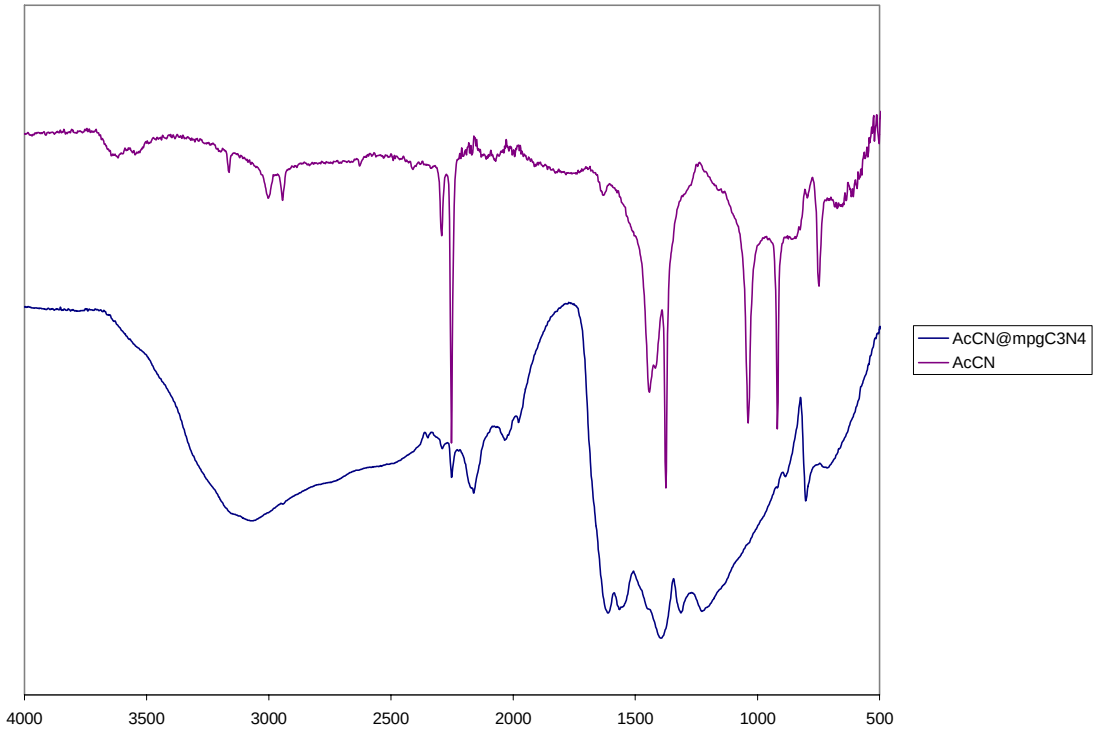
Supplementary Material (ESI) for New Journal of Chemistry

Supporting information for

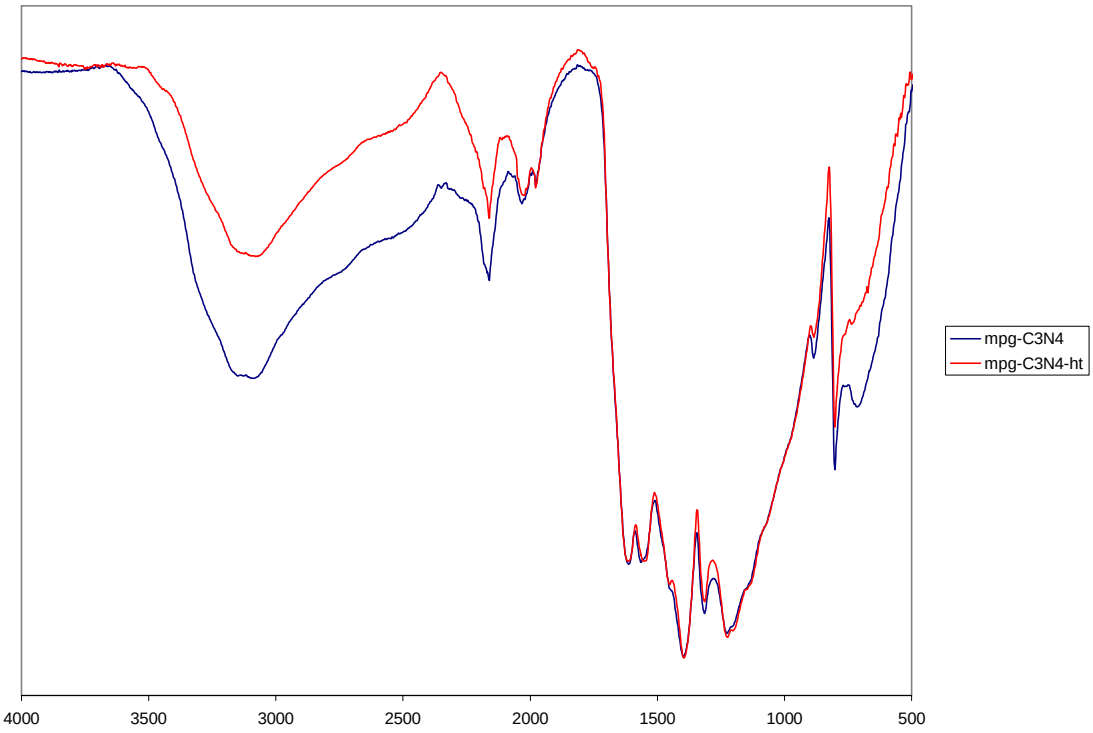
Mesoporous graphitic carbon nitride as a versatile, metal free, catalyst for the cyclotrimerization of functional nitriles and alkynes.

By Frederic Goettmann, Anna Fischer, Markus Antonietti and Arne Thomas.*

FT-IR spectra of mpg-C_3N_4, acetonitrile infiltrated mpg-C_3N_4 and heat treated mpg-C_3N_4.



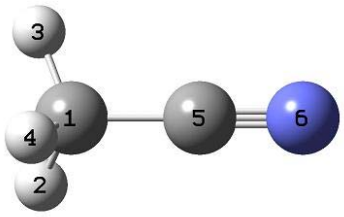
FT-IR spectra of mpg-C_3N_4 and mpg-C_3N_4-ht.



Computational details: All computations were performed using the Gaussian 03 suite of programs[1] and gradient-corrected density functional theory by using the B3Lyp functional.[2] Optimizations were carried out using the 6-311 basis set.

