

NBO Fock matrix:

NBO	1	2	3	4	5	6	7	8
1. C 1(cr)	-11.0415	0.0481	0.0445	-0.5703	-0.5874	-0.5891	-0.5891	0.0096
2. N 2(cr)	0.0481	-15.2590	-0.6352	-0.9339	-0.0204	-0.0260	-0.0260	-0.8090
3. N 2(lp)	0.0445	-0.6352	-0.4475	-0.1233	0.0645	-0.0200	-0.0200	-0.1200
4. C 1- N 2	-0.5703	-0.9339	-0.1233	-0.8974	-0.1326	-0.1304	-0.1304	-0.2193
5. C 1- H 3	-0.5874	-0.0204	0.0645	-0.1326	-0.6926	-0.1372	-0.1372	-0.0180
6. C 1- H 4	-0.5891	-0.0260	-0.0200	-0.1304	-0.1372	-0.6891	-0.1338	0.0413
7. C 1- H 5	-0.5891	-0.0260	-0.0200	-0.1304	-0.1372	-0.1338	-0.6891	-0.0229
8. N 2- H 6	0.0096	-0.8090	-0.1200	-0.2193	-0.0180	0.0413	-0.0229	-0.8093
9. N 2- H 7	0.0096	-0.8090	-0.1200	-0.2193	-0.0180	-0.0229	0.0413	-0.1957
10. C 1- N 2*	-0.0387	-0.0303	0.0011	-0.0023	-0.0030	0.0067	0.0067	0.0011
11. C 1- H 3*	-0.0214	-0.0154	-0.0846	-0.0083	0.0033	-0.0157	-0.0157	0.0097
12. C 1- H 4*	-0.0246	-0.0113	0.0363	-0.0156	-0.0183	-0.0023	-0.0240	-0.0585
13. C 1- H 5*	-0.0246	-0.0113	0.0363	-0.0156	-0.0183	-0.0240	-0.0023	0.0159
14. N 2- H 6*	-0.0545	0.0203	-0.0018	-0.0108	-0.0051	-0.0574	0.0002	0.0017
15. N 2- H 7*	-0.0545	0.0203	-0.0018	-0.0108	-0.0051	0.0002	-0.0574	0.0022
16. C 1(ry)	0.0045	0.1399	0.0217	0.0118	-0.0028	-0.0009	-0.0009	0.0278
17. C 1(ry)	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0006	0.0006	0.0219
18. C 1(ry)	-0.0025	0.1049	0.0203	0.0054	-0.0007	0.0006	0.0006	-0.0077
19. C 1(ry)	0.0030	-0.0297	-0.0025	-0.0001	0.0022	0.0031	0.0031	-0.0014
20. N 2(ry)	0.0040	0.0692	0.0026	0.0041	0.0377	-0.0231	-0.0231	0.0033
21. N 2(ry)	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0275	0.0275	-0.0001
22. N 2(ry)	0.0799	-0.0572	-0.0015	-0.0025	-0.0145	-0.0152	-0.0152	-0.0028
23. N 2(ry)	-0.0257	0.0314	0.0026	-0.0010	-0.0096	-0.0036	-0.0036	0.0015
24. H 3(ry)	0.1157	0.0135	-0.0111	-0.0133	0.0030	-0.0159	-0.0159	0.0026
25. H 4(ry)	0.1217	0.0131	0.0106	-0.0094	-0.0115	0.0041	-0.0129	-0.0023
26. H 5(ry)	0.1217	0.0131	0.0106	-0.0094	-0.0115	-0.0129	0.0041	0.0002
27. H 6(ry)	0.0161	0.0889	-0.0026	-0.0216	-0.0089	-0.0001	-0.0096	0.0002
28. H 7(ry)	0.0161	0.0889	-0.0026	-0.0216	-0.0089	-0.0096	-0.0001	-0.0108

