	0.00600	0.84436	
33. BD*(1) C 4- H 6	0.04859	0.65027	
Total Lewis	23.64454	(98.5189%)	
Valence non-Lewis	0.32134	(1.3389%)	
Rydberg non-Lewis	0.03413	(0.1422%)	
Total unit 1	24.00000	(100.0000%)	
Charge unit 1	0.00000		