Optimized structures of the nitriles, NBO analysis:

Acetonitrile



Input orientation:

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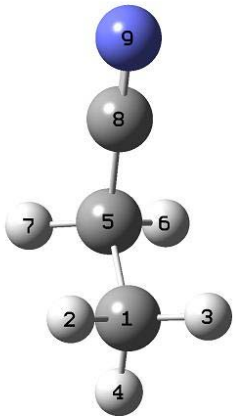
3	6	0	0.000000	0.000000	-1.179253
4	1	0	0.000000	1.020159	-1.564409
5	1	0	0.883484	-0.510080	-1.564409
6	1	0	-0.883484	-0.510080	-1.564409

Summary of Natural Population Analysis:

		Natural	Natural Population			
Atom	No	Charge	Core	Valence	Rydberg	Total
N	1	-0.33118	1.99963	5.32219	0.00937	7.33118
C	2	0.29168	1.99943	3.68021	0.02869	5.70832
C	3	-0.67861	1.99915	4.67586	0.00361	6.67861
H	4	0.23937	0.00000	0.75955	0.00107	0.76063
H	5	0.23937	0.00000	0.75955	0.00107	0.76063
H	6	0.23937	0.00000	0.75955	0.00107	0.76063

Propionitrile



Input orientation:

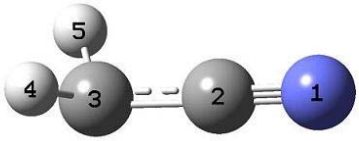
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.001472	-0.006154	0.001075
2	1	0	0.002320	-0.007095	1.090973
3	1	0	1.036515	-0.007507	-0.340367
4	1	0	-0.474226	-0.925193	-0.342379
5	6	0	-0.762597	1.215644	-0.551398
6	1	0	-0.779242	1.184010	-1.643891
7	1	0	-1.805294	1.183961	-0.224863
8	6	0	-0.181354	2.491914	-0.131048
9	7	0	0.291146	3.500838	0.210665

Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.55189	1.99929	4.54805	0.00456	6.55189
H	2	0.20336	0.00000	0.79507	0.00157	0.79664
H	3	0.20335	0.00000	0.79508	0.00157	0.79665
H	4	0.20258	0.00000	0.79618	0.00124	0.79742
C	5	-0.47817	1.99912	4.47330	0.00575	6.47817
H	6	0.23118	0.00000	0.76693	0.00189	0.76882
H	7	0.23118	0.00000	0.76693	0.00189	0.76882
C	8	0.29000	1.99938	3.67585	0.03477	5.71000
N	9	-0.33160	1.99963	5.32277	0.00920	7.33160
* Total *		0.00000	7.99741	21.94014	0.06245	30.00000

Chloroacetonitrile



Input orientation:

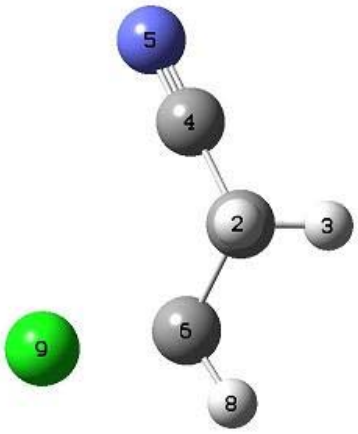
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.929828	-0.790083	-0.003098
2	6	0	0.765343	-0.784881	-0.002411
3	6	0	-0.678828	-0.799417	-0.004479
4	1	0	-1.077506	-1.139173	-0.954048
5	1	0	-1.077358	-1.391005	0.812375
6	17	0	-1.393037	0.940439	0.243447

Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
N	1	-0.26493	1.99962	5.25721	0.00810	7.26493
C	2	0.25183	1.99934	3.71747	0.03136	5.74817
C	3	-0.41473	1.99884	4.40872	0.00716	6.41473
H	4	0.24183	0.00000	0.75528	0.00288	0.75817
H	5	0.24183	0.00000	0.75529	0.00288	0.75817
Cl	6	-0.05583	9.99987	7.05030	0.00566	17.05583
* Total *		0.00000	15.99769	21.94427	0.05804	38.00000

Chloropropionitrile



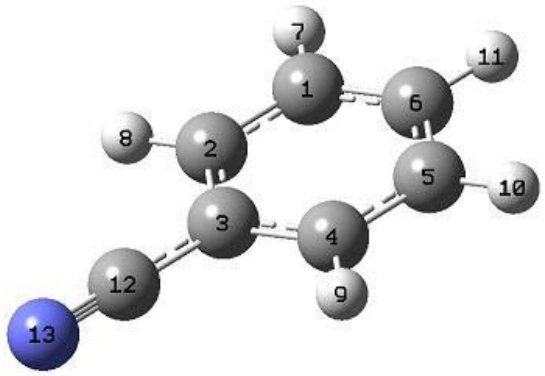
Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.053607	0.035403	-0.014356
2	1	0	-0.078151	0.044915	1.076924
3	1	0	1.002944	0.018494	-0.303869
4	6	0	-0.657276	1.266118	-0.523394
5	7	0	-1.129181	2.249038	-0.931402
6	6	0	-0.702426	-1.243667	-0.534743
7	1	0	-0.829567	-1.242767	-1.610603
8	1	0	-0.153066	-2.118763	-0.208024
9	17	0	-2.442104	-1.461041	0.173959

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	-0.50895	1.99905	4.50131	0.00859	6.50895
H	2	0.24963	0.00000	0.74784	0.00254	0.75037
H	3	0.24809	0.00000	0.74971	0.00220	0.75191
C	4	0.28299	1.99937	3.68121	0.03643	5.71701
N	5	-0.30320	1.99962	5.29483	0.00874	7.30320
C	6	-0.28913	1.99903	4.28042	0.00968	6.28913
H	7	0.21063	0.00000	0.78591	0.00345	0.78937
H	8	0.20853	0.00000	0.78853	0.00295	0.79147
Cl	9	-0.09859	9.99987	7.09261	0.00611	17.09859
* Total *		0.00000	17.99694	27.92237	0.08069	46.00000

Benzonitrile



Input orientation:

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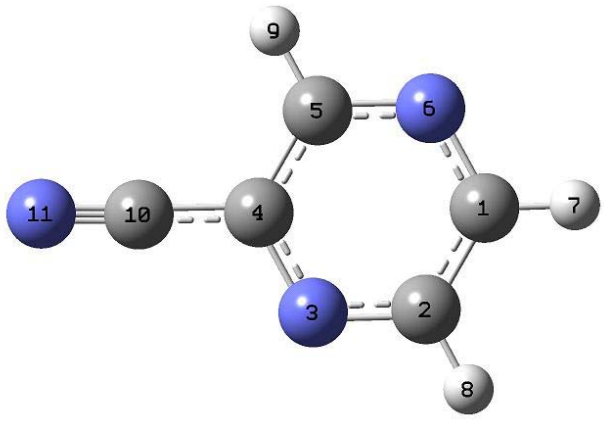
1	6	0	-0.003011	0.000050	0.011438
2	6	0	-0.008946	0.000627	1.405288
3	6	0	1.207937	0.000090	2.111617
4	6	0	2.424933	-0.000945	1.405388
5	6	0	2.419129	-0.001481	0.011575
6	6	0	1.208075	-0.001014	-0.686911
7	1	0	-0.940137	0.000431	-0.527743
8	1	0	-0.942043	0.001435	1.950413
9	1	0	3.357945	-0.001332	1.950658
10	1	0	3.356278	-0.002298	-0.527565
11	1	0	1.208153	-0.001435	-1.768328
12	6	0	1.207921	0.000655	3.543622
13	7	0	1.207940	0.001118	4.711548

Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	-0.19555	1.99915	4.18322	0.01317	6.19555
C	2	-0.15230	1.99909	4.14124	0.01197	6.15230
C	3	-0.16828	1.99888	4.15883	0.01057	6.16828
C	4	-0.15230	1.99909	4.14124	0.01197	6.15230
C	5	-0.19555	1.99915	4.18322	0.01317	6.19555
C	6	-0.17822	1.99916	4.16579	0.01327	6.17822
H	7	0.21119	0.00000	0.78756	0.00124	0.78881
H	8	0.21750	0.00000	0.78069	0.00181	0.78250
H	9	0.21750	0.00000	0.78069	0.00181	0.78250
H	10	0.21119	0.00000	0.78756	0.00124	0.78881
H	11	0.20877	0.00000	0.79002	0.00121	0.79123
C	12	0.27946	1.99926	3.68518	0.03610	5.72054
N	13	-0.30341	1.99962	5.29587	0.00792	7.30341
* Total *		0.00000	15.99342	37.88112	0.12546	54.00000

Pyrazine carbonitrile



Input orientation:

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1	6	0	0.007979	0.000010	0.019424
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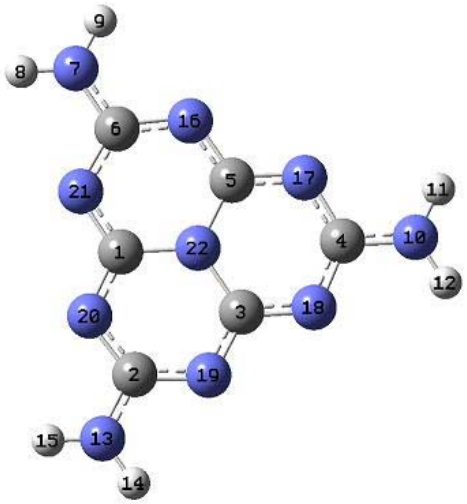
3	7	0	1.143586	0.000004	2.127893
4	6	0	2.304975	0.000006	1.425811
5	6	0	2.312991	0.000008	0.023287
6	7	0	1.163632	0.000011	-0.679346
7	1	0	-0.906170	0.000014	-0.555139
8	1	0	-0.919438	0.000010	1.981096
9	1	0	3.235853	0.000006	-0.537664
10	6	0	3.527534	-0.000006	2.171532
11	7	0	4.539350	-0.000015	2.750809

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	0.02300	1.99922	3.95892	0.01886	5.97700
C	2	0.01544	1.99921	3.96680	0.01856	5.98456
N	3	-0.37027	1.99943	5.36084	0.01000	7.37027
C	4	0.03926	1.99893	3.94666	0.01515	5.96074
C	5	0.05677	1.99914	3.92548	0.01861	5.94323
N	6	-0.39663	1.99948	5.38634	0.01081	7.39663
H	7	0.20667	0.00000	0.79166	0.00167	0.79333
H	8	0.20839	0.00000	0.78993	0.00168	0.79161
H	9	0.21322	0.00000	0.78522	0.00156	0.78678
C	10	0.26846	1.99928	3.69738	0.03489	5.73154
N	11	-0.26431	1.99962	5.25694	0.00775	7.26431
* Total *		0.00000	15.99431	37.86616	0.13953	54.00000

Melem



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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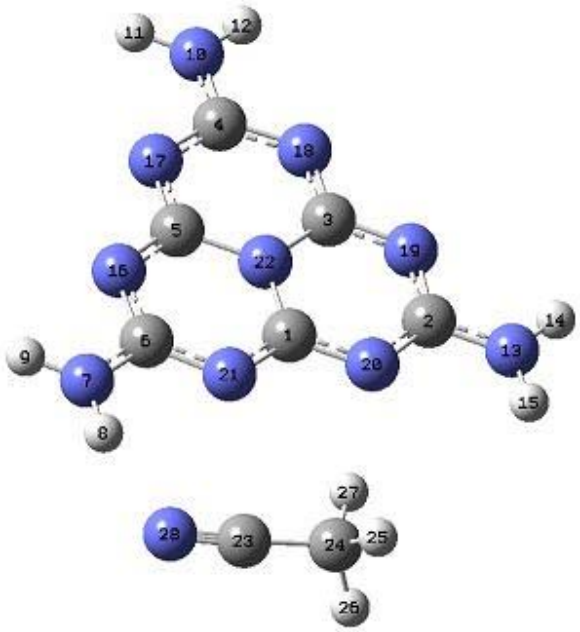
3	6	0	2.162178	-0.047631	1.323640
4	6	0	4.148891	-0.093624	0.155996
5	6	0	2.247367	-0.002279	-1.143247
6	6	0	0.244260	0.089239	-2.279846
7	7	0	-0.388160	0.134133	-3.467701
8	1	0	-1.390894	0.169510	-3.489229
9	1	0	0.153332	0.131455	-4.312660
10	7	0	5.493773	-0.141025	0.201591
11	1	0	6.014526	-0.142373	-0.656325
12	1	0	5.953983	-0.175403	1.092776
13	7	0	-0.627108	0.006260	3.464521
14	1	0	-0.145079	-0.027965	4.344097
15	1	0	-1.628980	0.042260	3.418199
16	7	0	1.602418	0.042710	-2.314521
17	7	0	3.582769	-0.049869	-1.079135
18	7	0	3.498872	-0.094702	1.349956
19	7	0	1.438103	-0.044950	2.448613
20	7	0	-0.622670	0.052478	1.162986
21	7	0	-0.542209	0.095410	-1.171035
22	7	0	1.492947	0.000258	0.066085