NBO	9	10	11	12	13	14	15	16
1. C 1(cr)	0.0096	-0.0387	-0.0214	-0.0246	-0.0246	-0.0545	-0.0545	0.0045
2. N 2(cr)	-0.8090	-0.0303	-0.0154	-0.0113	-0.0113	0.0203	0.0203	0.1399
3. N 2(lp)	-0.1200	0.0011	-0.0846	0.0363	0.0363	-0.0018	-0.0018	0.0217
4. C 1- N 2	-0.2193	-0.0023	-0.0083	-0.0156	-0.0156	-0.0108	-0.0108	0.0118
5. C 1- H 3	-0.0180	-0.0030	0.0033	-0.0183	-0.0183	-0.0051	-0.0051	-0.0028
6. C 1- H 4	-0.0229	0.0067	-0.0157	-0.0023	-0.0240	-0.0574	0.0002	-0.0009
7. C 1- H 5	0.0413	0.0067	-0.0157	-0.0240	-0.0023	0.0002	-0.0574	-0.0009
8. N 2- H 6	-0.1957	0.0011	0.0097	-0.0585	0.0159	0.0017	0.0022	0.0278
9. N 2- H 7	-0.8093	0.0011	0.0097	0.0159	-0.0585	0.0022	0.0017	0.0278
10. C 1- N 2*	0.0011	0.5701	-0.0140	-0.0227	-0.0227	-0.0377	-0.0377	0.1612
11. C 1- H 3*	0.0097	-0.0140	0.6870	0.0050	0.0050	-0.0289	-0.0289	0.1081
12. C 1- H 4*	0.0159	-0.0227	0.0050	0.6961	0.0084	0.0246	-0.0334	-0.0034
13. C 1- H 5*	-0.0585	-0.0227	0.0050	0.0084	0.6961	-0.0334	0.0246	-0.0034
14. N 2- H 6*	0.0022	-0.0377	-0.0289	0.0246	-0.0334	0.6804	-0.0321	0.0179
15. N 2- H 7*	0.0017	-0.0377	-0.0289	-0.0334	0.0246	-0.0321	0.6804	0.0179

NAOs in the AO basis:

	AO	1	2	3	4	5	6	7	8
1.	C 1 (s)	1.0034	-0.2133	0.0566	0.0038	-0.0021	0.0002	0.0004	0.0000
2.	C 1 (s)	0.0713	0.4291	1.9952	-0.0046	-0.0060	0.0002	0.0018	0.0000
3.	C 1 (px)	-0.0001	-0.0058	0.0465	0.6995	0.9612	-0.0007	-0.0002	0.0000
4.	C 1 (py)	0.0000	0.0001	0.0056	-0.0017	-0.0052	0.7135	0.9737	0.0000
5.	C 1 (pz)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.7141
6.	C 1 (s)	-0.0968	1.4485	-4.2594	-0.0488	-0.0788	-0.0034	-0.0092	0.0000
7.	C 1 (px)	-0.0001	-0.0137	0.0875	0.7289	-1.7206	0.0047	0.0304	0.0000
8.	C 1 (py)	0.0000	-0.0009	0.0019	0.0026	0.0198	0.6876	-2.0439	0.0000
9.	C 1 (pz)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.6837
10.	N 2 (s)	0.0022	0.0381	-0.0447	-0.0380	0.0197	-0.0021	0.0011	0.0000
11.	N 2 (s)	0.0003	-0.0472	-0.0184	0.0470	-0.0466	0.0020	-0.0060	0.0000
12.	N 2 (px)	-0.0070	-0.1364	0.0692	0.1283	-0.0640	0.0109	-0.0062	0.0000
13.	N 2 (py)	-0.0006	-0.0007	0.0054	0.0001	0.0018	-0.0645	0.0445	0.0000
14.	N 2 (pz)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0650
15.	N 2 (s)	-0.0024	-0.2350	0.7845	0.2798	-0.5791	0.0155	-0.0338	0.0000
16.	N 2 (px)	-0.0162	-0.2370	0.5883	0.2200	-0.3794	0.0191	-0.0323	0.0000
17.	N 2 (py)	-0.0011	-0.0047	-0.0162	0.0097	0.0502	-0.0811	0.3618	0.0000
18.	N 2 (pz)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	-0.0833
19.	H 3 (s)	-0.0047	-0.1770	0.2491	-0.0478	0.0405	-0.1779	0.2337	0.0000
20.	H 3 (s)	-0.0097	-0.2691	0.8378	-0.0564	0.2103	-0.1998	0.9808	0.0000
21.	H 4 (s)	-0.0047	-0.1755	0.2413	-0.0626	0.0558	0.0841	-0.1057	-0.1508
22.	H 4 (s)	-0.0098	-0.2693	0.8455	-0.0717	0.3005	0.0926	-0.4776	-0.1665
23.	H 5 (s)	-0.0047	-0.1755	0.2413	-0.0626	0.0558	0.0841	-0.1057	0.1508
24.	H 5 (s)	-0.0098	-0.2693	0.8455	-0.0717	0.3005	0.0926	-0.4776	0.1665
25.	H 6 (s)	0.0008	-0.0240	-0.0016	0.0304	-0.0565	-0.0030	-0.0200	0.0078
26.	H 6 (s)	0.0006	-0.0182	0.1138	0.0224	-0.1574	0.0040	0.0129	-0.0063
27.	H 7 (s)	0.0008	-0.0240	-0.0016	0.0304	-0.0565	-0.0030	-0.0200	-0.0078
28.	H 7 (s)	0.0006	-0.0182	0.1138	0.0224	-0.1574	0.0040	0.0129	0.0063

	AO	9	10	11	12	13	14	15	16
1.	C 1 (s)	0.0000	0.0023	0.0361	-0.0609	0.0209	-0.0440	-0.0010	0.0020
2.	C 1 (s)	0.0000	0.0000	-0.0459	-0.1894	-0.0502	-0.0549	0.0012	0.0122
3.	C 1 (px)	0.0000	0.0038	0.1247	-0.1442	0.1061	-0.1618	-0.0025	-0.0163
4.	C 1 (py)	0.0000	0.0002	0.0077	0.0025	0.0083	-0.0197	-0.0642	0.0205
5.	C 1 (pz)	0.9766	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
6.	C 1 (s)	0.0000	-0.0012	-0.2357	1.3521	-0.2084	1.2795	-0.0039	-0.0033
7.	C 1 (px)	0.0000	0.0082	0.2438	-0.6773	0.1714	-0.7484	0.0052	0.0410
8.	C 1 (py)	0.0000	0.0005	0.0171	0.0144	0.0135	-0.0739	-0.0762	0.4837
9.	C 1 (pz)	-2.0634	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
10.	N 2 (s)	0.0000	1.0045	-0.1946	0.0028	-0.0073	0.0339	-0.0135	0.0389
11.	N 2 (s)	0.0000	0.0770	0.3210	1.8596	0.0199	0.0365	0.0238	0.0261
12.	N 2 (px)	0.0000	0.0008	0.0416	0.0454	0.6180	1.0309	-0.0211	0.0073
13.	N 2 (py)	0.0000	0.0003	0.0554	0.0347	-0.0216	0.0036	0.5513	1.0442
14.	N 2 (pz)	0.0432	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
15.	N 2 (s)	0.0000	-0.1227	1.2502	-3.1178	0.0423	-0.4470	0.0891	-0.3954
16.	N 2 (px)	0.0000	0.0016	0.0508	-0.4778	0.7319	-1.8991	-0.0222	0.1740
17.	N 2 (py)	0.0000	0.0006	0.0866	-0.3948	-0.0232	0.1663	0.6720	-1.2957
18.	N 2 (pz)	0.3524	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
19.	H 3 (s)	0.0000	0.0006	-0.0034	-0.1065	-0.0126	-0.0656	0.0062	-0.0896