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	0.61522	1.99915	3.36315	0.02248	5.38478
C	2	0.58822	1.99924	3.38438	0.02816	5.41178

C	3	0.61524	1.99915	3.36313	0.02248	5.38476
C	4	0.58828	1.99924	3.38433	0.02815	5.41172
C	5	0.61526	1.99915	3.36311	0.02248	5.38474
C	6	0.58825	1.99924	3.38436	0.02815	5.41175
N	7	-0.71749	1.99939	5.71018	0.00792	7.71749
H	8	0.40289	0.00000	0.59548	0.00163	0.59711
H	9	0.40286	0.00000	0.59550	0.00163	0.59714
N	10	-0.71750	1.99939	5.71019	0.00792	7.71750
H	11	0.40288	0.00000	0.59549	0.00163	0.59712
H	12	0.40288	0.00000	0.59549	0.00163	0.59712
N	13	-0.71745	1.99939	5.71014	0.00793	7.71745
H	14	0.40287	0.00000	0.59550	0.00163	0.59713
H	15	0.40288	0.00000	0.59548	0.00163	0.59712
N	16	-0.56435	1.99932	5.55514	0.00988	7.56435
N	17	-0.56431	1.99932	5.55510	0.00988	7.56431
N	18	-0.56432	1.99932	5.55512	0.00989	7.56432
N	19	-0.56434	1.99932	5.55513	0.00989	7.56434
N	20	-0.56432	1.99932	5.55511	0.00989	7.56432
N	21	-0.56433	1.99932	5.55512	0.00988	7.56433
N	22	-0.48933	1.99917	5.48225	0.00791	7.48933
* Total *		0.00000	31.98843	79.75887	0.25270	112.00000

Melem + Acetonitrile



Input orientation:

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3	6	0	2.090874	0.000960	1.324023
4	6	0	4.078053	0.003832	0.157230

5	6	0	2.176141	0.000273	-1.146858
6	6	0	0.169911	-0.003374	-2.294488
7	7	0	-0.457533	-0.005147	-3.476529
8	1	0	-1.469300	-0.007061	-3.523282
9	1	0	0.099069	-0.004813	-4.312586
10	7	0	5.423355	0.005937	0.207853
11	1	0	5.946849	0.006514	-0.648364
12	1	0	5.881317	0.006931	1.100776
13	7	0	-0.699278	-0.002684	3.465934
14	1	0	-0.210005	-0.001600	4.342137
15	1	0	-1.701570	-0.004188	3.429875
16	7	0	1.533096	-0.001196	-2.316332
17	7	0	3.513710	0.002533	-1.077462
18	7	0	3.426279	0.003043	1.352922
19	7	0	1.362491	0.000090	2.447846
20	7	0	-0.697103	-0.003562	1.158612
21	7	0	-0.611040	-0.004237	-1.171793
22	7	0	1.422404	-0.000513	0.065720
23	6	0	-3.742927	-0.013552	-1.931554
24	6	0	-3.993615	-0.013599	-0.500217
25	1	0	-4.562670	0.869252	-0.206644
26	1	0	-4.554821	-0.901028	-0.205349
27	1	0	-3.034814	-0.009037	0.024567
28	7	0	-3.480694	-0.013330	-3.066299

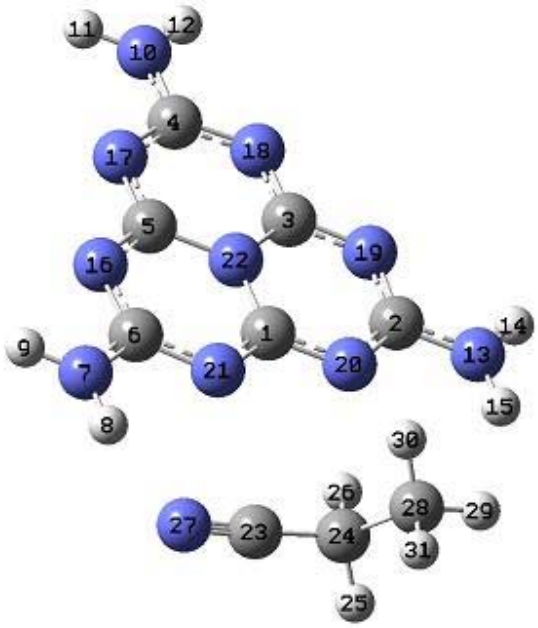
Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.61680	1.99915	3.36152	0.02253	5.38320
C	2	0.59127	1.99924	3.38146	0.02804	5.40873
C	3	0.61575	1.99915	3.36264	0.02247	5.38425
C	4	0.58819	1.99924	3.38443	0.02814	5.41181
C	5	0.61407	1.99915	3.36428	0.02250	5.38593
C	6	0.59403	1.99923	3.37993	0.02681	5.40597
N	7	-0.70810	1.99935	5.70070	0.00804	7.70810
H	8	0.42993	0.00000	0.56696	0.00311	0.57007
H	9	0.40026	0.00000	0.59821	0.00153	0.59974
N	10	-0.71679	1.99939	5.70947	0.00793	7.71679
H	11	0.40327	0.00000	0.59511	0.00162	0.59673
H	12	0.40290	0.00000	0.59548	0.00163	0.59710
N	13	-0.72067	1.99939	5.71344	0.00784	7.72067
H	14	0.40399	0.00000	0.59437	0.00165	0.59601
H	15	0.39888	0.00000	0.59952	0.00160	0.60112
N	16	-0.56112	1.99932	5.55206	0.00973	7.56112
N	17	-0.56374	1.99932	5.55451	0.00991	7.56374
N	18	-0.56387	1.99932	5.55466	0.00989	7.56387
N	19	-0.56632	1.99932	5.55716	0.00984	7.56632
N	20	-0.59612	1.99933	5.58656	0.01024	7.59612
N	21	-0.58135	1.99932	5.57143	0.01060	7.58135
N	22	-0.48932	1.99916	5.48222	0.00793	7.48932
C	23	0.36828	1.99939	3.60372	0.02860	5.63172
C	24	-0.69686	1.99911	4.69366	0.00408	6.69686

H	25	0.23400	0.00000	0.76489	0.00111	0.76600
H	26	0.23402	0.00000	0.76487	0.00111	0.76598
H	27	0.28622	0.00000	0.71078	0.00300	0.71378
N	28	-0.41758	1.99953	5.40808	0.00996	7.41758
* Total *		0.00000	37.98642	95.71211	0.30147	134.00000

Melem + Propionitirle



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.022839	-0.051157	0.000320
2	6	0	-0.023641	-0.056801	2.309187
3	6	0	2.059217	0.007617	1.320885
4	6	0	4.049749	0.069820	0.161467
5	6	0	2.153557	0.012052	-1.149621
6	6	0	0.152549	-0.046134	-2.304930
7	7	0	-0.469413	-0.066101	-3.489581
8	1	0	-1.480680	-0.093695	-3.541529
9	1	0	0.090892	-0.051651	-4.323107
10	7	0	5.394191	0.112090	0.217036
11	1	0	5.920625	0.129002	-0.637261
12	1	0	5.848664	0.125816	1.111689
13	7	0	-0.737161	-0.082697	3.452396
14	1	0	-0.251215	-0.072220	4.330443
15	1	0	-1.738789	-0.115632	3.412401
16	7	0	1.515270	-0.007400	-2.321396
17	7	0	3.490192	0.052949	-1.075246
18	7	0	3.393889	0.048535	1.354664

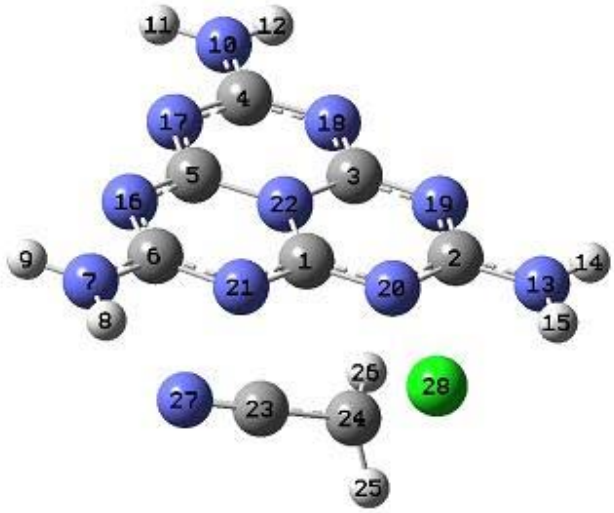
19	7	0	1.327265	-0.016303	2.441985
20	7	0	-0.727022	-0.073668	1.145321
21	7	0	-0.632586	-0.065981	-1.185176
22	7	0	1.395525	-0.010920	0.060109
23	6	0	-3.764940	-0.070078	-1.976540
24	6	0	-4.030208	-0.004944	-0.542769
25	1	0	-4.692375	-0.830269	-0.267970
26	1	0	-3.073686	-0.167769	-0.036723
27	7	0	-3.494753	-0.106087	-3.109549
28	6	0	-4.639420	1.341677	-0.099501
29	1	0	-4.798807	1.331928	0.979042
30	1	0	-3.966567	2.165786	-0.334848
31	1	0	-5.597344	1.529199	-0.585438

Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.61673	1.99915	3.36150	0.02262	5.38327
C	2	0.59089	1.99924	3.38178	0.02809	5.40911
C	3	0.61571	1.99915	3.36267	0.02247	5.38429
C	4	0.58817	1.99924	3.38445	0.02815	5.41183
C	5	0.61403	1.99915	3.36432	0.02250	5.38597
C	6	0.59396	1.99923	3.38000	0.02681	5.40604
N	7	-0.70807	1.99935	5.70066	0.00805	7.70807
H	8	0.43004	0.00000	0.56684	0.00312	0.56996
H	9	0.40020	0.00000	0.59826	0.00154	0.59980
N	10	-0.71689	1.99939	5.70958	0.00793	7.71689
H	11	0.40325	0.00000	0.59513	0.00163	0.59675
H	12	0.40287	0.00000	0.59550	0.00163	0.59713
N	13	-0.72082	1.99939	5.71358	0.00786	7.72082
H	14	0.40392	0.00000	0.59444	0.00165	0.59608
H	15	0.39881	0.00000	0.59955	0.00164	0.60119
N	16	-0.56125	1.99932	5.55219	0.00974	7.56125
N	17	-0.56386	1.99932	5.55463	0.00991	7.56386
N	18	-0.56402	1.99932	5.55480	0.00989	7.56402
N	19	-0.56640	1.99932	5.55723	0.00985	7.56640
N	20	-0.59490	1.99933	5.58534	0.01023	7.59490
N	21	-0.58158	1.99932	5.57169	0.01057	7.58158
N	22	-0.48954	1.99917	5.48243	0.00794	7.48954
C	23	0.36702	1.99935	3.59882	0.03482	5.63298
C	24	-0.49730	1.99907	4.49192	0.00631	6.49730
H	25	0.22599	0.00000	0.77216	0.00185	0.77401
H	26	0.27982	0.00000	0.71641	0.00377	0.72018
N	27	-0.41710	1.99953	5.40775	0.00981	7.41710
C	28	-0.55044	1.99929	4.54671	0.00444	6.55044
H	29	0.19938	0.00000	0.79925	0.00137	0.80062
H	30	0.20415	0.00000	0.79403	0.00182	0.79585
H	31	0.19723	0.00000	0.80116	0.00161	0.80277
* Total *		0.00000	39.98561	101.69478	0.31961	142.00000

Melem + Chloroacetonitrile



Input orientation:

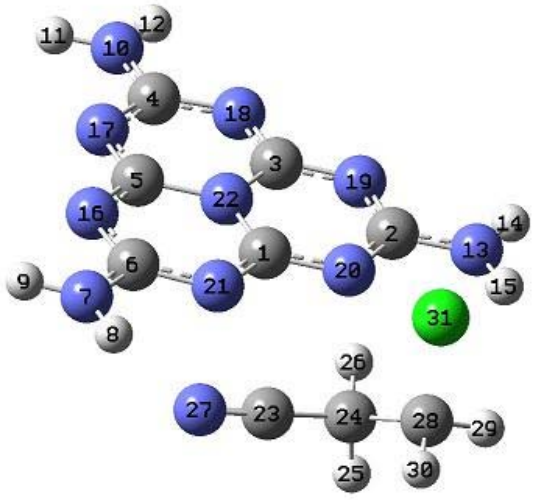
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.027309	-0.001173	-0.060538
2	6	0	-0.075745	0.031657	2.249067
3	6	0	2.026894	0.003511	1.296741
4	6	0	4.037901	-0.024351	0.171460
5	6	0	2.165073	-0.015021	-1.173773
6	6	0	0.183452	-0.002476	-2.362177
7	7	0	-0.425313	0.015464	-3.555257
8	1	0	-1.433625	0.044674	-3.613562
9	1	0	0.141196	0.024115	-4.384532
10	7	0	5.380715	-0.037539	0.249544
11	1	0	5.922069	-0.047337	-0.595663
12	1	0	5.820850	-0.034378	1.151606
13	7	0	-0.811232	0.064952	3.375846
14	1	0	-0.341789	0.088280	4.262842
15	1	0	-1.812573	0.096949	3.319339
16	7	0	1.544490	-0.011851	-2.357108
17	7	0	3.498979	-0.027183	-1.075931
18	7	0	3.360620	-0.008683	1.353013
19	7	0	1.273019	0.023246	2.403499
20	7	0	-0.755502	0.010036	1.068616
21	7	0	-0.619112	-0.008990	-1.255446
22	7	0	1.386298	-0.002377	0.023239
23	6	0	-3.673457	0.033708	-1.857029
24	6	0	-3.791151	-0.089136	-0.423673
25	1	0	-4.274967	-1.016708	-0.137702
26	1	0	-2.817322	0.017362	0.052877
27	7	0	-3.509334	0.104912	-3.007407
28	17	0	-4.884797	1.285412	0.303062

Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.61964	1.99915	3.35895	0.02226	5.38036
C	2	0.59617	1.99924	3.37711	0.02748	5.40383
C	3	0.61616	1.99915	3.36228	0.02241	5.38384
C	4	0.58894	1.99924	3.38380	0.02802	5.41106
C	5	0.61499	1.99915	3.36342	0.02245	5.38501
C	6	0.59641	1.99923	3.37760	0.02675	5.40359
N	7	-0.70823	1.99936	5.70100	0.00787	7.70823
H	8	0.42588	0.00000	0.57149	0.00264	0.57412
H	9	0.40264	0.00000	0.59586	0.00150	0.59736
N	10	-0.71365	1.99939	5.70635	0.00791	7.71365
H	11	0.40432	0.00000	0.59409	0.00159	0.59568
H	12	0.40405	0.00000	0.59436	0.00159	0.59595
N	13	-0.71606	1.99939	5.70895	0.00773	7.71606
H	14	0.40556	0.00000	0.59285	0.00159	0.59444
H	15	0.40219	0.00000	0.59640	0.00140	0.59781
N	16	-0.55921	1.99932	5.55021	0.00967	7.55921
N	17	-0.56078	1.99932	5.55157	0.00989	7.56078
N	18	-0.56072	1.99932	5.55153	0.00987	7.56072
N	19	-0.56335	1.99932	5.55430	0.00974	7.56335
N	20	-0.60788	1.99932	5.59817	0.01039	7.60788
N	21	-0.59180	1.99932	5.58154	0.01095	7.59180
N	22	-0.48772	1.99916	5.48063	0.00793	7.48772
C	23	0.32212	1.99930	3.64623	0.03234	5.67788
C	24	-0.42340	1.99877	4.41693	0.00771	6.42340
H	25	0.23495	0.00000	0.76234	0.00271	0.76505
H	26	0.29473	0.00000	0.70017	0.00510	0.70527
N	27	-0.35247	1.99955	5.34430	0.00861	7.35247
Cl	28	-0.08348	9.99987	7.07820	0.00541	17.08348
* Total *		0.00000	47.98587	101.70064	0.31349	150.00000

Melem + Chloropropionitrile



Input orientation:

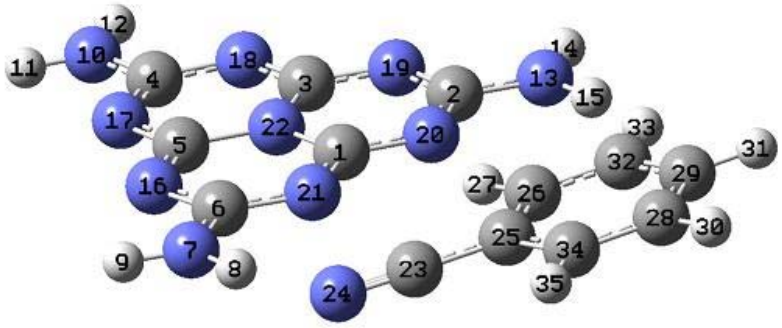
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.030594	0.098919	-0.035741
2	6	0	0.008374	0.174033	2.272132
3	6	0	2.096126	0.001849	1.306431
4	6	0	4.093024	-0.169745	0.169264
5	6	0	2.213166	-0.066578	-1.162212
6	6	0	0.227287	0.044745	-2.338582
7	7	0	-0.381761	0.077321	-3.530302
8	1	0	-1.388054	0.158479	-3.592955
9	1	0	0.185402	0.037685	-4.358312
10	7	0	5.433609	-0.265940	0.239202
11	1	0	5.966746	-0.323919	-0.609175
12	1	0	5.879424	-0.274830	1.138320
13	7	0	-0.711843	0.270144	3.406917
14	1	0	-0.231795	0.281305	4.288295
15	1	0	-1.709424	0.360623	3.358290
16	7	0	1.586672	-0.045540	-2.340793
17	7	0	3.545623	-0.159929	-1.073361
18	7	0	3.427362	-0.091950	1.354705
19	7	0	1.355187	0.086140	2.418617
20	7	0	-0.684042	0.173949	1.100581
21	7	0	-0.567864	0.104246	-1.227436
22	7	0	1.445151	0.013592	0.038827
23	6	0	-3.658553	0.190890	-1.988003
24	6	0	-3.868599	0.082752	-0.548304
25	1	0	-4.059115	-0.969508	-0.307157
26	1	0	-2.929088	0.341174	-0.050862
27	7	0	-3.432321	0.250739	-3.128232
28	6	0	-5.033712	0.900945	-0.008170
29	1	0	-5.182432	0.709027	1.047995
30	1	0	-5.954237	0.752551	-0.560669
31	17	0	-4.691180	2.761163	-0.121324

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population Core	Valence	Rydberg	Total
C	1	0.61842	1.99915	3.36000	0.02243	5.38158
C	2	0.59257	1.99924	3.38028	0.02791	5.40743
C	3	0.61593	1.99915	3.36247	0.02244	5.38407
C	4	0.58848	1.99924	3.38419	0.02809	5.41152
C	5	0.61443	1.99915	3.36395	0.02248	5.38557
C	6	0.59524	1.99923	3.37879	0.02674	5.40476
N	7	-0.70756	1.99936	5.70025	0.00796	7.70756
H	8	0.42764	0.00000	0.56940	0.00296	0.57236
H	9	0.40131	0.00000	0.59717	0.00152	0.59869
N	10	-0.71571	1.99939	5.70840	0.00792	7.71571
H	11	0.40365	0.00000	0.59474	0.00161	0.59635
H	12	0.40329	0.00000	0.59510	0.00161	0.59671
N	13	-0.71940	1.99939	5.71220	0.00782	7.71940

H	14	0.40464	0.00000	0.59373	0.00163	0.59536
H	15	0.39836	0.00000	0.60005	0.00160	0.60164
N	16	-0.56030	1.99932	5.55125	0.00972	7.56030
N	17	-0.56263	1.99932	5.55341	0.00990	7.56263
N	18	-0.56274	1.99932	5.55354	0.00988	7.56274
N	19	-0.56524	1.99932	5.55610	0.00982	7.56524
N	20	-0.59903	1.99933	5.58955	0.01016	7.59903
N	21	-0.58549	1.99932	5.57548	0.01069	7.58549
N	22	-0.48876	1.99916	5.48168	0.00792	7.48876
C	23	0.35746	1.99933	3.60614	0.03707	5.64254
C	24	-0.53160	1.99900	4.52298	0.00963	6.53160
H	25	0.24722	0.00000	0.75055	0.00222	0.75278
H	26	0.30030	0.00000	0.69525	0.00445	0.69970
N	27	-0.38832	1.99954	5.37956	0.00922	7.38832
C	28	-0.28581	1.99902	4.27756	0.00923	6.28581
H	29	0.20485	0.00000	0.79214	0.00301	0.79515
H	30	0.20570	0.00000	0.79085	0.00345	0.79430
Cl	31	-0.10685	9.99987	7.10104	0.00594	17.10685
* Total *		0.00000	49.98514	107.67781	0.33706	158.00000

Melem + Benzonitrile



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.024314	-0.300374	-0.005878
2	6	0	0.035344	-0.427726	2.299804
3	6	0	2.086707	-0.036021	1.323532
4	6	0	4.048281	0.347403	0.176675
5	6	0	2.173080	0.099250	-1.141933
6	6	0	0.194346	-0.168438	-2.307248
7	7	0	-0.411845	-0.221221	-3.498247
8	1	0	-1.409186	-0.380682	-3.574499
9	1	0	0.150875	-0.097590	-4.321229
10	7	0	5.375387	0.566776	0.239328
11	1	0	5.892295	0.694107	-0.611414
12	1	0	5.826424	0.598605	1.135203
13	7	0	-0.660931	-0.617808	3.438718
14	1	0	-0.174177	-0.595482	4.316092
15	1	0	-1.645497	-0.802528	3.394696

16	7	0	1.540987	0.048723	-2.314913
17	7	0	3.493075	0.314147	-1.061077
18	7	0	3.404171	0.181243	1.364737
19	7	0	1.369234	-0.215750	2.439612
20	7	0	-0.665471	-0.468771	1.135594
21	7	0	-0.582646	-0.336515	-1.193519
22	7	0	1.427119	-0.080555	0.061432
23	6	0	-4.038134	-0.609566	-2.465380
24	7	0	-3.404156	-0.621698	-3.444641
25	6	0	-4.774993	-0.581117	-1.240045
26	6	0	-4.076539	-0.509592	-0.019857
27	1	0	-2.994587	-0.487367	-0.012271
28	6	0	-6.886122	-0.577157	-0.054199
29	6	0	-6.196345	-0.502057	1.160375
30	1	0	-7.967003	-0.603727	-0.064643
31	1	0	-6.746838	-0.468893	2.091056
32	6	0	-4.799011	-0.468371	1.172046
33	1	0	-4.265508	-0.405427	2.110443
34	6	0	-6.181804	-0.615740	-1.255561
35	1	0	-6.707012	-0.671033	-2.198792

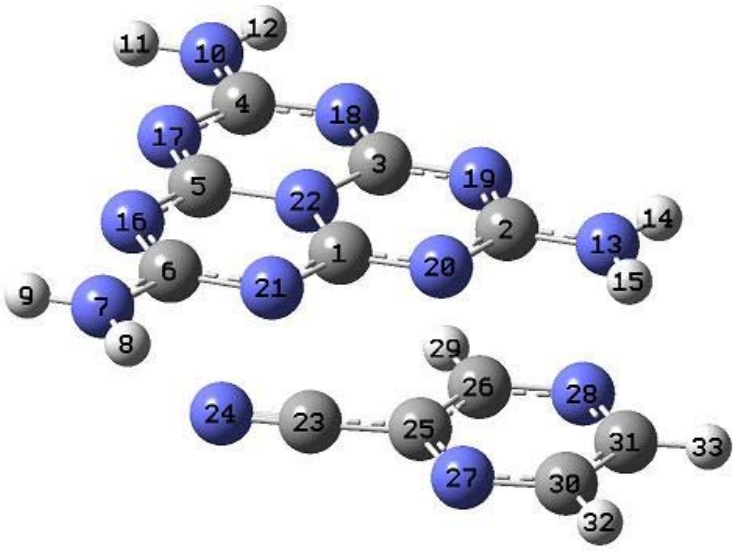
Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.61721	1.99915	3.36133	0.02231	5.38279
C	2	0.59164	1.99924	3.38129	0.02783	5.40836
C	3	0.61574	1.99915	3.36263	0.02248	5.38426
C	4	0.58799	1.99924	3.38460	0.02817	5.41201
C	5	0.61376	1.99915	3.36458	0.02251	5.38624
C	6	0.59343	1.99923	3.38056	0.02679	5.40657
N	7	-0.70733	1.99935	5.69981	0.00817	7.70733
H	8	0.43072	0.00000	0.56657	0.00271	0.56928
H	9	0.39959	0.00000	0.59885	0.00156	0.60041
N	10	-0.71777	1.99939	5.71045	0.00793	7.71777
H	11	0.40294	0.00000	0.59542	0.00164	0.59706
H	12	0.40255	0.00000	0.59581	0.00164	0.59745
N	13	-0.72228	1.99939	5.71478	0.00811	7.72228
H	14	0.40368	0.00000	0.59462	0.00170	0.59632
H	15	0.39765	0.00000	0.60043	0.00192	0.60235
N	16	-0.56195	1.99932	5.55285	0.00978	7.56195
N	17	-0.56461	1.99932	5.55537	0.00992	7.56461
N	18	-0.56470	1.99932	5.55548	0.00990	7.56470
N	19	-0.56667	1.99932	5.55750	0.00985	7.56667
N	20	-0.59353	1.99932	5.58404	0.01017	7.59353
N	21	-0.57799	1.99932	5.56889	0.00977	7.57799
N	22	-0.48961	1.99917	5.48253	0.00792	7.48961
C	23	0.35046	1.99923	3.61550	0.03480	5.64954
N	24	-0.38282	1.99951	5.37410	0.00921	7.38282
C	25	-0.18077	1.99887	4.17136	0.01055	6.18077
C	26	-0.14224	1.99905	4.13087	0.01232	6.14224
H	27	0.26013	0.00000	0.73665	0.00321	0.73987
C	28	-0.20147	1.99915	4.18902	0.01329	6.20147
C	29	-0.17628	1.99916	4.16411	0.01302	6.17628

H	30	0.20972	0.00000	0.78905	0.00124	0.79028
H	31	0.20613	0.00000	0.79261	0.00126	0.79387
C	32	-0.19830	1.99914	4.18618	0.01298	6.19830
H	33	0.20311	0.00000	0.79409	0.00280	0.79689
C	34	-0.15275	1.99909	4.14173	0.01193	6.15275
H	35	0.21461	0.00000	0.78351	0.00188	0.78539
* Total *		0.00000	47.98158	117.63716	0.38127	166.00000

Melem + Pyrazinecarbonitrile



Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.287844	-0.033461	0.046403
2	6	0	0.359738	-0.176121	2.352731
3	6	0	2.405474	-0.225308	1.284688
4	6	0	4.349501	-0.258698	0.045745
5	6	0	2.410539	-0.077030	-1.188726
6	6	0	0.366666	0.100492	-2.256142
7	7	0	-0.310883	0.207141	-3.406755
8	1	0	-1.320784	0.262551	-3.396206
9	1	0	0.202381	0.230438	-4.269525
10	7	0	5.693580	-0.333428	0.047146
11	1	0	6.187644	-0.308421	-0.826093
12	1	0	6.180111	-0.412919	0.921307
13	7	0	-0.334175	-0.206972	3.504706
14	1	0	0.160389	-0.286739	4.374353
15	1	0	-1.338862	-0.149629	3.475403
16	7	0	1.725947	0.029569	-2.331681
17	7	0	3.746865	-0.152411	-1.167518
18	7	0	3.739325	-0.297975	1.262676
19	7	0	1.714208	-0.255922	2.432575
20	7	0	-0.371241	-0.066997	1.211512
21	7	0	-0.371616	0.072503	-1.107861

22	7	0	1.701491	-0.112041	0.049165
23	6	0	-3.852362	0.298102	-1.718641
24	7	0	-3.367026	0.335806	-2.776567
25	6	0	-4.376381	0.246190	-0.384673
26	6	0	-3.509670	0.133842	0.713179
27	7	0	-5.723962	0.309654	-0.238901
28	7	0	-4.003375	0.084846	1.971834
29	1	0	-2.433745	0.082287	0.608487
30	6	0	-6.198272	0.259547	1.020556
31	6	0	-5.344424	0.147917	2.120013
32	1	0	-7.271011	0.310079	1.135048
33	1	0	-5.725135	0.107855	3.130060

Summary of Natural Population Analysis:

Natural Population

Atom	No	Natural Charge	Core	Valence	Rydberg	Total
C	1	0.61752	1.99914	3.36116	0.02218	5.38248
C	2	0.59776	1.99924	3.37591	0.02709	5.40224
C	3	0.61608	1.99915	3.36230	0.02247	5.38392
C	4	0.58835	1.99924	3.38427	0.02814	5.41165
C	5	0.61486	1.99915	3.36350	0.02249	5.38514
C	6	0.59389	1.99923	3.37995	0.02692	5.40611
N	7	-0.71126	1.99936	5.70387	0.00803	7.71126
H	8	0.42985	0.00000	0.56787	0.00228	0.57015
H	9	0.40065	0.00000	0.59783	0.00153	0.59935
N	10	-0.71638	1.99939	5.70906	0.00793	7.71638
H	11	0.40331	0.00000	0.59507	0.00162	0.59669
H	12	0.40308	0.00000	0.59530	0.00162	0.59692
N	13	-0.71881	1.99938	5.71156	0.00786	7.71881
H	14	0.40226	0.00000	0.59611	0.00163	0.59774
H	15	0.41309	0.00000	0.58402	0.00289	0.58691
N	16	-0.56222	1.99932	5.55324	0.00966	7.56222
N	17	-0.56360	1.99932	5.55439	0.00989	7.56360
N	18	-0.56363	1.99932	5.55441	0.00989	7.56363
N	19	-0.56467	1.99932	5.55573	0.00962	7.56467
N	20	-0.60603	1.99931	5.59494	0.01178	7.60603
N	21	-0.58354	1.99932	5.57418	0.01004	7.58354
N	22	-0.48824	1.99916	5.48116	0.00792	7.48824
C	23	0.33420	1.99926	3.63312	0.03342	5.66580
N	24	-0.33837	1.99953	5.32977	0.00908	7.33837
C	25	0.02878	1.99891	3.95679	0.01551	5.97122
C	26	0.06459	1.99908	3.91776	0.01857	5.93541
N	27	-0.37283	1.99943	5.36340	0.01000	7.37283
N	28	-0.42633	1.99949	5.41427	0.01258	7.42633
H	29	0.26719	0.00000	0.72958	0.00323	0.73281
C	30	0.00749	1.99921	3.97456	0.01874	5.99251
C	31	0.02478	1.99922	3.95706	0.01894	5.97522
H	32	0.20575	0.00000	0.79257	0.00167	0.79425
H	33	0.20242	0.00000	0.79588	0.00170	0.79758
* Total *		0.00000	47.98249	117.62056	0.39695	166.00000

(1) Frisch, M. J., et al. *Gaussian 98, Revision A-11*, Gaussian Inc.: Pittsburgh (PA), 1998.

(2) Becke, A. D., *J. Chem. Phys.***1993,** *98*, 5648-5652.